AD/A-005 221

COMPUTER SIMULATION OF THE CONTINUOUS TNT PROCESS. VOLUME 1: THE NITRATION SECTION

Raymond Goldstein

Picatinny Arsenal
Dover, New Jersey

January 1975

DISTRIBUTED BY:

NTIS
National Technical Information Service
U. S. DEPARTMENT OF COMMERCE

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE	READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER: Technical Report 4684	2. GOVT ACCESSION NO.
3. RECIPIENT'S CATALOG NUMBER: AD/A-005221	
4. TITLE (and Subtitle): COMPUTER SIMULATION OF THE CONTINUOUS TNT PROCESS. VOLUME I: THE NITRATION SECTION	5. TYPE OF REPORT & PERIOD COVERED
	6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s): Raymond Goldstein	8. CONTRACT OR GRANT NUMBER(s)
9. PERFORMING ORGANIZATION NAME AND ADDRESS: Manufacturing Technology Directorate, Picatinny Arsenal, Dover, New Jersey	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
11. CONTROLLING OFFICE NAME AND ADDRESS	12. REPORT DATE: JANUARY 1975
	13. NUMBER OF PAGES: 447
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)	15. SECURITY CLASS. (of this report): UNCLASSIFIED
	15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

DDC RECEIVED FEB 10 1975 D

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Mathematical model	Continuous multistage processes	mass transfer
Computer simulation	Steady state analysis	equilibrium
Nitration	Digital computer	optimization
TNT manufacture	Kinetics	process control

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The development of a mathematical model of the nitration section of a continuous process for the manufacture of TNT is described. Implementation of the model on a high-speed digital computer is also discussed, as are the steady state and dynamic studies that were conducted on the resulting computer simulation. The way in which optimized process operating conditions and improved process control strategies were developed using the simulation is illustrated.

DD FORM 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

PRICES SUBJECT TO CHANGE

Reproduced by NATIONAL TECHNICAL INFORMATION SERVICE U S Department of Commerce Springfield VA 22151

19. (Cont'd)

Parameter fitting
Numerical methods
Transient analysis

ACKNOWLEDGMENT

The author wishes to acknowledge the contributions made to this report by members of the engineering staff of Imperial Chemical Industries, U. S. (ICIUS) at Volunteer Army Ammunition Plant including Messrs. John Williams*, Fred Michlink**, Richard Chiang, and Kenneth Malone as well as Drs. Cecil L. Smith and Armand B. Corripio of Louisiana State University who, functioning in the capacity of consultants to ICIUS, are directly responsible for many of the accomplishments of the TNT process simulation effort.

* Current Address: Eastern Airlines, Miami, Florida
** Current Address: Industrial Nucleonics, Columbus, Ohio

TABLE OF CONTENTS

	Page No.
Summary	1
Introduction	2
The Chemistry of TNT Nitration - A Brief Description	3
Process Description	6
Development of the Mathematical Model	7
The Single Vessel Model	7
Formulation of the Overall Nitration Section Model from the Single Vessel Model	33
Computer Implementation of the Mathematical Model - the Simulation	38
The Dynamic Simulation	38
The Steady State Simulation	50
Parameter Fitting	65
Application of the Simulation	66
Steady State Applications	66
Dynamic Applications	69
Conclusion	70
References	71
Distribution List	447
Appendices	
A Vessel Equations	73
B Dynamic Simulation--Program Listing and Output	83

C	Dynamic Simulation--Program Flowchart	187
D	Dynamic Simulation--Program Nomenclature	227
E	Dynamic Simulation--Input Data Format	265
F	Steady State Simulation--Program Listing and Output	269
G	Steady State Simulation--Program Flowchart	335
H	Steady State Simulation--Program Nomenclature	373
I	Steady State Simulation--Input Data Format	417
J	Parameter Fitting	421
K	Steady State Optimization	429

Figures

1	Isomers formed during toluene nitration	434
2	Oxidation of trinitrotoluene	435
3	TNT nitration flow scheme (inter-vessel relationship)	436
4	Nitrator-separator combination	437
5	Generalized nitrator	438
6	Simplified nitrator	439
7	Chemical components considered in the model	440
8	Diffusion in the nitration process	441
9	The separation process	442
10	Acid concentration control--variables operated on	443

11	Acid concentration control--schematic diagram	444
12	Open loop response of dynamic simulation	445
13	Response of dynamic simulation under acid concentration control	446

SUMMARY

The development of a mathematical model of the nitration section of a continuous process for the manufacture of TNT is described. Implementation of the model on a high-speed digital computer is also discussed, as are the steady state and dynamic studies that were conducted on the resulting computer simulation. The way in which optimized process operating conditions and improved process control strategies were developed using the simulation is illustrated.

INTRODUCTION

Computer simulation of a chemical process, simply defined, is a procedure by which a mathematical model of the process' relevant chemical and physical characteristics is first constructed, after which the resultant system of equations is programmed for solution on a high speed computer. Such a model is usually based upon a combination of prevailing theory and empirical relationships, and, when properly formulated, will predict all process input/output relationships. The applicability of such a model depends heavily upon the ratio of theory to empiricism employed in model development. For example, a totally empirical model such as a least squares polynomial approximation is useful only within the boundaries of experimental observation, whereas a totally theoretical model, for example Newton's Laws of Motion as a description of projectile trajectories, will apply under virtually all conditions. For most complex systems (such as a chemical process) an optimum balance between theory and observation must be sought.

Upon completion of mathematical modeling and computer programming, the resulting computer simulation can then, after verification against real process data, be used to study the process without incurring the cost, time loss, and (especially in the case of explosives manufacturing processes) the risk involved in pilot plant or full-scale plant experimentation. Most often, studies of both the static and dynamic states of the process are carried out, the objective of the former being optimization of operating and design conditions, and the objective of the latter being development and testing of control strategies.

It has always been possible to develop mathematical models of complex physical systems. However, the value of such models remained questionable until the application of digital, analog, and hybrid computers made possible the rapid solution of the complex equations which usually resulted. It has only been in the last 10 to 15 years that mathematical modeling of complex processes has yielded significant accomplishments. Most notable among these have been the simulations used in the aerospace industry, especially in the manned space flight program.

Although employed successfully as a process study tool for a number of years in private industry, the application of chemical process simulation to the U. S. Army Armament Command's explosive and propellant manufacturing processes is just now beginning to be appreciated. For the past three and a half years, the Chemical Process Technology Division of the

Manufacturing Technology Directorate at Picatinny Arsenal has been engaged in an extensive effort to improve, via the application of computer simulation, a continuous process for TNT manufacturing. This work has been carried out jointly with Imperial Chemical Industries, U. S. (ICIUS) the operating contractor at Volunteer Army Munition Plant in Chattanooga, Tennessee, and has to date gone through three distinct phases: Phase I, initial development of a kinetics and mass transfer model of the nitration section with subsequent implementation on a hybrid computer; Phase II, conversion of the hybrid nitration model to a pure digital model, followed by improvement of the nitration model based on new plant data and additional theoretical considerations, simulation of nitration section hydraulics, and development of a simulation of the purification section of the process; and Phase III, extensive exploitation of the nitration and purification computer models.

Project summary reports (Ref 1, 2, 3) have previously been prepared covering these efforts. However, no unified text has been generated which ties together all the interrelated tasks and provides a much needed explanation of the present structure, capabilities, and limitations of various models developed. The purpose of this report is to satisfy these needs as well as to clarify material in the existing reports which has either become outdated or which the author feels is unclear as presently stated.

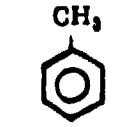
Because of the extensive amount of information which is presented, the report has been prepared in three volumes. Volume I describes the modeling and simulation effort that has been carried out on the nitration section of the process, including a description of the process chemistry and equipment. Volume II deals exclusively with the purification section model, and Volume III involves the simulation of the hydraulic phenomena occurring in a nitration stage.

THE CHEMISTRY OF TNT NITRATION - A BRIEF DESCRIPTION

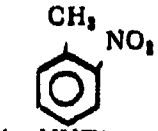
The production of TNT is essentially carried out via a three-step reaction in which toluene and its mono- and dinitro-substituted derivatives are contacted with mixtures of nitric and sulfuric acid called mixed acid. Each step in the reaction corresponds to the successive electrophilic substitution of a hydrogen ion (H^+) by a nitronium ion (NO_2^+) on the aromatic ring of the toluene molecule. The nitric acid serves as the source of NO_2^+ ions, while the sulfuric acid acts as both a catalyst and dehydrating agent, first reacting with the nitric acid to generate NO_2^+ ions and then picking up the water which forms as a product of the nitration reaction.

A simplified scheme for the mononitration of toluene in mixed acid can be written as follows:

$$HNO_3 + H_2SO_4 \rightleftharpoons NO_2^+ + HSO_4^- + H_2O \qquad (1)$$


(Toluene)

$$+ NO_2^+ + HSO_4^-$$

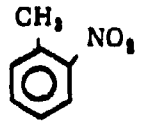

(o-MNT)

$$+ H_2SO_4 \qquad (2)$$

Adding reactions 1 and 2 gives the overall reaction:

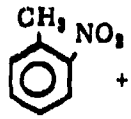


$$+ HNO_3 \xrightarrow{H_2SO_4}$$

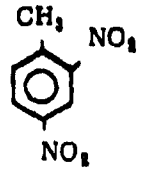


$$+ H_2O \qquad (3)$$

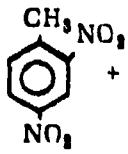
Similarly, when toluene is replaced by mononitrotoluene (MNT) or dinitrotoluene (DNT), the stoichiometric reactions are written as



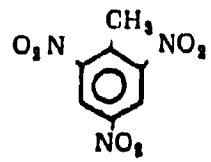
$$+ HNO_3 \xrightarrow{H_2SO_4}$$


(2,4-DNT)

$$+ H_2O \qquad (4)$$



$$+ HNO_3 \xrightarrow{H_2SO_4}$$


(α-TNT)

$$+ H_2O \qquad (5)$$

The temperature as well as the composition of mixed acid required to efficiently carry out each of the above reactions is different, reflecting the relative ease with which nitration is accomplished. Thus, Reaction 3 is usually conducted at relatively low temperatures (40° to 50°C) with weak acid solutions, while reactions 4 and 5 require progressively higher temperatures (60° to 100°C) and stronger acid mixtures to be driven to the desired degree of completion.

The strength of mixed acid is usually determined by the amount of water present. In aqueous media Reaction 1 controls the generation of nitronium ions. However, when nitration is conducted in an anhydrous medium, the acid mixture consists of nitric acid and oleum (100% H_2SO_4 in which SO_3 dissolved) and the controlling nitronium ion generation equilibria are:

$$HNO_3 + 2H_2S_2O_7 \rightleftharpoons NO_2^+ + HS_2O_7^- + 2H_2SO_4 \qquad (6)$$

$$HNO_3 + HS_2O_7^- \rightleftharpoons NO_2^+ + 2HSO_4^- \qquad (7)$$

It is also worth noting that Reactions 3, 4, and 5 are highly exothermic.

Although not shown in Reactions 3 through 5, a significant amount of isomerism occurs, resulting in the production of a variety of nitrated components in addition to the desired α-TNT. A complete description of the isomerism in toluene nitration with relative amounts of each component formed is given in Figure 1. The relative amounts of isomers formed depend upon nitrating temperature and acid composition. Thus Figure 1 must be viewed as a typical distribution only. In the continuous TNT process at Radford Army Ammunition Plant, only the α, β, γ, and ε isomers have been positively identified, although by the analytical technique used on process samples, it is not possible to separate the α and η isomers (Ref 4).

In addition to its function as a nitrating agent, nitric acid also plays the role of an oxidant under the usual conditions found in toluene nitration reactions. All nitrated components are capable of undergoing some form of oxidation. Two types of oxidation reactions are observed: those which result in destruction of the aromatic ring, yielding gaseous products, and those which result in oxidation of the methyl group or hydroxylation of the aromatic ring, yielding stable organic compounds. Typically, MNT undergoes hydroxylation to the cresol which is later destructively oxidized to gaseous products; DNT undergoes complete ring destruction

to yield CO_2, CO, NO, NO_2 and tetranitromethane (TNM); and TNT undergoes methyl group oxidation to yield a variety of organic products as shown in Figure 2.

In a typical nitration of toluene to TNT, isomerism and oxidation account for a yield loss of about 8 to 10% based on molar feed of toluene.

PROCESS DESCRIPTION

The continuous TNT process, which is the subject of the simulation study, is an adaptation of technology developed by Canadian Industries Limited and is currently the only continuous process for manufacture of TNT operating in the United States.

Nitration is carried out in a series of six reaction stages, each consisting of a 425-gallon nitrator and a 150-gallon separator, except for Stages 1 and 3 which have two nitrators. Because of the ratios of mixed acid to toluene employed in the process, a two-phase system results, with nitration occurring in the acid phase as diffusion and solubility phenomena establish equilibrium concentrations of the organic species in that phase. Separation of organic and acid phases is carried out after each nitration stage and enables countercurrent flow of the reactants to be maintained. A flow diagram of the nitration section of the process is shown in Figure 3, and a detailed diagram of a nitrator/separator nitration stage is shown in Figure 4.

In the countercurrent process, all of the toluene is introduced into the first stage, where mononitration and a small amount of dinitration occurs. After separation, this so-called "nitrobody" stream moves forward through the reactor train, becoming more highly nitrated as it progresses from vessel to vessel. Oleum is fed to Stage 6 and by means of the mixed acid recycle streams, moves in the opposite direction, decreasing in strength as it flows toward Stage 1. Nitric acid is added to each stage in order to maintain the correct mixed acid composition. Mixed acid recycle streams also contain some dissolved nitrobody as well as nitrosylsulfuric acid ($HNOSO_4$) which forms as a result of the oxidation side reactions.

As pointed out previously, nitration becomes progressively more difficult as the number of nitro groups on the aromatic ring of the substrate increases. Thus, the temperature as well as the mixed acid strength

must increase from Stage 1 to Stage 6. Nominal temperatures for the eight nitrators are 55, 50, 70, 80, 85, 90, 95, and 100°C respectively.

From Figure 4 it is seen that a nitrator is a cylindrically shaped vessel with an agitator fitted inside a draft tube at the center. The agitator provides the required interphase mixing in the nitrator and also creates a head difference between material on either side of the draft tube which in turn provides the motive force for fluid flow. There are no pumps in the system. Rapid internal circulation of material over the nitrator's cooling coils is maintained. There is also a recycle of acid between the separator and its own nitrator (internal recycle). Flow of this stream can be adjusted to maintain proper cooling in the separator or to change the acid-to-nitrobody ratio and residence time in the nitrator.

The acid stream flowing from a separator to the previous nitration stage (external recycle) passes through a weir-like device called a decanter. By adjusting this apparatus, the nitrobody/acid interface in the separator can be regulated to insure adequate phase separation. However, under normal operating conditions of 55 tons per day TNT production, a significant amount of entrainment still occurs, especially in Separator 3.

The crude TNT leaving Separator C flows to the purification section where residual nitrating acid and asymmetrical isomers are removed prior to final packaging of the product.

DEVELOPMENT OF THE MATHEMATICAL MODEL

The Single Vessel Model

The majority of the work conducted under the TNT process computer simulation effort has been devoted to the construction of a mathematical model which describes the nitration section of the process in terms of the kinetic and mass transfer phenomena which are believed to occur there and account for most of the process' behavior. As previously indicated, models of the purification section and of the hydraulic phenomena which govern fluid flow in a given nitration stage have also been developed but will not be discussed in this volume.

The kinetic and mass transfer model of the nitration section of the process (hereafter called the nitration section model) is the end product of numerous refinements and improvements which have been made to a first-generation model developed for Picatinny Arsenal in May 1970 by Kinotrol, Inc. of Houston, Texas, functioning as a consultant to ICIUS at Volunteer Army Ammunition Plant in Chattanooga, Tennessee. The structure and contents of the original nitration section model can be found in Reference 1.

As in the original, a fundamental approach was taken in developing the present nitration section model. Wherever possible, theoretical equations are employed to represent the chemical and physical phenomena which govern the nitration process. The use of empirically derived equations and correlations is kept to a minimum and has been resorted to only after exhaustive research for theoretical alternatives proved fruitless. Phenomena described by the model include kinetics of nitration and oxidation of organic species, diffusion of the organic species between the acid and organic phases, solubility of organic species in the acid phase, and solubility of nitric acid in the organic phase. The way in which real plant data was used in the development of the nitration section model will be described when parameter fitting is explained in a later section of this report.

The easiest way to explain the nitration section model is to take a single vessel in the nitration train (there are 14 vessels in series) and develop a complete material balance for each component in both acid and organic phases. The generalized nitrator in Figure 5 showing actual stream flows could be used for this purpose. However, the analysis is far simpler if each stream is broken down into its acid and organic phases with the subsequent addition of similar phases, so that the vessel input and output consist of a single acid phase, A, a single organic phase P, and a gas phase, G. Figure 6 illustrates this simplifying concept. Thus, for component i in the acid phase, a mole balance can be written as:

(Rate of moles i in with A_o) +

(Rate of generation of moles i in the acid phase within nitrator n) − (Rate of moles i out with A_n) = (Rate of accumulation of moles i within the acid of nitrator n) (1)

The balance for component i in the organic phase follows the same form as Equation 1. For the gas phase, the balance is simplified by the fact that products of the gaseous reaction are insoluble in both the acid and organic phases. Thus,

(Rate of generation of gaseous species i in nitrator n) = (Rate of gaseous i out with G_n) (2)

For a specific component, say α-TNT, the molar balances for vessel n are written as:

$$A^{o}_{n,\alpha\text{-TNT}} + \Sigma S^{A}_{n,\alpha\text{-TNT}} - A_{n,\alpha\text{-TNT}} = \frac{dA_{n,\alpha\text{-TNT}}}{dt} \quad (3)$$

for the acid phase, where S^A is the acid phase generation term, and

$$P^{o}_{n,\alpha\text{-TNT}} + \Sigma S^{P}_{n,\alpha\text{-TNT}} - P_{n,\alpha\text{-TNT}} = \frac{dP_{n,\alpha\text{-TNT}}}{dt} \quad (4)$$

for the organic phase, where S^P is an organic phase generation term. The assumption of a perfectly backmixed reactor allows for the equivalency of the reactor contents and the reactor outflow.

Equations similar to 3 and 4 can be written for all the components in each phase for every vessel in the nitration train. In the current version of the nitration section model, 10 chemical components are considered in the organic phase, 14 in the acid phase, and 3 in the gaseous effluent (see Figure 8). Before proceeding further, a few comments on these components are in order. First, all nitrobody components originating from m-MNT have been lumped together in the m-DNT and m-TNT terms in order to simplify the kinetics of the asymmetrical isomer reactions. Secondly, a single term, TNBX, is used to represent all components other than TNB formed from methyl group oxidation of TNT. This includes trinitrobenzyl alcohol, trinitrobenzaldehyde, and trinitrobenzoic acid. Lumping of oxidation products into one term was necessitated by a lack of process data for these components, and is justified considering the small concentration of each component which is present.

Thus, from Equations 3 and 4, it can be seen that for a given vessel the model consists essentially of a series of first order, non-linear, coupled, ordinary differential equations which make up the vessel's material balance.

The way in which the individual vessels are connected and the procedure for generating the flow and composition of the actual process streams from the ideal phases will be discussed at length in later sections of this report.

The heart of the vessel material balance equations and therefore the heart of the nitration section model is the generation terms. These terms are actually equations which represent the kinetic, mass transfer, and solubility processes occurring within a given vessel. For each component balance equation, three generation terms exist: reaction rate ($R_{n,i}$), diffusion ($D_{n,i}$), and bulk mass transport ($M_{n,i}$).

Thus Equation 3 can be rewritten as:

$$A^{O}_{n,\alpha TNT} + R^{A}_{n,\alpha TNT} + D^{A}_{n,\alpha TNT} + M^{A}_{n,\alpha TNT} - A_{n,\alpha TNT} = \frac{dA_{n,\alpha TNT}}{dt} \quad (5)$$

Since it is widely accepted that all reactions occur in the acid phase, it follows that $R^{P}_{n,i} = 0$. Also mass transfer into the acid phase must be at the expense of material in the organic phase so that $D^{P}_{n,\alpha TNT} = -D^{A}_{n,\alpha TNT}$ and $M^{P}_{n,\alpha TNT} = -M^{A}_{n,\alpha TNT}$. Thus, Equation 4 can be written as:

$$P^{O}_{n,\alpha TNT} - D_{n,\alpha TNT} - M_{n,\alpha TNT} - P_{n,\alpha TNT} = \frac{dP_{n,\alpha TNT}}{dt} \quad (6)$$

Note that there is no longer a need for acid and organic phase superscripts on the mass transfer terms. Development of the generation terms $R^{A}_{n,i}$, $D_{n,i}$, and $M_{n,i}$ will now be discussed in detail.

Reaction Kinetics

Reaction rate expressions have been developed to represent the nitration and oxidation of toluene and its nitro-substituted derivatives at each stage in the reactor train. The stoichiometric reations which are considered in the nitration section model include:

Nitration

$$\text{Toluene} + HNO_3 \longrightarrow \alpha MNT + H_2O \qquad \text{(Reaction 1)}$$
$$\text{Toluene} + HNO_3 \longrightarrow mMNT + H_2O \qquad \text{(Reaction 2)}$$

$$\alpha MNT + HNO_3 \longrightarrow \alpha DNT + H_2O \qquad \text{(Reaction 3)}$$
$$mMNT + HNO_3 \longrightarrow mDNT + H_2O \qquad \text{(Reaction 4)}$$

$$\alpha DNT + HNO_3 \longrightarrow \alpha TNT + H_2O \qquad \text{(Reaction 5)}$$
$$mDNT + HNO_3 \longrightarrow mTNT + H_2O \qquad \text{(Reaction 6)}$$

Oxidation

$$DNT + 13HNO_3 + 11H_2SO_4 \longrightarrow TNM + 6CO_{1.5} + 11HNOSO_4 + 15H_2O \qquad \text{(Reaction 7)}$$

$$DNT + 12\tfrac{1}{2}HNO_3 + 14\tfrac{1}{2}H_2SO_4 \longrightarrow 7CO_{1.5} + 14\tfrac{1}{2}HNOSO_4 + 16\tfrac{1}{2}H_2O \qquad \text{(Reaction 8)}$$

$$HNOSO_4 + \left(\frac{r+2}{3}\right) H_2O + r\,[O] \longrightarrow H_2SO_4 + \left(\frac{2-2r}{3}\right) NO + \left(\frac{1+2r}{3}\right) HNO_3 \qquad \text{(Reaction 9)}$$

$$4TNT + 9HNO_3 + 9H_2SO_4 \longrightarrow TNBOH + TNBAL + TNBA + TNB + CO_2 + 12H_2O + 9HNOSO_4 \qquad \text{(Reaction 10)}$$

It is pointed out that Reactions 1 through 10 are not mechanistic equations but rather stoichiometric equations which account for the appearance and disappearance of the various chemical components during the nitration process.

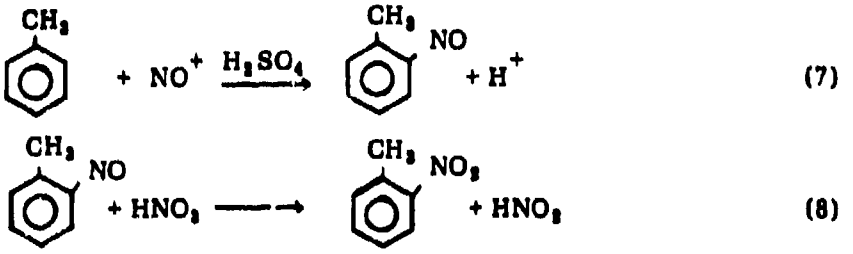
As mentioned briefly in the section on process chemistry, aromatic nitration in mixed acid occurs via electrophillic substitution, where in most instances the electrophile has been proven to be the nitronium ion.

However, it has also been well established (Ref 6) that as the molar ration of water to sulfuric acid in the mixed acid increases to unity, the

concentration of NO_2^+ falls off rapidly to nearly spectroscopically undetectable levels. Thus, in the case where $[H_2O]/[H_2SO_4] > 1$ (the weak acid region) and nitration is still seen to occur at a rapid rate, either the aromatic substrate is reactive enough to require only trace amounts of nitronium ion for reaction to proceed, or another nitration mechanism, say one dependent on molecular nitric acid is in effect. The former is more likely but the latter cannot be ruled out.

In the continuous TNT process, all of the monitration and a significant amount of dinitration occurs in mixed acid where $[H_2O]/[H_2SO_4] > 1$, so that in developing a kinetics model for this weak acid region one of the two mechanism hypothesis must be chosen . It was first decided to test both hypotheses against actual process performance data. While the nitronium ion mechanism was eventually shown to be preferable and was subsequently included in the overall nitration section model, a detailed description at the weak acid model based on molecular nitric acid is nevertheless also presented here for reasons of completeness.

The molecular nitric dependent weak acid kinetics model was based on the work of Kobe and Lakemeyer (Ref 7) and McKinley and White (Ref 8) who investigated the factors affecting the mononitration of toluene in mixed acid where the molar ratio of water to sulfuric acid was greater than two. A mechanism is proposed whereby the nitrosonium ion, NO^+, is first formed, then attacks the benzene ring and is subsequently oxidized by nitric acid to yield the mononitrated product. This mechanism can be represented as follows:



(7)

(8)

Although not definitively stated in the literature, Equation 8 appears to be the rate limiting step since data taken by McKinley and White show a strong dependence on the concentration of molecular nitric acid in the acid phase. McKinley and White's nitration studies also indicate that the sulfuric acid concentration has a significant influence on the rate of toluene

nitration in weak acid. Finally, Kobe and Lakemeyer demonstrated that the presence of nitrosylsulfuric acid in weak nitrating acid mixtures causes a maximum in the rate at 4 mole % $HNOSO_4$.

All of the above observed behavior was combined to yield an expression for the bimolecular rate constant for nitration in weak acid. This expression should be applicable to toluene, MNT, or DNT as long as the conditions of a weak acid nitrating medium are met. The form of this expression is:

$$\text{Rate}_N = \frac{d[N]}{dt} = k_2 \, [HNO_3] \, [M] \qquad (9)$$

$$k_2 = [H_2SO_4]^c \, 10^{-a^2 (x_{HNOSO_4} - .04)^2} \qquad (10)$$

where [M] is the concentration of the organic reactant in the acid phase;
[N] is the concentration of the organic product in the acid phase;
x_{HNOSO_4} is the mole fraction nitrosylsulfuric acid in the acid phase;
and a and c are adjustable parameters.

The dependence of weak acid nitration reactions on temperature was expressed through an Arrhenius-type relationship and, reaction was limited to the acid phase. Thus, Equations 9 and 10 can be restated as:

$$\text{Rate}_N = \frac{d[N]}{dt} = k_N \, e^{-\frac{E_n}{R}\left(\frac{1}{T} - \frac{1}{T_R}\right)} \, [M] \, \delta \qquad (11)$$

$$\delta = V_a \, [HNO_3] \, [H_2SO_4]^c \, 10^{-a^2 (X_{HNOSO_4} - .04)^2} \qquad (12)$$

where V_a is the volume of the acid phase;

k_N is the Arrhenius frequency factor;

E_N is the activation energy; and

T_R is a reference temperature.

Plant data for the continuous process at Radford indicates that toluene will react to mononitrotoluene just as fast as it can diffuse into the acid phase. Thus for Reactions 1 and 2, mass transfer is the limiting factor and the weak acid kinetics developed above are of academic interest only. However, for conversion of MNT to DNT in weak acid, the weak acid mechanism would apply.

The above model is obviously based on rather unstable theoretically grounds and even though a reasonably good fit to plant data was achieved with it, it was scraped in favor of a more theoretically consistent nitronium ion dependent system of equations.

In this approach the reaction rate is still expressed as in Equation 9; however the expression for k_2 is simply:

$$k_2 = V_a K_N Q \tag{12a}$$

where:

$$K_N = k_N e^{-\frac{E_N}{R}\left(\frac{1}{T} - \frac{1}{T_R}\right)} \tag{12b}$$

$$Q = \frac{[NO_2^+]}{[HNO_3]} \tag{12c}$$

Utilization of this model depends on the ability to compute the nitronium concentration from the equilibrium reactions which are in effect. The controlling equilibria are chosen to be (Ref 18):

$$HNO_3 + H_2SO_4 \rightleftharpoons NO_2^+ + HSO_4^- + H_2O \tag{12d}$$

$$H_2O + H_2SO_4 \rightleftharpoons H_3O^+ + HSO_4^- \tag{12e}$$

The procedure by which the NO_2^+ concentration is calculated follows below.

In the weak acid region, the initial and equilibrium concentrations are given as:

Component	Initial	At Equilibrium
HNO_3	$[HNO_3]_o$	$[HNO_3]$
H_2SO_4	$[H_2SO_4]_o$	$[H_2SO_4]$
H_2O	$[H_2O]_o$	$[H_2O]$
NO_2^+	0	$[NO_2^+]$
H_3O^+	0	$[H_3O^+]$
HSO_4^-	0	$[HSO_4^-]$

By writing material balances for each chemical element, a system of equations can be developed which, in conjunction with the equilibrium Equations 12d and 12e, can be used to solve for the desired NO_2^+ concentration at equilibrium. The elemental material balances are based on the necessary equivalance of the moles of chemical elements present initially and the moles of chemical elements present at equilibrium.

For Nitrogen:

$$[HNO_3]_o = [HNO_3] + [NO_2^+] \qquad (12f)$$

For Sulfur:

$$[H_2SO_4]_o = [H_2SO_4] + [HSO_4^-] \qquad (12g)$$

For Oxygen:

$$[H_2O]_o + 3[HNO_3]_o + 4[H_2SO_4]_o = [H_2O]$$

$$+ 3[\quad\quad 4[H_2SO_4] + 2[NO_2^+]$$

$$+ 4[HSO_4^-] + [H_3O^+] \qquad (12h)$$

Making use of Equations 12f and 12g in Equation 12h gives:

$$[H_2O]_o + [NO_2^+] = [H_2O] + [H_3O^+] \qquad (12i)$$

For Hydrogen:

$$2[H_2O]_o + [HNO_3]_o + 2[H_2SO_4]_o = 2[H_2O]$$

$$+ [HNO_3] + 2[H_2SO_4] + [HSO_4^-]$$

$$+ 3[H_3O^+] \qquad (12j)$$

Multiplying Equation 12i by 2 and subtracting from Equation 12j gives:

$$[HNO_3]_o - 2[NO_2^+] + 2[H_2SO_4]_o = [HNO_3]$$

$$+ 2[H_2SO_4] + [HSO_4^-] + [H_3O^+] \qquad (12k)$$

And subtracting Equations 12f and g from Equation 12k and gives:

$$[HSO_4^-] = [H_3O^+] + [NO_2^+] \qquad (12l)$$

Now, let the initial concentrations be given as:

$$[H_2O]_o = W$$

$$[H_2SO_4]_o = S$$

$$[HNO_3]_o = F$$

and the equilibrium concentrations of nitronium and bisulfate ions be given as x and y respectively. Then at equilibrium, the concentration of the remaining components can be expressed as:

$[HNO_3] = F-x$ (from Eq 12f)

$[H_2SO_4] = S-y$ (from Eq 12g)

$[H_3O^+] = y-x$ (from Eq 12ℓ)

$[H_2O] = W + x - (y-x)$ (from Eq 12i)

The equilibrium constant for Equation 12d is given by:

$$K_1 = \frac{[NO_2^+]\,[HSO_4^-]\,[H_2O]}{[H_2SO_4]\,[HNO_3]} = \frac{(x)\,(y)\,(W+2x-y)}{(s-y)\,(F-x)} \qquad (13)$$

and that for Equation 12e by:

$$K_2 = \frac{[H_3O^+]\,[HSO_4^-]}{[H_2O]\,[H_2SO_4]} = \frac{(y-x)\,(y)}{(W+2x-y)\,(S-y)} \qquad (14)$$

Based on the impossibility of negative concentrations, the assumed existence of all possible components at equilibrium, the following constraints must apply:

$0 < x < y$ if $y < F$

$0 < x < F$ if $F < y$

$0 < y < (W+2x)$ if $(W+2x) < S$

$0 < y < S$ if $S < (W+2x)$

Knowing K_1, K_2, F, W, and S, and utilizing the above constraints, Equations 13 and 14 can be solved for x, the nitronium ion concentration at equilibrium. From Equation 14,

$$x = \frac{y^2 - K_2\,(S-y)\,(W-y)}{2K_2\,(S-y) + y} \qquad (15)$$

Equation 15 can be solved for x and y by an interval halving procedure after which the solution values can be substituted in Equation 13 to give

a value of K_1. If convergence on K_1 is not achieved, the procedure is repeated using the current value of y to adjust the upper or lower boundary of the solution interval for x. In actual execution of the model, between 20 and 40 iterations are required to converge on K_1 for each pass through the vessel equations.

Before moving on to the strong acid region it should be pointed out that a general mechanism for aromatic nitration in aqueous mixed acid has been proposed (Ref 9) based on activity coefficients, but lack of data prevented using it in the nitration section model. An attempt was made, however, to do without any theoretically based weak acid mechanism and just use a curve fit of laboratory data developed by Vinnik (Ref 10) for nitration of p-MNT in mixed acid. The lower end of the curve had to be extrapolated since no data was provided for H_2SO_4 concentrations less than 80%. In all cases, the weak acid mechanism of Equations 9, 12a, 12b and 12c gave far better agreement with observed plant behavior, and it is these equations that constitute the current model.

For strong acid nitration (i.e. $[H_2O]/[H_2SO_4] < 1$) it is firmly established that the nitronium ion is the active nitrating species. Bennett (Ref 11) developed an expression for the bimolecular nitration rate constant, k_2, in the reaction

$$\frac{d[TNT]}{dt} = k_2 [HNO_3][DNT] \qquad (16)$$

where the dependence on the NO_2^+ ion concentration as well as the concentration of proton acceptor components (HSO_4^-, H_2SO_4, and $HS_2O_7^-$) are considered. Bennett's expression is given as follows:

$$k_2 = Q\left(k' [HSO_4^-] + k'' [H_2SO_4]\, k''' [HS_2O_7^-]\right) \qquad (17)$$

where $Q = \dfrac{[NO_2^+]}{[HNO_3]}$

In order to use Bennett's equation to represent strong acid nitration it is necessary to determine the nitronium and proton acceptor ion concentrations throughout the nitration section of the process. In the model, four strong acid regions are defined in which these ions should exist, and

then equilibrium equations are established which allow calculation of the ionic component concentrations. The first two regions are exactly those dealt with by Bennett. However the third and fourth regions have apparently never been examined experimentally so that the hypothesis presented below constitutes an extension of existing theory.

The first region (aqueous region) is characterized by the presence of water subject to the constraint $[H_2O]/[H_2SO_4] < 1$. The equilibria established in this situation are exactly those of Equations 12d and 12e for which the procedure to determine the equilibrium concentrations has been given.

The remaining three regions are water free, with nitric, sulfuric, and pyrosulfuric ($H_2S_2O_7$) acids making up the nitrating acid. These will be referred to as oleum regions.

In the first oleum region (nitric limited), pyrosulfuric acid is in large excess of the nitric acid to the extent that

$$[HNO_3] \leq .5\,[H_2S_2O_7]$$

This is the strong oleum region described by Bennett. The equilibria governing concentrations in this region are:

$$HNO_3 + 2H_2S_2O_7 \rightleftharpoons NO_2^+ + HS_2O_7^- + 2H_2SO_4 \qquad (18)$$

$$H_2SO_4 + H_2S_2O_7 \rightleftharpoons H_3SO_4^+ + HS_2O_7^- \qquad (19)$$

Equation 18 is believed to go completely to the right, thus leaving Equation 19 as the limiting equilibrium. A two-step reaction occurs, the nitric acid first completely dissociating to nitronium ions via Equation 18, followed by the establishment of equilibrium among sulfuric, pyrosulfuric acids and their ionic counterparts via Equation 19. The concentrations are represented as follows:

	Initial	After 18	After 19 (Equilibrium)
HNO_3	$[HNO_3]_o$	0	0
$H_2S_2O_7$	$[H_2S_2O_7]_o$	$[H_2S_2O_7]_o - 2[HNO_3]_o$	$[H_2S_2O_7]_o - 2[HNO_3]_o - Y$
H_2SO_4	$[H_2SO_4]_o$	$[H_2SO_4]_o + 2[HNO_3]_o$	$[H_2SO_4]_o + 2[HNO_3]_o - Y$
$HS_2O_7^-$	0	$[HNO_3]_o$	$[HNO_3]_o + Y$
NO_2^+	0	$[HNO_3]_o$	$[HNO_3]_o$
$H_2SO_4^+$	0	0	Y

where Y is the concentration of $HS_2O_7^-$ formed via Equation 19. The mass action expression for Equation 19 is:

$$K_{eq} = \frac{[H_2SO_4^+]\ [HS_2O_7^-]}{[H_2SO_4][H_2S_2O_7]} \qquad (20)$$

Substitution of the tabulated values yields:

$$K_{eq} = \frac{Y([HNO_3]_o + Y)}{([H_2SO_4]_o + 2[HNO_3]_o - Y)\ ([H_2S_2O_7]_o - 2[HMO_3]_o - Y)} \qquad (21)$$

If K_{eq} and initial concentrations are known, Y can be found by successive iterations of Equation 21. Bennett has suggested a value of 1.0 for K_{eq}.

In the second oleum region (intermediate), the pyrosulfuric acid is in moderate excess of the nitric such that:

$$.5[H_2S_2O_7] < [H_{\ \ ,}] \leq [H_2S_2O_7]$$

The dominant equilibria in effect here are (Ref 19):

$$HNO_3 + 2H_2SO_7 \rightleftharpoons NO_2^+ + HS_2O_7^- + 2H_2SO_4 \qquad (22)$$

$$HNO_3 + 2H_2SO_4 \rightleftharpoons NO_2^+ + H_3O^+ + 2HSO_4^- \qquad (23)$$

$$H_3O^+ + HS_2O_7^- \rightleftharpoons 2H_2SO_4 \qquad (24)$$

Again it is assumed that Equation 22 goes completely to the right. Because of the limits imposed on the nitric acid concentration, it must be true that the nitric acid remaining undissociated after reacting with $H_2S_2O_7$ (Eq 22) must always be less than the $HS_2O_7^-$ formed by the same reaction. Thus, there will always be enough $HS_2O_7^-$ present to soak up all of the H_3O^+ formed via equilibrium Equation 23. This continuously drives Equation 23 to the right until all the remaining nitric acid is completely converted to nitronium ions. Equations 23 and 24 can be added to give

$$HNO_3 + HS_2O_7^- \longrightarrow NO_2^+ + 2HSO_4^- \qquad (25)$$

In effect a two-step reaction occurs. Nitric acid reacts with the pyrosulfuric acid via Equation 22, and then the remaining undissociated nitric acid reacts completely with the $HS_2O_7^-$ produced from the first reaction. Both reactions go to completion and no equilibria are in effect. Concentrations are as follows:

	Initial	After 22	After 25
$H_2S_2O_7$	$[H_2S_2O_7]_0$	0	0
H_2SO_4	$[H_2SO_4]_0$	$[H_2SO_4]_0 + [H_2S_2O_7]_0$	$[H_2SO_4]_0 + [H_2S_2O_7]_0$
NO_2^+	0	$.5[H_2S_2O_7]_0$	$[HNO_3]_0$
$HS_2O_7^-$	0	$.5[H_2S_2O_7]_0$	$[H_2S_2O_7]_0 - [HNO_3]_0$
HSO_4^-	0	0	$2[HNO_3]_0 - [H_2S_2O_7]_0$
HNO_3	$[HNO_3]_0$	$[HNO_3]_0 - .5[H_2S_2O_7]_0$	0

While Gillespie maintains that Equation 25 is completely to the right, there is some basis for the occurrance of the reverse reaction (Ref 20). For this reason, the model has been structured so that, as an option, Equation 25 can be treated as an equilibrium with

$$K_{eq} = \frac{[HNO_3][HS_2O_7^-]}{[NO_2^+][HSO_7^-]^2} \qquad (25a)$$

Initial concentrations are assumed to be those existing after Equation 25 has gone completely to right at which time NO_2^+ and HSO_4^- begin to recombine via the reverse reaction. Equilibrium concentrations are found by assuming a value for K_{eq} and solving Equation 25a by interval halving.

In the third oleum region (oleum limited), nitric acid exists in excess of pyrosulfuric acid, i.e. $[HNO_3] > [H_2S_2O_7]$. The same equilibria are in effect here as in the intermediate region, but now Equation 25 can apply only until the $HS_2O_7^-$ produced by Equation 22 is completely dissipated. There will still be some undissociated nitric remaining which must then undergo equilibrium dissociation via Equation 23. In effect, a three-step reaction takes place: 1) Nitric acid → NO_2^+ in the presence of $H_2S_2O_7$, 2) Nitric acid → NO_2^+ via Equation 25 until all the $HS_2O_7^-$ is dissipated, and 3) Equilibrium dissociation of the remaining nitric acid via Equation 23. Concentrations are as follows:

	Initial	After 22	After 25	After 23 (Equilibrium)
HNO_3	$[HNO_3]_0$	$[HNO_3]_0 - .5[H_2S_2O_7]_0$	$[HNO_3]_0 - [H_2S_2O_7]_0$	$[HNO_3]_0 - [H_2S_2O_7]_0 - z$
$H_2S_2O_7$	$[H_2S_2O_7]_0$	0	0	0
H_2SO_4	$[H_2SO_4]_0$	$[H_2SO_4]_0 + [H_2S_2O_7]_0$	$[H_2SO_4]_0 + [H_2S_2O_7]_0$	$[H_2SO_4]_0 + [H_2S_2O_7]_0 - 2z$
NO_2^+	0	$.5[H_2S_2O_7]_0$	$[H_2S_2O_7]_0$	$[H_2S_2O_7]_0 + z$
$HS_2O_7^-$	0	$.5[H_2S_2O_7]_0$	0	0
HSO_4^-	0	0	$[H_2S_2O_7]_0$	$[H_2S_2O_7]_0 + 2z$
H_3O^+	0	0	0	z

where z is the concentration of nitronium ions formed via the equilibrium Equation 23.

As before, the mass action expression for Equation 23 is:

$$K_{eq} = \frac{[NO_2^+][H_3O^+][HSO_4^-]^2}{[HNO_3][H_2SO_4]^2} \qquad (26)$$

Substitution of the appropriate tabulated values into Equation 26 gives:

$$K_{eq} = \frac{([H_2S_2O_7]_o - z)(z)([H_2S_2O_7]_o + 2z)^2}{([HNO_3]_o - [H_2S_2O_7]_o - z)([H_2SO_4]_o + [H_2S_2O_7]_o - 2z)^2} \qquad (27)$$

If K_{eq} and the initial concentrations are known, z can be found by successive iteration of Equation 27.

As was done for the second oleum region, provision has been made to consider recombination of NO_2^+ and HSO_4^- via Equation 25. If this option is chosen in the model, Equations 23 and 25a must be solved simultaneously to give the equilibrium concentrations of the various ionic species. A procedure analogous to that used in the weak acid region to solve Equations 12d and 12e is employed.

Now, knowing initial concentrations, and having solved for the appropriate concentrations at equilibrium, Bennett's proposed rate expression can be applied to strong acid nitration as follows:

$$\frac{d[N]}{dt} = (k'[HSO_4^-] + k''[H_2SO_4] + k'''[HS_2O_7^-])[M][HNO_3]_o Q \qquad (28)$$

where Q is the fraction of nitric acid existing as nitronium ions;
[M] is the concentration of nitrotoluene reactant;
[N] is the concentration of nitrotoluene product; and
k', k'', and k''' are rate constants.

It is emphasized that Equation 28 is continuous over the four strong acid regions previously described.

The influence of temperature upon reaction rate is taken into account by assuming, as Bennett did, that the constants k', k'', and k''' exhibit an Arrhenius dependence.

Thus, Equation 28 can be rewritten as:

$$\frac{d[N]}{dt} = k_N \, e^{\frac{-E_N}{R}\left(\frac{1}{T} - \frac{1}{T_R}\right)} (k_a [HSO_4^-] + k_b [H_2SO_4]$$

$$+ k_c [HS_2O_7^-]) [M] [HNO_3]_o \, Q \qquad (29)$$

and Equation 29 can be further simplified,

$$\text{Rate}_N = k_N \, e^{\frac{-E_N}{R}\left(\frac{1}{T} - \frac{1}{T_R}\right)} [M] \, \gamma \qquad (30)$$

$$\gamma = V_a (k_a [HSO_4^-] + k_b [H_2SO_4] + k_c [HS_2O_7^-]) [HNO_3]_o \, Q \qquad (31)$$

where k_N and E_N are the velocity coefficient and activation energy associated with the nitration reaction:

$$M + HNO_3 \rightarrow N + H_2O$$

and V_a is the volume of the acid phase.

Subsequent to Bennett's work, strong experimental evidence was uncovered which contradicted a portion of his basic hypothesis. Melander demonstrated that proton departure from the transition compound during nitration is kinetically insignificant (Ref 12). Therefore, Bennett's contention that DNT nitration in mixed acid is a termolecular process dependent on both the nitronium ion and the proton acceptor ions, is most likely incorrect. In addition, for two-phase nitration systems, no maximum in

the rate at 92% H_2SO_4 has been noted.

Returning to Equations 16 and 17, it appears that there is sufficient justification to eliminate the proton acceptor component concentration terms from the expression for k_2 so that

$$k_2 = k' \frac{[NO_2^+]}{[HNO_3]} \qquad \text{and} \qquad (31a)$$

$$\gamma = V_a k_2 [HNO_3] \qquad (31b)$$

with the dependence of nitration on the concentrations of SO_3, H_2SO_4, and H_2O considered only in so far as those concentrations affect nitronium ion equilibria.

Although the nitration section simulation has been modified to utilize this simpler strong acid nitration model, the option to use Bennett's mechanism has been retained.

Far less is known about the kinetic mechanisms that govern the oxidation reactions which always occur to some extent during TNT manufacture along with the desired nitration reactions. With regard to oxidation, three key assumptions are made in the model: (1) oxidation reactions occur exclusively in the acid phase and therefore compete with the nitration reactions, (2) the controlling component in oxidation is the same as that which governs nitration (NO_2^+ ion), and (3) oxidation reactions exhibit bimolecular kinetics and are thus subject to the same reaction mechanisms as nitration. Also, because of a lack of plant data on cresol formation, oxidation of MNT 's not represented in the model. This however, is not a critical shortcoming since cresols are eventually destructively oxidized to gaseous products and their contribution to overall yield loss can be compensated for by adjustment of the DNT oxidation rates. Equations A-42 through A-55 are employed in the model to represent oxidation.

Diffusion

Diffusion, as employed in the nitration section model, is the process by which the nitrobody components move between the two phases after their acid phase saturation solubility has been reached. This phenomenon depends solely upon the concentration gradients of the nitrobody species

across each phase and on the fluid properties of the medium as reflected by the mass transfer coefficient.

At steady state, diffusion of components toward the acid/organic interface must be equal to that away from it.

Thus,

$$D_i = \eta_\varphi \ (y_i - y_i^*) = \eta_A \ (x_i^* - x_i) \tag{32}$$

where

$$x_i = \frac{A_i}{A_T} \text{ and } y_i = \frac{\varphi_i}{\varphi_T} \approx \frac{\varphi_i}{\varphi_{nb}} \tag{33}$$

(See Figure 8 for an explanation of the nomenclature.)

Now, if we assume that the acid phase is always saturated with nitrobody,

$$A_{nb} = X_{eq}^{A} \ A_T \tag{34}$$

$$A_T = \frac{A_{NB}}{X_{eq}^{A}} \tag{35}$$

so that by substitution of Equation 35 into Equation 33 we get

$$x_i = \frac{A_i}{A_{nb}} \ X_{eq}^{A} \tag{36}$$

At the interface, the two phases must be in equilibrium. The equilibrium relationship assumed to be in effect is that the mole fraction nitrobody component in the organic phase must be equal to the acid-free mole fraction of that component in the acid phase.

Thus, at the interface,

$$\frac{\varphi_i^*}{\varphi_{nb}^*} = \frac{A_i^*}{A_{nb}^*} \tag{37}$$

but $$A_{nb}^* = X_{eq}^A \, A_T^*$$

so that $$\frac{\varphi_i^*}{\varphi_{nb}^*} = \frac{A_i^*}{X_{eq}^A \, A_T^*} \tag{38}$$

or $$y_i^* = x_i^* / X_{eq}^A \tag{39}$$

Substitution of the expressions for y_i and y_i^* into Equation 32 gives

$$D_i = \eta_\varphi \left(\frac{\varphi_i}{\varphi_{nb}} - \frac{x_i^*}{X_{eq}^A} \right) \tag{40}$$

but also from Equation 32,

$$x_i^* = \frac{D_i}{\eta_A} + x_i \tag{41}$$

so that

$$D_i = \eta_\varphi \left[\frac{\varphi_i}{\varphi_{nb}} - \frac{\left(\frac{D_i}{\eta_A} + x_i \right)}{X_{eq}^A} \right] \tag{42}$$

$$D_i = \eta_\varphi \left(\frac{\varphi_i}{\varphi_{nb}} - \frac{D_i}{\eta_A X_{eq}^A} - \frac{x_i}{X_{eq}^A} \right) \qquad (43)$$

$$\frac{D_i}{\eta_\varphi} + \frac{D_i}{\eta_A X_{eq}^A} = \left(\frac{\varphi_i}{\varphi_{nb}} - \frac{x_i}{X_{eq}^A} \right) = \left(\frac{\varphi_i}{\varphi_{nb}} - \frac{A_i}{A_T X_{eq}^A} \right) \qquad (44)$$

$$D_i \left(\frac{1}{\eta_\varphi} + \frac{1}{\eta_A X_{eq}^A} \right) = \frac{\varphi_i}{\varphi_{nb}} - \frac{A_i}{A_{nb}} \qquad (45)$$

Now let $$\frac{1}{\eta} = \left(\frac{1}{\eta_\varphi} - \frac{1}{\eta_A X_{eq}^A} \right) \qquad (46)$$

so that $$D_i = \eta \left(\frac{\varphi_i}{\varphi_{nb}} - \frac{A_i}{A_{nb}} \right) \qquad (47)$$

Equation 47 is true for all organic components except toluene. For toluene, the reaction to MNT is so fast that it is assumed to occur at the interface, which eliminates the acid phase diffusion of toluene and forces A_{Tol} to be zero. Also the extremely rapid movement of toluene to the inter face warrants a separate mass transfer coefficient. Thus,

$$D_{Tol} = \eta_{Tol} \frac{\varphi_{Tol}}{\varphi_{nb}} \qquad (48)$$

As indicated previously, the rate of conversion of toluene to MNT via Reactions 1 and 2 is solely dependent upon the rate of toluene diffusion so that

$$R_1 + R_2 = D_{Tol}$$

$$\frac{R_1}{R_2} = \frac{D_{Tol}}{R_2} - 1 \tag{49}$$

However, the ratio of aMNT to mMNT produced is dependent on the kinetic expressions:

$$\frac{aMNT}{mMNT} = \frac{R_1}{R_2} = \frac{k_1 \, e^{-\frac{E_1}{R}\left(\frac{1}{T} - \frac{1}{T_R}\right)}}{k_2 \, e^{-\frac{E_2}{R}\left(\frac{1}{T} - \frac{1}{T_R}\right)}} \tag{50}$$

$$\frac{R_1}{R_2} = \left(\frac{k_1}{k_2}\right) e^{\left[-\frac{E_1}{R}\left(\frac{1}{T} - \frac{1}{T_R}\right) + \frac{E_2}{R}\left(\frac{1}{T} - \frac{1}{T_R}\right)\right]} \tag{51}$$

$$\frac{R_1}{R_2} = \left(\frac{k_1}{k_2}\right) e^{-\frac{(E_1 - E_2)}{R}\left(\frac{1}{T} - \frac{1}{T_R}\right)} \tag{52}$$

$$\frac{R_1}{R_2} = k_{12} \, e^{-\frac{(E_1 - E_2)}{R}\left(\frac{1}{T} - \frac{1}{T_R}\right)} \tag{53}$$

Substitution of Equation 49 into Equation 53 gives

$$\frac{D_{Tol}}{R_2} - 1 = k_{12}\, e^{-\frac{(E_1 - E_2)}{R}\left(\frac{1}{T} - \frac{1}{T_R}\right)} \qquad (54)$$

$$\frac{1}{R_2} = \frac{1 + k_{12}\, e^{-\frac{(E_1 - E_2)}{R}\left(\frac{1}{T} - \frac{1}{T_R}\right)}}{D_{Tol}} \qquad (55)$$

Now, since $k_{12}\, e^{-\frac{(E_1 - E_2)}{R}\left(\frac{1}{T} - \frac{1}{T_R}\right)} >>> 1$, we can rewrite Equation 55 as

$$R_2 = \frac{D_{Tol}}{k_{12}\, e^{-\frac{(E_1 - E_2)}{R}\left(\frac{1}{T} - \frac{1}{T_R}\right)}} \qquad (56)$$

$$R_2 = \frac{D_{Tol}}{k_{12}}\, e^{(E_1 - E_2)/R\left(\frac{1}{T} - \frac{1}{T_R}\right)} = \frac{D_{Tol}}{k_{12}}\, e^{-(E_2 - E_1)/R\left(\frac{1}{T} - \frac{1}{T_R}\right)} \qquad (57)$$

At this point, it should also be noted that while chemical reactions occur in both the nitrators and separators due to the ever present solubilised organic components in the acid phase, diffusion is assumed to be nonexistent in the separators because of the drastic reduction in interface area which occurs there.

Bulk Mass Transfer and Solubility

The remaining generation terms in the material balance equations (Equations 5 and 6) are those for bulk mass transfer. Bulk mass transfer, is in effect,the means by which equilibrium nitrobody solubility is enforced on the acid phase. At any point in the nitration section, the equilibrium amount of nitrobody in the acid phase is given by

$$A_{nb} = X_{eq}^{A} A_T \tag{58}$$

where X_{eq}^{A} has a value dependent on the local temperature as well as the local acid phase composition. For a given vessel, nitrobody is present in the acid phase by virtue of that which entered with the incoming acid phase, A_{nb}^{o}, that which diffused in from the organic phase, $\sum_{i=nb} D_i$, and that which resulted from a change in solubility created by combination of various vessel input streams which are obviously not in equilibrium. The last of these is considered the bulk mass transfer. Thus, to enforce equilibrium on the acid phase leaving the vessel, it must be true that

$$X_{eq}^{A} A_T = A_{nb}^{o} + \sum_{i=nb} D_i + M_{nb} \tag{59}$$

and

$$M_{nb} = X_{eq}^{A} A_T - A_{nb}^{o} - \sum_{i=nb} D_i \tag{60}$$

where M_{nb} represents the bulk movement of nitrobody into the acid phase which must occur in order to maintain equilibrium solubility. Negative values of M_{nb} are reasonable and indicate nitrobody dropping out of solution at the new vessel conditions. The individual component bulk mass transfer rates are computed from the overall bulk nitrobody transfer rate as follows:

$$M_i = \begin{cases} \dfrac{A_i}{A_{nb}} M_{nb} & \text{if } M_{nb} < 0 \\ \dfrac{\varphi_i}{\varphi_{nb}} M_{nb} & \text{if } M_{nb} \geq 0 \end{cases}$$

where the index i represents each nitrobody component. The change in acid phase nitrobody composition due to reaction is not included in the bulk mass transfer term since reaction only converts one nitrobody component to another and does not result in a net molar change.

An expression for the equilibrium solubility of bulk nitrobody in the acid phase has been developed by subjecting a limited quantity of published solubility data to a multiple regression procedure.* Solubility is correlated against temperature and acid phase composition to give:

$$x_{eq}^{A} = 10^{p} \tag{61}$$

where

$$p = 3.62 + .01023T - 3.808\, x_{H_2O} + 7.716\, x_{MNT} - 8.452\, x_{TNT} - 6.292\, x_{HNO_3} \tag{62}$$

*Laboratory solubility data for TNT, DNT, and MNT in mixed acid at various temperatures is currently being generated. This data, being more extensive than what is used for the existing solubility correlation, will be regressed to generate a new nitrobody solubility expression which is expected to significantly improve the nitration section model.

where

T is temperature in °K

x_{H_2O} is mole fraction water in acid phase

x_{MNT} is mole fraction MNT in acid phase

x_{TNT} is mole fraction TNT in acid phase

x_{HNO_3} is mole fraction nitric acid in acid phase

Finally, an expression has been developed to represent the solubility of nitric acid in the organic phase. It is the only acid component that shows any appreciable solubility in the organic phase. The expression used in the model is:

$$y_{HNO_3} = 1.51\, X_{H_2O}\left(\frac{x_{HNO_3}}{x_{H_2SO_4}}\right) \qquad (63)$$

Expressions for all of the terms in the vessel material balance equations (Equations 5 and 6) have now been developed so that if all vessel inputs are known and can be divided into acid and organic phase components, simultaneous solution of the vessel equations will give the output of that vessel in terms of moles per hour each component in each phase.

The vessel equations can be solved either for the transient state, in which case integration of the first order ordinary differential equations is required, or for the steady state, in which case the derivative terms are set equal to zero, resulting in a system of non-linear, simultaneous, coupled, algebraic equations. Both of these cases have been solved and the solution procedures including the computer programs generated will be described in detail in subsequent sections of this report.

Formulation of the Overall Nitration Section Model from the Single Vessel Model

Up to this point, discussion has centered around the details of the single vessel model without any regard to the way in which the complete 14-vessel nitration train (8 nitrators and 6 separators) is actually simulated. "Connection" of the individual vessels in the nitration section is

made possible by use of a physical separation model which takes the ideally separated organic and acid phses computed by the separator vessel model and constructs the three reel streams which actually flow to other vessels. These include the organic stream forward to the next nitrator, the internal acid recycle stream, and the external acid recycle stream to the previous nitration stage. Because the separation process is not ideal, a portion of the acid phase is entrained in the organic stream leaving the separator and similarly, a portion of the organic phase is entrained in the two exiting acid streams.

In developing the equations for the physical separation model, the entrainments are defined as follows:

e_{oa} = molar fraction of the acid recycle stream, both internal and external, which is entrained organic phase.

e_{ao} = molar fraction of the organic stream which is entrained acid phase.

The following assumptions are also made: (1) the composition of entrained material is the same as that of the bulk phase from which it originated, (2) the composition of the internal and external recycle streams are identical, and (3) the values for e_{oa} and e_{ao} are constant for a given separator.*

The separation process is described schematically in Figure 9. It is again stressed that this physical separation model operates on the contents of a separator after the kinetic and mass transfer processes in that separator have transpired.

*An option exists in the model whereby e_{oa} and e_{ao} can be computed based on correlations that were developed using linear multiple regression techniques. However, because of the relatively high standard error of estimate associated with the correlation coefficients, e_{oa} and e_{ao} are usually assigned their constant values.

Now, let

A_i = moles/hr of acid phase in Stream i

φ_i = moles/hr of organic phase in Stream i

Note that the flow rates A_0 and φ_0 of the acid and organic phases in the input stream are known.

First consider the separation of Stream 0 into Streams 1 and 2. From the definition of e_{oa} and e_{ao}:

$$e_{oa} = \frac{\varphi_1}{A_1 + \varphi_1} \tag{64}$$

$$e_{oa} = \frac{A_2}{A_2 + \varphi_2} \tag{65}$$

These can be converted into molar ratios as follows:

$$e'_{oa} = \frac{\varphi_1}{A_1} = \frac{e_{oa}}{1-e_{ao}} = \text{molar ratio of organic phase to acid phase in recycle streams.} \tag{66}$$

$$e'_{oa} = \frac{A_2}{\varphi_2} = \frac{e_{ao}}{1-e_{ao}} = \text{molar ratio of acid phase to organic phase in organic stream.} \tag{67}$$

Material balances around node A yield:

$$\varphi_0 = \varphi_1 + \varphi_2 \tag{68}$$

$$A_0 = A_1 + A_2 \tag{69}$$

Substituting Equation 66 for φ_1 and Equation 67 for A_2 gives:

$$\varphi_o = A_1 e'_{oa} + \varphi_2 \tag{70}$$

$$A_o = A_1 + \varphi_2 e'_{oa} \tag{71}$$

Eliminating φ_2 and rearranging, gives

$$f_{ar} = \frac{A_1}{A_2} = \frac{1-e'_{ao}\,\varphi_o/A_o}{1-e'_{ao}\,e'_{oa}} = \text{fraction of the entering acid phase that appears in the acid recycle stream.} \tag{72}$$

Solving Equation 70 for φ_2, substituting Equation 72, and rearranging gives:

$$f_{po} = \frac{\varphi_2}{\varphi_o} = 1 - f_{ar}\, e'_{oa}\, A_o/\varphi_o \tag{73}$$

From f_{po} and f_{ar} the composition of each component in the organic stream can readily be calculated. Let A_{ij} be the moles/hr of Component j in the acid phase of Stream i. Define φ_{ij} analogously to be the moles/hr of Component j in the organic phase of Stream i. For Stream 2, these can be computed as follows:

$$A_{2j} = (1-f_{ar})\, A_{oj} \tag{74}$$

$$\varphi_{2j} = f_{po}\, \varphi_{oj} \tag{75}$$

Stream 1 must now be separated into its internal and external recycle portions. The volumes of the entering phases (Stream 0)

can be computed from their compositions:

$Q_{\varphi o}$ = ft^3/hr of organic phase in Stream 0

Q_{Ao} = ft^3/hr of acid phase in Stream 0

$Q_{To} = Q_{\varphi o} + Q_{Ao}$ = total ft^3/hr for Stream 0.

The total flow of Stream 1 can be computed as:

$$Q_{T_1} = f_{ar} Q_{Ao} + (1-f_{po}) Q_{\varphi o} \qquad (76)$$

The fraction of Stream 1 that appears in Stream 3 (internal acid recycle) is:

$$f_{ir} = \frac{Q_{T3}}{Q_{T1}} = \frac{Q_{max} f(N)}{f_{ar} Q_{Ao} + (1-f_{po}) Q_{\varphi o}} \qquad (77)$$

where Q_{max} = maximum ft^3/hr of internal recycle (a known constant),

N = notch setting on a gate valve in the internal recycle line which is modeled as an equal percentage valve,

f(N) = fraction of maximum flow corresponding to the notch setting.

The flow rates of the individual components in each phase of Streams 3 and 4 can be computed as follows:

$$A_{3j} = f_{ir} f_{ar} A_{oj} \qquad (78)$$

$$\varphi_{3j} = f_{ir} (1-f_{po}) \varphi_{oj} \qquad (79)$$

$$A_{4j} = (1-f_{ir}) f_{ar} A_{oj} \qquad (80)$$

$$\varphi_{4j} = (1-f_{ir}) (1-f_{po}) \varphi_{oj} \qquad (81)$$

Thus it is seen that the composition of the separator outlet streams can be calculated by the physical separation model from the results of the separator vessel model and that this in turn forms the basis for connection of the six nitration stages. The way in which the stages are connected will become clearer in the next section of the report, which deals with the implementation of the vessel and physical separation models on a digital computer to form the complete nitration section simulation.

COMPUTER IMPLEMENTATION OF THE MATHEMATICAL MODEL - THE SIMULATION

Separate computer programs have been prepared to simulate both the dynamic and steady states of the nitration process. While differing in solution procedure, there is no difference in their basic structures; both are ways to solve the vessel equations to give vessel outputs for known inputs. In fact, the solution obtained by running the dynamic simulation long enough to reach steady state is exactly that obtained by executing the steady state simulation, within the limits of numerical accuracy. A complete list of the vessel equations (the mathematical model of any nitration section vessel) ordered according to a logical solution sequence is given in Appendix A.

The Dynamic Simulation

The dynamic simulation is a computer program which, for a given set of nitration section independent variables including (1) feed rates (lb/hr), (2) composition of raw materials (wt%), (3) nitrator temperatures (^{o}C), and (4) recycle notch settings, will operate upon the vessel and physical separation equations to give the composition and flow rate (moles/hr) of the exiting streams from each of the 14 process vessels as functions of time. A numerical integration technique known as Euler's Method is employed to solve the differential equations. Although this is the simplest of the many numerical integration algorithms available, its efficiency in solving the vessel equations is satisfactory.

Formulation of the Equations

In order to solve the unsteady state vessel equations via Euler's Method, it is first necessary to reformulate the continuous differential equations (Equations 5 and 6) into their discrete numerical equivalents.

For Component 1 (αMNT)*, Equation 5 is

$$A^{o}_{n,1} + R^{A}_{n,1} - R^{A}_{n,2} + D_{n,1} + M_{n,1} - A_{n,1} = \frac{d\,A_{n,1}}{dt} \quad (82)$$

and Equation 6 is

$$P^{o}_{n,1} - D_{n,1} - M_{n,1} - P_{n,1} = \frac{d\,P_{n,1}}{dt} \quad (83)$$

Equations 82 and 83 are not exactly correct since the units of all terms on the left side are moles/hr while those on the right are moles/hr^2. To correct for this, the derivatives are rewritten as:

$$\frac{d}{dt}\ (V_n\, f_A\, \rho_A\, x_{n,1}) \text{ for } \frac{d\,A_{n,1}}{dt}$$

and

$$\frac{d}{dt}\ (V_n\, (1-f_A)\, \rho_P\, y_{n,1}) \text{ for } \frac{d\,P_{n,1}}{dt}$$

where V_n is the vessel volume (ft^3)

f_A is the volume fraction acid phase in the vessel

ρ_A is the density of the acid phase (moles/ft^3)

ρ_P is the density of the organic phase (moles/ft^3)

x_1 is the mole fraction of α MNT in the acid phase

y_1 is the mole fraction of α MNT in the organic phase.

Therefore Equations 82 and 83 can be rewritten as:

$$A_o + R_1 - R_2 + D_1 + M_1 - A_1 = \frac{d}{dt}\ (V f_A\, \rho_A\, x_1) \approx \frac{V_A f_A \rho_A}{A_T}\ \frac{d\,A_1}{dt} \quad (84)$$

*See Appendix A for component number assignments

$$P_o - D_1 - M_1 - P_1 = \frac{d}{dt}\left[V(1-f_A)\,\rho_P\,y_1\right] \approx \frac{V(1-f_A)\,\rho_o}{A_T}\,\frac{dP_1}{dt} \qquad (85)$$

Note that in Equations 84 and 85 the vessel subscripts have been dropped and the assumption that fraction acid, density, and total moles change little with time has been made.

The numerical approximations for the continuous derivatives are:

$$\frac{d\,A_1}{dt} = \frac{A_1^{\,t+\Delta t} - A_1^{\,t}}{\Delta t} \qquad (86a)$$

$$\frac{d\,P_1}{dt} = \frac{P_1^{\,t+\Delta t} - P_1^{\,t}}{\Delta t} \qquad (86b)$$

where the superscript t represents a quantity evaluated at the current time and t+Δt indicated computation at the end of a time step. Substitution into Equations 84 and 85 yields:

$$\left[A_1^{\,o} + R_1 - R_2 + D_1 + M_1 - A_1\right]^t = \frac{Vf_A\,\rho_A}{A_T\Delta t}\left[A_1^{\,t+\Delta t} - A_1^{\,t}\right] \qquad (87)$$

$$\left[P_1^{\,o} - D_1 - M_1 - P_1\right]^t = \frac{V(1-f_A)\,\rho_P}{P_T\,\Delta t}\left[P_1^{\,t+\Delta t} - P_1^{\,t}\right] \qquad (88)$$

Solving for $A_1^{\,t+\Delta t}$ and $P_1^{\,t+\Delta t}$ we get:

$$A_1^{\,t+\Delta t} = A_1^{\,t} + \left[A_1^{\,o} + (R_1 - R_2) + D_1 + M_1 - A_1\right]^t \Delta t_A \qquad (89)$$

$$P_1^{\,t+\Delta t} = P_1^{\,t} + \left[P_1^{\,o} - D_1 - M_1 - P_1\right]^t \Delta t_P \qquad (90)$$

where

$$\Delta t_A = \frac{A_T \Delta t}{V f_A \rho_A} \qquad \text{(dimensionless)}$$

$$\Delta t_P = \frac{P_T \Delta t}{V(1-f_A)\rho_P} \qquad \text{(dimensionless)}$$

Equations analogous to 89 and 90 may now be written for all components in the organic phase (except P_s which is given by Equation 83) and for all components in the acid phase, and then solved via the Euler algorithm. This procedure was incorporated into the original computer program which was written to solve the unsteady state equations. Although the procedure is theoretically and numerically consistent, it was found that because of the large numerical values of the diffusion terms, a very small integration step size (Δt) was required in order to obtain numerical stability and generate convergent solutions. This was not acceptable, since use of an extremely small Δt resulted in intolerably long computer runs. To avoid this difficulty, an alternate solution procedure was devised based on the fact that the accumulation of nitrobody in the acid phase is small compared to that in the organic phase. This allows the integration of the nitrobody components to be carried out over the combined total amount of nitrobody in both phases, while the integration of the acid components in the acid phase is conducted as before. The concentration of the individual nitrobody components in the acid phase can then be obtained by solving the appropriate steady state equations after the integration has been carried out. In effect, it is assumed that the nitrobody in the acid phase is in equilibrium with that in the organic phase. Implementation of the procedure described above is carried out by first adding Equations 84 and 85 to give:

$$P_i^o + A_i^o + R_i - R_s \cdot (P_i + A_i) = \frac{V(1-f_A)\rho_P}{P_T} \frac{d P_i}{dt} + \frac{V f_A \rho_A}{A_T} \frac{d A_i}{dt} \qquad (91)$$

(Note that the troublesome mass transfer terms have dropped out of Equation 91.)

Now, let the total nitrobody in both phases be given by:

$$T_1 = P_1 + A_1 \tag{92}$$

so that

$$P_1 = T_1 - A_1 \tag{93}$$

Substitution of Equations 92 and 93 into Equation 91 yields:

$$P_1^{\,o} + A_1^{\,o} + R_1 - R_s - T_1 = \frac{V(1-f_A)\rho_P}{P_T}\frac{dT_1}{dt} - \frac{V(1-f_A)\rho_P}{P_T}\frac{dA_1}{dt}$$

$$+ \frac{Vf_A\rho_A}{A_T}\frac{dA_1}{dt} \tag{94}$$

$$P_1^{\,o} + A_1^{\,o} + R_1 - R_s - T_1 = \frac{V(1-f_A)\rho_P}{P_T}\frac{dT_1}{dt} + \left[\frac{Vf_A\rho_A}{A_T}\right.$$

$$\left. - \frac{V(1-f_A)\rho_P}{P_T}\right]\frac{dA_1}{dt} \tag{95}$$

Since $$\frac{dA_1}{dt} <<< \frac{dT_1}{dt}$$

we can write:

$$P_1^{\,o} + A_1^{\,o} + R_1 - R_s - T_1 \cong \frac{V(1-f_A)\rho_P}{P_T}\frac{dT_1}{dt} \tag{96}$$

In terms of discrete quantities:

$$T_1^{\,t+\Delta t} = T_1^{\,t} + \Delta t_p\,[P_1^{\,o} + A_1^{\,o} + R_1 - R_s - T_1]^t \tag{97}$$

Equation 97 is called the normal or forward difference form of the discrete equation, where the term in brackets is evaluated at the beginning of the interval. However, the efficiency and stability of the numerical integration procedure is enhanced if the backward difference form is used, in which case the bracketed term is evaluated at the end of the interval. In this case:

$$T_1^{t+\Delta t} = T_1^{t} + \Delta t_p \, [P_1^{o} + A_1^{o} + R_1 - R_s - T_1]^{t+\Delta t} \tag{98}$$

Solving for $T^{t+\Delta t}$, we get:

$$T_1^{t+\Delta t} = \frac{T_1^{t} + \Delta t_p \, [P_1^{o} + A_1^{o} + R_1 - R_s]^{t+\Delta t}}{1 + \Delta t_p} \tag{99}$$

But (from Appendix A),

$$R_s = A_1 \, (G_s \delta + G_{ss} \, \gamma \,) = A_1 \, F_s \tag{100}$$

From the steady state equation

$$A_1^{o} + R_1 - R_s + D_1 + M_1 = A_1 = 0 \tag{101}$$

we can determine a value for A_1 as follows:

$$A_1 = A_1^{o} + R_1 - G_s \delta A_1 - G_{ss} \gamma A_1 + \eta \left(\frac{P_1}{P_{nb}} - \frac{A_1}{A_{nb}} \right) + M_{nb} \left(\frac{P_1}{P_{NB}} + \frac{A_1}{A_{nb}} \right) \tag{102}$$

$$\left(1 + G_s \delta + G_{ss} \gamma + \frac{\eta}{A_{nb}} - \frac{M_{nb}}{A_{nb}} \right) A_1 = A_1^{o} + R_1 + P_1 \left(\frac{\eta}{P_{nb}} + \frac{M_{nb}}{P_{nb}} \right) \tag{103}$$

But $P_1 = T_1 - A_1$ so that

$$\left(1 + G_s\delta + G_{ss}\gamma + \frac{\eta}{A_{nb}} - \frac{M_{nb}}{A_{nb}}\right) A_1 = A_1^{o} + R_1$$

$$+ T_1 \left(\frac{\eta}{P_{nb}} + \frac{M_{nb}}{P_{nb}}\right) - A_1 \left(\frac{\eta}{P_{nb}} + \frac{M_{nb}}{P_{nb}}\right) \qquad (104)$$

$$\left(1 + G_s\delta + G_{ss}\gamma + \frac{\eta}{A_{nb}} - \frac{M_{nb}}{A_{nb}} + \frac{\eta}{P_{nb}} + \frac{M_{nb}}{P_{nb}}\right) A_1 = A_1^{o}$$

$$+ R_1 + T_1\left(\frac{\eta}{P_{nb}} + \frac{M_{nb}}{P_{nb}}\right) \qquad (105$$

$$A_1 = \frac{A_1^{o} + R_1 + T_1\left(\frac{\eta}{P_{nb}} + \frac{M_{nb}}{P_{nb}}\right)}{\left(1 + G_s\delta + G_{ss}\gamma + \frac{\eta}{A_{nb}} - \frac{M_{nb}}{A_{nb}} + \frac{\eta}{P_{nb}} + \frac{M_{nb}}{P_{nb}}\right)} \qquad (106)$$

$$A_1 = \frac{A_1^{o} + R_1 + T_1\ (C_x)}{F_s + C_s} \qquad (107)$$

where:

$$C_x = (\eta/P_{nb} + M_{nb}/P_{nb})$$

$$C_s = (1 + \eta/A_{nb} - M_{nb}/A_{nb} + C_x)$$

$$F_s = G_s\delta + G_{ss}\gamma$$

Substitution of Equations 100 and 107 into Equation 99 gives:

$$T_1^{t+\Delta t} = \frac{T_1^{t} + \Delta t_p \left[A_1^{o} + P_1^{o} + R_1 - \frac{F_s}{F_s + C_z}\left(A_1^{o} + R_1 + C_x T_1^{t+\Delta t}\right)\right]^{t+\Delta t}}{1 + \Delta t_p} \tag{108}$$

Rearrangement of Equation 108 yields:

$$T_1^{t+\Delta t} = \frac{T_1^{t} + \Delta t_p X}{1 + \Delta t_p Y} \tag{109}$$

where

$$X = \left[P_1^{o} + (R_1 + A_1^{o})\left(1 - \frac{F_s}{F_s + C_z}\right)\right] \tag{110}$$

$$Y = \left[1 + \left(\frac{F_s}{F_s + C_z}\right) C_x\right] \tag{111}$$

The value of $A_s^{t+\Delta t}$ can now be computed from Equation 107 using the value of T determined in Equation 109. A_{nb}, M_{nb}, γ, and δ in Equation 107 are computed using the values of A_1^{t} and P_1^{t} rather than $A_1^{t+\Delta t}$ and and $P_1^{t+\Delta t}$, but this has not posed any problems in the execution of the program. Equations similar to 109 can now be written to determine $T_2^{t+\Delta t}$ through $T_6^{t+\Delta t}$ with $A_2^{t+\Delta t}$ through $A_6^{t+\Delta t}$ being calculated from equations analogous to 107.

For the acid components in the acid phase, forward difference integration is employed.

$$A_6^{t+\Delta t} = A_6^{t} + [A_6^{o} + P_6^{o} - P_6 - R_1 - R_2 - R_3 - R_4 - R_5 - R_6$$

$$- 13\,R_7 - 12.5\,R_8 - 9\,R_{10} - 12.5\,R_{9C} + (.33 + .67\,RP)\,R_9$$

$$- A_6]^{t}\,\Delta t_A \tag{112}$$

$$AL^{t+\Delta t} = AL^{t} + [A_{13}^{o} - A_{14}^{o} + R_1 + R_2 + R_3 + R_4 + R_5 + R_6$$

$$+ 15\ R_7 + 16.5\ R_8 + 12\ R_{10} + 16.5\ R_{9G} - (.33\ RP + .67)\ R_9$$

$$- AL]^{t}\ \Delta t_A \qquad (113)$$

where $$AL^{t+\Delta t} = A_{13}^{t+\Delta t} - A_{14}^{t+\Delta t} \qquad (114)$$

If $AL < 0$ $\quad A_{13} = 0$, $A_{14} = AL$

and if $AL \geq 0$ $\quad A_{13} = AL$, $A_{14} = 0$

$$A_{13}^{t+\Delta t} = A_{13}^{t} + [A_{13}^{o} + (11\ R_7 + 14.5\ R_8 + 9\ R_{10} + 14.5\ R_{9G})\ (1-FD)$$

$$- A_{13}]^{t}\ \Delta t_A \qquad (115)$$

$$A_{SO}^{t+\Delta t} = A_{SO_4}^{t} + [A_{11}^{o} + A_{14}^{o} - (11\ R_7 + 14.5\ R_8 + 9\ R_{10}$$

$$+ 14.5\ R_{9G})\ (1-F_D) - A_{SO_4}]^{t}\ \Delta t_A \qquad (116)$$

$$A_{11}^{t+\Delta t} = A_{SO_4}^{t+\Delta t} - A_{14}^{t+\Delta t} \qquad (117)$$

Solution Procedure for Dynamic Simulation

The primary sequence of operations which must be executed in order to obtain the unsteady state solution of the nitration section equations is as follows:

Step 1: Enter the initial steady state of the process. This includes the composition and flow rates of the ideally separated acid and organic phases from each of the 14 process vessels, as well as the corresponding feed rates, compositions, nitrator temperatures, and notch settings.

Step 2: Process the initial conditions through the physical separation equations for all six separators to get initial conditions on the recycle streams.

Step 3: Read in the perturbations to the independent variables which constitute the deviations from steady state.

Step 4: Begin execution of the vessel equations for Vessel 1 (Nitrator 1A) by making up the terms required to compute the generation expressions D_i, M_i, and R_i.

Step 5: Integrate using Equations 107 to 117 to get the values of P_i and A_i at the end of the first time step.

Step 6: Store these values as the current outputs from Nitrator 1A, and use them to make up the inputs to Nitrator 1B.

Step 7: Repeat Steps 4 and 5 for Nitrator 1B.

Step 8: Store these values as the current outputs from Nitrator 1B and use them to make up the inputs to Separator 1.

Step 9: Repeat Steps 4 and 5 for Separator 1.

Step 10: Store these values as the current ideally separated outputs from Separator 1.

Step 11: Process the current values of the ideally separated output from Separator 1 through the physical separation equations to give the current composition and flow of the three streams leaving Separator 1.

Step 12: Store these values for use in making up inputs to other vessels.

Step 13: Begin execution of vessel equations for Nitrator 2 and continue the procedure for all remaining vessels through Separator 6.

At this point, one complete pass will have been made across the entire nitration reactor train for the first time step with the values of each vessel's output used to make up the necessary inputs for execution during the second time step. This procedure is now repeated for n time steps as desired. The program currently employs a time step of .01 hours (36 seconds). Thus, to simulate 12 hours of process operation, 1200 time steps must be executed. Typically, the execution time required for such a case is about 120 seconds on the CDC 6500 computer giving an average of 0.1 second of machine time per time step.

Program Description

The nitration section dynamic simulation consists of a main program, four subroutine subprograms, and one function subprogram. Appendix B presents a complete program listing; Appendix C shows the program flow chart; Appendix D gives the program nomenclature; and Appendix E presents the input data format.

All programs are written in FORTRAN IV for compilation on the CDC FORTRAN extended (FTN) compiler, version 3.0 and require 65K (octal) words on the CDC 6500 computer for complete execution. Word length on the CDC 6500 is 60 bits. Since there are no machine-dependent routines, the program should execute on any comparable computer with only minor modifications. It should be noted that a number of library subroutines (NANCY, NUCHAR, and NANCYM) are used to plot desired output.

The MAIN program reads in all data and parameter values, monitors and controls the sequential execution of the vessel and physical separation equations, and keeps track of all vessel inputs and outputs. The program also computes the values of a number of process performance indicators from the current values the vessel outflows at various times during the run and plots them as a function of time. These performance indicators constitute the primary output of the dynamic simulation and include: concentration of DNT in the crude TNT (wt %), flow rate of crude TNT (lb/hr); concentration of nitrobody in the spent acid (wt %), the fraction DNT in the spent acid nitrobody (wt %), concentration of water in the spent

acid (wt %), flow rate of spent acid (lb/hr), total carbon and nitrogen oxides in the off-gas (lb-moles/hr), heat loads in each nitrator (BTU/hr), concentration of nitric acid in the external recycle from each separator (wt % actual nitric), ratio of nitric to sulfuric acid in each nitrator, the amount of nitration occurring in each nitrator, and the specific gravities of the external acid recycle and organic streams leaving each separator. The values of e'_{oa} and e'_{oa} for each separator given by Equations 66 and 67 are also computed in the main program for later use in the physical separation equations.

Subroutine INPUT is called by the main program to read in the starting values of the independent variables including raw material feed rates and compositions, nitrator temperatures, and internal recycle notch setting, as well as to read in the magnitude and time of the desired perturbations to these quantities. Since feed rate data is entered in lb/hr, the subroutine makes the appropriate conversions to molar units. Also, the exponential factors in the rate equations (e.g.,

$$K_i \exp \left[- \frac{F_i}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right) \right]$$

are precomputed in INPUT in order to increase the efficiency with which the vessel equations are executed.

The heart of the dynamic simulation is subroutine SUB. Here, all of the vessel and physical separation equations are executed and integrated each time the subroutine is called by the main program as it steps through the reactor train. In effect, the main program provides the necessary input data to SUB (i.e. the main program tells SUB whether it is a nitrator or separator and then which one it is in the reactor train; it provides vessel constants for that vessel such as volume and notch setting; it provides the input and output phase compositions for the vessel from the previous time step). SUB then generates the output of the vessel and returns. SUB also computes a temperature rise for each separator based on the adiabatic heat generated by the small amount of reaction which takes place there.

Subroutine SUB1 computes the change in the calculated values of the phase compositions for each vessel from one iteration to the next. An iteration is defined as the execution of m time steps where m is specified at the beginning of the run. SUB1 also flags that component in each vessel which shows the maximum change between iterations.

Subroutine SUB2 executes the physical separation equations for each separator using the steady state phase compositions of the input data. SUB2 is called by the main program prior to execution of the first time step only in order to initialize the recycle flows. The physical separation equations are thereasfter executed in subroutine SUB as the run progresses.

The final subprogram in the dynamic simulation is function ENTH. This function is used in conjunction with the nitrator heat balance calculations executed by the main program. Its purpose is to calculate the enthalpy of any specified flow stream in the process by interpolating enthalpy-composition data which exits as a data table within the function. The enthalpies of the input and output streams are combined with the heats of reaction and heats of mixing to compute each nitrator's heat duty.

The Steady State Simulation

The steady state simulation is a computer program which, for a given set of nitration section independent variables, will execute the vessel and physical separation equations to give the steady state values of the composition and flow rates (moles/hr) of the exiting streams from each of the 14 process vessels. In addition, the values of a number of process performance functions are computed.

At steady state, the accumulation terms in Equations A-57 to A-82 go to zero so that differential equation system of the dynamic case becomes one of simultaneous algebraic equations. Because of the implicit nature of these equations, and also because of the presence of numerous recycle streams, a multilevel (nested) iteration procedure is used along with a simultaneous equation solving technique to arrive at the final solution.

Formulation of Equations

For the nitrobody components in the acid phase, the following system of steady state equations can be written:

For component 1: $A_1^0 - R_3 + D_1 + M_1 - A_1 = 0$ (118)

$$A_1 + R_3 - D_1 - M_1 = A_1^0 \quad (119)$$

Substitution of Equations 16, 20, 21, and 38 from Appendix A into Equation 119 gives

$$A_1 + (G_3\delta + G_3 S\gamma)\, A_1 - \eta\left(\frac{P_1}{P_{nb}} - \frac{A_1}{A_{nb}}\right) - M_{nb}\frac{A_1}{A_{nb}} - M_{nb}\frac{P_1}{P_{nb}} = A_1^{\,o} \tag{120}$$

Simplifying,

$$A_1\,(1 + G_3\delta + G_3 S\gamma) - C_1\left(\frac{P_1}{P_{nb}} - \frac{A_1}{A_{nb}}\right) - C_A A_1 - C_R P_1 = A_1^{\,o} \tag{121}$$

where: $C_1 = \eta$

$$C_A = \frac{M_{nb}}{A_{nb}} \text{ for } M_{nb} < 0 \qquad C_A = 0 \text{ for } M_{nb} \geq 0$$

$$C_R = \frac{M_{nb}}{P_{nb}} \text{ for } M_{nb} \geq 0 \qquad C_R = 0 \text{ for } M_{nb} < 0$$

Further rearrangement of Equation 121 yields:

$$(1 + G_3\delta + G_3 S\delta + \frac{C_1}{A_{nb}} - C_A)\, A_1 - \left(\frac{C_1}{P_{nb}} + C_R\right) P_1 = A_1^{\,o} \tag{122}$$

Similarly, for component 2:

$$A_2^{\,o} - R_4 + D_2 + M_2 - A_2 = 0 \tag{123}$$

$$A_2 + R_4 - D_2 - M_2 = A_2^{\,o} \tag{124}$$

Appropriate substitution from Appendix A yields:

$$A_2 + (G_4\delta + G_4S\,\gamma)\,A_2 - \frac{C_1}{P_{nb}}\,P_2 + \frac{C_1}{A_{nb}}\,A_2 - C_A A_2 - C_R P_2 = A_2^{\,o} \tag{125}$$

$$A_2\left(1 + G_4\delta + G_4S\,\gamma + \frac{C_1}{A_{nb}} - C_A\right) - \left(\frac{C_1}{P_{nb}} + C_R\right) P_2 = A_2^{\,o} \tag{126}$$

For component 3:

$$A_3 + R_3 - R_5 - R_7A - R_8A - R_9A + D_3 + M_3 - A_3 = 0 \tag{127}$$

$$A_3 - R_3 + R_5 + R_7A - R_8A + R_9A - D_3 - M_3 = A_3^{\,o} \tag{128}$$

$$A_3 - (G_3\delta + G_3S\,\gamma)\,A_1 + G_5\gamma A_2 + G_7\gamma A_3 + \frac{VG_8f_AA_2}{Q_A^2}\,A_3 + G_9\gamma A_3$$

$$- \frac{C_1}{P_{NB}}\,P_3 + \frac{C_1}{A_{NB}}A_3 - C_A A_3 - C_R P_3 = A_3^{\,o} \tag{129}$$

$$A_3\left(1 + G_5\gamma + G_7\gamma + \frac{VG_8f_AA_2}{Q_A^2} + G_9\gamma + \frac{C_1}{A_{nb}} - C_A\right) - \left(\frac{C_1}{P_{nb}} + C_R\right) P_3$$

$$= A_3^{\,o} + (G_3\delta + G_3S\,\gamma)\,A_1 \tag{130}$$

For component 4:

$$A_4^{\,o} + R_4 - R_6 - R_7M - R_8M - R_9M + D_4 + M_4 - A_4 = 0 \tag{131}$$

$$A_4 - R_4 + R_6 + R_7M + R_8M + R_9M - D_4 - M_4 = A_4^0 \quad (132)$$

$$A_4 - (G_4\delta + G_{48}\gamma)\, A_8 + G_8\gamma A_4 + \frac{VG_8 f_A A_8}{Q_A^2} A_4 + G_9\gamma A_4$$

$$- \frac{C_1}{P_{nb}} P_4 + \frac{C_1}{A_{nb}} A_4 - C_A A_4 - C_R P_4 = A_4^0 \quad (133)$$

$$A_4 \left(1 + G_6\gamma + G_7\gamma + \frac{VG_8 f_A A_8}{Q_A^2} + G_9\gamma + \frac{C_1}{A_{nb}} - C_A\right)$$

$$- \left(\frac{C_1}{P_{nb}} + C_R\right) P_4 = A_4^0 + (G_4\delta + G_{48}\gamma) A_8 \quad (134)$$

For component 5:

$$A_5^0 + R_5 - R_{10}A + D_5 + M_5 - A_5 = 0 \quad (135)$$

$$A_5 - R_5 + R_{10}A - D_5 - M_5 = A_5^0 \quad (136)$$

$$A_5 - G_5\gamma A_5 + \frac{VG_{10} f_A A_{17}}{Q_A^2} A_5 - \frac{C_1}{P_{nb}} P_5 + \frac{C_1}{A_{nb}} A_5 - C_A A_5$$

$$- C_R P_5 = A_5^0 \quad (137)$$

$$A_5 \left(1 + \frac{VG_{10} f_A A_{17}}{Q_A^2} + \frac{C_1}{A_{nb}} - C_A\right) - \left(\frac{C_1}{P_{nb}} + C_R\right) P_5$$

$$= A_5^0 - G_5\gamma A_5 \quad (138)$$

For component 6:

$$A_6^{\,o} + R_6 - R_{10M} + D_6 + M_6 - A_6 = 0 \tag{138}$$

$$A_6 - R_6 + R_{10M} - D_6 - M_6 = A_6^{\,o} \tag{140}$$

$$A_6 - G_6\gamma A_4 + \frac{VG_{10}f_A A_{17}}{Q_A'} A_6 - \frac{C_1}{P_{nb}} P_6 + \frac{C_1}{A_{nb}} A_6 \cdot C_A A_6$$

$$- C_R P_6 = A_6^{\,o} \tag{141}$$

$$A_6 \left(1 + \frac{VG_{10}f_A A_{17}}{Q_A'} + \frac{C_1}{A_{nb}} - C_A \right) - \left(\frac{C_1}{P_{nb}} + C_R \right) P_6$$

$$= A_6^{\,o} + G_6\gamma A_4 \tag{142}$$

For component 7:

$$A_7^{\,o} + R_{10} + D_7 + M_7 - A_7 = 0 \tag{143}$$

$$A_7 - R_{10} - D_7 - M_7 = A_7^{\,o} \tag{144}$$

$$A_7 - \frac{VG_{10}f_A A_{17}}{Q_A'} (A_6 + A_6) - \frac{C_1}{P_{nb}} P_7 + \frac{C_1}{A_{nb}} A_7 - C_A A_7$$

$$- C_R P_7 = A_7^{\,o} \tag{145}$$

$$A_7 \left(1 + \frac{C_1}{A_{nb}} - C_A \right) - \left(\frac{C_1}{P_{nb}} + C_R \right) P_7 = A_7^{\,o}$$

$$+ \frac{VG_{10}f_A A_{17}}{Q_A'} (A_6 + A_6) \tag{146}$$

For component 8:

$$A_8^{\circ} + 3R_{10} + D_8 + M_8 - A_8 = 0 \tag{147}$$

$$A_8 - 3R_{10} - D_8 - M_8 = A_8^{\circ} \tag{148}$$

$$A_8 - \frac{3VG_{10}f_A A_{17}}{Q_A^I}(A_8 + A_8) - \frac{C_1}{P_{nb}}P_8 + \frac{C_1}{A_{nb}}A_8 - C_A A_8$$

$$- C_R P_8 = A_8^{\circ} \tag{149}$$

$$A_8\left(1 + \frac{C_1}{A_{nb}} - C_A\right) - \left(\frac{C_1}{P_{nb}} + C_R\right)P_8 = A_8^{\circ}$$

$$+ \frac{3VG_{10}f_A A_{17}}{Q_A^I}(A_8 + A_8) \tag{150}$$

For the nitrobody species in the organic phase, the steady state vessel equations can be written as follows:

$$P_1^{\circ} + R_1 - M_1 - D_1 - P_1 = 0 \tag{151}$$

$$P_1 - R_1 + M_1 + D_1 = P_1^{\circ} \tag{152}$$

$$P_1 - D_{10}(1 - G_1) + C_A A_1 + C_R P_1 + \frac{C_1}{P_{nb}}P_1 - \frac{C_1}{A_{nb}}A_1 = P_1^{\circ} \tag{153}$$

$$\text{but} \quad D_{10} = \eta_{Tol}\frac{P_{10}}{P_{nb}} = C_1' P_{10} \tag{154}$$

so that,

$$P_1 - C_1' P_{10} (1-G_1) + A_1 \left(C_A - \frac{C_1}{A_{nb}}\right) + P_1 \left(C_R + \frac{C_1}{P_{nb}}\right) = P_1^o \tag{155}$$

$$\left(C_A - \frac{C_1}{A_{nb}}\right) A_1 + \left(1 + C_R + \frac{C_1}{P_{nb}}\right) P_1 = P_1^o$$

$$+ C_1' P_{10} (1 - G_1) \tag{156}$$

For component 2:

$$P_2^o + R_2 - M_2 - D_2 - P_2 = 0 \tag{157}$$

$$P_2 - R_2 + M_2 + D_2 = P_2^o \tag{158}$$

$$P_2 - C_1' P_{10} G_1 + C_A A_2 + C_R P_2 + \frac{C_1}{P_{nb}} P_2 - \frac{C_1}{A_{nb}} A_2 = P_2^o \tag{159}$$

$$\left(C_A - \frac{C_1}{A_{nb}}\right) A_2 + \left(1 + C_R + \frac{C_1}{P_{nb}}\right) P_2 = P_2^o + C_1' P_{10} G_1 \tag{160}$$

For component 3:

$$P_3^o - M_3 - D_3 - P_3 = 0 \tag{161}$$

$$P_3 + M_3 + D_3 = P_3^o \tag{162}$$

$$P_3 + C_A A_3 + C_R P_3 + \frac{C_1}{P_{nb}} P_3 - \frac{C_1}{A_{nb}} A_3 = P_3^o \tag{163}$$

$$(C_A - \frac{C_1}{A_{nb}}) A_3 + (1 + C_R + \frac{C_1}{P_{nb}}) P_3 = P_3^o \quad (164)$$

For component 4:

$$P_4^o - M_4 - D_4 - P_4 = 0 \quad (165)$$

$$P_4 + M_4 + D_4 = P_4^o \quad (166)$$

$$(C_A - \frac{C_1}{A_{nb}}) A_4 + (1 + C_R + \frac{C_1}{P_{nb}}) P_4 = P_4^o \quad (167)$$

Similarly, for components 5 through 8:

$$C_{21} A_5 + C_{22} P_5 = P_5^o \quad (168)$$

$$C_{21} A_6 + C_{22} P_6 = P_6^o \quad (169)$$

$$C_{21} A_7 + C_{22} P_7 = P_7^o \quad (170)$$

$$C_{21} A_8 + C_{22} P_8 = P_8^o \quad (171)$$

where:

$$C_{21} = C_A - \frac{C_1}{A_{nb}} \text{ and } C_{22} = (1 + C_R + \frac{C_1}{P_{nb}})$$

Now, for toluene:

$$P_{10}^o - D_{10} P_{10} = 0 \quad (172)$$

$$P_{10} + D_{10} = P_{10}^o \quad (173)$$

$$P_{10} (1 + C_1') = P_{10}^o \quad (174)$$

$$P_{10} = P_{10}^o / (1 + C_1') \quad (175)$$

For the acid species in the acid phase, the steady state vessel equations are written as follows:

$$A_9^{\,o} + P_9^{\,o} - P_9 - D_{10} - R_3 - R_4 - R_5 - R_6 - 13R_7 - 12.5R_8$$

$$- 9R_{10} - 12.5R_9G + (.33 + .67\,RP)\,R_9 - A_9 = 0 \quad (176)$$

Making the appropriate substitutions from Appendix A gives:

$$A_9 + P_9 + C_1' P_{10} + (G_3\delta + G_3g\gamma)\,A_1 + (G_4\delta + G_4g\gamma)A_2 + G_5\gamma A_3$$

$$+ G_6\gamma A_4 + 13G_7\gamma\,(A_3 + A_4) + 12.5\left(\frac{VG_9f_A}{Q_A}\;[HNO_3]\right)(A_3 + A_4)$$

$$+ 12.5G_8\gamma\,(A_3 + A_4) + 9\left(\frac{VG_{10}f_A}{Q_A}\;[NO_3^+]\right)(A_3 + A_4)$$

$$- (.33 + .67RP)F_DC_9 = A_9^{\,o} + P_9^{\,o}$$

$$A_9 + P_9 + C_1'P_{10} + F_9A_1 - F_4A_2 + \left(G_3\gamma + 13G_7\gamma + 12.5\frac{VG_9f_A}{Q_A}\;[HNO_3]\right.$$

$$\left. + 12.5\,G_8\gamma\right)\;A_3 + \left(G_6\gamma + 13G_7\gamma + 12.5\frac{VG_9f_A}{Q_A}\;[HNO_3] + 12.5G_8\gamma\right)A_4$$

$$+ 9\,\frac{VG_{10}f_A}{Q_A}\;[NO_3^+]\,A_3 + 9\,\frac{VG_{10}f_A}{Q_A}\;[NO_3^+]\,A_4 - (.33 + .67RP)F_DG_9$$

$$= A_9^{\,o} + P_9^{\,o} \quad (177)$$

Also, $$P_8 = \left(\frac{1.51\,A_{18}P_T}{A_T A_{11}}\right) A_8 \qquad (178)$$

$$A_{11}^{o} + A_{14}^{o} - C_8P - A_{SO_4} = 0 \qquad (179)$$

$$A_{SO_4} + (1 - F_D)C_8 = A_{11}^{o} + A_{14}^{o} \qquad (180)$$

$$A_{18}^{o} + C_8P - A_{18} = 0 \qquad (181)$$

$$A_{18} - C_8P = A_{18}^{o} \qquad (182)$$

$$A_{18}^{o} - A_{14}^{o} + R_1 + R_2 + R_3 + R_4 + R_5 + 15R_7 + 16.5R_8 + 12R_{10}$$

$$+ 16.5R_9G - (.33R_P + .67)R_9 - A_L = 0 \qquad (183)$$

$$A_L - C_1' P_{10} - F_3A_1 - F_4A_2 - \left(G_8\gamma + 15G_1 - 16.5\,\frac{VG_8f_A}{Q_A}\,[HNO_3]\right.$$

$$\left. + 16.5G_9\gamma\right) A_3 - \left(G_8\gamma + 15G_7\gamma + 16.5\,\frac{VG_8f_A}{Q_A}\,[HNO_3]\right.$$

$$\left. + 16.5G_9\gamma\right) A_4 - 12\,\frac{VG_{10}f_A}{Q_A}\,[NO_2^+]\,A_5 - 12\,\frac{VG_{10}f_A}{Q_A}\,[NO_2^+]\,A_6$$

$$+ (.33RP + .67)\,F_DC_8 = A_{18}^{o} + A_{14}^{o} \qquad (184)$$

Equations 122, 126, 130, 134, 138, 142, 146, 150, 156, 160, 164, 167, 168, 169, 170, 171, 175, 177, 178, 179, 182, and 184 are linear in the following unknowns: A_1 through A_8, A_{SO_4}, A_{18}, A_L, and P_1 through P_{10}. This

constitutes a system of 22 equations and 22 unknowns which is solvable provided the coefficients of all the unknown terms can be determined.

Solution Procedure for the Steady State Simulation

Execution of the steady state simulation consists mainly of the simultaneous solution of the 22 vessel equations for each of the 14 vessels in the nitration train. Although these equations could be solved simultaneously via Gauss reduction, it was decided that because of the sparcity of the coefficient matrix, a straightforward direct substitution approach would be more efficient. This will become clear as the step-by-step solution procedure is outlined below. The physical separation equations must also be employed here as in the dynamic case to convert computed pure phase outputs to real stream outputs. As mentioned previously, a multilevel or nested iterative procedure is used because of (1) the implicit nature of the vessel equations (the coefficients of the linear unknowns are functions of these unknowns), and (2) the numerous recycle streams in the process.

The primary sequence of operations which must be executed in order to obtain the steady solution is as follows:

Step 1: Enter an assumed solution for the phase outputs from each of the 14 process vessels.

Step 2: Enter the values of the process's independent variables for which the steady state solution is desired.

Step 3: Using the assumed solution for the vessel phase outputs, compute the flow rates and compositions of all recycle streams in the process via the physical separation equations.

Step 4: Begin the iterative solution of the vessel equations for the first vessel (Nitrator #1A). Start by computing the values of all coefficients of the 22 x 22 vessel equation matrix from the assumed solution for that vessel. Also, make up the correct phase inputs to Nitrator 1A.

Step 5: Solve Equation 175 for P_{10}.

Step 6: Solve Equations 122 and 156 simultaneously for values of A_1 and F_1.

Step 7: Solve Equations 126 and 160 simultaneously for values of A_3 and P_3.

Step 8: Solve Equations 130 and 164 simultaneously for values of A_5 and P_5.

Step 9: Solve Equations 134 and 167 simultaneously for values of A_4 and P_4.

Step 10: Solve Equations 138 and 168 simultaneously for values of A_6 and P_6.

Step 11: Solve Equations 142 and 169 simultaneously for values of A_8 and P_8.

Step 12: Solve Equations 146 and 170 simultaneously for values of A_7 and P_7.

Step 13: Solve Equations 150 and 171 simultaneously for values of A_8 and P_8.

Step 14: Solve Equations 176 and 178 simultaneously for values of A_9 and P_9.

Step 15: Solve Equation 182 for A_{13}.

Step 16: Solve Equation 184 for A_L.

Step 17: Use the logic of Equations A-70 and A-71 to determine values for A_{12} and A_{14}.

Step 18: If computed values and assumed values differ by more than a predetermined amount, repeat Steps 5 through 17 using newly computed values for the A_i's and P_i's.

Step 19: Repeat Step 18 until convergence is achieved on Nitrator 1A.

Step 20: Using the converged solution for Nitrator 1A, and the previously assumed recycle stream flows, make up the correct phase inputs to Nitrator 1B and then repeat Step 4 for Nitrator 1B.

Step 21: Repeat Steps 5 through 17 for Nitrator 1B.

Step 22: Repeat Step 18 for Nitrator 1B.

Step 23: Repeat Step 22 until convergence is achieved on Nitrator 1B.

Step 24: Using the converged solution for Nitrator 1B as the input to Separator 1 and the initially assumed phase outputs, execute Steps 4 through 19 for Separator 1.

Step 25: Process the converged outputs for Separator 1 through the physical separation equations to get the flow rates and compositions of the recycle streams leaving that separator.

Step 26: Compare the calculated recycle stream between Separator 1 and Nitrator 1B (internal recycle) to that assumed when the inputs to Nitrator 1B were made up. If they differ by a preset amount, use the newly calculated recycle stream, and the previously converged values of the outputs from Nitrators 1A and 1B to repeat Steps 4 through 19 for Nitrator 1B.

Step 27: Repeat Steps 24 through 26 until convergence on the internal recycle stream is achieved.

Step 28: Using the converged Separator 1 outputs and the originally assumed Nitrator 2 output and Separator 3 recycle stream values, execute Steps 4 through 19 for Nitrator 2.

Step 29: Repeat Steps 24 through 27 for Separator 2.

Step 30: Repeat Steps 28 and 29 for Stages 3 through 6 until convergence on all internal recycle streams is achieved. Note, although a converged solution for each stage will have been obtained at this point, no attempt at linking the six stages together through their external recycle streams has yet been made. This must now be done in order to obtain the complete steady state solution for the 14-vessel reactor train.

Step 31: Begin with the external recycle between Separator 6 and Nitrator 5. Using the previously converged outputs from Separators 4, 5, and 6 as Nitrator 5 inputs and the previously converged Nitrator 5 output, execute Steps 4 through 19 for Nitrator 5.

Step 32: Repeat Steps 24 through 27 for Separator 5.

Step 33: Execute Steps 4 through 19 for Nitrator 6 using the newly converged Separator 5 output and previously converged Separator 6 and Nitrator 6 outputs.

Step 34: Repeat Steps 24 through 27 for Separator 6.

Step 35: Compare the newly calculated external acid recycle stream from Separator 6 to that employed in Step 31. If they differ by a preset amount, use the newly calculated value as well as the most recently converged values for the other required flows to repeat Steps 31 through 34.

Step 36: Repeat Step 35 until convergence on the external recycle from Separator 6 is achieved.

Step 37: Continue with this stagewise iteration procedure until the remaining external recycle streams (and thus the entire nitration reactor train) have been converged.

Typically, a steady state run requires approximately 5000 iterations of the vessel equations with convergence limits set at .05 mole/hr for overall vessel composition, .02 moles/hr for components in the internal recycle, and .02 moles/hr for components in the external recycle. Under these conditions, program execution time is approximately 30 seconds on the CDC 6500. Obviously, if tighter convergence is desired, run time increases significantly.

Program Description

The nitration section steady state simulation consists of a main program, two subroutine subprograms, and one function subprogram. A complete steady state run including the program listing is presented in Appendix F. Appendix G shows the program flow chart; Appendix H gives the program nomenclature; and Appendix I illustrates the input data format.

All programs are written in FORTRAN IV for compilation on the CDC FORTRAN extended (FTN) compiler, version 3.0, and will compile and execute in 55,000 (octal) words on the CDC 6500. Since there are no machine-dependent routines, the program should execute on any comparable computer with only minor modifications. A brief description of the main program and the three subprograms will now be given.

The main program (TNTSIM) reads in all data and parameter values which form the fixed data base for the steady state simulation. Included in this data base is an initial guess at the steady state solution. Also, the program is responsible for reading the particular set of values for the independent process input variables for which the steady state output is desired. All feed streams which are entered as lb/hr are converted to moles/hr and the Arrhenius factors are precomputed for later use in the rate expressions as are values for e'_{ao} and e'_{oa}. However, the primary function of the main program is to monitor and control the execution of the three-level convergence procedure employed to arrive at the steady state solution. The program is actually responsible for external recycle convergence and calls the appropriate subroutines for internal recycle or vessel convergence. The program also assigns and updates vessel identification parameters so that it can correctly sequence through the reactor system. After overall convergence is achieved, the main program prints out the steady state values of the ideal phase and actual stream compositions and flow rates from each nitrator and separator in the process (including the off-gas streams) and then proceeds to compute and print out the values of a number of process performance indicators including vessel time constants (hours), overall molar yield, flow rate of crude TNT (lb/hr), DNT in the crude TNT (wt %), raw material cost ($/lb TNT), spent acid flow (lb/hr) and composition, extent of nitration in each stage, acid composition in each stage (in units similar to those generated by plant operators during control checks), nitrobody density in each stage (lb/ft^3), and heat duty in each nitrator. An elemental material balance is also run to check the consistency of the converged solution. The complete steady state printout is shown in Appendix F.

Subroutine NITSEP is employed to carry out the internal recycle convergence procedure. It is called by the main program during individual stage convergence and then again during total process convergence. The subroutine compares the current and previously computed values for the internal acid recycle leaving a given separator and does the required updating if the difference exceeds a predetermined value.

The heart of the steady state simulation program is subroutine VESSEL. Here, all of the vessel and physical separation equations are solved to give the output of each nitrator and separator during execution of the nested iteration convergence procedure. The subroutine is thus responsible for the execution and convergence of the primary iteration loop, i.e. the individual vessel. VESSEL is called by the main program and by subroutine NITSEP during the uncoupled stage convergence

procedure and then again by subroutine NITSEP during total process convergence. The calling program provides the necessary input data to VESSEL, such as whether it is to simulate a nitrator or a separator, the values of all input streams and the currently assumed output of the vessel. VESSEL will then execute Steps 4 through 19 of the solution procedure and, if the vessel has been flagged as a separator, process the converged vessel output through the physical separation equations. A modified direct substitution procedure is used, whereby a percentage of the difference between quantities calculated during successive iterations is added to the newly calculated quantity.

The final subprogram in the steady state simulation is function ENTH. It serves the same purpose here as it did in the dynamic simulation.

Parameter Fitting

As has been illustrated, the vessel equations are interspersed with a number of constants. These include terms associated with kinetic phenomena such as frequency factors, activation energies, and concentration exponents, as well as mass transfer coefficients, equilibrium constants, and solubility factors. In most cases, the appearance of these constants in the vessel equations is theoretically consistent and not simply a function of empirical supposition. An attempt was made to use published, experimentally determined values of constants when such values were available. However, because many needed values were simply not available, and, because most of those that were had been developed under laboratory conditions not comparable to the state of the actual nitration process, it was necessary to fit the constants (parameters) to steady state process operating data (steady state snapshots).

The parameter fitting procedure consisted of (1) assuming an initial value for each of the 27 parameters, (2) executing the steady state simulation with these parameter values and input variables values corresponding to specific data snapshots, (3) comparing computed outputs (molar component flows of all process streams) with observed snapshot values, and (4) making appropriate changes in parameter values to give better agreement between calculated and observed quantities.

A total of 14 steady state snapshots were available for parameter fitting. This data was obtained during normal operations at the production facility located at the Radford Army Ammunition Plant. A typical snapshot is shown in Table I of Appendix J. Of the 14 snapshots, seven were used for fitting with the remaining sets being employed to check the validity of the final fit.

In order to use the snapshot data (which is essentially stream compositions in weight %) for fitting purposes, it was first necessary to convert from units of composition to units of molar flow rate for each component. This was accomplished by processing the snapshot data through a material balance program, the details of which can be found in Reference 1. With the snapshot data in correct form for comparison with the individual stage outputs calculated by the simulation, it was simply required to make repetitive steady state runs and after each run, to evaluate an objective function. This function was in effect a measure of the total weight deviation from observed conditions in all nitration stages. Changes were then made to the parameter set which drove the objective function toward a minimum.

Minimization of the objective function was accomplished systematically by using a pattern search algorithm which was added to the steady state simulation as a subroutine and controlled program execution. The pattern search technique will be described in detail in the next section of the report when steady state optimization is discussed. A list of parameters with their final fit values is included in Table II of Appendix J.

APPLICATION OF THE SIMULATION

The computer simulation of the nitration section has been used to carry out a variety of studies on the nitration process. Most significant among these has been the use of the steady state simulation to develop optimized operating conditions and the development of a multivariable control procedure for vessel acid composition using the dynamic simulation to generate the process transfer function.

It is not intended that this report serve as the documentary record of the exploitation of the nitration section simulation. Detailed technical reports on specific studies using the nitration section simulation have been prepared (see Ref 15 to 17). However, it is desired in this volume to give the reader some feeling for the way in which the nitration section simulation can be used. With this in mind, the following description of two major areas of exploitation is presented.

Steady State Applications

Steady state optimization was carried out by making multiple steady state runs under the control of the same pattern search algorithm that was used during parameter fitting. The pattern search method is one of a number of direct climing (Ref 13) techniques which will move toward an extremum of a multidimensional objective function based on previous information

about the response surface. The particular pattern search algorithm used was an adaptation of a procedure developed by Hooke and Jeeves (Ref 14) which employs accelerated climing and has ridge-following properties.

For each steady state run made under control of the pattern search subroutine, an objective function, defined as the raw material cost per pound of TNT, was evaluated. The independent variables over which the search was made included feed composition, feed flow rate, nitrator temperature and internal recycle rate. The feed rate of toluene to the process (and therefore the production rate) was not varied during steady state optimization so that what was sought was the set of independent variables which gave the minimum raw material cost per pound of α -TNT produced at a fixed production rate. The fixed toluene rate employed during optimization was 2350 lb/hr, which corresponds to a TNT production rate of approximately 57 tons/day based on an 87% α -yield. The raw material cost per pound of TNT was calculated from the equation:

$$C = \frac{(TxC_T) + (SxC_S) + (NxC_N) + (WxC_W)}{(TxY)} \qquad (185)$$

where:

- C = raw material cost ($/lb TNT)
- T = toluene flow rate (lb/hr)
- S = oleum flow rate (lb/hr)
- N = strong nitric acid flow rate (lb/hr)
- W = weak nitric acid flow rate (lb/hr)
- C_T = cost of toluene ($/lb toluene)
- C_S = cost of oleum ($/lb)
- C_N = cost of strong nitric acid (98.5% HNO_3) ($/lb)
- C_W = cost of weak nitric acid (61.0% HNO_3) ($/lb)
- Y = yield (lb TNT/lb toluene)

Values of cost factor employed were based on data supplied by Radford Army Ammunition Plant and thus reflected that plant's raw material cost as of July 1972. Specific values used were: C_T = .0293, C_S = .01192, C_W = .01061, C_N = .01714.

Rather than consider all independent variables simultaneously, a sensitivity analysis was carried out which enabled ranking these variables in the order in which perturbations in them affected the objective function. Only main effect sensitivities were determined. Although the possibility of significant higher order effects could not be discounted, it was felt that the complexity of multiple-effect analysis (including increased machine time requirements) was not justified.

The independent variables were thus divided into five blocks according to their effects on the objective function, and pattern searches were conducted separately over each block. Since the number of variables per search was reduced by this procedure, the pattern search algorithm functioned more efficiently and saved computer time. The complete list of independent variables, ranked in decreasing order of their effects on the objective function and broken down into their search blocks, is shown in Table I of Appendix K.

Because of physical limitations in the actual process, a number of constraints on the independent variables had to be included in the objective function to insure that only feasible sets of process operating conditions were considered. This was accomplished by assigning penalty values to the objective function whenever a constraint value of one or more of the independent variables was under consideration of the search routine. This "brute force" method worked satisfactorily in keeping the search within feasible areas of the response surface. The constraints employed were based on information supplied by plant operating personnel at Radford and are listed in Table II of Appendix K.

As the optimization proceeded, it became evident that a substantial reduction in oleum was being made by the search program. Because of the magnitude of the predicted reduction (nearly 50% of the baseline feed rate), the validity of the model in a region so far from conditions under which parameters were fit came into question. Also, even if the simulation's predictions were correct, it was felt that plant operating personnel would never agree to such a drastic reduction in oleum flow. But the qualitative result was clear--cut back on oleum flow.

Consequently, the oleum flow rate was treated as a parameter, with sets of optimum conditions being developed for oleum flow rates of 11,000, 10,000, 9,000, 8,000, and 7,000 lb/hr. Of course, the lowest unit cost of TNT is predicted for the lowest oleum flow rate. Predicted optimum conditions for 10,000 lb/hr oleum are shown in Table K3 of Appendix K. For the interested reader, a more complete description of certain aspects of the steady state optimization studies can be found in Reference 3. In general, however, steady state optimization studies have resulted in the development of operating conditions which predict savings on the order of 20% in the raw material cost per pound of TNT.

Dynamic Applications

The primary application of the dynamic simulation has been its use in conjunction with the design of a supervisory control strategy for acid composition in each stage of nitration. The need to control the composition of the acid phase in each nitration stage is a result of the critical effect which this variable has on the extent of reaction. The object of the control study was thus to develop a procedure whereby predicted optimum acid concentrations could be maintained throughout the process in view of uncontrollable fluctuations in such things as raw material acid composition, internal flows, mixing characteristics, and heat transfer coefficients, as well as step changes in production rate.

It was determined that the way to accomplish this was to control specific indicators of acid concentration in all six external recycle streams and in the emulsion stream flowing from Nitrator 3A to Nitrator 3B by manipulating the seven primary nitric acid feeds and the yellow waterfeeds to the process. A system of nine manipulated and nine controlled variables results. The specific indicator of acid composition is optional and can be either total acidity, actual nitric acid, or nitric to sulfuric acid ratio. Control strategies employing various combinations of these controlled variables have been tested and shown to be feasible and the most promising approach appears to be control of total acidity and actual nitric acid in Stages 1 and 2 with the nitric to sulfuric ratio being controlled at the remaing five locations. Controlled variables with their proposed manipulated variables are listed in Figure 10.

The details of control strategy development have been documented elsewhere (Ref 15), although a number of significant points should be noted here. Because of the many recycle streams in the process, it was necessary

to develop a decoupling mechanism in order to counteract the disturbances created in adjacent nitrators when a feed change is made. Secondly, because of difficulties in obtaining real time measurements of the controlled variables, it was also necessary to develop a computational scheme to estimate the values of the desired controlled variables from measurable data and certain assumed constant values generated by the steady state program. A block diagram of the overall scheme for acid concentration control is shown in Figure 11. Note that the process simulation provides the necessary process dynamics in the same way, as an assumed transfer function (e.g., a first order lag plus dead time) would have, had not a detailed process model been used.

A number of runs were made with the simulated control scheme in order to develop reasonable values for controller tuning parameters. The open and closed loop responses of the system to a 10% step change in oleum flow are shown in Figures 12 and 13, respectively, for a typical run.

The dynamic simulation was also used in conjunction with a simulation of the nitrator temperature cascade control loop which is included in the software package provided by the Foxboro Company as part of the Volunteer AAP direct digital computer control system, scheduled to begin operation in late 1974. Performance of the temperature control system was tested for normal continuous operation on a single nitrator simulation and also for start-up operations on the complete six-stage nitration section simulation. The details and significant results of this effort can be found in Reference 16.

CONCLUSION

The modeling and simulation study of the continuous TNT process has resulted in much being learned about the chemical and physical phenomena which govern the process's behavior. Quantification of process interactions has made possible the generation of optimum operating conditions, improvements in the process design, and has allowed the development of a supervisory control strategy. Implementation of the results of the simulation effort is anticipated during calendar year 1974 when new computer-controlled TNT lines will be started up at Volunteer Army Ammunition Plant in Chattanooga, Tennessee. Only after verification of model predictions on the actual process and use of the model-developed process control strategies, will the full benefit of the simulation undertaking be realized. While simulation studies on other processes are planned, much will depend on the successful implementation of the TNT process simulation study's results.

REFERENCES

1. Williams, J. E., *Computer Simulation of the Continuous TNT Manufacturing Process,* Volunteer Army Ammunition Plant Technical Report PE-AAP-01, Vol 1 (Dec 1970)

2. Williams, J. E. and Michlink, F. P., *Computer Simulation of the Continuous TNT Process,* Volunteer Army Ammunition Plant Technical Report PE-AAP-01C, Vols 1, 2, and 3 (Dec 1971)

3. Michling F. P., *Computer Simulation of the Continuous TNT Process,* Volunteer Army Ammunition Plant Technical Report PE-AAP-01D, Vol 1 (Oct 1972)

4. Chandler, C. D. and Kohlbeck, J. A., *Continuous TNT Process Characterization Study,* Radford Army Ammunition Plant Technical Report RAD-240.10 (Nov 1972), p 13

5. Hoggett, et al, *Nitration and Aromatic Reactivity,* Cambridge University Press (1971), Great Britain, p 48

6. *"Ibid,"* p 19

7. Kobe, K. A. and Lakemeyer, J. L., *Effect of Nitrosylsulfuric Acid on the Rate of Mononitration of Toluene,* Ind and Eng Chem (50), No. 11, pp 1691-1694

8. McKinley, C. and White, R.R., Trans Am Inst Chem Engrs (40), (1944) p 143-175

9. Hogget, op cit, p 17

10. Vinnik, M.I., et al *Kinetics of the Nitration of p-Nitrotoluene, p-Chloronitrobenzene and o-Chloronitrobenzene in Mixtures of Sulfuric and Nitric Acids,* Russell J. Phys Chem (41), No. 5, (1967) p 580-583

11. Bennet, G. M., et al *Nitration in Sulfuric Acid. Part IV. Kinetics of the Nitration of 2,4-Dinitrotoluene,* J. Chem Society (1947) p 474-492

12. Hughes, E. D., et al, *Kinetics and Mechanism of Aromatic Nitration. Part II,* J. Chem Society (1950) p 2400-2440

13. Wilde, D. J. and Beightler, C. S., *Foundations of Optimization,* Prentice Hall (1967), Englewood Cliffs, N. J., p 271-344

14. Hooke, R. and Jeeves, T. A., *Direct Search Solution of Numerical and Statistical Problems,* J. Assn Comp Mach (8) No. 2, (Apr 1961) p 212-219

15. Smith, C. L., *Development and Application of a Supervisory Control System for the Continuous TNT Process,* Report to Imperial Chemical Industries, VAAP, (July 1973)

16. Corripio, A. B., *Single Nitrator Model for the Study of Local Control of Nitrator Temperature,* Report to Imperial Chemical Industries, VAAP, (November 1972)

17. Smith, C. L., *Solubility of TNT in Mixed Acids,* Report to Imperial Chemical Industries, VAAP, (February 1973)

18. Gillespie, R. J., and Graham, J., *Cryoscopic Measurements in Sulfuric Acid. Part III,* J. Chem Society, 1949

19. Gillespie, R. J., and Graham, J. *Cryoscopic Measurements in Sulfuric Acid. Part IV,* J. Chem Society, 1949

20. Ross, D. L., Personal Correspondence, (Dec 1973)

APPENDIX A

Vessel Equations

The following is an ordered set of equations which make up the kinetics and mass transfer model for any vessel in the nitration section of the continuous TNT process. The order in which they are listed represents the logical sequence of calculation employed in SUBROUTINE SUB of the dynamic simulation and SUBROUTINE VESSEL of the steady state simulation program.

Component Index Assignments

Component	Index (i)
αMNT	1
mMNT	2
αDNT	3
mDNT	4
αTNT	5
mTNT	6
TNB	7
TNBX	8
HNO_3	9
Toluene	10
H_2SO_4	11
$HNOSO_4$	12
H_2O	13
SO_3	14
Not used	15
Not used	16
NO_2^+	17

Equations

$$A_{NB} = \sum_{i=1}^{8} A_i \qquad \text{(A-1)}$$

$$P_{NB} = \sum_{i=1}^{8} P_i + P_{10} \qquad \text{(A-2)}$$

$$A_T = A_{NB} = A_9 + A_{11} + A_{12} + A_{13} + A_{14} \qquad \text{(A-3)}$$

$$P_T = P_{NB} + P_9 \qquad \text{(A-4)}$$

$$Q_A = \sum_{i=1}^{14} \frac{A_i}{\rho_i} \qquad \text{(A-5)}$$

$$Q_P = \sum_{i=1}^{10} \frac{P_i}{\rho_i} \qquad \text{(A-6)}$$

$$F_A = \frac{Q_A}{Q_A + Q_P} \qquad \text{(A-7)}$$

$$F_P = 1 - F_A \qquad \text{(A-8)}$$

When vessel is a separator, $F_A = .755$ (A-8a)

$$X_i = \frac{A_i}{A_T} \qquad \text{(A-9)}$$

$$X_{eq}^{A} = 10^{P} \qquad \text{(A-10)}$$

Where:

$$P = 3.62 + 0.01023\,T - 3.608\,X_{10} + 7.716\,(X_1 + X_2) - 8.452\,(X_3 + X_8) - 6.292\,X_9 \qquad \text{(A-11)}$$

$$\eta_A = VF_P\,kma \qquad \text{(A-12)}$$

$$\eta_P = VF_P\,(kma)_P \qquad \text{(A-13)}$$

$$\eta_{Tol} = VF_P\,(kma)_{Tol} \qquad \text{(A-14)}$$

$$\eta = \left(\frac{1}{\frac{1}{\eta_P} + \frac{1}{\eta_A X_{eq}^{A}}} \right) \qquad \text{(A-15)}$$

$$D_i = \eta \left(\frac{P_i}{P_{NB}} - \frac{A_i}{A_{NB}} \right) \quad i = 1,8 \qquad \text{(A-16)}$$

$$D_{10} = \eta_{Tol} \left(\frac{P_{10}}{P_{NB}} \right) \qquad \text{(A-17)}$$

$$A_{NB} = (X_{eq}^{A})\, A_T \qquad \text{(A-18)}$$

$$M_{NB} = A_{NB} - A_{NB}^{o} - \sum_{i=1}^{8} D_i \qquad \text{(A-19)}$$

$$\text{If } M_{NB} < 0: \quad M_i = M_{NB} \left(\frac{A_i}{A_{NB}} \right) \quad i = 1,8 \qquad \text{(A-20)}$$

$$\text{If } M_{NB} \geq 0: \quad M_i = M_{NB} \left(\frac{P_i}{P_{NB}} \right) \qquad \text{(A-21)}$$

$$\gamma = \frac{Vf_A}{Q_A} [NO_2^+] \left(k_a [HSO_4^-] + k_b [H_2SO_4] + k_c [HS_2O_7^-] \right) \qquad \text{(A-22)}$$

or

$$\gamma = k_8 \frac{Vf_A}{Q_A} [NO_2^+] \qquad \text{(A-23)}$$

All concentrations are equilibrium values resulting from dissociations according to the mechanisms outlined in Section V, Volume I of this report.

$$Z = - \frac{1}{R} \left(\frac{1}{T} - \frac{1}{T_R}\right) \qquad \text{(A-24)}$$

$$G_1 = \frac{1}{k_{18}} \exp (E_{81} Z) \qquad \text{(A-25)}$$

$$G_2 = k_{2W} \exp (E_{2W} Z) \qquad \text{(A-26)}$$

$$G_{2S} = k_{2S} \exp (E_{2W} Z) \qquad \text{(A-27)}$$

$$G_4 = k_{4W} \exp (E_{4W} Z) \qquad \text{(A-28)}$$

$$G_{4S} = k_{4S} \exp (E_{4S} Z) \qquad \text{(A-29)}$$

$$G_{5S} = k_{5S} \exp (E_{5S} Z) \qquad \text{(A-30)}$$

$$G_6 = k_{6S} \exp (E_{6S} Z) \qquad \text{(A-31)}$$

$$G_7 = k_7 \exp (E_7 Z) \qquad \text{(A-32)}$$

$$G_8 = k_8 \exp (E_8 Z) \qquad \text{(A-33)}$$

$$G_9 = k_9 \exp (E_9 Z) \quad \text{(not used)} \qquad \text{(A-34)}$$

$$G_{10} = k_{10} \exp(E_{10} Z) \quad \text{(A-35)}$$

$$R_2 = D_{10} G_1 \quad \text{(A-36)}$$

$$R_1 = D_{10} - R_2 \quad \text{(A-37)}$$

$$R_3 = (G_{38}\gamma)A_1 \quad \text{(A-38)}$$

$$R_4 = (G_{48}\gamma)A_2 \quad \text{(A-39)}$$

$$R_5 = G_5 \gamma A_3 \quad \text{(A-40)}$$

$$R_6 = G_6 \gamma A \quad \text{(A-41)}$$

$$R_7 A = G_7 \frac{Vf_A}{Q_A} [NO_2^+] A_3 \; ; \; R_7 M = G_7 \frac{Vf_A}{Q_A} [NO_2^+] A_4 \quad \text{(A-42)}$$

$$R_7 = R_7 A + R_7 M \quad \text{(A-43)}$$

$$R_8 A = \frac{VG_8 f_A}{Q_A} [NO_2^+] A_3 \quad \text{(A-44)}$$

$$R_8 M = \frac{VG_8 f_A}{Q_A} [NO_2^+] A_4 \quad \text{(A-45)}$$

$$R_8 = R_8 A + R_8 M \quad \text{(A-46)}$$

$$R_9 A = G_9 \gamma A_3 \quad \text{(A-47)}$$

$$R_9 M = G_9 \gamma A_4 \quad \text{(A-48)}$$

$$R_9 G = R_9 A + R_9 M \quad \text{(A-49)}$$

(not used)

$$R_{10A} = \frac{VG_{10}f_A}{Q_A} [NO_2^+] A_8 \quad \text{(A-50)}$$

$$R_{10M} = \frac{VG_{10}f_A}{Q_A} [NO_2^+] A_8 \quad \text{(A-51)}$$

$$R_{10} = -R_{10A} + R_{10M} \quad \text{(A-52)}$$

$$C_8 = 11R_7 + 14.5R_8 + 9R_{10} + 14.5R_9G \quad \text{(A-53)}$$

$$R_9 = (F_D)(C_8) \quad \text{(A-54)}$$

$$C_{8p} = C_8 - R_9 = C_8 (1-F_D) \quad \text{(A-55)}$$

$$\tau_A = \frac{Vf_{A\rho A}}{A_T} \quad \text{(A-56)}$$

$$A_1^o = R_2 + D_1 + M_1 - A_1 = \tau_A \frac{dA_1}{dt} \quad \text{(A-57)}$$

$$A_2^o = -R_4 + D_2 + M_2 - A_2 = \tau_A \frac{dA_2}{dt} \quad \text{(A-58)}$$

$$A_3^o + R_3 - R_5 - R_7A - R_8A - R_9A + D_3 + M_3 - A_3 = \tau_A \frac{DA_3}{dt} \quad \text{(A-59)}$$

$$A_4^o + R_4 - R_6 - R_7M - R_8M - R_9M + D^4 + M_4 - A_4 = \tau_A \frac{dA_4}{dt} \quad \text{(A-60)}$$

$$A_5^{o} + R_5 - R_{10A} + D^5 + M_5 - A_5 = \tau_A \frac{dA_5}{dt} \quad \text{(A-61)}$$

$$A_6^{o} + R_6 - R_{10M} + D_6 + M_6 - A_6 = \tau_A \frac{dA_6}{dt} \quad \text{(A-62)}$$

$$A_7^{o} + R_{10} + D_7 + M_7 - A_7 = \tau_A \frac{dA_7}{dt} \quad \text{(A-63)}$$

$$A_8^{o} + 3R_{10} + D_8 + M_8 - A_8 = \tau_A \frac{dA_8}{dt} \quad \text{(A-64)}$$

$$A_9^{o} + P_9^{o} - P_9 - D_{10} - R_3 - R_4 - R_5 - R_6 - 13R_7 - 12.5R_8 - 9R_{10} - 12.5R_{9G} + (.33 + .67\,RP)\,R_9 - A_9 = \tau_A \frac{dA_9}{dt} \quad \text{(A-65)}$$

$$A_{10} = 0 \quad \text{(A-66)}$$

$$A_{11}^{o} + A_{14}^{o} - C_{5P} - A_{SO_4} = \tau_A \frac{dA_{SC_A}}{dt} \quad \text{(A-67)}$$

$$A_{12}^{o} + C_{5P} - A_{14} = \tau_A \frac{dA_{12}}{dt} \quad \text{(A-68)}$$

$$A_{13}^{o} - A_{14}^{o} + P_1 + R_2 + R_3 + R_4 + R_5 + R_6 + 15R_7 + 16.5R_8 + 12R_{10} + 16.5R_{9G} - (.33R_p + .67)\,R_9 - A_L = \tau_A \frac{dA_L}{dt} \quad \text{(A-69)}$$

If $A_L < 0$ (A-70)

$A_{13} = 0$

$A_{14} = A_L$

If $A_L > 0$ (A-71)

$A_{13} = A_L$

$A_{14} = 0$

$$A_{11} = A_{SO_4} - A_{14} \quad \text{(A-72)}$$

$$\tau_P = \frac{V\,(1-f_A)}{P_T}\,\rho_P \quad \text{(A-73)}$$

$$P_1^{\,0} + R_1 - M_1 - D_1 - P_1 = \frac{dP_1}{dt} \quad \text{(A-74)}$$

$$P_2^{\,0} + R_2 - M_2 - D_2 - P_2 = \tau_P \frac{dP_2}{dt} \quad \text{(A-75)}$$

$$P_3^{\,0} - M_3 - D_3 - P_3 = \tau_P \frac{dP_3}{dt} \quad \text{(A-76)}$$

$$P_4^{\,0} - M_4 - D_4 - P_4 = \tau_P \frac{dP_4}{dt} \quad \text{(A-77)}$$

$$P_5 - M_5 - D_5 - P_5 = \tau_P \frac{dP_5}{dt} \quad \text{(A-78)}$$

$$P_6^{\,0} - M_6 - D_6 - P_6 = \tau_P \frac{dP_6}{dt} \quad \text{(A-79)}$$

$$P_7^{\,0} - M_7 - D_7 - P_7 = \tau_P \frac{dP_7}{dt} \quad \text{(A-80)}$$

$$P_8^0 - M_8 - D_8 - P_8 = \tau_P \frac{dP_8}{dt} \quad \text{(A-81)}$$

$$P_{10}^0 - D_{10} - P_{10} = \tau_P \frac{dP_{10}}{dt} \quad \text{(A-82)}$$

$$P_8 = 1.81\left(\frac{A_{10}\,A_8}{A_{11}}\right)\left(\frac{P_T}{A_T}\right) \quad \text{(A-83)}$$

$$G_{CO_{1.8}} = R_{10} + 6R_7 + 7R_8 + 7R_8 G \quad \text{(A-84)}$$

$$G_{NO} = .67R_8\,(1 - R_P) \quad \text{(A-85)}$$

$$G_{TNM} = R_7 \quad \text{(A-86)}$$

Appendix B

Dynamic Simulation--Program Listing and Output

SOURCE PROGRAM LISTING

```
      PROGRAM TNTSIM(INPUT,TAPE5=INPUT,OUTPUT,TAPE6=OUTPUT,PUNCH,TAPE7      TNTDY    2
     C=PUNCH)                                                               TNTDY    3
      REAL MM                                                               TNTDY    4
      DIMENSION TACDTY(150,2)                                               TNTDY    5
      DIMENSION RMSS(150,6)                                                 TNTDY    6
      DIMENSION SPENT(150)                                                  TNTDY    7
      DIMENSION MM(17),AMT(17,8),PMT(17,8)                                  TNTDY    8
      DIMENSION RHO(14),TEMP(8),WKR(8),FV(8),E0A(6),EA0(6),E0AP(6),         TNTDY    9
     C  EA0P(6),     A5(17,6),P5(17,6),FA(6),HP(6),FACID(6),F0(6),          TNTDY   10
     C FORG(6),FR(6),FRC(6),AA(14,6),ATR(6),ATW(6),AWL(6),TM(3),            TNTDY   11
     C TW(3),TWL(3)                                                         TNTDY   12
      DIMENSION P1A(17),P1B(17),P1S(17),P2(17),P2S(17),P3A(17),             TNTDY   13
     C P3R(17),P3S(17),P4(17),P4S(17),P5(17),P5S(17),P6(17),P6S(17)         TNTDY   14
      DIMENSION A(17),P(17),AI(17),PI(17)                                   TNTDY   15
      DIMENSION A1A(17),A1B(17),A1S(17),A2(17),A2S(17),A3A(17),             TNTDY   16
     C A3R(17),A3S(17),A4(17),A4S(17),A5(17),A5S(17),A6(17),A6S(17)         TNTDY   17
      DIMENSION ARRAY(17,8)                                                 TNTDY   18
      DIMENSION XX(150,8),X(150)                                            TNTDY   19
      DIMENSION CONT(150),CRANE(150),CWBSA(150),CWSA(150),CONTSA(150),      TNTDY   20
     CON(150,8),TTCOX(150),TYWOX(150),AN(150,6) ,RMS(150,8)                 TNTDY   21
     C,ANA(150,8),AWR(150,8),MENE(150,6)                                    TNTDY   22
      DIMENSION MENSA(150,6)                                                TNTDY   23
      COMMON EX,BT,IPRNT,JACK,NM,NN,TTME,ICALL,MP,TCOX,TWOX,RATES(8,10)      TNTDY   24
     C,TSEP(6)                                                              TNTDY   25
      COMMON/PAR/G1(8),G3(8),G4(8),G3S(8),G4S(8),G5(8),G6(8),G7(8),         TNTDY   26
     C G8(8),G10(8),G9(8)                                                   TNTDY   27
      COMMON/VECT/AV(14,17),PV(14,17),IVSL,CHANXO,DFANXO,CHPNXO,OFPNXO      TNTDY   28
      COMMON/X/                    A1AI(17),A1PI(17),A2I(17),A3AI(17),      TNTDY   29
     C  A3RI(17),AAI(17),A5I(17),AAI(17),PIAI,PIRI                          TNTDY   30
      COMMON/VECTOR/A,P,T,FWKN,FRAC,NOTCH,ITYPE,FAR,FPO,ISTGE,IV            TNTDY   31
     C,EAP,E0P                                                              TNTDY   32
      COMMON/ORG/ARY(14),XYY(14)                                            TNTDY   33
      COMMON/SEP/T1A,T1R,T2,T3A,T3R,T4,T5,T6,FWKN1A,FWKN1R,FWKN2,           TNTDY   34
     C FWKN3A,FWKN3R,FWKN4,FWKN5,FWKN6,E0AP1,E0AP2,E0AP3,E0AP4,E0AP5,       TNTDY   35
     C E0AP6,FA(P1),FA0P2,FA0P3,EAMP4,EA0P5,EAMP6,FA1,FA2,FA3,FA4,FA5,      TNTDY   36
     C FA6,FRC(1),FRC(2),FRC(3),FRC(4),FRC(5),FRC(6),F01,F02,F03,F04,       TNTDY   37
     C F05,F06,FRAC1,FRAC2,FRAC3,FRAC4,FRAC5,FRAC6,FR1,FR2,FR3,FR4,FR5,     TNTDY   38
     C FR6,A1S,A2S,A3S,A4S,A5S,A6S,P1S,P2S,P3S,P4S,P5S,P6S,                 TNTDY   39
     C A1P(14),A1R(14),AF(14),PIR(14),PRR(14),PF(14)                        TNTDY   40
     C ,M1,M2,M3,M4,M5,M6,FORG1,FORG2,FORG3,FORG4,FORG5,FORG6               TNTDY   41
      COMMON/AMNT/A1A,A1B,A2,A3A,A3R,A4,A5,A6                               TNTDY   42
     C,P1A,P1R,P2,P3A,P3R,P4,P5,P6                                          TNTDY   43
      EQUIVALENCE (AMT(1,1),A1A(1))                                         TNTDY   44
     C,(PMT(1,1),P1A(1))                                                    TNTDY   45
      COMMON /INPUT/AI,PI,TI                                                TNTDY   46
      COMMON/FRR/FR(17,8)                                                   TNTDY   47
      COMMON/RHO/R(10)                                                      TNTDY   48
      COMMON/70/RHO1,RHO2,RHO3,RHO4,RHO5,RHO6,RHO7,RHO8,RHO9,RHO10,        TNTDY   49
     C RHO11,RHO12,RHO13,RHO14,CP(14),DH(10),AK12,AK3W,AK4W,AK5S,AK6S,      TNTDY   50
     C AK7S,AK4S,E7S,E4S,                                                   TNTDY   51
     C AK7,AKR,AK10,E2I,E3W,E4W,E5S,F6S,E7,E8,E10,FD,AKHA,AKHATL,SA,SB,     TNTDY   52
     C SC,SD,SF,SG,SH,SI,SJ,RP,TR,FWI,RP                                   TNTDY   53
      EQUIVALENCE (T1A,TEMP(1)),(FWKN1A,FV  (1)),(E0AP1,E0AP(1)),           TNTDY   54
     C  (EA0P1,E0P(1)),(A1,R0(1)),(A1S(1),AS(1)),(P1S(1),PS(1)),            TNTDY   55
     C(FA1,FA(1)),(FACID1,FACID(1)),(F01,F0(1)),(FORG1,FORG(1)),            TNTDY   56
     C  (FR1,FR(1)),(FRAC1,FRC(1)),(AA(1,1),AIR(1))                         TNTDY   57
      EQUIVALENCE (IC ,ICOUNT)                                              TNTDY   58
```

```
      EQUIVALENCE (RMO1,RMO(1)),(FMIN,FMAX)                              TNTDV      59
      EQUIVALENCE (ARRAY(1,1),A1&I(1))                                   TNTDV      60
      EQUIVALENCE (AK9,SE),(F9,SG)                                       TNTDV      61
      DATA FWN,EFW,EYW,EOL/-89.,-87.,-45.,104./                          TNTDV      62
      DATA PW/2*137.,2*182.,2*227.,213.,258.,63.,92.,98.,127.,18.,88.,   TNTDV1      1
     C 3*1./                                                             TNTDV      64
      DATA IMAGEN,FMAX,IQUIT/7,418.,6/                                   TNTDV      65
      READ(5,1)AK12,AK3W,AK4W,AK5S,AK6S,AK7,AK8,AK10                     TNTDV      67
      READ(5,1)AK3S,AK4S,E3S,E4S                                         TNTDV      68
    1 FORMAT(8F10.0)                                                     TNTDV      69
      READ(5,1) E21,E3W,E4W,F5S,E6S,E7,E8,E10                            TNTDV      70
      READ(5,1)S4,S8,SC,SD,SF,SG,SH,SI                                   TNTDV      71
      READ(5,1) SJ,RR,TP,AKMA,AKMATE,FMAX,FB,PP                          TNTDV3     1
      READ(5,1)DM                                                        TNTDV      73
      READ(5,1)RMO                                                       TNTDV      74
      READ(5,1)CP                                                        TNTDV      75
      READ(5,2)A1A,P1A,A1B,P1B,A1S,P1S,        A2,P2,A2S,P2S,A3A,P3A,    TNTDV      76
     C A3W,P3W,A3S,P3S,A4,P4,A4S,P4S,A5,P5,A5S,P5S,A6,P6,A6S,P6S         TNTDV      77
      READ(5,4)N1,N2,N3,N4,N5,N6                                         TNTDV      78
    4 FORMAT(6I)                                                         TNTDV      79
      READ(5,1)EA0                                                       TNTDV      80
      READ(5,1)E0A                                                       TNTDV      81
      READ(5,1)VKN,VKMS                                                  TNTDV      82
      READ(5,1)TEMP                                                      TNTDV      83
      READ(5,1)EX                                                        TNTDV      84
    2 FORMAT(5E16.7/5E16.7/4F16.7,3F2.0)                                 TNTDV1     2
      WRITE(6,5)A1A,P1A,A1B,P1B,A1S,P1S,       A2,P2,A2S,P2S,A3A,P3A,    TNTDV      86
     C A3W,P3W,A3S,P3S,A4,P4,A4S,P4S,A5,P5,A5S,P5S,A6,P6,A6S,P6S         TNTDV      87
    5 FORMAT( 12H0INPUT COMP</(1X,10F12.4/1X7F12.4))                     TNTDV      88
      DO 179 I=1,37                                                      TNTDV      89
      A(I)=0.                                                            TNTDV      90
      P(I)=0.                                                            TNTDV      91
      AV(1,I)=A1A(I)                                                     TNTDV      92
      AV(2,I)=A1B(I)                                                     TNTDV      93
      AV(3,I)=A1S(I)                                                     TNTDV      94
      AV(4,I)=A2 (I)                                                     TNTDV      95
      AV(5,I)=A2S(I)                                                     TNTDV      96
      AV(6,I)=A3A(I)                                                     TNTDV      97
      AV(7,I)=A3P(I)                                                     TNTDV      98
      AV(8,I)=A3S(I)                                                     TNTDV      99
      AV(9,I)=A4 (I)                                                     TNTDV     100
      AV(10,I)=A4S(I)                                                    TNTDV     101
      AV(11,I)=A5 (I)                                                    TNTDV     102
      AV(12,I)=A5S(I)                                                    TNTDV     103
      AV(13,I)=A6 (I)                                                    TNTDV     104
      AV(14,I)=A6S(I)                                                    TNTDV     105
      PV(1,I)=P1A(I)                                                     TNTDV     106
      PV(2,I)=P1B(I)                                                     TNTDV     107
      PV(3,I)=P1S(I)                                                     TNTDV     108
      PV(4,I)=P2 (I)                                                     TNTDV     109
      PV(5,I)=P2S(I)                                                     TNTDV     110
      PV(6,I)=P3A(I)                                                     TNTDV     111
      PV(7,I)=P3W(I)                                                     TNTDV     112
      PV(8,I)=P3S(I)                                                     TNTDV     113
      PV(9,I)=P4 (I)                                                     TNTDV     114
      PV(10,I)=P4S(I)                                                    TNTDV     115
      PV(11,I)=P5 (I)                                                    TNTDV     116
```

```
                      PV(12,I)=PSS(I)                                                   TNTDY  117
                      PV(13,I)=PG (I)                                                   TNTDY  118
                      PV(14,I)=PGS(I)                                                   TNTDY  119
                  179 CONTINUE                                                          TNTDY  120
                      DO170I=1,6                                                        TNTDY  121
                      EAMP(I)=EA0(I)/(1.-EA0(I))                                        TNTDY  122
                      FOMP(I)=E0A(I)/(1.-E0A(I))                                        TNTDY  123
                  170 CONTINUE                                                          TNTDY  124
                      FWKMS=  WKMS                                                      TNTDY  125
                      DO171I=1,8                                                        TNTDY  126
                      PV(I)=WKM(I)                                                      TNTDY  127
                  171 CONTINUE                                                          TNTDY  128
                      WRITE(6,303)AK12,AK13,AK14,AK15,AK45,AK55,AK65,AK7,AK8,AK10,E21,  TNTDY  129
                     C E31,E41,E51,E45,E55,E65,E7,E8,E10,SA,SB,SC,SD,SE,SG,S1,SI,SJ,AM,  TNTDY  130
                     C TP,AKMA,AKMATL,FO,MP                                             TNTDY  131
                      WRITE(6,301) (I,MU(I),AMO(I),CP(I),I=1,NM)(I,I=1,10)              TNTDY  132
                      WRITE(6,302) (I,MU(I),AMO(I),CP(I),)I=11,14)                      TNTDY  133
                  300 FORMAT( 1H1,20X 20H*****INPUT DATA*****/ 15HRATE CONSTANTS/12X    TNTDY  134
                     C 3HK12,7X,3HK13,7X,3HK14,7X,3HK15,7X,3HK45,7X,3HK55,7X,3HK65,7X,  TNTDY  135
                     C 2HK7,8X,2HK8,8X,3HK10/4X10F10.2/20HREACTIVATION ENERGIES/12X,3HE21 TNTDY  136
                  175 C,7X,3HE31,7X,3HE41,7X,3HE51,7X,3HE45,7X,3HE55,7X,3HE65,7X,2HE7,8X, TNTDY  137
                     C 2HE8,8X,3HE10/6X10F1                                             TNTDY  138
                     C0,8/ 19HCONSTANTS/11X 1HA,7X 1HB,7X 1HC,  7X 1HD,7X 1HE,7 TNTDY  139
                     CX 1HG,7X 1HH,7X 1HI,7X 1HJ/6X9F8.2/6X 18HGAS LAW CONSTANT =,      TNTDY  140
                     C  F5.2/6X 27HREFERENCE TEMPERATURE =.F8.2,    6H DEG K/           TNTDY  141
                  180 C  5X 17HMASS TX. COEFF, =.F10.1/6X 23HMASS TX. COEFF. (TOL) =.F10. TNTDY  142
                     C1/ 4X,46H CONVERSION OF MnOSO4 DECOMPOSITION REACTION =.F6.4/     TNTDY  143
                     C 6X,29HOXYGEN COEFFICIENT =.F8.4)                                 TNTDY  144
                  301 FORMAT( 29H0PHYSICAL PROPERTIES/6X 9HCOMPONENT,5X 6HMOL. WT.,     TNTDY  145
                     C      5X 7HDENSITY,5X 4HVNT, CAP.,10X 8HREACTION,5X 15HVP. OF     TNTDY  146
                  185 CREACTION/       (6X15,F14.1,F12.2,F13.2,I16,F20.0))              TNTDY  147
                  302 FORMAT(6X15,F16.1,F12.2,F13.2)                                    TNTDY  148
                      307 J=1                                                           TNTDY  149
                      WRITE(6,190)                                                      TNTDY  150
                  190 FORMAT( 1H1)                                                      TNTDY  151
                  190 DO187I=1,6                                                        TNTDY  152
                      WRITE(6,191)I                                                     TNTDY  153
                  191 FORMAT( 6HOSTAGE,I2)                                              TNTDY  154
                      IF(I.NE.1.AND.I.NE.3)GOTO192                                      TNTDY  155
                      WRITE(6,193)I,I,VKM(J),VKM(J+1),TEMP(J),TEMP(J+1)                 TNTDY  156
                  195 FORMAT(6X  8HNITRATOR,I2,  1HA,19X  8HNITRATOR,I2,  1HB/          TNTDY  157
                     C       6X  6HVOL. =,F5.1,19X,  6HVOL. =,F5.1/6X  6HTEMP.=,F5.1,  TNTDY  158
                     C            19X  6HTEMP,=,F5.1)                                  TNTDY  159
                      J=J+1                                                             TNTDY  160
                      GOTO194                                                           TNTDY  161
                  192 WRITE(6,195)I,VKM(J),TEMP(J)                                      TNTDY  162
                  195 FORMAT(6X  8HNITRATOR,I2/6X  6HVOL. =,F5.1/6X  6HTEMP.=,F5.1)     TNTDY  163
                  194 J=J+1                                                             TNTDY  164
                      WRITE(6,196)I,VKMS,MO(I),E0A(I),EA0(I)                            TNTDY  165
                  196 FORMAT( 1H0,5X,  9HSEPARATOR,I2/6X  6HVOL. =F5.1/                 TNTDY  166
                  165 C       6X 15HNOTCH SETTING =,I2/6X 11HENTRAINMENT/11X 15HORGANIC I TNTDY  167
                     CN ACID,      FA.5/11X 15HACID IN ORGANIC =F8.5)                   TNTDY  168
                  187 CONTINUE                                                          TNTDY  169
                      CALL SUB2(A15,P15,N1,FOAC1,EOAP1,EAOP1,FA1,F01,FAC101,FOAG1)      TNTDY  170
                      CALL SUB2(A25,P25,N2,FOAC2,EOAP2,EAOP2,FA2,F02,FAC102,FOAG2)      TNTDY  171
                  170 CALL SUB2(A35,P35,N3,FOAC3,EOAP3,EAOP3,FA3,F03,FAC103,FOAG3)      TNTDY  172
                      CALL SUB2(A45,P45,N4,FOAC4,EOAP4,EAOP4,FA4,F04,FAC104,FOAG4)      TNTDY  173
```

```
                      CALL SUB2(AS5,PS5,AS,FRAC5,EXP5,EXP5,FA5,F05,FACID5,FUN05)      TWTDY   174
                      CALL SUB2(AS6,PS6,AS,FRAC6,EXP6,EXP6,FA6,F06,FACID6,FUN06)      TWTDY   175
                      FP1=1.-FRAC1                                                    TWTDY   176
  175                 FP2=1.-FRAC2                                                    TWTDY   177
                      FP3=1.-FRAC3                                                    TWTDY   178
                      FP4=1.-FRAC4                                                    TWTDY   179
                      FP5=1.-FRAC5                                                    TWTDY   180
                      FP6=1.-FRAC6                                                    TWTDY   181
  180                 ICALL=0                                                         TWTDY   182
                      TIME=3.                                                         TWTDY   183
                      CALL INPT                                                       TWTDY   184
                      ICOUNT=0                                                        TWTDY   185
                      NOTJACK=1.-AM                                                   TWTDY   186
  185                 YCOX=0.                                                         TWTDY   187
                      YNO=0.                                                          TWTDY   188
                      J=JACK-(JACK/AM)*AM+AM                                          TWTDY   189
                      TIME=TIME+DT                                                    TWTDY   190
                      IF(J.EQ.AM)WRITE(6,390)TIME                                     TWTDY   191
  190           900   FORMAT(1H1,5X,23H******SOLUTION AT TIME =,F6.3,11H HOURS*****) TWTDY   192
                      CALL INPT                                                       TWTDY   193
                      IVSL=1                                                          TWTDY   194
                      DFP=A0=0.                                                       TWTDY   195
                      DFA=A0=0.                                                       TWTDY   196
  195                 CHP=A0=0.                                                       TWTDY   197
                      CHA=A0=0.                                                       TWTDY   198
                    3006 FORMAT(1X15)                                                 TWTDY   199
                      ITYPE=0                                                         TWTDY   200
                      ISTGE=1                                                         TWTDY   201
  200                 IV=1                                                            TWTDY   202
                      T=T1A                                                           TWTDY   203
                      FWDX=FWDX1A                                                     TWTDY   204
                      DD400I=1.14                                                     TWTDY   205
                      A1(I)=A1A1(I)+FR2*A2S(I)*FA2                                    TWTDY   206
  205                 P1(I)=FOMG2**2S(I)*FR2                                          TWTDY   207
                      A(I)=A1A(I)                                                     TWTDY   208
                  600 P(I)=P1A(I)                                                     TWTDY   209
                      P1(10)=P1(10)+P1A1                                              TWTDY   210
                      CALL SUB                                                        TWTDY   211
  210                 IF(J.NE.AM) GO TO 499                                           TWTDY   212
                      WRITE(6,500)                                                    TWTDY   213
                  500 FORMAT(1?HNITRATOR 1A)                                          TWTDY   214
                      WRITE(6,401)                                                    TWTDY   215
                      CALL SUB1(8.?,A1,P1)                                            TWTDY   216
  215               499 CONTINUE                                                      TWTDY   217
                      FWDX=FWDX18                                                     TWTDY   218
                      T=T1A                                                           TWTDY   219
                      IV=?                                                            TWTDY   220
                      DD61P1=1.14                                                     TWTDY   221
  220                 A1A(I)=A(I)                                                     TWTDY   222
                      P1A(I)=P(I)                                                     TWTDY   223
                      A(I)=A10(I)                                                     TWTDY   224
                      P(I)=P10(I)                                                     TWTDY   225
                      A1(I)=A1M1(I)+FRAC1*A1C(I)+FA1*A1A(I)                           TWTDY   226
  225                 P1(I)=      P1A(I)+FOMG1*P1S(I)                                 TWTDY   227
                      P1(10)=P1(10)+P101                                              TWTDY   228
                      CALL SUB                                                        TWTDY   229
                      IF(J.EQ.AM)WRITE(6,501)                                         TWTDY   230
```

```
                  501  FORMAT( 12H0ITERATOR I4)                                  TWTDY   231
          230          IF(J.EQ.NN)WRITE(6,401)                                   TWTDY   232
                       IF(J.EQ.NN)CALL SUBI(A,P,AI,PI)                           TWTDY   233
                       EAP=EAPP1                                                 TWTDY   234
                       EOP=FOAP1                                                 TWTDY   235
                       WRITE(NN)I                                                TWTDY   236
          235          FWRD=FWDPS                                                TWTDY   237
                       ITYPE=1                                                   TWTDY   238
                       DO670I=1,14                                               TWTDY   239
                       AIB(I)=A(I)                                               TWTDY   240
                       PIB(I)=P(I)                                               TWTDY   241
          240          A(I)=AIS(I)                                               TWTDY   242
                       P(I)=PIS(I)                                               TWTDY   243
                       AI(I)=AIB(I)                                              TWTDY   244
                       PI(I)=PIB(I)                                              TWTDY   245
                  620  CONTINUE                                                  TWTDY   246
          245          CALL SUM                                                  TWTDY   247
                       IF(J.NE.NN) GOTO62I                                       TWTDY   248
                       WRITE(6,502)                                              TWTDY   249
                  502  FORMAT( 12H0SEPARATOR )                                   TWTDY   250
                       WRITE(6,401)                                              TWTDY   251
          250          CALL SUBI(A,P,AI,PI)                                      TWTDY   252
                  621  CONTINUE                                                  TWTDY   253
                       ITYPE=0                                                   TWTDY   254
                       FBAC1=FBAC                                                TWTDY   255
                       FB1=1.-FBAC1                                              TWTDY   256
          255          FA1=FAB                                                   TWTDY   257
                       FB1=FPB                                                   TWTDY   258
                       FACI01=1.-FA1                                             TWTDY   259
                       FOPG1=1.-FB1                                              TWTDY   260
                       ISTEE=2                                                   TWTDY   261
          260          IV=3                                                      TWTDY   262
                       FWRD=FWDP2                                                TWTDY   263
                       T=T2                                                      TWTDY   264
                       DO430I=1,14                                               TWTDY   265
                       AIS(I)=A(I)                                               TWTDY   266
          265          PIS(I)=P(I                                                TWTDY   267
                       A(I)=A2(I)                                                TWTDY   268
                       P(I)=P2(I)                                                TWTDY   269
                       AI(I)=A2I(I)*FACIDI*PAI<(I)*FB3*A3S(I)*FA3                TWTDY   270
                      C *FBAC2*A2S(I)*FA2                                        TWTDY   271
          270         670  PI(I)=P1S(I)*FO1*FB3*P1S(I)*FOBG3*FBAC2*P2S(I)*FOBG2  TWTDY   272
                       IF(IQUIT.EQ.1)GOTO)                                       TWTDY   273
                       CALL SUM                                                  TWTDY   274
                       IF(J.EQ.NN)WRITE(6,503)                                   TWTDY   275
                  503  FORMAT( 1I*0ITERATOR 2)                                   TWTDY   276
          275          IF(J.EQ.NN)WRITE(6,401)                                   TWTDY   277
                       IF(J.EQ.NN)CALL SUBI(A,P,AI,PI)                           TWTDY   278
                       EAP=EAPP2                                                 TWTDY   279
                       EOP=EOAP2                                                 TWTDY   280
                       WRITE(NN)I                                                TWTDY   281
          280          FWRD=FWDP5                                                TWTDY   282
                       ITYPE=1                                                   TWTDY   283
                       DO640I=1,14                                               TWTDY   284
                       A2(I)=A(I)                                                TWTDY   285
                       P2(I)=P(I)                                                TWTDY   286
          285          A(I)=A2S(I)                                               TWTDY   287
```

```
                      P(I)=P2S(I)                                                TWIST4   288
                      A1(I)=A2 (I)                                               TWIST4   289
                      P1(I)=P2 (I)                                               TWIST4   290
                  640 CONTINUE                                                   TWIST4   291
          290         CALL SUB                                                   TWIST4   292
                      IF(J.NE.JMX) GOTO641                                       TWIST4   293
                      WRITE(6,506)                                               TWIST4   294
                  506 FORMAT( 12HQSE-MATOR >)                                    TWIST4   295
                      WRITE(6,401)                                               TWIST4   296
          295         CALL SUB1(A,P,A1,P1)                                       TWIST4   297
                  641 CONTINUE                                                   TWIST4   298
                      ITYPE=0                                                    TWIST4   299
                      FRAC2=FRAC                                                 TWIST4   300
                      FR2=1.-FRAC2                                               TWIST4   301
          300         FA2=FA0                                                    TWIST4   302
                      F02=FP0                                                    TWIST4   303
                      FAC1R2=1.-F12                                              TWIST4   304
                      F0RC2=1.-F02                                               TWIST4   305
                      ISTATE=1                                                   TWIST4   306
          305         IY=4                                                       TWIST4   307
                      FYOLD=FYOLD                                                TWIST4   308
                      T=T0A                                                      TWIST4   309
                      DO460I=1,14                                                TWIST4   310
                      A2S(I)=A(I)                                                TWIST4   311
C0          310         P2S(I)=P(I)                                              TWIST4   312
                      A(I)=A0A(I)                                                TWIST4   313
                      P(I)=P0A(I)                                                TWIST4   314
                      A1(I)=A3A1(I)+FAC1R2*A2S(I)+FRA*DAS(I)*FAA                 TWIST4   315
                      P1(I)=F02*P2S(I)+FRA*PAS(I)*F0R6A                          TWIST4   316
          315     650 CONTINUE                                                   TWIST4   317
                      IF(IOUT.EQ.2)GOTO3                                         TWIST4   318
                      CALL SUP                                                   TWIST4   319
                      IF(J.NE.JMX)GOTO651                                        TWIST4   320
                      WRITE(6,505)                                               TWIST4   321
          320         FORMAT( 12HQUITRATOR >)                                    TWIST4   322
                      WRITE(6,401)                                               TWIST4   323
                      CALL SUB1(A,P,A1,P1)                                       TWIST4   324
                  651 CONTINUE                                                   TWIST4   325
                      FYOLD=FYOLD                                                TWIST4   326
          325         T=T0                                                       TWIST4   327
                      IY=5                                                       TWIST4   328
                      DO64PI=1,14                                                TWIST4   329
                      A3A(I)=A(I)                                                TWIST4   330
                      P3A(I)=P(I)                                                TWIST4   331
          330         A(I)=A0A(I)                                                TWIST4   332
                      P(I)=P0A(I)                                                TWIST4   333
                      A1(I)=A3P1(I)+FRAC3*A3*(I-*A3-A3A(I)                       TWIST4   334
                  660 P1(I)=P3A(I)+FRAC3*P3S(I)-FRAC3                            TWIST4   335
                      CALL SUB                                                   TWIST4   336
          335         IF(J.NE.JMX)GOTO661                                        TWIST4   337
                      WRITE(6,506)                                               TWIST4   338
                  506 FORMAT( 12HQUITRATOR 3>)                                   TWIST4   339
                      WRITE(6,401)                                               TWIST4   340
                      CALL SUB1(A,P,A1,P1)                                       TWIST4   341
          340     661 CONTINUE                                                   TWIST4   342
                      EXP=EXP3                                                   TWIST4   343
                      EXP=EXP3                                                   TWIST4   344
```

```
                NOTCH=N3                                                        INTDY   345
                FVKH=FVKHS                                                      INTDY   346
      345       ITYPE=1                                                         INTDY   347
                DO670I=1,14                                                     INTDY   348
                A3S(I)=A(I)                                                     INTDY   349
                P3S(I)=P(I)                                                     INTDY   350
                A(I)=A3S(I)                                                     INTDY   351
      350       P(I)=P3S(I)                                                     INTDY   352
                AI(I)=A3R(I)                                                    INTDY   353
                PI(I)=P3R(I)                                                    INTDY   354
            670 CONTINUE                                                        INTDY   355
                CALL SUB                                                        INTDY   356
      355       IF(J.NE.NN) GOTO671                                             INTDY   357
                WRITE(6,507)                                                    INTDY   358
            507 FORMAT( 12H0SEPARATOR 3)                                        INTDY   359
                WRITE(6,401)                                                    INTDY   360
                CALL SUB1(A,P,AI,PI)                                            INTDY   361
      360       CONTINUE                                                        INTDY   362
            671 ITYPE=0                                                         INTDY   363
                FRAC3=FRAC                                                      INTDY   364
                FR3=1.-FRAC3                                                    INTDY   365
                FA3=FAR                                                         INTDY   366
      365       F03=FPO                                                         INTDY   367
                FAC03=1.-FA3                                                    INTDY   368
                FORG3=1.-F03                                                    INTDY   369
                ISTGE=4                                                         INTDY   370
                IV=6                                                            INTDY   371
      370       T=T4                                                            INTDY   372
                FVKH=FVKH4                                                      INTDY   373
                DO680I=1,14                                                     INTDY   374
                A3S(I)=A(I)                                                     INTDY   375
                P3S(I)=P(I)                                                     INTDY   376
      375       A(I)=A4(I)                                                      INTDY   377
                P(I)=P4(I)                                                      INTDY   378
                AI(I)=A4I(I)*FAC03*A3S(I)*FR3*A3S(I)*FA3*    A4S(I)*FA4*FRAC4    INTDY   379
            680 PI(I)=F03*P3S(I)+FR3*P3S(I)*FORG3*FRAC4*P4S(I)*FORG4            INTDY   380
                IF(IQUIT.EQ.3)GOTO3                                             INTDY   381
      390       CALL SUB                                                        INTDY   382
                IF(J.NE.NN)GOTO681                                              INTDY   383
                WRITE(6,508)                                                    INTDY   384
            508 FORMAT( 11H0ITRATOR 4)                                          INTDY   385
                WRITE(6,401)                                                    INTDY   386
      395       CALL SUB1(A,P,AI,PI)                                            INTDY   387
            681 CONTINUE                                                        INTDY   388
                EOP=EOAP4                                                       INTDY   389
                EAP=EAOP4                                                       INTDY   390
                NOTCH=N4                                                        INTDY   391
      390       FVKH=FVKHS                                                      INTDY   392
                ITYPE=1                                                         INTDY   393
                DO690I=1,14                                                     INTDY   394
                A4(I)=A(I)                                                      INTDY   395
                P4(I)=P(I)                                                      INTDY   396
      395       A(I)=A4S(I)                                                     INTDY   397
                P(I)=P4S(I)                                                     INTDY   398
                AI(I)=A4 (I)                                                    INTDY   399
                PI(I)=P4 (I)                                                    INTDY   400
            690 CONTINUE                                                        INTDY   401
```

```
      CALL SUM                                                          TNTDY   402
      IF(J.NE.NN) GOTO691                                               TNTDY   403
      WRITE(6,509)                                                      TNTDY   404
509   FORMAT( 12H0SEPARATOR 4)                                          TNTDY   405
      WRITE(6,401)                                                      TNTDY   406
      CALL SUB1(A,P,AI,PI)                                              TNTDY   407
691   CONTINUE                                                          TNTDY   408
      ITYPE=0                                                           TNTDY   409
      FRAC4=FRAC                                                        TNTDY   410
      FP4=1.-FRAC4                                                      TNTDY   411
      FA4=FAR                                                           TNTDY   412
      FO4=FPO                                                           TNTDY   413
      FACID4=1.-FA4                                                     TNTDY   414
      FORG4=1.-FO4                                                      TNTDY   415
      ISTGE=5                                                           TNTDY   416
      IV=7                                                              TNTDY   417
      T=T5                                                              TNTDY   418
      FVK4=FVKM5                                                        TNTDY   419
      DO700I=1,14                                                       TNTDY   420
      A4S(I)=A(I)                                                       TNTDY   421
      P4S(I)=P(I)                                                       TNTDY   422
      A(I)=A5(I)                                                        TNTDY   423
      P(I)=P5(I)                                                        TNTDY   424
      AI(I)=A5I(I)+FACID4*A4S(I)+FR6*A6S(I)*FA4+FRAC5*A5S(I)*FA5        TNTDY   425
      PI(I)=FO4*P4S(I)+FR6*P6S(I)*FORG6+FRAC5*P5S(I)*FORG5              TNTDY   426
700   CONTINUE                                                          TNTDY   427
      IF(IQUIT.EQ.4)GOTO3                                               TNTDY   428
      CALL SUB                                                          TNTDY   429
      IF(J.NE.NN)GOTO701                                                TNTDY   430
      WRITE(6,510)                                                      TNTDY   431
510   FORMAT( 11H0NITRATOR 5)                                           TNTDY   432
      WRITE(6,401)                                                      TNTDY   433
      CALL SUM1(A,P,AI,PI)                                              TNTDY   434
701   CONTINUE                                                          TNTDY   435
      EOP=EOAP5                                                         TNTDY   436
      EAP=EAOP5                                                         TNTDY   437
      NOTCM=NM5                                                         TNTDY   438
      FVKM=FVKM5                                                        TNTDY   439
      ITYPE=1                                                           TNTDY   440
      DO710I=1,14                                                       TNTDY   441
      A5(I)=A(I)                                                        TNTDY   442
      P5(I)=P(I)                                                        TNTDY   443
      A(I)=A5S(I)                                                       TNTDY   444
      P(I)=P5S(I)                                                       TNTDY   445
      AI(I)=A5 (I)                                                      TNTDY   446
      PI(I)=P5 (I)                                                      TNTDY   447
710   CONTINUE                                                          TNTDY   448
      CALL SUM                                                          TNTDY   449
      IF(J.NE.NN) GOTO711                                               TNTDY   450
      WRITE(6,511)                                                      TNTDY   451
511   FORMAT( 12H0SEPARATOR 5)                                          TNTDY   452
      WRITE(6,401)                                                      TNTDY   453
      CALL SUM1(A,P,AI,PI)                                              TNTDY   454
711   CONTINUE                                                          TNTDY   455
      ITYPE=0                                                           TNTDY   456
      FRAC5=FRAC                                                        TNTDY   457
      FP5=1.-FRAC5                                                      TNTDY   458
```

```
                      FA5=FAR                                                    TNTDY   459
                      FO5=FPO                                                    TNTDY   460
                      FACIO5=1.-FA5                                              TNTDY   461
      460             FORG5=1.-FO5                                               TNTDY   462
                      ISTGE=6                                                    TNTDY   463
                      IV=8                                                       TNTDY   464
                      T=T6                                                       TNTDY   465
                      FVKM=FVKM6                                                 TNTDY   466
      465             DO720I=1,14                                                TNTDY   467
                      A5S(I)=A6(I)                                               TNTDY   468
                      P5S(I)=P6(I)                                               TNTDY   469
                      A6(I)=A6S(I)                                               TNTDY   470
                      P6(I)=P6S(I)                                               TNTDY   471
      470             AI(I)=A6I(I)*FACIO5*A5S(I)+FRAC6*A6S(I)*FA6                TNTDY   472
                      PI(I)=FO5*P5S(I)+FRAC6*P6S(I)*FORG6                        TNTDY   473
                720   CONTINUE                                                   TNTDY   474
                      IF(IQUIT.EQ.5)GOTO3                                        TNTDY   475
                      CALL SUB                                                   TNTDY   476
      475             IF(J.NE.MM)GOTO721                                         TNTDY   477
                      WRITE(6,512)                                               TNTDY   478
                512   FORMAT( 11H0NITRATOR 6)                                    TNTDY   479
                      WRITE(6,401)                                               TNTDY   480
                      CALL SUB1(A,P,AI,PI)                                       TNTDY   481
      480             GOTO721                                                    TNTDY   482
                      EOP=EOAP6                                                  TNTDY   483
                      EAP=EAOP6                                                  TNTDY   484
                      NOTCH=N6                                                   TNTDY   485
                      FVKM=FVKM5                                                 TNTDY   486
                      ITYPE=1                                                    TNTDY   487
      485             DO770I=1,14                                                TNTDY   488
                      A6(I)=A(I)                                                 TNTDY   489
                      P6(I)=P(I)                                                 TNTDY   490
                      A(I)=A6S(I)                                                TNTDY   491
      490             P(I)=P6S(I)                                                TNTDY   492
                      AI(I)=A6 (I)                                               TNTDY   493
                      PI(I)=P6 (I)                                               TNTDY   494
                770   CONTINUE                                                   TNTDY   495
                      CALL SUB                                                   TNTDY   496
      495             FRAC6=FRAC                                                 TNTDY   497
                      FP6=1.-FRAC6                                               TNTDY   498
                      FA6=FAR                                                    TNTDY   499
                      FO6=FPO                                                    TNTDY   500
                      FORG6=1.-FO6                                               TNTDY   501
      500             FACIO6=1.-FA6                                              TNTDY   502
                      IF(J.NE.NN) GOTO731                                        TNTDY   503
                      WRITE(6,513)                                               TNTDY   504
                513   FORMAT( 12H0SEPARATOR 6)                                   TNTDY   505
                      WRITE(6,401)                                               TNTDY   506
      505             CALL SUB1(A,P,AI,PI)                                       TNTDY   507
                      WRITE(6,247)CHANIO,CHPWIO,DFAWIO,DFPWIO                    TNTDY   508
                247 FORMAT(1H0,6HCONVERGENCE TESTS,/,60X,4HACID,4X,8HORGANIC,/   TNTDY   509
                    1 50HMAXIMUM PERCENT ERROR  FROM STEADY STATE EQUATIONS,2F10.3,/  TNTDY   510
                    2 6X,46HMAXIMUM PERCENT CHANGE FROM PREVIOUS ITERATION,3X,2F10.3)  TNTDY   511
      510             WRITE(6,246) (I,I=1,6),FACID,FORG,FRC                      TNTDY   512
                246   FORMAT( 40H3PARAMETERS USED IN RECYCLE CALCULATIONS/6X  STAGE,  TNTDY   513
                    C     27X6I8/6X 34HFRACTION ACID PHASE IN ORG. STREAM,6F8.5/  TNTDY   514
                    C       6X 34HFRACTION ORG. PHASE IN ACID STREAM,6F8.5/      TNTDY   515
```

```
      C        6X 25HFRACTION INTERNAL RECYCLE,9X6F8.5)                    TNTDY  516
  515       DO219IV=1,6                                                    TNTDY  517
            DO211J=1,14                                                    TNTDY  518
            AIR(J)=AS(J,IV)*FA(IV)*FRC(IV)                                 TNTDY  519
            AXR(J)=AS(J,IV)*FA(IV)*FR (IV)                                 TNTDY  520
            AF(J)=AS(J,IV)*FACID(IV)                                       TNTDY  521
  520       PIR(J)=PS(J,IV)*FORG(IV)*FRC(IV)                               TNTDY  522
            PXR(J)=PS(J,IV)*FORG(IV)*FR (IV)                               TNTDY  523
        211 PF(J)=PS(J,IV)*FO(IV)                                          TNTDY  524
            WRITE(6,400)IV                                                 TNTDY  525
          C COMPUTE FLOW DATA                                              TNTDY  526
  525       DO212J=1,6                                                     TNTDY  527
            ATM(J)=0.                                                      TNTDY  528
            ATW(J)=0.                                                      TNTDY  529
            AVL(J)=0.                                                      TNTDY  530
            DO213I=1,14                                                    TNTDY  531
  530       ATM(J)=ATM(J)+AA(I,J)                                          TNTDY  532
            ATW(J)=ATW(J)+AA(I,J)*WW(I)                                    TNTDY  533
        213 AVL(J)=AVL(J)+AA(I,J)/WWO(I)                                   TNTDY  534
        212 CONTINUE                                                       TNTDY  535
            WRITE(6,401)                                                   TNTDY  536
  535       DO214I=1,3                                                     TNTDY  537
            K=I+3                                                          TNTDY  538
            TP(I)=ATM(I)+ATM(K)                                            TNTDY  539
            TW(I)=ATW(I)+ATW(K)                                            TNTDY  540
        214 TVL(I)=AVL(I)+AVL(K)                                           TNTDY  541
  540       WRITE(6,402)AF,(PF(I),I=1,10),ATM(3),ATP(6),TM(3),ATW(3),ATW(6), TNTDY  542
          C TW(3),AVL(3),AVL(6),TVL(3)                                     TNTDY  543
        400 FORMAT( 10H0SEPARATOR,I2/6X 28HORGANIC STREAM TO NEXT STAGE)   TNTDY  544
        401 FORMAT(13X  4HAMNT,4X  4HMMNT,4X  4HADNT,4X  4HMDNT,4X  4HATNT,4X TNTDY  545
          C 4HMTNT,      4X  3HTNA, 5X  4HTMRA,4X 4H4NO3,4X  3HTOL,4X 13H42SO4 TNTDY  546
          C  HNOSO4,4X  3HH2O,       5X  3HSO3)                            TNTDY  547
  545   402 FORMAT(  9H ACID PH,,14F8.3/  9H ORG, PH,,10F8.3/21X  8HACID PH,, TNTDY  548
          C        7X  8HORG, PH,,7X  5HTOTAL/6X  5HMOLES,3X3F15.3/         TNTDY  549
          C             6X  4HMASS,4X3F15.3/6X  8HVOLUME  3F15.3)           TNTDY  550
            WRITE(6,403)                                                   TNTDY  551
  550       FORMAT(  1H0,5X 21HNEXTFINAL ACID RECYCLE)                     TNTDY  552
            WRITE(6,401)                                                   TNTDY  553
            WRITE(6,402) AXR,(PXR(I),I=1,10),ATM(2),ATM(5),TW(2),ATW(2),   TNTDY  554
          C  ATW(5),TW(2),AVL(2),AVL(5),TVL(2)                             TNTDY  555
            WRITE(6,404)                                                   TNTDY  556
  555       FORMAT(  1H0,5X 21HINTFINAL ACID RECYCLE)                      TNTDY  557
            WRITE(6,401)                                                   TNTDY  558
            WRITE(6,402) AIR,(PIR(I),I=1,10),ATM(1),ATM(4),TM(1),ATW(1),ATW(4) TNTDY  559
          C ,TW(1),AVL(1),AVL(4),TVL(1)                                    TNTDY  560
        210 CONTINUE                                                       TNTDY  561
  560    731 DO740I=1,14                                                   TNTDY  562
            A6S(I)=A(I)                                                    TNTDY  563
        740 P6S(I)=P(I)                                                    TNTDY  564
            IF((JACK/NP)*NP.NE.JACK)GOTO3                                  TNTDY  565
            ICOUNT=ICOUNT+1                                                TNTDY  566
  565       TONT=((P6S(3)+P6S(4))*FO6+(A6S(3)+A6S(4))*FACID6)*182.         TNTDY  567
            SUM=0.                                                         TNTDY  568
            DO 75 I=1,8                                                    TNTDY  569
         75 SUM=SUM+(A6S(I)*FACID6+P6S(I)*FO6)*WW(I)                       TNTDY  570
            CONT(ICOUNT)=100.*TONT/SUM                                     TNTDY  571
  570       DO 76 I=9,14                                                   TNTDY  572
```

```
                74 SUM=SUM+(A6S(I)*FACID6.P6S(I)*F06)*MW(I)                          TNTDY    573
                   CRUDE(ICOUNT)=SUM                                                 TNTDY    574
                   SPA=0.                                                            TNTDY    575
                   FAFR=FA1*FR1                                                      TNTDY    576
          575      DO 77 I=1,8                                                       TNTDY    577
                77    SPA=SPA+A1S(I)*FAFR*MW(I)                                    TNTDY    578
                   SPO=SPA                                                           TNTDY    579
                   DO 78 I=9,14                                                      TNTDY    580
                78 SPA=SPA+A1S(I)*FAFR*MW(I)                                        TNTDY    581
          580      SPENT(ICOUNT)=SPA                                                 TNTDY    582
                   CWBSA(ICOUNT)=100.*SPO/SPA                                        TNTDY    583
                   CWSA(ICOUNT)=100.*A1S(13)*FAFR*10./SPA                            TNTDY    584
                   CONTSA(ICOUNT)=100.*(A1S(3)+A1S(4))*MW(3)*FAFR/SPO                TNTDY    585
                   DO 79 IS=1,6                                                      TNTDY    586
          585      RWSS(ICOUNT,IS)=AS(9,IS)/(AS(11,IS)+AS(14,IS))                    TNTDY    587
                   TLBS=0.                                                           TNTDY    588
                   DO 80 I=9,14                                                      TNTDY    589
                80 TLBS=TLBS+AS(1,IS)*MW(I)                                         TNTDY    590
                   IF(IS.GT.2) GO TO 79                                              TNTDY    591
          590      TACDTY(ICOUNT,IS)=100.*((AS(14,IS)+AS(11,IS))*MW(11)*0.7718*     TNTDY    592
                  1(AS(9,IS)*MW(9)+0.4959*AS(12,IS)*MW(12)))/TLBS                    TNTDY    593
                79 AN(ICOUNT,IS)=6300.*AS(9,IS)/TLBS                                TNTDY    594
                   DO 81 IN=1,8                                                      TNTDY    595
                   RWS(ICOUNT,IN)=ANT(9,IN)/(ANT(11,IN)+ANT(14,IN))                  TNTDY    596
          595   81 CONTINUE                                                         TNTDY    597
                   TTCOX(ICOUNT)=TCOX                                                TNTDY    598
                   TTNOX(ICOUNT)=TNOX                                                TNTDY    599
                   DO6I=1,6                                                          TNTDY    600
                   OP=0.                                                             TNTDY    601
          600      PP=0.                                                             TNTDY    602
                   DO7J=1,10                                                         TNTDY    603
                   OP=OP+PS(J,I)/RMO(J)                                              TNTDY    604
                7  PP=PP+PS(J,I)*MW(J)                                              TNTDY    605
                6  DENS(IC,I)=PP/(OP*62.4)                                          TNTDY    606
          605      DO 50 I=1,8                                                       TNTDY    607
                   ANAC=0.                                                           TNTDY    608
                   ANMC=0.                                                           TNTDY    609
                   DO40J=1,5,2                                                       TNTDY    610
                   ANAC=ANAC+RATES(I,J)                                              TNTDY    611
          610   40 ANMC=ANMC+RATES(I,J+1)                                           TNTDY    612
                   ANA(ICOUNT,I)=ANAC                                                TNTDY    613
                   ANM(ICOUNT,I)=ANMC                                                TNTDY    614
                   Q=0.                                                              TNTDY    615
                   DO 51 J=1,10                                                      TNTDY    616
          615   51 Q=Q+RATES(I,J)*DH(J)                                             TNTDY    617
                   Q=Q+(FIN(1,I)*EWN+FIN(2,I)*EFR+FIN(3,I)*EYW+FIN(5,I)*EQL)*.252    TNTDY    618
                   GOTO(31,32,33,34,35,36,37,38),I                                   TNTDY    619
                31 Q=Q+ENTH(A2S,FA2,FR2,P2S,FORG2,FR2,TSEP(2))                       TNTDY    620
                  C -ENTH(A1A,1.,1.,P1A,1.,1.,T1A)                                   TNTDY    621
          620      GOTO50                                                            TNTDY    622
                32 Q=Q+ENTH(A1A,1.,1.,P1A,1.,1.,T1A)                                TNTDY    623
                  C +ENTH(A1S,FA1,FRAC1,P1S,FORG1,FRAC1,TSEP(1))                     TNTDY    624
                  C -ENTH(A3B,1.,1.,P1B,1.,1.,T1B)                                  TNTDY    625
                   DLT=TSEP(1)-20.                                                   TNTDY    626
          625      DO39J=1,10                                                        TNTDY    627
                39 Q=Q+CP(J)*P1S(J)*FORG1*FR1*DLT                                   TNTDY    628
                   GOTO50                                                            TNTDY    629
```

```
      37   Q=Q+ENTH(A1S,FACID1,1.,P1S,FO1,1.,TSEP(1))                        TNTDY   630
           C +ENTH(A3S,FA3,FR3,P3S,FORG3,FR3,TSEP(3))                        TNTDY   631
           C +ENTH(A2S,FA2,FRAC2,P2S,FORG2,FRAC2,TSEP(2))                    TNTDY   632
           C -ENTH(A7,1.,1.,P2,1.,1.,T2)                                     TNTDY   633
            GOTO50                                                           TNTDY   634
      34   Q=Q+ENTH(A2S,FACID2,1.,P2S,FO2,1.,TSEP(2))                        TNTDY   635
           C +ENTH(A4S,FA4,FR4,P4S,FORGA,FR4,TSEP(4))                        TNTDY   636
           C -ENTH(A3A,1.,1.,P3A,1.,1.,T3A)                                  TNTDY   637
            GOTO50                                                           TNTDY   638
      35   Q=Q+ENTH(A3A,1.,1.,P3A,1.,1.,T3A)                                 TNTDY   639
           C +ENTH(A3S,FA3,FRAC3,P3S,FORG3,FRAC3,TSEP(3))                    TNTDY   640
           C -ENTH(A3B,1.,1.,P3B,1.,1.,T3B)                                  TNTDY   641
            GOTO50                                                           TNTDY   642
      36   Q=Q+ENTH(A3S,FACID3,1.,P3S,FO3,1.,TSEP(3))                        TNTDY   643
           C +ENTH(A5S,FA5,FR5,P5S,FORG5,FR5,TSEP(5))                        TNTDY   644
           C +ENTH(A4S,FA4,FRAC4,P4S,FORG4,FRAC4,TSEP(4))                    TNTDY   645
           C -ENTH(A4,1.,1.,P4,1.,1.,T4)                                     TNTDY   646
            GOTO50                                                           TNTDY   647
      37   Q=Q+ENTH(A4S,FACID4,1.,P4S,FO4,1.,TSEP(4))                        TNTDY   648
           C +ENTH(A6S,FA6,FR6,P6S,FORG6,FR6,TSEP(6))                        TNTDY   649
           C +ENTH(A5S,FA5,FRAC5,P5S,FORG5,FRAC5,TSEP(5))                    TNTDY   650
           C -ENTH(A5,1.,1.,P5,1.,1.,T5)                                     TNTDY   651
            GOTO50                                                           TNTDY   652
      38   Q=Q+ENTH(A5S,FACID5,1.,P5S,FO5,1.,TSEP(5))                        TNTDY   653
           C +ENTH(A6S,FA6,FRAC6,P6S,FORG6,FRAC6,TSEP(6))                    TNTDY   654
           C -ENTH(A6,1.,1.,P6,1.,1.,T6)                                     TNTDY   655
        50 ON(ICOUNT,I)=Q/.252                                               TNTDY   656
            DO 678 I=1,6                                                     TNTDY   657
            AS(10,I)=0                                                       TNTDY   658
            QA=0.                                                            TNTDY   659
            PA=0.                                                            TNTDY   660
            DO 679 J=1,14                                                    TNTDY   661
            QA=QA+AS(J,I)/RHO(J)                                             TNTDY   662
       679  PA=PA+AS(J,I)*MW(J)                                              TNTDY   663
       678  DENSA(IC,I)=PA/(QA*62.4)                                         TNTDY   664
         3  CONTINUE                                                         TNTDY   665
            WRITE(6,8) (CONT(I),CRUDE(I,CNBSA(I),CWSA(I),CONTSA(I),TTCOX(I), TNTDY   666
           C TTNOX(I),SPENT(I),I=1,IC)                                       TNTDY   667
         8  FORMAT(*1       CONT        CRUDE        CNBSA         CWSA       CONT TNTDY   668
           CSA        TTCOX        TTNOX           SPENT*/(1XF12.5,F12.1,F12.5, TNTDY   669
           C2F12.3,2F12.4,F16.2))                                            TNTDY   670
            WRITE(6,9) (I,I=1,8),((QN(J,I),I=1,8),J=1,IC)                    TNTDY   671
         9  FORMAT(*1HFAT LOADS*/1X(8,7I12/(1X8F12.1)))                      TNTDY   672
            WRITE(6,10) (I,I=1,6),((I,I=1,6),((AN(J,I),I=1,6),(DENS(J,I),I=1,6) TNTDY   673
           C ,J=1,IC)                                                        TNTDY   674
        10   FORMAT(*1*,24X,*ACTUAL NITRIC*,58X,*SPECIFIC GRAVITY*/1XI6,5I10, TNTDY   675
           C 10X,6I10/(1X,6F10,4,10X,6F10,5))                                TNTDY   676
            WRITE(6,15) (I,I=1,6),((RNSS(J,I),I=1,6),J=1,IC)                 TNTDY   677
        15 FORMAT(*1NITRIC/SULFURIC RATIO IN EXTERNAL ACID RECYCLE FROM EACH TNTDY   678
           1SEPARATOR*/1X,I8,5I12/(1X6F12.5))                                TNTDY   679
            WRITE(6,11) (I,I=1,8),((RNS(J,I),I=1,8),J=1,IC)                  TNTDY   680
        11  FORMAT(*1NITRIC/SULPHURIC RATIO IN EACH NITRATOR*/1X,I8,7I12/    TNTDY   681
           C (1X8F12.5))                                                     TNTDY   682
            WRITE(6,12) (I,I=1,8),((ANA(J,I),I=1,8),J=1,IC)                  TNTDY   683
        12  FORMAT(*1A-NITRATION IN EACH NITRATOR*/1X,I8,7I12/(1X8F12.5))    TNTDY   684
            WRITE(6,13) (I,I=1,8),((ANN(J,I),I=1,8),J=1,IC)                  TNTDY   685
        13  FORMAT(*1N-NITRATION IN EACH NITRATOR*/1XI8,7I12/(1X8F12.5))     TNTDY   686
```

```
                      DTPR=+P*DT*60.                                                    TNTDY     687
                      WRITE(6,14) DTPR                                                  TNTDY     688
                14    FORMAT(*0TIME BETWEEN POINTS =*,F10.5,*  MINUTES*)                TNTDY     689
                      DO 777 I=1,ICOUNT                                                 TNTDY     690
                 777  X(I)=DT*I*MP                                                      TNTDY     691
          690         DO 778 J=1,8                                                      TNTDY     692
                      DO 779 I=1,150                                                    TNTDY     693
                 779  ZZ(I,J)=X(I)                                                      TNTDY     694
                 778  CONTINUE                                                          TNTDY     695
                      DO 780 I=1,IC                                                     TNTDY     696
          695         CWSA(I)=CWASA(I)*100.                                             TNTDY     697
                      DO781J=5,8                                                        TNTDY     6
                      AMA(IC,J)=AMA(IC,J)*10.                                           TNTDY     699
                 781  AMP(IC,J)=AMP(IC,J)*10.                                           TNTDY     700
                 780  CRUDE(I)=CRUDE(I)/2000.                                           TNTDY     701
          700         CALL NUCHAR(1,1HO)                                                TNTDY     702
                      CALL NUCHAR(2,1HT)                                                TNTDY     703
                      CALL NUCHAR(3,1HC)                                                TNTDY     704
                      CALL NUCHAR(4,1HN)                                                TNTDY     705
                      CALL NAMCYL(4HTIME,7H(HOURS),10HPCT. ONT,T,10HNT,COX,HOX)         TNTDY2      1
          705         CALL NAMCY4(X,CONT,IC ,X,CRUDE,IC ,X,TTCOX,IC ,X,TTNOX,IC,TTME,0.,,  TNTDY     706
                     ( 10.,0.,1,1 )                                                     TNTDY     707
                      CALL NUCHAR(1,1H1)                                                TNTDY     709
                      CALL NUCHAR(2,1H2)                                                TNTDY     710
                      CALL NUCHAR(3,1H3)                                                TNTDY     711
          710         CALL NUCHAR(4,1H4)                                                TNTDY     712
                      CALL NUCHAR(5,1H5)                                                TNTDY     713
                      CALL NUCHAR(6,1H6)                                                TNTDY     714
                      CALL NUCHAR(7,1H7)                                                TNTDY     715
                      CALL NUCHAR(8,1H8)                                                TNTDY     716
          715         CALL NAMCYL(4HTIME,7H(HOURS),10HTOTL ACDTY,10H(WT. PCT.))         TNTDY2      2
                      CALL NAMCY*(XX,TACDTY,IC,2,TTME,0.,,100.,0.,50.,0.,1,1,150,0)     TNTDY     717
                      CALL NAMCYL(4HTIME,7H(HOURS),10HHNO3/H2SO4,7H(STAGE))             TNTDY2      3
                      CALL NAMCY*(XX,PHSS,IC,4,TTME,0.,,0.,4,0.,1,1,1,150,0)            TNTDY     719
                      CALL NAMCYL(4HTIME,7H(HOURS),10HHNO3/H2SO4,10H(VFSSEL  ))         TNTDY2      4
          720         CALL NAMCY*(XX,PHS,IC,4,TTME,0.,,0.,4,,1,1,1,150,0)               TNTDY     721
                      CALL NAMCYL(4HTIME,7H(HOURS),10HSEN. HEAT , 6H(BTUS))             TNTDY2      5
                      CALL NAMCY*(XX,QN,IC,8,TTME,0.,,2500000.,,0.,,1,1,150,0)          TNTDY     723
                      CALL NAMCYL(4HTIME,7H(HOURS),10HA-NITRATIO,10HN (NITR  ))         TNTDY2      6
                      CALL NAMCY*(XX,ANA,IC,4,TTME,0.,,50.,,0.,,1,1,150,0)              TNTDY     725
          725         CALL NAMCYL(4HTIME,7H(HOURS),10HM-NITRATIO,10HN (NITR  ))         TNTDY2      7
                      CALL NAMCY*(XX,ANM,IC,4,TTME,0.,,2.,,0.,,1,1,150,0)               TNTDY     727
                      CALL NAMCYL(4HTIME,7H(HOURS),10HACT,NIT*IC,10H(STAGE   ))         TNTDY2      8
                      CALL NAMCY*(XX,AN,IC,6,TTME,0.,,20.,,0.,,1,1,150,0)               TNTDY     729
                      CALL NAMCYL(4HTIME,7H(HOURS),10HSP. GRAV. ,10H(STAGE)   )         TNTDY2      9
          730         CALL NAMCY*(XX,DENS,IC,4,TTME,0.,,1.,6,,1.,,1,1,150,0)            TNTDY     731
                      CALL NAMCYL(4HTIME,7H(HOURS), 10HSP. GRAV. ,10H(STAGE)   )        TNTDY2     10
                      CALL NAMCY*(XX ,DFNSA,IC,6,TTME,0.,,2.,0,1.,0,1,1,150,0)          TNTDY     733
                      CALL NUCHAR(1,1HS)                                                TNTDY     735
                      CALL NAMCYL(4HTIME,7H(HOURS),10HSPENT ACID,9H (LBS/HR))           TNTDY2     11
          735         CALL NAMCY1(X,SPL  ,IC,TTME,0.,,20000.,,10000.,,1,1)              TNTDY     736
                      CALL NUCHAR(1,1HO)                                                TNTDY     738
                      CALL NUCHAR(2,1HN)                                                TNTDY     739
                      CALL NUCHAR(3,1HH)                                                TNTDY     740
                      CALL NAMCYL(4HTIME,7H(HOURS),10HONT,H2O,NB,10H(WT. PCT.))         TNTDY2     12
          740         CALL NAMCY3(X,CONTSA,IC ,X,CWSA,IC,X,CNBSA,IC,TTME,0.,,100.,,0.,,1,1) TNTDY     741
                      STOP                                                              TNTDY3      2
```

END TNTSV 744

SYMBOLIC REFERENCE MAP (R=1)

ENTRY POINTS
6153 TNTSIN

VARIABLES	SN	TYPE	RELOCATION							
0	A	REAL	ARRAY	VECTOR	406	AA	REAL	ARRAY	SEP
442	AF	REAL	ARRAY	SEP	0	AI	REAL	ARRAY	INPUT
404	AIP	REAL	ARRAY	SEP	73	AKMA	REAL		ZD
74	AK**ATL	REAL		ZD	61	AK10	REAL		ZD
46	AK12	REAL		ZD	53	AK3S	REAL		ZD
47	AK3W	REAL		ZD	54	AK4S	REAL		ZD
50	AK4W	REAL		ZD	51	AK5S	REAL		ZD
52	AK6S	REAL		ZD	57	AK7	REAL		ZD
60	AK8	REAL		ZD	101	AK9	REAL		ZD
25323	AN	REAL	ARRAY		31407	ANA	REAL	ARRAY	
13465	ANAC	REAL			33647	ANN	REAL	ARRAY	
13466	ANNC	REAL			0	ANT	REAL	ARRAY	ANNT
0	APPAY	REAL	APPAY	X	72	AS	REAL	ARRAY	SEP
16250	ATN	REAL	ARRAY		16256	ATW	REAL	ARRAY	
0	AV	REAL	ARRAY	VECT	16264	AVL	REAL	ARRAY	
424	AXP	REAL	APPAY	SEP	0	A1A	REAL	ARRAY	ANNT
0	A1AI	REAL	ARRAY	X	21	A1B	REAL	ARRAY	ANNT
21	A1BI	REAL	ARRAY	X	72	A1S	REAL	ARRAY	SEP
42	A2	REAL	ARRAY	ANNT	42	A2I	REAL	ARRAY	X
115	A2S	REAL	ARRAY	SEP	63	A3A	REAL	ARRAY	ANNT
63	A3AI	REAL	ARRAY	X	104	A3P	REAL	ARRAY	ANNT
104	A3BI	REAL	ARRAY	X	134	A3S	REAL	ARRAY	SEP
125	A4	REAL	ARRAY	ANNT	125	A4I	REAL	ARRAY	X
155	A4S	REAL	ARRAY	SEP	146	A5	REAL	ARRAY	ANNT
146	A5I	REAL	ARRAY	X	176	A5S	REAL	ARRAY	SEP
167	A6	REAL	ARRAY	ANNT	167	A6I	REAL	ARRAY	X
217	A6S	REAL	ARRAY	SEP	21011	CONT	REAL	ARRAY	
22141	CONTSA	REAL	ARRAY		735	CHANXO	REAL		VECT
737	CNP**10	REAL		VECT	21465	CNRSA	REAL	ARRAY	
14	CP	REAL	ARRAY	ZD	21237	CPUDE	REAL	ARRAY	
21713	CWSA	REAL	ARRAY		36147	DENS	REAL	ARRAY	
37753	DENSA	REAL	ARRAY		736	DFANXO	REAL		VECT
740	DFP**10	REAL		VECT	34	DH	REAL	ARRAY	ZD
13470	DLT	REAL			1	DT	REAL		/ /
13473	DTPP	REAL			16242	EAO	REAL	ARRAY	
26	FAOP	REAL	ARRAY	SEP	26	EAOP1	REAL		SEP
27	FAOP2	REAL		SEP	30	EAOP3	REAL		SEP
31	FAOP4	REAL		SEP	32	EAOP5	REAL		SEP
33	FAOP6	REAL		SEP	53	EAP	REAL		VECTOR
11714	FFP	REAL			16234	EOA	REAL	ARRAY	
20	FOAP	REAL	ARRAY	SEP	20	EOAP1	REAL		SEP
21	FOAP2	REAL		SEP	22	EOAP3	REAL		SEP
23	FOAP	REAL		SEP	24	EOAP5	REAL		SEP
25	FOAP6	REAL		SEP	11716	EOL	REAL		
54	FOP	REAL		VECTOR	11713	EWR	REAL		
0	FX	REAL		/ /	11715	EYW	REAL		
71	F10	REAL		ZD	42	E2I	REAL		ZD
55	F3S	REAL		ZD	63	E3W	REAL		ZD
56	F4S	REAL		ZD	64	E4W	REAL		ZD
65	F5S	REAL		ZD	66	E6S	REAL		ZD
67	F7	REAL		ZD	70	E8	REAL		ZD

88

VARIABLES	SN	TYPE		RELOCATION
182	F0	REAL		Z0
42	FACIB	REAL	ARRAY	SEP
43	FACIB2	REAL		SEP
45	FACIB4	REAL		SEP
47	FACIB6	REAL		SEP
47	FAR	REAL		VECTOR
35	FA2	REAL		SEP
37	FA4	REAL		SEP
41	FA6	REAL		SEP
0	FIN	REAL	ARRAY	FIN
110	FMX	REAL		Z0
540	FOPG	REAL	ARRAY	SEP
541	FOPG2	REAL		SEP
543	FOPG4	REAL		SEP
545	FOPG6	REAL		SEP
51	F02	REAL		SEP
53	F04	REAL		SEP
55	F06	REAL		SEP
64	FR	REAL	ARRAY	SEP
56	FRAC1	REAL		SEP
60	FRAC3	REAL		SEP
62	FRAC5	REAL		SEP
56	FRC	REAL	ARRAY	SEP
65	FR2	REAL		SEP
67	FR4	REAL		SEP
71	FR6	REAL		SEP
43	FVFR	REAL		VECTOR
10	FVKH1A	REAL		SEP
12	FVKH2	REAL		SEP
14	FVKH3B	REAL		SEP
16	FVKH5	REAL		SEP
0	G1	REAL	ARRAY	PAR
10	G3	REAL	ARRAY	PAR
20	G4	REAL	ARRAY	PAR
50	G5	REAL	ARRAY	PAR
70	G7	REAL	ARRAY	PAR
120	G9	REAL	ARRAY	PAR
13474	IC	INTEGER		
13674	ICOUNT	INTEGER		
11717	IPNCH	INTEGER		
11720	IQUIT	INTEGER		
51	ISTGE	INTEGER		VECTOR
52	IV	INTEGER		VECTOR
13450	I	INTEGER		
13452	K	INTEGER		
4	KM	INTEGER		/ /
532	M0	INTEGER	ARRAY	SEP
10	MP	INTEGER		/ /
533	M2	INTEGER		SEP
535	M4	INTEGER		SEP
537	M6	INTEGER		SEP
13472	PA	REAL		
21	PI	REAL	ARRAY	INPUT
210	PMT	REAL	ARRAY	AMNT
240	PS	REAL	ARRAY	SEP
476	PSR	REAL	ARRAY	SEP
210	P1A1	REAL		X
34	FA	REAL	ARRAY	SEP
42	FACIB1	REAL		SEP
44	FACIB3	REAL		SEP
46	FACIB5	REAL		SEP
13456	FAFR	REAL		
34	FA1	REAL		SEP
36	FA3	REAL		SEP
40	FA5	REAL		SEP
72	FD	REAL		Z0
110	FMAX	REAL		Z0
50	F0	REAL	ARRAY	SEP
540	FOPG1	REAL		SEP
542	FOPG3	REAL		SEP
544	FOPG5	REAL		SEP
50	F01	REAL		SEP
52	F03	REAL		SEP
54	F05	REAL		SEP
50	FP0	REAL		VECTOR
44	FPAC	REAL		VECTOR
57	FRAC2	REAL		SEP
61	FRAC4	REAL		SEP
63	FRAC6	REAL		SEP
54	FR1	REAL		SEP
66	FR3	REAL		SEP
70	FR5	REAL		SEP
10	FV	REAL	ARRAY	SEP
13447	FVKMS	REAL		
11	FVKH1R	REAL		SEP
13	FVKH3A	REAL		SEP
15	FVKH4	REAL		SEP
17	FVKH6	REAL		SEP
110	G10	REAL	ARRAY	PAR
30	G3S	REAL	ARRAY	PAR
40	G4S	REAL	ARRAY	PAR
60	G6	REAL	ARRAY	PAR
100	G8	REAL	ARRAY	PAR
13446	I	INTEGER		
7	ICALL	INTEGER		/ /
13462	IN	INTEGER		
2	IPRNT	INTEGER		/ /
13460	IS	INTEGER		
46	ITYPE	INTEGER		VECTOR
734	IVSL	INTEGER		VECT
3	JACK	INTEGER		/ /
13475	KN	REAL	ARRAY	
5	KN	INTEGER		/ /
45	NOTCH	INTEGER		VECTOR
532	M1	INTEGER		SEP
534	M3	INTEGER		SEP
536	M5	INTEGER		SEP
21	P	REAL	ARRAY	VECTOR
514	PF	REAL	ARRAY	SEP
460	PIR	REAL	ARRAY	SEP
13464	PP	REAL		
356	PV	REAL	ARRAY	VECT
210	P1A	REAL	ARRAY	AMNT
231	P1B	REAL	ARRAY	AMNT

VARIABLES SN TYPE RELOCATION

211	P1BI	REAL		X	240	P1S	REAL	ARRAY	SEP
252	P2	REAL	ARRAY	ANNT	261	P2S	REAL	ARRAY	SEP
273	P3A	REAL	ARRAY	ANNT	314	P3B	REAL	ARRAY	ANNT
302	P3S	REAL	ARRAY	SEP	335	P4	REAL	ARRAY	ANNT
323	P4S	REAL	ARRAY	SEP	356	P5	REAL	ARRAY	ANNT
344	P5S	REAL	ARRAY	SEP	377	P6	REAL	ARRAY	ANNT
365	P6S	REAL	ARRAY	SEP	13467	Q	REAL		
13471	QA	REAL			22367	QM	REAL	ARRAY	
13463	QP	REAL			0	QY	REAL	ARRAY	000
0	R	REAL	ARRAY	DUM	13	RATES	REAL	ARRAY	/ /
0	RM0	REAL	ARRAY	ZD	0	RM01	REAL		ZD
11	RM010	REAL		ZD	12	RM011	REAL		ZD
13	RM012	REAL		ZD	14	RM013	REAL		ZD
15	RM014	REAL		ZD	1	RM02	REAL		ZD
2	RM03	REAL		ZD	3	RM04	REAL		ZD
4	RM05	REAL		ZD	5	RM06	REAL		ZD
6	RM07	REAL		ZD	7	RM08	REAL		ZD
10	RM09	REAL		ZD	27127	RMS	REAL	ARRAY	
14172	RMSS	REAL	ARRAY		111	RP	REAL		ZD
104	RR	REAL		ZD	75	SA	REAL		ZD
74	SB	REAL		ZD	77	SC	REAL		ZD
100	SD	REAL		ZD	101	SE	REAL		ZD
102	SG	REAL		ZD	103	SH	REAL		ZD
104	SI	REAL		ZD	105	SJ	REAL		ZD
13455	SPA	REAL			15776	SPENT	REAL	ARRAY	
13457	SPO	REAL			13454	SUP	REAL		
42	T	REAL		VECTOR	13516	TACDTY	REAL	ARRAY	
11	TCOX	REAL		/ /	13453	TDNT	REAL		
0	TEMP	REAL	ARRAY	SEP	42	TI	REAL		INPUT
13451	TIME	REAL			13461	TLPS	REAL		
16272	TN	REAL	ARRAY		12	TNOX	REAL		/ /
107	TR	REAL		ZD	133	TSEP	REAL	ARRAY	/ /
24647	TTCOX	REAL	ARRAY		6	TTME	REAL		/ /
25075	TTNOX	REAL	ARRAY		16330	TVL	REAL	ARRAY	
16275	TW	REAL	ARRAY		0	T1A	REAL		SEP
1	T1B	REAL		SEP	2	T2	REAL		SEP
3	T3A	REAL		SEP	4	T3B	REAL		SEP
5	T4	REAL		SEP	6	T5	REAL		SEP
7	T6	REAL		SEP	16224	VKN	REAL	ARRAY	
13445	VKMS	REAL			20563	X	REAL	ARRAY	
16303	XX	REAL	ARRAY		16	XYY	REAL	ARRAY	000

FILE NAMES MODE

0	INPUT		2041	OUTPUT	4102	PUNCH	0	TAPE5 FNT
2041	TAPE6	FNT	4102	TAPE7				

EXTERNALS TYPE ARGS

FNTH	REAL	7	INPT	0	
NANCYL		4	NANCYM	12	
NANCY1		9	NANCY3	15	
NANCY4		18	NUCHAR	2	
SUR		0	SUB1	4	
SUB2		10			

STATEMENT LABELS

11745	1	FNT	12140	2	FNT	10237	3	
12104	4	FNT	12203	5	FNT	0	6	

STATEMENT LABELS

0	7			13206	8	FMT		13237	9	FMT	
13260	10	FMT		13325	11	FMT		13345	12	FMT	
13364	13	FMT		13377	14	FMT		13382	15	FMT	
10046	31			10055	32			10101	33		
10116	34			10130	35			10142	36		
10157	37			10174	38			0	39		
0	48			10206	58			0	51		
0	75			0	76			0	77		
0	78			7726	79			0	80		
0	81			0	170			0	171		
0	179			0	187			12417	190	FMT	
12425	191	FMT		6373	192			12441	193	FMT	
6491	194			12463	195	FMT		12501	196	FMT	
0	210			0	211			0	212		
0	213			0	214			12774	246	FMT	
12741	247	FMT		12382	300	FMT		12370	301	FMT	
12418	302	FMT		0	307		INACTIVE	12523	390	FMT	
13045	400	FMT		13054	401	FMT		13071	402	FMT	
13112	403	FMT		13143	404	FMT		6520	499		
12537	500	FMT		12550	501	FMT		12561	502	FMT	
12572	503	FMT		12603	504	FMT		12614	505	FMT	
12625	506	FMT		12636	507	FMT		12647	508	FMT	
12660	509	FMT		12671	510	FMT		12702	511	FMT	
12713	512	FMT		12724	513	FMT		0	600		
0	610			0	620			6617	621		
0	630			0	640			6735	641		
0	650			7010	651			0	660		
7046	661			0	670			7101	671		
0	678			0	679			0	680		
7162	681			0	690			7215	691		
0	700			7275	701			0	710		
7338	711			0	720			7403	721		
0	730			7566	731			0	740		
0	777			0	778			0	779		
0	780			0	781			12532	3006	FMT	NO REFS

COMMON BLOCKS	LENGTH
/ /	97
PAR	88
VECT	401
X	13A
VECTOR	45
000	28
SEP	35A
AMNT	272
INPUT	35
FNN	5A
NUM	10
70	74

STATISTICS

PROGRAM LENGTH	336140	14229
BUFFER LENGTH	61439	7171
COMMON LENGTH	70618	15A5
BLANK COMMON	1418	97

```
      SUBROUTINE SUB                                                    TNTDY   745
      DIMENSION P(17),A(17),AT(17),PI(17)                               TNTDY   746
      DIMENSION FF(5),RATE(10)                                          TNTDY   747
      COMMON/PRTS/P1,P2,P3,P4,P5,P6,P7,P8,P9,P10                        TNTDY   748
      COMMON FX,QT,IPRNT,JACK,NM,NN,TIME,ICALL,NP,TCOX,TNOX,RATES(8,10) TNTDY   749
     C,TSEP(6)                                                          TNTDY   750
      COMMON/VECTOR/A1,A2,A3,A4,A5,A6,A7,A8,A9,A10,A11,A12,A13,A14,     TNTDY   751
     C A15,A16,A17,P1,P2,P3,P4,P5,P6,P7,P8,P9,P10,P11,P12,P13,          TNTDY   752
     C P14,P15,P16,P17,T,FVKM, FRAC,NOTCH,ITYPE,FAR,FPO,ISTGE,IV       TNTDY   753
     C,EAOP,FOAP                                                        TNTDY   754
      COMMON/PAR/G1(8),G3(8),G4(8),G7S(8),G4S(8),G5(8),G6(8),G7(8),     TNTDY   755
     C G8(8),G10(8),G9(8)                                               TNTDY   756
      COMMON/INPUT/A11,A12,A13,A14,A15,A16,A17,A18,A19,A110,A111,       TNTDY   757
     C  A112,A113,A114,A115,A116,A117, P11,P12,P13,P14,P15,P16,P17,P18, TNTDY   758
     C  P19,P110,P111,P112,P113,P114,P115,P116,P117,TI                  TNTDY   759
      COMMON/OOO/GY(14),YY(14)                                          TNTDY   760
      COMMON/ZO/RHO1,RHO2,RHO3,RHO4,RHO5,RHO6,RHO7,RHO8,RHO9,RHO10,     TNTDY   761
     C RHO11,RHO12,RHO13,RHO14,CP(14),DH(10),AK12,AK3W,AK4W,AK5S,AK6S,  TNTDY   762
     C AK7S,AK4S,E7S,E4S,                                               TNTDY   763
     C AK7,AKA,AK10,E21,E3W,F4W,E5S,E6S,E7,E8,E10,FD,AKMA,AKMATL,SA,SB, TNTDY   764
     C SC,SD,SE,SG,SH,SI,SJ,SR,TR,FMX,RP                               TNTDY   765
      EQUIVALENCE (P(1),P1),(A(1),A1)                                   TNTDY   766
     C ,(AI(1),AT1),(PI(1),PT1)                                         TNTDY   767
      EQUIVALENCE (AKMAP,SA)                                            TNTDY   768
      EQUIVALENCE(RATE(1),R1)                                           TNTDY   769
      EQUIVALENCE (AKE03,SJ),(AKF04,SC)                                 TNTDY4    1
      DATA AKA,AKB,AKC,AKEO,AKEOOV,FOV/.2,.10116,.2491,50.0,1.495,      TNTDY1    3
     C 1./                                                              TNTDY   771
      AKE01=SH                                                          TNTDY1    4
      AKE02=AKEO                                                        TNTDY1    5
      DATA FF/.06547,.16547,.29179,.42941,.57059/                       TNTDY   772
      IF(IPRNT.EQ.1)WRITE(6,1)IV,A,P,AI,PI                             TNTDY   773
    1 FORMAT( 17H0SUB CALLED, IV =,I5                                   TNTDY   774
     C                        /(1X10F12.6/1X7F12.6))                    TNTDY   775
      TKEL=T+273.1                                                      TNTDY   776
C     COMPUTE TOTAL FLOWS                                               TNTDY   777
      ANR=A1+A2+A3+A4+A5+A6                                             TNTDY   778
     C +A7+AR                                                           TNTDY   779
      PNR=P1+P2+P3+P4+P5+P6+P10                                         TNTDY   780
     C +P7+PR                                                           TNTDY   781
      AT=ANR+A9+A11+A12+A13+A14                                         TNTDY   782
      PT=PNR+PR                                                         TNTDY   783
C     COMPUTE DENSITIES                                                 TNTDY   784
      QA=A1/RHO1+A2/RHO2+A3/RHO3+A4/RHO4+A5/RHO5+A6/RHO6+A9/RHO9+       TNTDY   785
     C A11/RHO11+A12/RHO12+A13/RHO13+A14/RHO14                          TNTDY   786
     C +A7/RHO7+AR/RHO8                                                 TNTDY   787
      IF(QA.LT.1.) QA=1.                                                TNTDY   788
      QP=P1/RHO1+P2/RHO2+P3/RHO3+P4/RHO4+P5/RHO5+P6/RHO6+P9/RHO9        TNTDY   789
     C +P10/RHO10                                                       TNTDY   790
     C +P7/RHO7+PR/RHO8                                                 TNTDY   791
      IF(QP.LT.1.) QP=1.                                                TNTDY   792
C     COMPUTE FRACTION ACID AND FRACTION ORGANIC                        TNTDY   793
      IF(ITYPE)11,11,12                                                 TNTDY   794
   11 FA=QA/(QA+QP)                                                     TNTDY   795
      GOTO13                                                            TNTDY   796
   12 FA=.755                                                           TNTDY   797
   13 FP=1.-FA                                                          TNTDY   798
```

```
      C     COMPUTE MOLE FRACTIONS                                          TNTDY    790
            IF(A9.LT.2.) A9=2.                                              TNTDY    800
   60       ATI=1./AT                                                       TNTDY    801
            X13=A13*ATI                                                     TNTDY    802
            X1=A1*ATI                                                       TNTDY    803
            X2=A2*ATI                                                       TNTDY    804
            X5=A5*ATI                                                       TNTDY    805
   65       X6=A6*ATI                                                       TNTDY    806
            X9=A9*ATI                                                       TNTDY    807
            X14=A14*ATI                                                     TNTDY    808
            IF(IPRNT.EQ.1)                                                  TNTDY    809
           CWRITE(6,1000)TKEL,ANB,PNB,AT,PT,QA,QP,FA,FP,ATI,X13,X1,X2,      TNTDY    810
   70      C  X5,X6,X9,X14                                                 TNTDY    811
     1000 FORMAT(1X8F10.2)                                                  TNTDY    812
      C     COMPUTE XEQA                                                    TNTDY    813
            PP=-7.620+0.01023*TKEL-1.888*X13+7.716*(X1+X2)-0.452*(X5+X6)-   TNTDY    814
           C 5.592*X9                                                       TNTDY3     3
   75       IF(PP.GT.300.) PP=300.                                          TNTDY    816
            IF(PP.LT.-250.) PP=-250.                                        TNTDY    817
            XEQA=10.**PP                                                    TNTDY    818
      C     COMPUTE ETA                                                     TNTDY    819
      C     COMPUTE D                                                       TNTDY    820
   80       IF(ITYPE)15,15,16                                               TNTDY    821
     15     ETAA=FVKM*FP*AKMA                                               TNTDY    822
            ETAP=FVKM*FP*AKMAP                                              TNTDY    823
            ETATL=FVKM*FP*AKMATL                                            TNTDY    824
            ETA=1./(1./ETAP+1./(ETAA*XEQA))                                 TNTDY    825
   85       ZA=ETA/PNB                                                      TNTDY    826
            ZP=ETA/ANB                                                      TNTDY    827
            D1=ZA*P1-ZP*A1                                                  TNTDY    828
            D2=ZA*P2-ZP*A2                                                  TNTDY    829
            D3=ZA*P3-ZP*A3                                                  TNTDY    830
   90       D4=ZA*P4-ZP*A4                                                  TNTDY    831
            D5=ZA*P5-ZP*A5                                                  TNTDY    832
            D6=ZA*P6-ZP*A6                                                  TNTDY    833
            D7=ZA*P7-ZP*A7                                                  TNTDY    834
            D8=ZA*P8-ZP*A8                                                  TNTDY    835
   95       D10=ETATL*P10/PNB                                               TNTDY    836
            GOTO17                                                          TNTDY    837
     16     D1=0.                                                           TNTDY    838
            ZA=0.                                                           TNTDY    839
            ZP=0.                                                           TNTDY    840
  100       D2=0.                                                           TNTDY    841
            D3=0.                                                           TNTDY    842
            D4=0.                                                           TNTDY    843
            D5=0.                                                           TNTDY    844
            D6=0.                                                           TNTDY    845
  105       D7=0.                                                           TNTDY    846
            D8=0.                                                           TNTDY    847
            D10=0.                                                          TNTDY    848
     141    FAR=(1.-FAOP*PT/AT)/(1.-EOAP*EAOP)                              TNTDY    849
            IF(FAR)142,143,143                                              TNTDY    850
  110       FAR=0.                                                          TNTDY    851
     143    IF(FAR.GT.1.)FAR=1.                                             TNTDY    852
            FPO=1.-FAR*EOAP*AT/PT                                           TNTDY    853
            IF(FPO)144,145,145                                              TNTDY    854
     144    FPO=0.                                                          TNTDY    855
```

```
                      IF(FPO.GT.1.)FPO=1.                                        TNTDY    856
                      OT=OA*FAR*(1.-FPO1*OP                                      TNTDY    857
                      FRAC=F*X*FF(NOTCH)/OT                                      TNTDY    858
                      IF(FRAC.GT.1.)FRAC=1.                                      TNTDY    859
                17    CONTINUE                                                   TNTDY    860
                      IF(IPRNT.EQ.1)                                             TNTDY    861
                     CWRITE(6,1000)PP,XEQA,ETA,D1,D2,D3,D4,D5,D6,D10             TNTDY    862
                C     COMPUTE M                                                  TNTDY    863
                      AINR=AI1+AI2+AI3+AI4+AI5+AI6                               TNTDY    864
                     C +AI7+AI8                                                  TNTDY    865
                      AN9=AT*XEQA                                                TNTDY    866
                      AMNR=AT*XECA-AINR-D1-D2-D3-D4-D5-D6-D7-D8                  TNTDY    867
                      IF(AMNR)20,21,21                                           TNTDY    868
                20    YA=AMNR/AN9                                                TNTDY    869
                      YP=0.                                                      TNTDY    870
                      GOTO22                                                     TNTDY    871
                21     YP=AMNR/PNB                                               TNTDY    872
                      YA=0.                                                      TNTDY    873
                22    CONTINUE                                                   TNTDY    874
                      AM1=YP*P1+YA*A1                                            TNTDY    875
                      AM2=YP*P2+YA*A2                                            TNTDY    876
                      AM3=YP*P3+YA*A3                                            TNTDY    877
                      AM4=YP*P4+YA*A4                                            TNTDY    878
                      AM5=YP*P5+YA*A5                                            TNTDY    879
                      AM6=YP*P6+YA*A6                                            TNTDY    880
                      AM7=YP*P7+YA*A7                                            TNTDY    881
                      AM8=YP*P8+YA*AR                                            TNTDY    882
                      IF(IPRNT.EQ.1) WRITE(6,1409)AINB,AMNB                      TNTDY    883
                1409 FORMAT( 10H0AINB,AMNB,2F14.4)                               TNTDY    884
                C     COMPUTE NITROGEN ION CONCENTRATION                         TNTDY3     4
                      F=A9/OA                                                    TNTDY3     5
                      W=A11/OA                                                   TNTDY    895
                      S=A11/OA                                                   TNTDY1     6
                      IF(A14.GT.0.) GO TO 1341                                   TNTDY    896
                C                                                                TNTDY    897
                C                                                                TNTDY    898
                C     SULPHURIC - WATER SYSTEM                                   TNTDY    899
                C                                                                TNTDY    900
                      YL=0.                                                      TNTDY3     6
                      YU=S                                                       TNTDY3     7
                      DO 1306 I=1,40                                             TNTDY3     8
                      Y=(YL+YU)/2.                                               TNTDY3     9
                      X=(Y*Y-AKE02*(S-Y)*(W-Y))/(2.*AKE02*(S-Y)+Y)               TNTDY3    10
                      IF(X.LE.0..OR.X.LE.(Y-W)/2.) GO TO 1305                    TNTDY3    11
                      GO TO 1306                                                 TNTDY3    12
                1305  YL=Y                                                       TNTDY3    13
                      GO TO 1308                                                 TNTDY3    14
                1306  IF(X.GE.F.OR.X.GE.Y) GO TO 1307                           TNTDY3    15
                      GO TO 1308                                                 TNTDY3    16
                1307  YU=Y                                                       TNTDY3    17
                      GO TO 1308                                                 TNTDY3    18
                1308  AK1=X*Y*(W+2.*X-Y)/((F-X)*(S-Y))                           TNTDY3    19
                      IF(ABS(AK1-AKE01).LT..0001) GO TO 1312                     TNTDY3    20
                      IF(AK1.LT.AKE01) GO TO 1310                                TNTDY3    21
                      YU=Y                                                       TNTDY3    22
                      GO TO 1308                                                 TNTDY3    23
                1310  YL=Y                                                       TNTDY3    24
```

```
                1300 CONTINUE                                                    TNTDY3    25
                1312 CNO2=X                                                      TNTDY3    26
                     CHSO4=Y                                                     TNTDY3    27
      175            CH2O=Y-X                                                    TNTDY3    28
                     CH2SO4=S-Y                                                  TNTDY3    29
                     CHNO3=F-X                                                   TNTDY3    30
                     CH2O=W*X-(Y-X)                                              TNTDY3    31
                     ALT=CNO2*OA                                                 TNTDY3    32
      180            O=X/F                                                       TNTDY3    33
                     KLM=2                                                       TNTDY     920
                     GO TO 2341                                                  TNTDY     921
                1341 F=A9/OA                                                     TNTDY     922
                     B=(A11-A16)/OA                                              TNTDY     923
      185            C=A14/OA                                                    TNTDY     924
                C                                                                TNTDY4      2
                C    SULFURIC - OLEUM SYSTEM (REGION 1)                          TNTDY4      3
                C                                                                TNTDY4      4
                     IF(A9.GT..5*A14) GO TO 2337                                 TNTDY4      5
      190            CNO2=F                                                      TNTDY4      6
                     CHNO3=0.                                                    TNTDY4      7
                     CH2SO4=B*F                                                  TNTDY4      8
                     CHS2O7=F                                                    TNTDY4      9
                     CHSO4=0.                                                    TNTDY4     10
      195            CH2O=0.                                                     TNTDY4     11
                     ALT=CNO2*OA                                                 TNTDY4     12
                     O=1.                                                        TNTDY4     13
                     GO TO 2341                                                  TNTDY4     14
                C                                                                TNTDY4     15
      200       C    SULFURIC - OLEUM SYSTEM (REGION 3)                          TNTDY4     16
                C                                                                TNTDY4     17
                2337 IF(A9.LE.A14) GO TO 3300                                    TNTDY4     18
                     XU=F                                                        TNTDY4     19
                     XL=.5*C                                                     TNTDY4     20
      205            RC=A+3.*C                                                   TNTDY4     21
                     CR=.5*A+1.5*C                                               TNTDY4     22
                     DO 233A I=1,40                                              TNTDY4     23
                     X=(XU+XL)/2.                                                TNTDY4     24
                     Y=AKEQ4*X*(2.*X-C)**2/(F-X)                                 TNTDY4     25
      210            IF(Y.LE.(C-X)) GO TO 2339                                   TNTDY4     26
                     GO TO 2340                                                  TNTDY4     27
                2339 XL=X                                                        TNTDY4     28
                     GO TO 233A                                                  TNTDY4     29
                2340 IF(Y.GE.(CR-X)) GO TO 2343                                  TNTDY4     30
      215            GO TO 2344                                                  TNTDY4     31
                2343 XU=X                                                        TNTDY4     32
                     GO TO 2338                                                  TNTDY4     33
                2344 AK3=X*(Y+X-C)*(2.*X-C)**2/((F-X)*(RC-2.*X-2.*Y)**2)        TNTDY4     34
                     IF(ABS(AK3-AKEQ3).LT.1.) GO TO 2348                         TNTDY4     35
      220            IF(AK3.LT.AKEQ3) GO TO 2345                                 TNTDY4     36
                     XU=X                                                        TNTDY4     37
                     GO TO 2338                                                  TNTDY4     38
                2345 XL=X                                                        TNTDY4     39
                233A CONTINUE                                                    TNTDY4     40
      225       2348 CNO2=X                                                      TNTDY4     41
                     CHS2O7=Y                                                    TNTDY4     42
                     CHNO3=F-X                                                   TNTDY4     43
                     CH2O=Y+X-C                                                  TNTDY4     44
```

```
                      CM2SO4=MC-2.*X-2.*Y                                        TNTDY4    45
      230             CMSO4=2.*X-C                                               TNTDY4    46
                      A17=CM02*QA                                                TNTDY4    47
                      Q=CM02/F                                                   TNTDY4    48
                      GO TO 2341                                                 TNTDY4    49
                C                                                                TNTDY4    50
      235       C     SULFURIC - OLEUM SYSTEM (REGION 2)                         TNTDY4    51
                C                                                                TNTDY4    52
                3300  XU=.5*F                                                    TNTDY4    53
                      IF((F-.5*C).LT.XU) XU=F-.5*C                               TNTDY4    54
                      XL=0.                                                      TNTDY4    55
      240             FC=2.*F-C                                                  TNTDY4    56
                      CF=C-F                                                     TNTDY4    57
                      DO 2350 I=1,20                                             TNTDY4    58
                      X=(XL+XU)/2.                                               TNTDY4    59
                      AK4=X*(CF+X)/((F-X)*(FC-2.*X)**2)                          TNTDY4    60
      245             IF(AK4.LT.AKEQ4) GO TO 2351                                TNTDY4    61
                      XU=X                                                       TNTDY4    62
                      GO TO 2350                                                 TNTDY4    63
                 2351 XL=X                                                       TNTDY4    64
                 2350 CONTINUE                                                   TNTDY4    65
      250             CM02=F-X                                                   TNTDY4    66
                      CM4O3=X                                                    TNTDY4    67
                      CM5207=CF+X                                                TNTDY4    68
                      CMSO4=FC-2.*X                                              TNTDY4    69
                      CM3O=0.                                                    TNTDY4    70
      255             CM2SO4=0+C                                                 TNTDY4    71
                      A17=CM02*QA                                                TNTDY4    72
                      Q=CM02/F                                                   TNTDY4    73
                 2341 GAMMA=FVKM*FA*Q*A9*AKA/(QA*QA)                             TNTDY1    36
                 2342 XYY(IV      )=Q*A9                                         TNTDY     902
      260             QY (IV      )=Q                                            TNTDY     903
                C     COMPUTE REACTION RATE COEFFICIENTS                         TNTDY     1000
                      F3=GAMMA*G3S(IV)                                           TNTDY3    34
                      IF(IPRNT.EQ.1)                                             TNTDY     1002
                     CWRITE(6,381) DELTA,FVKM,FA,ZD,SA,CB,A110A,SC,QA,G3(IV),G3S(IV),  TNTDY     1003
      265            C GAMMA,F3                                                 TNTDY     1004
                 381  FORMAT(' DELTA,FVKM,FA,ZD,SA,CB,A110A',E15.6,       6F10.4/  TNTDY     1005
                     C' SC,QA,G3,G3S,GAMMA,G3D',2F10.4,2E15.6,F10.6,F15.4)       TNTDY     1006
                      F4=GAMMA*G4S(IV)                                           TNTDY3    35
                      F5=GAMMA*G5(IV)                                            TNTDY     1008
      270             F6=GAMMA*G6(IV)                                            TNTDY     1009
                      F7A=G7(IV)*FVKM*FA*A17/(QA*QA)                             TNTDY3    36
                      F7M=F7A                                                    TNTDY3    37
                      F8A=G8(IV)*FVKM*FA*A17/(QA*QA)                             TNTDY3    38
                      F8M=F8A                                                    TNTDY3    39
      275             F9A=0.                                                     TNTDY3    40
                      F9M=0.                                                     TNTDY3    41
                      F10A=G10(IV)*FA*A17*FVKM/(QA*QA)                           TNTDY     1016
                      F10M=F10A                                                  TNTDY     1017
                      T1=A1*P1                                                   TNTDY     1018
      280             T2=P2*A2                                                   TNTDY     1019
                      T3=A3*P3                                                   TNTDY     1020
                      T4=A4*P4                                                   TNTDY     1021
                      T5=A5*P5                                                   TNTDY     1022
                      T6=A6*P6                                                   TNTDY     1023
      285             T7=A7*P7                                                   TNTDY     1024
```

```
      TP=A8*P8                                                          TNTDY  1025
      CX=ZA*YP                                                          TNTDY  1026
      CZ=ZB-YA*1.*CX                                                    TNTDY  1027
      C                                                                 TNTDY  1028
  290 C                                                                 TNTDY  1029
      C     BACKWARD DIFFERENCE INTEGRATION OF ORGANIC SPECIES           TNTDY  1030
      C                                                                 TNTDY  1031
      DTP=DP*DT/(FWKM*FP)                                               TNTDY  1032
      DTA=DA*DT/(FWKM*FA)                                               TNTDY  1033
  295 P10=(P10+DTP*P110)/(1.+DTP+ETATL*DTP/PMB)                         TNTDY  1034
      IF(IVPE.EQ.1) ETATL=0.                                            TNTDY  1035
      D10=ETATL*P10/PMB                                                 TNTDY  1036
      R2=D10*GI(IV)                                                     TNTDY  1037
      P1=D10-R2                                                         TNTDY  1038
  300 Z=F3/(F3+CZ)                                                      TNTDY  1039
      X=(1.-Z)*A11+P11+R1                                               TNTDY  1040
      Y=Z*CX+1.                                                         TNTDY  1041
      T1=(T1+DTP*X)/(1.+DTP*Y)                                          TNTDY  1042
      A1=(A11    +CX*T1)/(F3+CZ)                                        TNTDY  1043
  305 IF(A1.LT.0.) A1=0.                                                TNTDY  1044
      R3=F3*A1                                                          TNTDY  1045
      Z=F4/(F4+CZ)                                                      TNTDY  1046
      X=(1.-Z)*A12+P12+R2                                               TNTDY  1047
      Y=Z*CX+1.                                                         TNTDY  1048
  310 T2=(T2+DTP*X)/(1.+DTP*Y)                                          TNTDY  1049
      A2=(A12    +CX*T2)/(F4+CZ)                                        TNTDY  1050
      IF(A2.LT.0.) A2=0.                                                TNTDY  1051
      R4=F4*A2                                                          TNTDY  1052
      Z=F5+F7A+F8A+F9A                                                  TNTDY  1053
  315 Z=Z/(Z+CZ)                                                        TNTDY  1054
      X=A13+P13+R3-Z*(A13+R3)                                           TNTDY  1055
      Y=Z*CX+1.                                                         TNTDY  1056
      T3=(T3+DTP*X)/(1.+DTP*Y)                                          TNTDY  1057
      A3=(A13+R3+CX*T3)/(F5+F7A+F8A+F9A+CZ)                             TNTDY  1058
  320 IF(A3.LT.0.) A3=0.                                                TNTDY  1059
      R5=F5*A3                                                          TNTDY  1060
      R7A=F7A*A3                                                        TNTDY  1061
      R8A=F8A*A3                                                        TNTDY  1062
      R9A=F9A*A3                                                        TNTDY  1063
  325 Z=FA+F7M+F8M+F9M                                                  TNTDY  1064
      Z=Z/(Z+CZ)                                                        TNTDY  1065
      X=A14+P14+R4-Z*(A14+R4)                                           TNTDY  1066
      Y=Z*CX+1.                                                         TNTDY  1067
      T4=(T4+DTP*X)/(1.+DTP*Y)                                          TNTDY  1068
  330 A4=(A14+R4+CX*T4)/(F6+F7M+F8M+F9M+CZ)                             TNTDY  1069
      IF(A4.LT.0.) A4=0.                                                TNTDY  1070
      R6=F6*A4                                                          TNTDY  1071
      R7M=F7M*A4                                                        TNTDY  1072
      R8M=F8M*A4                                                        TNTDY  1073
  335 R9M=F9M*A4                                                        TNTDY  1074
      R7=R7A+R7M                                                        TNTDY  1075
      R8=R8A+R8M                                                        TNTDY  1076
      R9G=R9A+R9M                                                       TNTDY  1077
      Z=4.*F10A/(4.*F10A+CZ)                                            TNTDY  1078
  340 X=A15+P15+R5-Z*(A15+R5)                                           TNTDY  1079
      Y=Z*CX+1.                                                         TNTDY  1080
      T5=(T5+DTP*X)/(1.+DTP*Y)                                          TNTDY  1081
```

```
                A5=(A15+R5+CX*T5)/(4.*F10A+CZ)                                    TNTDY  1092
                IF(A5.LT.0.) A5=0.                                                TNTDY  1093
  345           R10A=A5*F10A                                                      TNTDY  1094
                Z=4.*F10M/(4.*F10M+CZ)                                            TNTDY  1095
                X=A16+P16+R6-Z*(A16+R6)                                           TNTDY  1096
                Y=Z*CX+1.                                                         TNTDY  1097
                T6=(T6+DTP*X)/(1.+DTP*Y)                                          TNTDY  1098
  350           A6=(A14+R6+CX*T6)/(4.*F10M+CZ)                                    TNTDY  1099
                IF(A6.LT.0.) A6=0.                                                TNTDY  1100
                R10M=A6*F10M                                                      TNTDY  1101
                P10=F10A+R10M                                                     TNTDY  1102
                X=A17+P17+R10                                                     TNTDY  1103
  355           T7=(T7+DTP*X)/(1.+DTP)                                            TNTDY  1104
                A7=(A17+P18+CX*T7)/CZ                                             TNTDY  1105
                IF(A7.LT.0.) A7=0.                                                TNTDY  1106
                X=A18+P18+3.*R10                                                  TNTDY  1107
                T8=(T8+DTP*X)/(1.+DTP)                                            TNTDY  1108
  360           A8=(A18+3.*R10+CX*T8)/CZ                                          TNTDY  1109
                IF(A8.LT.0.) A8=0.                                                TNTDY  1110
              C                                                                   TNTDY  1111
              C                                                                   TNTDY  1112
                A504=A13+A14                                                      TNTDY  1113
  365           CS=11.*R7+14.5 *R8+9.*R10+14.5*R9G                                TNTDY  1114
                R9=FD*CS                                                          TNTDY  1115
                CSP=CS-R9                                                         TNTDY  1116
                IF(IPRNT.EQ.1)                                                    TNTDY  1117
               CWRITE(6,1009)R1,R2,R3,R4,R5,R6,R7,R8,R9,R10                       TNTDY  1118
  370           AL=A13-A14                                                        TNTDY  1119
                IF(IPRNT.EQ.1)WRITE(6,1405)Q,DELTA,GAMMA                          TNTDY  1120
             1405 FORMAT( 14H0Q,DELTA,GAMMA,3F14.4)                               TNTDY  1121
                IF(IPRNT.NE.1)GOTO1790                                            TNTDY  1122
                DA1=      (A11+R1-R3+D1+AM1-A1)                                   TNTDY  1123
  375           DA2  =    (A12+R2-R4+D2+AM2-A2    )                               TNTDY  1124
                DA3  =    (A13+R3-R5+D3+AM3-R7A-R8A-A3-R9A)                       TNTDY  1125
                DA4  =    (A14+R4-R6+D4+AM4-R7M-R8M-A4-R9M)                       TNTDY  1126
                 DA5=     (A15+R5+D5+AM5-R10A-A5)                                 TNTDY  1127
                DA6=      (A16+R6+D6+AM6-R10M-A6)                                 TNTDY  1128
  380           DA7=      (A17+AM7+R10-A7)                                        TNTDY  1129
                DA8=      (A18+AM8+3.*R10-A8)                                     TNTDY  1130
                WRITE(6,1450) A19,P19,P9,D10,R3,R4,R5,R6,R7,R8,R10,RP,R9,A9,R9G   TNTDY  1131
             1450 FORMAT( 58H0A19,P19,P9,D10,R3,R4,R5,R6,R7,R8,R10,RP,R9,A9,R9G/  TNTDY  1132
               C   (1X,F12.4))                                                    TNTDY  1133
  385           WRITE(6,1451) A17,A16,AL,A11,A14,CSP,A504                       TNTDY  1134
             1451 FORMAT( 32H0A13,A14,AL,A11,A14,CSP,A504/1X,7F12.4)              TNTDY  1135
                DA9=      (A19+P19-P9-R10-R3-R4-R5-R6-13.*R7-12.5*R8-9.*R10+    TNTDY  1136
               C (.33+.67*RP)*R9-A9-12.5*R9G)                                     TNTDY  1137
                DAL=      ( A13-A14+R10+R3+R4+R5+R6+15.*R7+16.5*R8+12.*R10-     TNTDY  1138
  390           C(.33*RP+.67)*R9-AL+16.5*R9G)                                     TNTDY  1139
                DA504=        (A11+A14-CSP      -A504)                          TNTDY  1140
                DA12=       (A12+CSP      -A12)                                   TNTDY  1141
                DP1=      (P11-D1-AM1-P1)                                         TNTDY  1142
                DP2=      (P12-D2-AM2-P2)                                         TNTDY  1143
  395           DP3=      (P13-D3-AM3-P3)                                         TNTDY  1144
                DP4=      (P14-D4-AM4-P4)                                         TNTDY  1145
                 DP5=     (P15       -D5-AM5-P5)                                  TNTDY  1146
                DP6=      (P16-D6-AM6-P6)                                         TNTDY  1147
                DP7=      (P17-D7-AM7-P7)                                         TNTDY  1148
```

```
      DP9=       (P19-D9-AM8-P8)                                          TNTDV 1139
      DP10=        (P10-D10-P10)                                          TNTDV 1140
      WRITE(6,1790)DA1,DA2,DA3,DA4,DA5,DA6,DA7,DA8,DA9,DA12,DA5O4,DAL     TNTDV 1141
 1790 FORMAT( 3H0DA,6F15.6/3X6F15.6)                                       TNTDV 1142
      WRITE(6,1791)DP1,DP2,DP3,DP4,DP5,DP6,DP7,DP8,DP10                   TNTDV 1143
 1791 FORMAT( 3H0DP,6F15.6/3X3F15.6)                                       TNTDV 1144
 1799 CONTINUE                                                             TNTDV 1145
      A9=A9+DTA*(A19+P19-P9-D10-R3-R4-R5-R6-13.*R7-12.5*R8-9.*R10+        TNTDV 1146
     C (.33-.67*RP)*R9-A9-12.5*R9G)                                       TNTDV 1147
      AL=AL+DTA*( A113-A114+D10+R3+R4+R5+R6+15.*R7+16.5*R8+12.*R10-       TNTDV 1148
     C(.33*RP-.67)*R9-AL+16.5*R9G)                                        TNTDV 1149
      IF(IPRNT.EQ.1) WRITE(6,1402)AL,A1,A2,A3,A4,A5,A6,A7,A8,A9           TNTDV 1150
 1402 FORMAT( 3H0AL,A1,A2,A3,A4,A5,A6,A7,A8,A9/1X10F12.4)                  TNTDV 1151
      A10=0.                                                               TNTDV 1152
      A5O4=A5O4+DTA*(A111+A114-CSP      -A5O4)                             TNTDV 1153
      A12=A12+DTA*(A112+CSP      -A12)                                     TNTDV 1154
      IF(AL)30,31,31                                                       TNTDV 1155
   30 A11=0.                                                               TNTDV 1156
      A14=-AL                                                              TNTDV 1157
      GOTO32                                                               TNTDV 1158
   31 A11=AL                                                               TNTDV 1159
      A14=0.                                                               TNTDV 1160
   32 A11=A5O4-A14                                                         TNTDV 1161
      IF(IPRNT.EQ.1) WRITE(6,1401) A13,A14,A11,A12                         TNTDV 1162
 1401 FORMAT( 16H A13,A14,A11,A12/4F12.4)                                  TNTDV 1163
      P1=T1-A1                                                             TNTDV 1164
      P2=T2-A2                                                             TNTDV 1165
      P3=T3-A3                                                             TNTDV 1166
      P4=T4-A4                                                             TNTDV 1167
      P5=T5-A5                                                             TNTDV 1168
      P6=T6-A6                                                             TNTDV 1169
      P7=T7-A7                                                             TNTDV 1170
      P8=T8-A8                                                             TNTDV 1171
      AT=A1+A2+A3+A4+A5+A6+A7+A8+A9+A11+A12+A13+A14                        TNTDV 1172
      PT=P1+P2+P3+P4+P5+P6+P7+P8+P9+P10                                    TNTDV 1173
      P9=1.5*A13*A9*PT/(AT*A11)                                            TNTDV 1174
      IF(IPRNT.EQ.1)WRITE(6,1400) (P(I),I=1,10)                            TNTDV 1175
 1400 FORMAT( 12H0P(I),I=1,10/10F12.4)                                     TNTDV 1176
      R8=R8+R9G                                                            TNTDV 1177
      TCOX=R10+6.*R7+7.*R8+TCOX                                            TNTDV 1178
      TNOX=TNOX+R9*.67*(1.-RP)                                             TNTDV 1179
      IF(ITYPE.EQ.1)GOTO3                                                  TNTDV 1180
      DO21=1,10                                                            TNTDV 1181
    2 RATES(IV,I)=RATE(I)                                                  TNTDV 1182
      RETURN                                                               TNTDV 1183
    3 ZA=0.                                                                TNTDV 1184
      ZR=0.                                                                TNTDV 1185
      DO4I=1,10                                                            TNTDV 1186
      ZA=ZA+(P(I)+A(I))*CP(I)                                              TNTDV 1187
    4 ZR=ZR+DH(I)*RATE(I)                                                  TNTDV 1188
      DO5I=11,14                                                           TNTDV 1189
    5 ZA=ZA+A(I)*CP(I)                                                     TNTDV 1190
      TSEP(ISTGE)=T*ZR/ZA                                                  TNTDV 1191
      RETURN                                                               TNTDV 1192
      END                                                                  TNTDV 1193
```

SYMBOLIC REFERENCE MAP (R=1)

ENTRY POINTS
1 SUB

VARIABLES	SN	TYPE		RELOCATION					
0	A	REAL	ARRAY	VECTOR	0	AI	REAL	ARRAY	INPUT
2617	AINR	REAL			0	AI1	REAL		INPUT
11	AI10	REAL		INPUT	12	AI11	REAL		INPUT
13	AI12	REAL		INPUT	14	AI13	REAL		INPUT
15	AI14	REAL		INPUT	16	AI15	REAL		INPUT
17	AI16	REAL		INPUT	20	AI17	REAL		INPUT
1	AI2	REAL		INPUT	2	AI3	REAL		INPUT
3	AI4	REAL		INPUT	4	AI5	REAL		INPUT
5	AI6	REAL		INPUT	6	AI7	REAL		INPUT
7	AI8	REAL		INPUT	10	AI9	REAL		INPUT
1745	AKA	REAL			1746	AKP	REAL		
1747	AKC	REAL			1750	AKE0	REAL		
1751	AKFOOV	REAL			2352	AKE01	REAL		
2353	AKE02	REAL			105	AKE03	REAL		Z0
77	AKEQA	REAL		Z0	73	AKPA	REAL		Z0
76	AKPAP	REAL		Z0	74	AKPATL	REAL		Z0
1443	AK1	REAL			51	AK10	REAL		Z0
46	AK12	REAL		Z0	2463	AK3	REAL		
53	AK3S	REAL		Z0	47	AK3W	REAL		Z0
2466	AK4	REAL			54	AK4S	REAL		Z0
50	AK4W	REAL		Z0	51	AK5S	REAL		Z0
52	AK6S	REAL		Z0	57	AK7	REAL		Z0
40	AKR	REAL		Z0	2540	AL	REAL		
2420	AMAR	REAL			2423	AM1	REAL		
2424	AM2	REAL			2425	AM3	REAL		
2426	AM4	REAL			2427	AM5	REAL		
2430	AM6	REAL			2431	AM7	REAL		
2432	AMR	REAL			2355	AMP	REAL		
2535	ASQR	REAL			2357	AT	REAL		
2365	ATI	REAL			0	A1	REAL		VECTOR
11	A10	REAL		VECTOR	12	A11	REAL		VECTOR
2673	A110A	REAL	*UNDEF		13	A12	REAL		VECTOR
14	A13	REAL		VECTOR	15	A14	REAL		VECTOR
16	A15	REAL		VECTOR	17	A16	REAL		VECTOR
20	A17	REAL		VECTOR	1	A2	REAL		VECTOR
2	A3	REAL		VECTOR	3	A4	REAL		VECTOR
4	A5	REAL		VECTOR	5	A6	REAL		VECTOR
6	A7	REAL		VECTOR	7	A8	REAL		VECTOR
10	A9	REAL		VECTOR	2454	B	REAL		
2451	BC	REAL			2455	C	REAL		
2462	CR	REAL			2465	CF	REAL		
2450	CHR03	REAL			2445	CHS04	REAL		
2456	CHS207	REAL			2451	CH20	REAL		
2447	CH2S04	REAL			2446	CH30	REAL		
2444	CH07	REAL			16	CP	REAL	ARRAY	Z0
2517	CR	REAL			2520	CZ	REAL		
2536	CS	REAL			2537	CSP	REAL		
2552	DAL	REAL			2553	DAS64	REAL		
2541	DA1	REAL			2554	DA12	REAL		
2542	DA2	REAL			2543	DA3	REAL		
2544	DA4	REAL			2545	DA5	REAL		

VARIABLES SN TYPE RELOCATION

2546	%A6	REAL			2547	DA7	REAL		
2550	%A8	REAL			2551	DA9	REAL		
2471	DELTA	REAL	*UNDEF		34	DN	REAL	ARRAY	Z0
2555	%P1	REAL			2565	DP10	REAL		
2556	%P2	REAL			2547	DP3	REAL		
2560	%P4	REAL			2561	DP5	REAL		
2562	%P6	REAL			2563	DP7	REAL		
2564	%P9	REAL			1	DT	REAL		/ /
2522	DTA	REAL			2521	DTP	EAL		
2405	D1	REAL			2415	D10	*		
2406	D2	REAL			2407	D3			
2410	D4	REAL			2411	D5			
2412	D6	REAL			2413	D7	REA		
2414	D8	REAL			53	EADP	REAL		VECTOR
54	EDAP	REAL		VECTOR	2402	ETA	REAL		
2377	ETAA	REAL			2400	ETAP	REAL		
2401	ETATL	REAL			0	EX	REAL		/ /
71	F10	REAL		Z0	62	EZI	REAL		Z0
55	F3S	REAL		Z0	63	E3W	REAL		Z0
56	F4S	REAL		Z0	64	E4W	REAL		Z0
65	F5S	REAL		Z0	66	E6S	REAL		Z0
67	F7	REAL		Z0	70	E8	REAL		Z0
2433	F	REAL			2343	FA	REAL		
47	FAR	REAL		VECTOR	2464	FC	REAL		
72	FD	REAL		Z0	2566	FF	REAL	ARRAY	
110	FMX	REAL		Z0	1752	FOV	REAL		
2344	FP	REAL			50	FPB	REAL		VECTOR
44	FRAC	REAL		VECTOR	43	FVKH	REAL		VECTOR
2505	F1PA	REAL			2506	F1BR	REAL		
2470	F3	REAL			2474	F4	REAL		
2475	F5	REAL			2476	F6	REAL		
2477	F7A	REAL			2500	F7R	REAL		
2501	FRA	REAL			2502	FBR	REAL		
2503	FSA	REAL			2504	FSR	REAL		
2447	GAMMA	REAL			0	G1	REAL	ARRAY	PAR
110	G10	REAL	ARRAY	PAR	10	G3	REAL	ARRAY	PAR
30	G3S	REAL	ARRAY	PAR	20	G4	REAL	ARRAY	PAR
40	G4S	REAL	ARRAY	PAR	50	G5	REAL	ARRAY	PAR
60	G6	REAL	ARRAY	PAR	70	G7	REAL	ARRAY	PAR
100	GR	REAL	ARRAY	PAR	120	G9	REAL	ARRAY	PAR
2440	I	INTEGER			7	ICALL	INTEGER		/ /
7	IPRNT	INTEGER		/ /	51	ISTGE	INTEGER		VECTOR
46	ITYPE	INTEGER		VECTOR	52	IV	INTEGER		VECTOR
3	IACK	INTEGER		/ /	2453	KLM	INTEGER		
4	MM	INTEGER		/ /	5	MN	INTEGER		/ /
-5	NOTCH	INTEGER		VECTOR	10	NP	INTEGER		/ /
21	P	REAL	ARRAY	VECTOR	21	P1	REAL	ARRAY	INPUT
21	P11	REAL		INPUT	32	P110	REAL		INPUT
33	P111	REAL		INPUT	34	P112	REAL		INPUT
35	P113	REAL		INPUT	36	P114	REAL		INPUT
37	P115	REAL		INPUT	40	P116	REAL		INPUT
41	P117	REAL		INPUT	22	P12	REAL		INPUT
23	P13	REAL		INPUT	24	P14	REAL		INPUT
25	P15	REAL		INPUT	26	P16	REAL		INPUT
27	P17	REAL		INPUT	30	P18	REAL		INPUT
31	P19	REAL		INPUT	2356	PHB	REAL		
2375	PP	REAL			2360	PT	REAL		

VARIABLES	SN	TYPE	RELOCATION
21	P1	REAL	VECTOR
33	P11	REAL	VECTOR
35	P13	REAL	VECTOR
37	P15	REAL	VECTOR
41	P17	REAL	VECTOR
23	P3	REAL	VECTOR
25	P5	REAL	VECTOR
27	P7	REAL	VECTOR
31	P9	REAL	VECTOR
2361	PA	REAL	
2416	PT	REAL	
0	RATE	REAL	ARRAY RRTS
0	RN01	REAL	ZB
12	RN011	REAL	ZB
14	RN013	REAL	ZB
1	RN02	REAL	ZB
3	RN04	REAL	ZB
5	RN06	REAL	ZB
7	RN08	REAL	ZB
111	RP	REAL	ZB
0	R1	REAL	RRTS
2533	R10A	REAL	
1	R2	REAL	RRTS
3	R4	REAL	RRTS
5	R6	REAL	RRTS
2524	R7A	REAL	
7	R8	REAL	RRTS
2530	RBM	REAL	
2526	RMA	REAL	
2531	RMM	REAL	
75	SA	REAL	ZB
77	SC	REAL	ZB
101	SF	REAL	ZB
103	SH	REAL	ZB
105	SJ	REAL	ZB
11	TCBK	REAL	/ /
2354	TKEL	REAL	
107	TP	REAL	ZB
6	TTME	REAL	/ /
2510	T2	REAL	
2512	T4	REAL	
2514	T6	REAL	
2516	T8	REAL	
2442	U	REAL	
2460	VL	REAL	
14	VYY	REAL	ARRAY 000
2366	X13	REAL	
2370	X2	REAL	
2372	X4	REAL	
2441	Y	REAL	
2434	YL	REAL	
2437	YU	REAL	
2403	Z1	REAL	
2472	Z8	REAL	*UNDEF

VARIABLES	SN	TYPE	RELOCATION
32	P10	REAL	VECTOR
34	P12	REAL	VECTOR
36	P14	REAL	VECTOR
40	P16	REAL	VECTOR
22	P2	REAL	VECTOR
24	P4	REAL	VECTOR
26	P6	REAL	VECTOR
30	P8	REAL	VECTOR
2452	Q	REAL	
2362	QP	REAL	
0	QY	REAL	ARRAY 000
13	RATES	REAL	ARRAY / /
11	RN010	REAL	ZB
13	RN012	REAL	ZB
15	RN014	REAL	ZB
2	RN03	REAL	ZB
4	RN05	REAL	ZB
6	RN07	REAL	ZB
10	RN09	REAL	ZB
106	RR	REAL	ZB
11	R10	REAL	RRTS
2534	R10M	REAL	
2	R3	REAL	RRTS
4	R5	REAL	RRTS
6	R7	REAL	RRTS
2527	RTM	REAL	
2525	RWA	REAL	
10	R9	REAL	RRTS
2532	RWM	REAL	
2435	S	REAL	
76	SB	REAL	ZB
100	SD	REAL	ZB
102	SG	REAL	ZB
104	SI	REAL	ZB
42	T	REAL	VECTOR
42	TI	REAL	INPUT
12	TMBK	REAL	/ /
133	TSEP	REAL	ARRAY / /
2507	T1	REAL	
2511	T3	REAL	
2513	T5	REAL	
2515	T7	REAL	
2434	U	REAL	
2376	XEQA	REAL	
2457	XW	REAL	
2367	X1	REAL	
2374	X14	REAL	
2371	X5	REAL	
2373	X9	REAL	
2421	YA	REAL	
2422	YP	REAL	
2523	Z	REAL	
2404	ZB	REAL	

FILE NAMES MODE
TAPE6 FMT

INLINE FUNCTIONS TYPE ARGS
ABS REAL 1 INTEGER

STATEMENT LABELS

1763	1	FMT	0	2		1720	3			
0	4		0	5		0	11		INACTIVE	
127	12		131	13		0	15		INACTIVE	
253	14		316	17		0	20		INACTIVE	
350	21		353	22		0	30		INACTIVE	
1607	31		1611	32		0	141		INACTIVE	
0	142	INACTIVE	270	143		0	144		INACTIVE	
302	145		2065	301	FMT	2015	1000	FMT		
434	1300		440	1305		442	1306			
445	1307		450	1308		443	1310			
447	1312		504	1341		2306	140.	FMT		
2276	1401	FMT	2261	1402	FMT	2123	1405	FMT		
2041	1409	FMT	2151	1450	FMT	2173	1451	FMT		
2220	1790	FMT	2240	1791	FMT	1520	1798			
522	2117		574	2330		550	2339			
552	2340		662	2341		0	2342		INACTIVE	
555	2343		557	2344		573	2345			
577	2346		644	2350		443	2351			
614	2400									

COMMON BLOCKS LENGTH
BUFS 10
// 97
VECTOR 45
PSR 88
INPUT 35
OUT 28
ZQ 74

STATISTICS
PROGRAM LENGTH 25700 1483
COMMON LENGTH 4300 298
BLANK COMMON 1410 97

```
      SUBROUTINE SUB2(A0,P0,NOTCH,FRAC,EOAP,EAOP,FAR,FP0,FAR1,FP01)
      DIMENSION A0(17),P0(17),FF(5)
      COMMON/ZD/RHO(14),
     C                    CP(14),QN(10),AK12,AK34,AK44,AK55,AP65,
     5 C AK75,AK45,E35,E45,
     C AK7,AK9,AK10,E21,E34,F44,E55,E65,E7,E8,E10,FD,AOOA,AOOATL,SA,SB,
     C SC,SD,SF,SG,SH,SI,SJ,QP,TB,FWX,AP
      DATA FF/.06547,.16547,.29179,.42041,.57059/
      AT=A0(9)
      PT=P0(9)+P0(10)
     10 QA=AR(9)/RHO(9)
      QP=P0(9)/RHO(9)+P0(10)/RHO(10)
      DO 10 I=1,8
      AT=AT+A0(I)
      QP=QP+P0(I)/RHO(I)
     15 PT=PT+P0(I)
     10 QA=QA+A0(I)/RHO(I)
      DO 20 I=11,14
      AT=AT+A0(I)
     20 QA=QA+A0(I)/RHO(I)
      FAR=(1.-EAOP*PT/AT)/(1.-EOAP*EAOP)
      IF(FAR)30,40,40
     30 FAR=0.
     40 IF(FAR.GT.1.) FAR=1.
     25 FP0=1.-FAR*EOAP*AT/PT
      IF(FP0)50,60,60
     50 FP0=0.
     60 IF(FP0.GT.1.) FP0=1.
      FAR1=1.-FAR
     30 FP01=1.-FP0
      QT=QA*FAR*(1.-FP0)*QP
      FRAC=FWX*FF(NOTCH)/QT
      IF(FRAC.GT.1.) FRAC=1.
      WRITE(6,1)NOTCH,FRAC,EAOP,EOAP,FAR,FP0,FAR1,FP01
     35 1 FORMAT(  SH SUB2,I5,7F12.4)
      WRITE(6,2) PT,AT,QP,QA,FWX,FF(NOTCH),QT
     2 FORMAT(  PT,AT,QP,QA,FWX,FF,QT,          7F11.4/)
      RETURN
      END
```

SYMBOLIC REFERENCE MAP (R=1)

ENTRY POINTS
3 SUB2

VARIABLES	SN	TYPE		RELOCATION					
3	AKMA	REAL		Z0	74	AKMATL	REAL		Z0
61	AK10	REAL		Z0	46	AK12	REAL		Z0
53	AK5S	REAL		Z0	47	AK3W	REAL		Z0
54	AK4S	REAL		Z0	50	AK4W	REAL		Z0
51	AK6S	REAL		Z0	52	AK6S	REAL		Z0
57	AK7	REAL		Z0	60	AK8	REAL		Z0
0	AO	REAL	ARRAY	F.P.	147	AT	REAL		
16	CP	REAL	ARRAY	Z0	34	DH	REAL	ARRAY	Z0
0	FAMP	REAL		F.P.	0	EOMP	REAL		F.P.
71	F19	REAL		Z0	62	E21	REAL		Z0
55	F3S	REAL		Z0	63	E3W	REAL		Z0
56	F4S	REAL		Z0	64	E4W	REAL		Z0
65	F5S	REAL		Z0	66	E6S	REAL		Z0
67	F7	REAL		Z0	70	E8	REAL		Z0
0	FAR	REAL		F.P.	0	FAR1	REAL		F.P.
72	FD	REAL		Z0	155	FF	REAL	ARRAY	
110	FNX	REAL		Z0	0	FPO	REAL		F.P.
0	FPO1	REAL		F.P.	0	FRAC	REAL		F.P.
153	I	INTEGER			0	NOTCH	INTEGER		F.P.
0	PO	REAL	ARRAY	F.P.	150	PT	REAL		
151	PA	REAL			152	QP	REAL		
154	QT	REAL			0	PHO	REAL	ARRAY	Z0
111	RP	REAL		Z0	106	RR	REAL		Z0
75	SA	REAL		Z0	76	SB	REAL		Z0
77	SC	REAL		Z0	100	SD	REAL		Z0
101	SE	REAL		Z0	102	SG	REAL		Z0
103	SH	REAL		Z0	104	SI	REAL		Z0
105	SJ	REAL		Z0	107	TR	REAL		Z0

FILE NAMES MODE
TAPE6 FMT

STATEMENT LABELS
124 1 FMT 141 2 FMT 0 10
0 20 0 30 INACTIVE 50 40
0 50 INACTIVE 62 60

COMMON BLOCKS LENGTH
Z0 74

STATISTICS
PROGRAM LENGTH 1620 114
COMMON LENGTH 112B 74

```
      SUBROUTINE SUB1(AO,PO,AI,PI)                                          TNTDY  1233
      DIMENSION DFA(14),DFP(14)                                             TNTDY  1234
      DIMENSION AO(14),PO(10),PI(10),AI(14)                                 TNTDY  1235
      COMMON C,DT,IPRNT,JACK,NM,MM,TIME,ICALL,NP,TCOX,TNOX,RATES(8,10)      TNTDY  1236
     C,TSEP(6)                                                              TNTDY  1237
      COMMON/QQQ/QY(14),XYY(14)                                             TNTDY  1238
      COMMON/VECT/AV(14,17),PV(14,17),IVSL,CHAMXO,DFAMXO,CHPMXO,DFPMXO      TNTDY  1239
      COMMON/DUM/R1,R2,R3,R4,R5,R6,R7,R8,R9,R10                             TNTDY  1240
      COMMON/PAR/G1(8),G3(8),G4(8),G3S(8),G4S(8),G5(8),G6(8),G7(8),         TNTDY  1241
     C G9(8),G10(8),G9(8)                                                   TNTDY  1242
      COMMON/ZO/RHO1,RHO2,RHO3,RHO4,RHO5,RHO6,RHO7,RHO8,RHO9,RHO10,         TNTDY  1243
     C RHO11,RHO12,RHO13,RHO14,CP(14),DH(10),AK12,AK3W,AK4W,AK5S,AK6S,      TNTDY  1244
     C AK3S,AK4S,E3S,E4S,                                                   TNTDY  1245
     C AK7,AK8,AK10,E21,E3W,E4W,E5S,E6S,E7,E8,E10,FD,AKHA,AKHATL,SA,SB,     TNTDY  1246
     C SC,SD,SF,SG,SH,SI,SJ,RR,TR,FMX,RP                                   TNTDY  1247
      DFAMX=0.                                                              TNTDY  1248
      DO110I=1,14                                                           TNTDY  1249
  123 IF(AV(IVSL,I)-0.1)125,125,124                                         TNTDY  1250
  124 DFA(I)=(AO(I)-AV(IVSL,I))*100.      /(AV(IVSL,I)     )               TNTDY  1251
      GOTO126                                                               TNTDY  1252
  125 DFA(I)=0.                                                             TNTDY  1253
  126 IF(ABS(DFA(I)).GT.DFAMX) DFAMX=ABS(DFA(I))                            TNTDY  1254
  110 CONTINUE                                                              TNTDY  1255
      IF(DFAMX.GT.DFAMXO)DFAMXO=DFAMX                                       TNTDY  1256
      WRITE(6,A7) AI,AO,DFA,DFAMX,PI,PO                                     TNTDY  1257
   A7 FORMAT(  9H ACID IN ,14F8.3/  9H ACID OUT,14F8.3/                     TNTDY  1258
     C9H PCT CHNG, 14F8.3,2H (,F8.3,  1H)/                                  TNTDY  1259
     C                       9H@ORG. IN ,10F8.3/  9H ORG. OUT,10F8.3/ )     TNTDY  1260
      DFPMX=0.                                                              TNTDY  1261
      DO111I=1,10                                                           TNTDY  1262
  133 IF(PV(IVSL,I)-0.1)135,135,134                                         TNTDY  1263
  135 DFP(I)=0.                                                             TNTDY  1264
      GOTO136                                                               TNTDY  1265
  134 DFP(I)=(PO(I)-PV(IVSL,I))*100.     /(PV(IVSL,I)     )               TNTDY  1266
  136 IF(ABS(DFP(I)).GT.DFPMX)DFPMX=ABS(DFP(I))                             TNTDY  1267
  111 CONTINUE                                                              TNTDY  1268
      IF(DFPMX.GT.DFPMXO)DFPMXO=DFPMX                                       TNTDY  1269
      WRITE(6,112) (DFP(I),I=1,10),DFPMX                                    TNTDY  1270
  112 FORMAT ( 9H PCT CHNG,11F8.3,  2H (,F8.3,  1H))                        TNTDY  1271
      DO113I=1,17                                                           TNTDY  1272
      AV(IVSL,I)=AO(I)                                                      TNTDY  1273
  113 PV(IVSL,I)=PO(I)                                                      TNTDY  1274
      IVSL=IVSL+1                                                           TNTDY  1275
   86 CONTINUE                                                              TNTDY  1276
   80 RETURN                                                                TNTDY  1277
      END                                                                   TNTDY  1278
```

SYMBOLIC REFERENCE MAP (R=1)

ENTRY POINTS
3 SUB1

VARIABLES	SN	TYPE		RELOCATION
0	AI	REAL	ARRAY	F.P.
74	AKMATL	REAL		ZO
46	AK12	REAL		ZO
47	AK3W	REAL		ZO
50	AK4W	REAL		ZO
52	AK6S	REAL		ZO
60	AKA	REAL		ZO
0	AV	REAL	ARRAY	VECT
737	CHPMXO	REAL		VECT
134	DFA	REAL	ARRAY	
736	DFAMXO	REAL		VECT
133	DFPMX	REAL		
34	DH	REAL	ARRAY	ZO
0	EX	REAL		/ /
62	F21	REAL		ZO
63	F3W	REAL		ZO
64	F4W	REAL		ZO
66	F6S	REAL		ZO
70	F8	REAL		ZO
110	FMX	REAL		ZO
110	G10	REAL	ARRAY	PAR
30	G3S	REAL	ARRAY	PAR
40	G4S	REAL	ARRAY	PAR
60	G6	REAL	ARRAY	PAR
100	G8	REAL	ARRAY	PAR
132	I	INTEGER		
2	IPRNT	INTEGER		/ /
3	JACK	INTEGER		/ /
5	NN	INTEGER		/ /
0	PI	REAL	ARRAY	F.P.
356	PV	REAL	ARRAY	VECT
13	RATES	REAL	ARRAY	/ /
11	RHO10	REAL		ZO
13	RHO12	REAL		ZO
15	RHO14	REAL		ZO
2	RHO3	REAL		ZO
4	RHO5	REAL		ZO
6	RHO7	REAL		ZO
10	RHO9	REAL		ZO
106	RR	REAL		ZO
11	R10	REAL		DUM
2	R3	REAL		DUM
4	R5	REAL		DUM
6	R7	REAL		DUM
10	R9	REAL		DUM
76	SB	REAL		ZO
100	SD	REAL		ZO
102	SG	REAL		ZO
104	SI	REAL		ZO
11	TCOX	REAL		/ /
107	TR	REAL		ZO
73	AKMA	REAL		ZO
61	AK10	REAL		ZO
53	AK3S	REAL		ZO
54	AK4S	REAL		ZO
51	AK5S	REAL		ZO
57	AKT	REAL		ZO
0	AO	REAL	ARRAY	F.P.
735	CHAMXO	REAL		VECT
16	CP	REAL	ARRAY	ZO
131	DFARX	REAL		
152	DFP	REAL	ARRAY	
740	DFPMXO	REAL		VECT
1	DT	REAL		/ /
71	E10	REAL		ZO
55	E3S	REAL		ZO
56	E4S	REAL		ZO
55	E5S	REAL		ZO
67	E7	REAL		ZO
72	FD	REAL		ZO
0	G1	REAL	ARRAY	PAR
10	G3	REAL	ARRAY	PAR
20	G4	REAL	ARRAY	PAR
50	G5	REAL	ARRAY	PAR
70	G7	REAL	ARRAY	PAR
120	G9	REAL	ARRAY	PAR
7	ICALL	INTEGER		/ /
734	IVSL	INTEGER		VECT
4	MM	INTEGER		/ /
10	MP	INTEGER		/ /
0	PO	REAL	ARRAY	F.P.
0	QY	REAL	ARRAY	000
0	RHO1	REAL		ZO
12	RHO11	REAL		ZO
14	RHO13	REAL		ZO
1	RHO2	REAL		ZO
3	RHO4	REAL		ZO
5	RHO6	REAL		ZO
7	RHO8	REAL		ZO
111	RP	REAL		ZO
0	R1	REAL		DUM
1	R2	REAL		DUM
3	R4	REAL		DUM
5	R6	REAL		DUM
7	R8	REAL		DUM
75	SA	REAL		ZO
77	SC	REAL		ZO
101	SE	REAL		ZO
103	SH	REAL		ZO
105	SJ	REAL		ZO
12	TNDX	REAL		/ /
133	TSEP	REAL	ARRAY	/ /

```
VARIABLES     SN  TYPE            RELOCATION
     6  TIME      REAL              / /          16  XYY      REAL      ARRAY    000

FILE NAMES        MODE
     TAPE6        FMT

INLINE FUNCTIONS   TYPE   ARGS
     ABS           REAL      1  INTRIN

STATEMENT LABELS
     0  A0          INACTIVE              0  86          INACTIVE             101  87      FMT
     0  110                               0  111                              122  112     FMT
     0  113                               0  123         INACTIVE               0  124         INACTIVE
    17  125                              20  126                                0  133         INACTIVE
    43  134                               0  135         INACTIVE              45  136

COMMON BLOCKS   LENGTH
     / /          97
     000          2A
     VECT        481
     NUM          10
     PAR          8A
     70           74

STATISTICS
  PROGRAM LENGTH    1700     170
    COMMON LENGTH  12518     681
     BLANK COMMON   1418      97
```

```
      SUBROUTINE INPT                                                   TNTDY  1279
      REAL MW                                                           TNTDY  1280
      DIMENSION MW(17)                                                  TNTDY  1281
      DIMENSION NOTCH(6),TEMP(8)                                        TNTDY  1282
      DIMENSION ICH(50),IVS(50),DL(50),NTME(50),NTVL(50)                TNTDY  1283
      DIMENSION COMP(5,14)                                              TNTDY  1284
      COMMON/PAR/G1(8),G3(8),G4(8),G3S(8),G4S(8),G5(8),G6(8),G7(8),     TNTDY  1285
     C G8(8),G10(8),G9(8)                                               TNTDY  1286
      COMMON/ZO/PHO1,PHO2,PHO3,PHO4,PHO5,PHO6,PHO7,PHO8,PHO9,PHO10,     TNTDY  1287
     C PHO11,PHO12,PHO13,PHO14,CP(14),DH(18),AK12,AK3W,AK4W,AK5S,AK6S,  TNTDY  1288
     C AK7S,AK4S,E3S,E4S,                                               TNTDY  1289
     C AK7,AK8,AK19,E21,E3W,E4W,E5S,E6S,E7,E8,E10,FD,AKPA,AKMATL,SA,SB, TNTDY  1290
     C SC,SD,SE,SG,SH,SI,SJ,QQ,TQ,FWX,QP                               TNTDY  1291
      COMMON/FNN/FIN(7,8)                                               TNTDY  1292
      COMMON/SEP/T1A,T1B,T2,T3A,T3B,T4,T5,T6,FVKH1A,FVKH1B,FVKH2,       TNTDY  1293
     C FVKH3A,FVKH3B,FVKH4,FVKH5,FVKH6,EOAP1,EOAP2,EOAP3,EOAP4,EOAP5,  TNTDY  1294
     C EOAP6,EAOP1,EAOP2,EAOP3,EAOP4,EAOP5,EAOP6,FA1,FA2,FA3,FA4,FA5,  TNTDY  1295
     C FA6,FACID1,FACID2,FACID3,FACID4,FACID5,FACID6,F01,F02,F03,F04,   TNTDY  1296
     C F05,F06,FRAC1,FRAC2,FRAC3,FRAC4,FRAC5,FRAC6,FR1,FR2,FR3,FR4,FR5, TNTDY  1297
     C FR6,A1S,A2S,A3S,A4S,A5S,A6S,P1S,P2S,P3S,P4S,P5S,P6S,             TNTDY  1298
     C AIP(14),AXP(14),AF(14),PIR(14),PXR(14),PF(14)                    TNTDY  1299
     C ,N1,N2,N3,N4,N5,N6,FORG1,FORG2,FORG3,FORG4,FORG5,FORG6           TNTDY  1300
      COMMON/X/ARRAY(17,8),P1AI,P10I                                    TNTDY  1301
      COMMON/ EX,DT,IPRNT,JACK,NN,NN,TTME,ICALL,NP,TCOX,TNOX,RATES(8,10) TNTDY  1302
     C,TSEP(6)                                                          TNTDY  1303
      EQUIVALENCE(NOTCH(1),N1),(TEMP(1),T1A)                            TNTDY  1304
      EQUIVALENCE (AK9,SE),(F9,SG)                                      TNTDY  1305
      DATA MW/2*137.,2*182.,2*227.,213.,258.,63.,92.,98.,127.,18.,88.,  TNTDY1   37
     C 3*1./                                                            TNTDY  1307
      IF(ICALL.EQ.0) GOTO100                                            TNTDY  1308
      IKT=0                                                             TNTDY  1309
  779 CONTINUE                                                          TNTDY  1310
      IF(NCHNG.EQ.0)GOTO91                                              TNTDY  1311
      DO20K=1,NCHNG                                                     TNTDY  1312
      I=ICH(K)                                                          TNTDY  1313
      J=IVS(K)                                                          TNTDY  1314
      IF(JACK.LT.NTME(K    ))GOTO20                                     TNTDY  1315
      IF(JACK.GT.NTME(K    )+NTVL(K    ))GOTO20                        TNTDY  1316
      IF(I.GT.7)GOTO21                                                  TNTDY  1317
      IF(NTVL(  K  ).NE.0)GOTO30                                        TNTDY  1318
      FIN(I,J)=FIN(I,J)+DL(K)                                           TNTDY  1319
      GOTO20                                                            TNTDY  1320
   30 DDL=DL(K    )/FLOAT(NTVL(K    ))                                 TNTDY  1321
      FIN(I,J)=FIN(I,J)+DDL                                             TNTDY  1322
      GOTO20                                                            TNTDY  1323
   21 IF(I.NE.9)GOTO40                                                  TNTDY  1324
      NOTCH(J)=NOTCH(J)+INT(DL(K    ) +.1)                             TNTDY  1325
      GOTO20                                                            TNTDY  1326
   40 IF(NTVL(K    ).NE.0)GOTO45                                        TNTDY  1327
      TEMP(J)=TEMP(J)+DL(K)                                             TNTDY  1328
      IKT=1                                                             TNTDY  1329
      GOTO20                                                            TNTDY  1330
   45 DDL=DL(K    )/FLOAT(NTVL(K    ))                                 TNTDY  1331
      TEMP(J)=TEMP(J)+DDL                                               TNTDY  1332
      IKT=1                                                             TNTDY  1333
   20 CONTINUE                                                          TNTDY  1334
  777 CONTINUE                                                          TNTDY  1335
```

```
                IF(I.NE.0)GOTO770                                       TNTDY  1336
                DO171I=1,8                                              TNTDY  1337
                ZA=(1./TR-1./(TEMP(I)+273.3))/BR                        TNTDY  1338
40              G1(I)=EXP(E21*ZA)/AK12                                  TNTDY  1339
                G3(I)=AK3*EXP(E3*ZA)                                    TNTDY  1340
                G3S(I)=AK3S*EXP(E3S*ZA)                                 TNTDY  1341
                G4(I)=AK4*EXP(E4*ZA)                                    TNTDY  1342
45              G4S(I)=AK4S*EXP(E4S*ZA)                                 TNTDY  1343
                G5(I)=AK5S*EXP(E5S*ZA)                                  TNTDY  1344
                G6(I)=AK6S*EXP(ZA*E6S)                                  TNTDY  1345
                G7(I)=AK7*EXP(E7*ZA)                                    TNTDY  1346
                G8(I)=AK8*EXP(E8*ZA)                                    TNTDY  1347
                G9(I)=AK9*EXP(E9 *ZA)                                   TNTDY  1348
70              G10(I)=AK10*EXP(E10*ZA)                                 TNTDY  1349
                IF(I.LT.4) GOTO171                                      TNTDY  1350
                IF(G3 (I).GT.EX) G3 (I)=EX                              TNTDY  1351
                IF(G3S(I).GT.EX) G3S(I)=EX                              TNTDY  1352
75              IF(G4 (I).GT.EX) G4 (I)=EX                              TNTDY  1353
                IF(G4S(I).GT.EX) G4S(I)=EX                              TNTDY  1354
            171 CONTINUE                                                TNTDY  1355
            770 CONTINUE                                                TNTDY  1356
                P1A(I=FIN(6,I)/MW(10)                                   TNTDY  1357
80              P19(I=FIN(6,2)/MW(10)                                   TNTDY  1358
                IF(JACK.GE.500)  COMP(6,9)=95.0                         TNTDY  1359
                IF(JACK.GE.500)  COMP(4,13)=5.0                         TNTDY  1360
                DO79I=1,8                                               TNTDY  1361
                DO71J=1,14                                              TNTDY  1362
85              ARRAY(J,I)=0.                                           TNTDY  1363
                DO72K=1,5                                               TNTDY  1364
            72  ARRAY(J,I)=ARRAY(J,I)+FIN(K,I)*COMP(K,J)*.01/MW(J)      TNTDY  1365
            71  CONTINUE                                                TNTDY  1366
                ARRAY(13,I)=ARRAY(13,I)+FIN(7,I)/MW(13)                 TNTDY  1367
90          79  CONTINUE                                                TNTDY  1368
            91  IF((JACK/MW)*MW.NE.JACK) RETURN                         TNTDY  1369
                WRITE(6,709) ((FIN(I,J),J=1,8),I=1,7)                   TNTDY  1370
                WRITE(6,709) TEMP                                       TNTDY  1371
            709 FORMAT(*0TEMPERATURES   *,  8F10.2)                     TNTDY  1372
95              RETURN                                                  TNTDY  1373
            100 ICALL=1                                                 TNTDY  1374
                READ(5,1)((FIN(I,J),J=1,8),I=1,7)                       TNTDY  1375
            1   FORMAT(8F10.0)                                          TNTDY  1376
                READ(5,6)((COMP(J,I),I=1,14),J=1,5)                     TNTDY  1377
100         6   FORMAT(8F10.0/6F10.0)                                   TNTDY  1378
                READ(5,10)IPRNT,TIME,DT,DPRNT                           TNTDY  1379
                WRITE(6,110)TIME,DT,DPRNT                               TNTDY  1380
            110 FORMAT(*0TIME OF RUN, HRS*,F10.4/*0INTEGRATION INTERVAL, HRS*,  TNTDY  1381
               C F10.4/*0TIME BETWEEN PRINTOUT, HRS*,F10.4)             TNTDY  1382
105           10 FORMAT(I5,8F10.0)                                      TNTDY  1383
                NP=TIME/DT+.0001                                        TNTDY  1384
                NPRNT=DPRNT/DT+.0001                                    TNTDY  1385
                NP=8.01*TIME/DT+.5                                      TNTDY  1386
                NC=NG=1                                                 TNTDY  1387
110             WRITE(6,111)                                            TNTDY  1388
            111 FORMAT(*0/////PROCESS CHANGES//////*/                   TNTDY  1389
               C * VARIABLE   VESSEL     CHANGE        TIME       INTERVAL*)  TNTDY  1390
                READ(5,7) ICH(NCHNG),IVS(NCHNG),DL(NCHNG),TIME,TVL     TNTDY  1391
            7   FORMAT(2I5,3F10.0)                                      TNTDY  1392
```

```
                      IF(ICH(NCHNG).EQ.0)GOTO9                                    TNTDV  1393
                      WRITE(6,112) ICH(NCHNG),IVS(NCHNG),DL(NCHNG),TME,TVL        TNTDV  1394
                  112 FORMAT(1X,I5,I10,F14.2,F14.4,F16.4)                         TNTDV  1395
                      NTVL(NCHNG)=TVL/DT+.00001                                   TNTDV  1396
                      IF(NTVL(NCHNG).NE.0.) NTVL(NCHNG)=NTVL(NCHNG)-1             TNTDV  1397
                      NTMF(NCHNG)=TME/DT+.00001                                   TNTDV  1398
                      NCHNG=NCHNG+1                                               TNTDV  1399
                      GOTO9                                                       TNTDV  1400
                    8 NCHNG=NCHNG-1                                               TNTDV  1401
                      WRITE(6,304) (((COMP(I,J),J=1,14),I=1,5)                    TNTDV  1402
                  304 FORMAT(25H0ACID STRENGTHS, WT. PCT.,/6X,4HCOM.,7X,4HAMNT,2X,4HNMNT TNTDV  1403
                     C,2X,4HAMNT,2X,4HNMNT,2X,4HATNT,2X,4HPTNT,2X,4HTNBA,2X,3HTNP,3X,4HN TNTDV  1404
                     CMO3,2X,7HTVL,2X,17HH2SO4 HNO3 H2O.3X,3HSO3,/                TNTDV  1405
                     C 6X,10HWEAK NIT, ,14F6.2,/6X,3HFR,.7X,14F6.2,/6X,10HYELLOW WA,, TNTDV  1406
                     C 14F6.2,/6X,10HSTRONG NI,,14F6.2,/6X,5HOLEUM,5X,14F6.2)     TNTDV  1407
                  303 FORMAT( 13H0INPUT MATRIX/6X  6HVESSEL,10X  2HIA,8X  2HIB,9X  1H2,8 TNTDV  1408
                     CX  2H14,      6X  2H30,9X  1H4,9X  1H5,9X  1H6/6X 10HWEAK NIT, ,8F TNTDV  1409
                     C10.0/                 6X  3HFR,,7X,8F10.0/  6X 10HYELLOW WA,,8F10 TNTDV  1410
                     C.0/ 6X 10HSTRONG NI,,        8F10.0/6X  5HOLEUM,5X,8F10.0/6X  7HTO TNTDV  1411
                     CLUENE,7X,8F10.0/6X,10HWATER      ,8F10.0)                  TNTDV  1412
                      JACK=0                                                      TNTDV  1413
                      IXT=1                                                       TNTDV  1414
                      GOTO777                                                     TNTDV  1415
                      END                                                         TNTDV  1416
```

SYMBOLIC REFERENCE MAP (R=1)

ENTRY POINTS
1 INPT

VARIABLES	SN	TYPE		RELOCATION					
142	AF	REAL	ARRAY	SEP	106	AIP	REAL	ARRAY	SEP
73	AKMA	REAL		Z0	74	AKMATL	REAL		Z0
61	AK10	REAL		Z0	46	AK12	REAL		Z0
53	AK3S	REAL		Z0	47	AK3W	REAL		Z0
56	AK4S	REAL		Z0	50	AK4W	REAL		Z0
51	AK5S	REAL		Z0	52	AK6S	REAL		Z0
57	AK7	REAL		Z0	60	AK8	REAL		Z0
101	AK9	REAL		Z0	0	AMRAY	REAL	ARRAY	X
126	AXR	REAL	ARRAY	SEP	72	A1S	REAL		SEP
73	A2S	REAL		SEP	74	A3S	REAL		SEP
75	A4S	REAL		SEP	76	A5S	REAL		SEP
77	A6S	REAL		SEP	1275	COMP	REAL	ARRAY	
16	CP	REAL	ARRAY	Z0	655	DDL	REAL		
34	PH	REAL	ARRAY	Z0	1047	DL	REAL	ARRAY	
657	MPRMT	REAL			1	DT	REAL		/ /
26	FAOP1	REAL		SEP	27	EAOP2	REAL		SEP
30	FAOP3	REAL		SEP	31	EAOP4	REAL		SEP
32	FAOP5	REAL		SEP	33	EAOP6	REAL		SEP
20	FOAP1	REAL		SEP	21	EOAP2	REAL		SEP
22	FOAP3	REAL		SEP	23	EOAP4	REAL		SEP
24	FOAP5	REAL		SEP	25	EOAP6	REAL		SEP
0	FX	REAL		/ /	71	E10	REAL		Z0
62	F21	REAL		Z0	55	E3S	REAL		Z0
63	F3W	REAL		Z0	56	E4S	REAL		Z0
64	F4W	REAL		Z0	45	E5S	REAL		Z0
66	F6S	REAL		Z0	67	E7	REAL		Z0
70	F8	REAL		Z0	102	F9	REAL		Z0
42	FACIO1	REAL		SEP	43	FACIO2	REAL		SEP
44	FACIO3	REAL		SEP	45	FACIO4	REAL		SEP
46	FACIO5	REAL		SEP	47	FACIO6	REAL		SEP
34	FA1	REAL		SEP	35	FA2	REAL		SEP
36	FA3	REAL		SEP	37	FA4	REAL		SEP
40	FA5	REAL		SEP	41	FA6	REAL		SEP
72	FD	REAL		Z0	0	FIN	REAL	ARRAY	FWM
110	FWX	REAL		Z0	240	FOPG1	REAL		SEP
241	FOPG2	REAL		SEP	242	FOPG3	REAL		SEP
243	FOPG4	REAL		SEP	244	FOPG5	REAL		SEP
245	FOPG6	REAL		SEP	50	FO1	REAL		SEP
51	FO2	REAL		SEP	52	FO3	REAL		SEP
53	FO4	REAL		SEP	54	FO5	REAL		SEP
55	FO6	REAL		SEP	56	FRAC1	REAL		SEP
57	FRAC2	REAL		SEP	60	FRAC3	REAL		SEP
61	FRAC4	REAL		SEP	62	FRAC5	REAL		SEP
63	FRAC6	REAL		SEP	64	FR1	REAL		SEP
65	FR2	REAL		SEP	66	FR3	REAL		SEP
67	FR4	REAL		SEP	70	FR5	REAL		SEP
71	FR6	REAL		SEP	10	FWKN1A	REAL		SEP
11	FWKN1B	REAL		SEP	12	FWKN2	REAL		SEP
13	FWKN3A	REAL		SEP	14	FWKN3B	REAL		SEP
15	FWKN4	REAL		SEP	16	FWKN5	REAL		SEP
17	FWKN6	REAL		SEP	0	G1	REAL	ARRAY	PAP

VARIABLES	SN	TYPE	RELOCATION						
110	G10	REAL	ARRAY	PAR	18	G3	REAL	ARRAY	PAR
30	G3S	REAL	ARRAY	PAR	20	G4	REAL	ARRAY	PAR
40	G4S	REAL	ARRAY	PAR	50	G5	REAL	ARRAY	PAR
60	G6	REAL	ARRAY	PAR	70	G7	REAL	ARRAY	PAR
100	G8	REAL	ARRAY	PAR	120	G9	REAL	ARRAY	PAR
653	I	INTEGER			7	ICALL	INTEGER		/ /
743	ICH	INTEGER	ARRAY		650	IKT	INTEGER		
2	IPRNT	INTEGER		/ /	765	IVS	INTEGER	ARRAY	
654	J	INTEGER			3	JACK	INTEGER		/ /
652	K	INTEGER			642	NN	REAL	ARRAY	
651	NCHNG	INTEGER			4	NN	INTEGER		/ /
5	NN	INTEGER		/ /	232	NOTCH	INTEGER	ARRAY	SEP
10	NP	INTEGER		/ /	1131	NTME	INTEGER	ARRAY	
1213	NTVL	INTEGER	ARRAY		232	N1	INTEGER		SEP
233	N2	INTEGER		SEP	234	N3	INTEGER		SEP
235	N4	INTEGER		SEP	236	N5	INTEGER		SEP
237	N6	INTEGER		SEP	214	PF	REAL	ARRAY	SEP
160	PIP	REAL	ARRAY	SEP	176	PIP	REAL	ARRAY	SEP
210	PIAI	REAL		X	211	PIRI	REAL		X
100	P1S	REAL		SEP	101	P2S	REAL		SEP
102	P3S	REAL		SEP	103	P4S	REAL		SEP
104	P5S	REAL		SEP	105	P6S	REAL		SEP
13	PAYFS	REAL	ARRAY	/ /	0	RHO1	REAL		Z0
11	RHO10	REAL		Z0	12	RHO11	REAL		Z0
13	RHO12	REAL		Z0	14	RHO13	REAL		Z0
15	RHO14	REAL		Z0	1	RHO2	REAL		Z0
2	RHO3	REAL		Z0	3	RHO4	REAL		Z0
4	RHO5	REAL		Z0	5	RHO6	REAL		Z0
6	RHO7	REAL		Z0	7	RHO8	REAL		Z0
10	RHO9	REAL		Z0	111	RP	REAL		Z0
104	RR	REAL		Z0	75	SA	REAL		Z0
76	SB	REAL		Z0	77	SC	REAL		Z0
100	SD	REAL		Z0	101	SE	REAL		Z0
102	SG	REAL		Z0	103	SH	REAL		Z0
104	SI	REAL		Z0	105	SJ	REAL		Z0
11	TCHX	REAL		/ /	0	TEMP	REAL	ARRAY	SEP
660	TME	REAL			12	TNDX	REAL		/ /
107	TP	REAL		Z0	133	TSEP	REAL	ARRAY	/ /
6	TTME	REAL		/ /	661	TVL	REAL		
0	T1A	REAL		SEP	1	T1B	REAL		SEP
2	T2	REAL		SEP	3	T3A	REAL		SEP
4	T3B	REAL		SEP	5	T4	REAL		SEP
6	T5	REAL		SEP	7	T6	REAL		SEP
656	Z0	REAL							

FILE NAMES MODE

TAPES	FMT	TAPE6	FMT

EXTERNALS	TYPE	ARGS
FXP	REAL	1 LIBRARY

INLINE FUNCTIONS	TYPE	ARGS					
FLOAT	REAL	1	INTRIN	INT	INTEGER	1	INTRIN

STATEMENT LABELS

437	1	FMT	443	6	FMT	532	7	FMT
381	8		325	9		500	10	FMT

STATEMENT LABELS

51	20			33	21			25	30		
41	40			45	45			0	70		
0	71			0	72			217	91		
245	100			464	110	FMT		506	111	FMT	
545	112	FMT		152	171			611	383	FMT	
557	704	FMT		417	309	FMT		52	777		
195	778			0	779		INACTIVE				

COMMON BLOCKS LENGTH

BLO	48
70	74
FMT	54
CFP	166
Y	138
/ /	97

STATISTICS

PROGRAM LENGTH	14838	771	
COMMON LENGTH	10170	522	
BLANK COMMON	1418	97	

```
      FUNCTION ENTH(AK,XA1,XA2,PX,XP1,XP2,TP)                          TNTHDY  1417
      DIMENSION A(14),P(14),X(14),Y(14)                                TNTHDY  1418
      DIMENSION AX(14),PX(14)                                          TNTHDY  1419
      REAL LAS,LBSE                                                    TNTHDY  1420
      COMMON/ZB/RHO1,RHO2,RHO3,RHO4,RHO5,RHO6,RHO7,RHO8,RHO9,RHO10,    TNTHDY  1421
     C RHO11,RHO12,RHO13,RHO14,CP(14),BM(10),A 12,AK3W,AW4W,AK5S,AK6S,  TNTHDY  1422
     C AK7S,AK8S,E7S,E8S,                                              TNTHDY  1423
     C AK7,AK8,AK10,E21,E3W,F4W,E5S,E6S,E7,E8,E10,FB,AKPA,AKPATL,SA,SB, TNTHDY  1424
     C SC,SD,SE,SG,SH,SI,SJ,HP,TM,FMAX                                TNTHDY  1425
      EQUIVALENCE (CP(11),CP1),(CP(9),CP9),(CP(14),CP14),              TNTHDY  1426
     C (CP(13),CP13),(CP(12),CP12)                                     TNTHDY  1427
      DATA X/-12*.,-133.,-136.,-137.,-134.,-128.,-115.,-98.,-75.,-49.,  TNTHDY  1428
     C 0.,68.,168.,268./                                               TNTHDY  1429
      DATA Y/-127.,-127.,-129.,-130.,-126.,-120.,-108.,-91.,-72.,-47.,  TNTHDY  1430
     C -25.,-5.,20.,40./                                               TNTHDY  1431
      DO10I=1,14                                                       TNTHDY  1432
      A(I)=AX(I)*XA1*XA2                                               TNTHDY  1433
   10 P(I)=PX(I)*XP1*XP2                                               TNTHDY  1434
      BL1=TP-20.                                                       TNTHDY  1435
      LAS=90.*A(11)+63.*A(9)+18.*A(13)+80.*A(14)                       TNTHDY  1436
      ENTH=0.                                                          TNTHDY  1437
      IF(LAS.LT.1.)GOTO3                                               TNTHDY  1438
      LBSE=90.*(A(11)+A(14))+63.*A(9)                                  TNTHDY  1439
      WTA=LBSE/LAS                                                     TNTHDY  1440
      F=(WTA-.65)/.05                                                  TNTHDY  1441
      J=F                                                              TNTHDY  1442
      F=F-FLOAT(J)                                                     TNTHD   1443
      ENTH0=X(J)+(X(J+1)-X(J))*F                                       TNTHDY  1444
      ENTH2=Y(J)+(Y(J+1)-Y(J))*F                                       TNTHDY  1445
      WTN=53.*A(9)/LBSE                                                TNTHDY  1446
      ENTH=LAS*(ENTH0+(ENTH2-ENTH0)*WTN/.2)*.252                       TNTHDY  1447
     C +BLT*(A(11)*CP11+A(9)*CP9+A(13)*CP13+A(14)*CP14)                TNTHDY  1448
    3 DO1I=1,10                                                        TNTHDY  1449
      IF(I.EQ.9)GOTO2                                                  TNTHDY  1450
      T=A(I)*P(I)                                                      TNTHDY  1451
      GOTO1                                                            TNTHDY  1452
    2 T=P(I)                                                           TNTHDY  1453
    1 ENTH=ENTH+T*BLT*CP(I)                                            TNTHDY  1454
      ENTH=ENTH+BLT*CP12*A(12)                                         TNTHDY  1455
      RETURN                                                           TNTHDY  1456
      END                                                              TNTHDY  1457
```

SYMBOLIC REFERENCE MAP (R=1)

ENTRY POINTS
4 ENTH

VARIABLES	SN	TYPE	RELOCATION					
157	A	REAL	ARRAY		73	AKMA	REAL	20
74	AKMATL	REAL	20		61	AK10	REAL	20
44	AK12	REAL	20		53	AK35	REAL	20
47	AK14	REAL	20		54	AK45	REAL	20
50	AK4M	REAL	20		51	AK55	REAL	20
52	AK65	REAL	20		57	AK7	REAL	20
60	AK8	REAL	20		0	AL	REAL	ARRAY F.P.
14	CP	REAL	ARRAY 20		30	CP11	REAL	20
31	CP12	REAL	20		32	CP13	REAL	20
33	CP14	REAL	20		26	CP9	REAL	20
34	EH	REAL	ARRAY 20		147	ELT	REAL	
143	ENTH	REAL			153	ENTH0	REAL	
156	ENTH2	REAL			71	E10	REAL	20
62	F21	REAL	20		55	E35	REAL	20
63	F3M	REAL	20		56	E45	REAL	20
64	F4M	REAL	20		65	E55	REAL	20
66	F65	REAL	20		67	E7	REAL	20
70	F8	REAL	20		151	F	REAL	
72	F9	REAL	20		110	FMAX	REAL	20
146	I	INTEGER			152	J	INTEGER	
144	LBS	REAL			145	LOSE	REAL	
175	P	REAL	ARRAY		0	PX	REAL	ARRAY F.P.
0	PM01	REAL	20		11	PM010	REAL	20
12	PM011	REAL	20		13	PM012	REAL	20
14	PM013	REAL	20		15	PM014	REAL	20
1	PM02	REAL	20		2	PM03	REAL	20
3	PM04	REAL	20		4	PM05	REAL	20
5	PM06	REAL	20		6	PM07	REAL	20
7	PM08	REAL	20		10	PM09	REAL	20
106	PP	REAL	20		75	SA	REAL	20
76	SB	REAL	20		77	SC	REAL	20
100	SD	REAL	20		101	SE	REAL	20
102	SG	REAL	20		103	SH	REAL	20
104	SI	REAL	20		105	SJ	REAL	20
156	T	REAL			0	TP	REAL	F.P.
107	TH	REAL	20		150	UTA	REAL	
155	WTH	REAL			213	X	REAL	ARRAY
0	XA1	REAL	F.P.		0	XA2	REAL	F.P.
0	XP1	REAL	F.P.		0	XP2	REAL	F.P.
231	Y	REAL	ARRAY					

INLINE FUNCTIONS TYPE ARGS
FLOAT REAL 1 ENTH0N

STATEMENT LABELS
128 1 117 2 106 3
0 10

COMMON BLOCKS LENGTH
78 73

128

STATISTICS

PROGRAM LENGTH	2058	101
COMMON LENGTH	1119	73

24.8	2503330.	322403.	154.5	506.75	.275	1.33	.000001	
671000.	671000.	17200.	10600.					
88.9	26400.	17462.	9300	6500.	6300.	10000.	1.	
.44	5000.	4.27	1.547	2.0	7000.	4.95	60000.	
.363	.9	363.3	26000.	5000.	418.	.561		
15340.	15010.	15000.	14920.	11240.	14520.	237000.	321000.	
16300.	0.							
.503	.533	.457	.457	.406	.406	.404	.404	
1.454	.552	1.146	1.146	3.346	1.146			
33.8	33.8	33.8	33.8	33.8	33.8	33.8	33.8	
10.91	33.89	15.55	0.	8.16	14.3			
	.2348734E+00	.4791485E-02		.5060835E-01	.2864946E-02		.2671275E-01	
	.1374097E-02	.1256196E-00		.3798584E-00	.1774038E+02		0.	
	.9444754E+02	.7249987E+01		.1667845E+03	0.			
	.1359494E+0C	.8138158E+00		.4789531E+01	.1659479E+00		.2100827E+01	
	.1119533E+00	.1933934E-05		.3101501E-06	.5123718E+01		.8188324E-02	
0.		0.		0.	0.			
	.1625854E+00	.6495519E-02		.3483137E-01	.1229810E-02		.1621020E-01	
	.8275237E-03	.7642231E-04		.2232687E-04	.1834404E+02		0.	
	.1157935E+03	.9531445E+01		.2752697E+03	0.			
	.2229623E+02	.9141384E+00		.4774434E+01	.1644287E+00		.2220151E+01	
	.1134480E+00	.1847633E-06		.3142980E-04	.5279466E+01		.1086122E-02	
0.		0.		0.	0.			
	.1621752E+00	.6604514E-02		.3524373E-01	.1314953E-02		.1621014E-01	
	.8275165E-03	.7642225E-09		.2292667E-04	.1834363E+02		0.	
	.1157934E+03	.9531582E+01		.2752502E+03	0.			
	.2229423E+02	.9141384E+00		.4774434E+01	.1644297E+00		.2220151E+01	
	.1134480E+00	.1847633E-06		.3142980E-06	.5229362E+01		.1086122E-02	
0.		0.		0.	0.			
	.1551155E-01	.1244188E-02		.8947235E+00	.3156273E-01		.5307070E+00	
	.2469268E-01	.2535120E-07		.7665361E-07	.3200270E+02		0.	
	.1581240E+03	.1187897E+02		.1212359E+03	0.			
	.1134544E+01	.7014841E-01		.3112161E+02	.1095405E+01		.1067977E+02	
	.9337228E+00	.8919838E-06		.2675644E-05	.7483319E+01		.6159652E-06	
0.		0.		0.	0.			
	.2227773E-04	.3584281E-05		.8592117E+00	.2641471E-01		.5717639E+00	
	.1231243E-01	.2620984E-07		.7448813E-07	.3191367E+02		0.	
	.1588993E+03	.1111792E+02		.1213576E+03	0.			
	.1134544E+01	.7014842E-01		.3112401E+02	.1095480E+01		.1068130E+02	
	.9334129E+00	.8919568E-06		.2675464E-05	.7478155E+01		.6159652E-06	
0.		0.		0.	0.			
	.4254487E-04	.3781054E-05		.2887287E+01	.4550288E-01		.3047819E+01	
	.1627454E+00	.1675497E-05		.4427691E-06	.2365484E+02		0.	
	.5129213E+02	.5594558E+01		0.	.1816392E+02			
	.3622445E-02	.2233847E-03		.1846719E+02	.4655846E+00		.2891873E+02	
	.1517948E+01	.1382787E-05		.4149342E-05	0.		.2077269E-09	
0.		0.		0.	0.			
	.2536219E-06	.2685945E-07		.3269406E+01	.5617495E-01		.9000874E+01	
	.4572479E+00	.4182993E-06		.1256898E-05	.3789764E+02		0.	
	.1759089E+03	.1383586E+02		0.	.1443496E+02			
	.1354742E-04	.8856208E-06		.1487887E+02	.2672540E+00		.6891446E+02	
	.2879445E+01	.1991546E-05		.5784697E-05	0.		.1218848E-12	
0.		0.		0.	0.			
	.3954194E-10	.6697115E-11		.1745419E+01	.1678815E-01		.1019584E+02	
	.4838282E+00	.5168946E-06		.1558414E-05	.3522391E+02		0.	
	.1725596E+03	.1347882E+02		0.	.1235522E+02			
	.1356742E-04	.8856218E-06		.1492834E+02	.2676264E+00		.4113940E+02	
	.2892644E+01	.1912911E-05		.5734737E-05	0.		.1218898E-12	
0.		0.		0.	0.			
	.4435475E-10	.1503825E-10		.8549896E+00	.9238455E-07		.1116896E+02	
	.4941933E+00	.7037437E-06		.2111231E-05	.4480474E+02		0.	
	.1473105E+03	.7242.8E+01		0.	.7759742E+02			
	.3274722E-07	.2374022E-04		.3112652E+01	.3334174E-01		.4809364E+02	
	.1791431E+01	.2524453E-05		.7574845E-05	0.		.4224444E-16	

DATA DECK LISTING

0.	0.	0.	0.	
.1403989E-14	.1277687E-14	.2583020E+00	.1753939E-02	.1165264E+02
.4999380E+00	.8341209E-06	.2502363E-05	.6403065E+02	0.
.6799963E+03	.7448349E+01	0.	.7671505E+02	
.9574722E-07	.2374022E+00	.3114207E+01	.3390421E-01	.4017842E+02
.1795362E+01	.2530809E-05	.7502466E-05	0.	.4220444E-16
0.	0.	0.	0.	
.6699451E-13	.2476182E-13	.1248208E+00	.1814219E-02	.8152114E+01
.3498437E+00	.6631445E-06	.1989444E-05	.4115708E+02	0.
.9419395E+02	.1442115E+01	0.	.6356637E+02	
.7727[illegible]E-10	.5269769E-11	.6789083E+00	.5302040E-02	.4213463E+02
.1799117E+01	.3420364E-05	.1027897E-04	0.	.1301650E-19
0.	0.	0.	0.	
.4895084E-10	.8485717E-10	.2048656E-01	.1125311E-03	.8239840E+01
.3444081E+00	.8127625E-06	.2439288E-05	.4101106E+02	0.
.4491542E+02	.1494023E+01	0.	.6339585E+02	
.7777[illegible]E-10	.5269769E-11	.6710009E+00	.5303044E-02	.4214952E+02
.1799[illegible]E+01	.3427581E-05	.1024274E-04	0.	.1301650E-19
0.	0.	0.	0.	
.5551354E-16	.2714242E-16	.1711757E-01	.1822340E-03	.6550890E+01
.2772[illegible]E+00	.6154619E-06	.1832844E-05	.3456[illegible]E+02	0.
.7234431E+02	.2398897E+00	0.	.5388[illegible]E+02	
.1347[illegible]E-12	.9233648E-14	.7834895E-01	.4737591E-03	.2907539E+02
.1243[illegible]E+01	.2782175E-05	.8367124E-05	0.	.3165607E-23
0.	0.	0.	0.	
.1508731E-21	.4569297E-21	.1569769E-02	.6824803E-05	.6572169E+01
.2773724E+00	.7605184E-06	.2385557E-05	.3456758E+02	0.
.7241598E+02	.2447983E+00	0.	.5395[illegible]E+02	
.1347864E-12	.9233696E-14	.7894905E-01	.4737596E-03	.2907508E+02
.1243243E+01	.2782623E-05	.8367268E-05	0.	.3[illegible]5607E-23
0.	0.	0.	0.	

123431							
0.	.15615	.13918	.02421	.01950	.00477		
.09971	.82787	.09532	.03847	.04133	.04715		
52.1	52.1	48.1	53.5	52.1	53.5	68.2	68.2
20.1							
44.	24.	60.	7[illegible].	78.	92.	100.	105.
2[illegible]00.							
2900.		2980.					
500.							
	500.						
			253.	87.	475.	58.	1362.
							10044.
2999.	223.						
0.							
57.				43.			
0.							
55.				45.			
				.5			
5.5		18.		84.			
0.							
98.				2.			
0.							
5.23		57.1			37.67		
0	9.	.00950	4.5				
5	0	1000.	1.	0.			

CORE MAP 10.04.04. NORMAL CONTROL 000100 067525 067364 000141

---TIME---LOAD MODE --L1--L2-----TYPE----------USER-----+---CALL----------FWA LOAD--LWA LOAD--BLNK COMN--LENGTH--

FWA LOADER 123665 FWA TABLES 116403

-PROGRAM----ADDRESS-

NANCY	000570
NANC30	001413
NANCYM	003733
RTHETA	005076
NANCYL	005110
NANPLT	005221
NANCOY	005556
MMMX	005673
NUCHAR	005770
LABEL	006076
TITLE	006143
LYNNN	006226
SAVPLT	006234
TNTSIM	011341
SUB	053277
SUB2	056255
SUB1	056520
INPT	056773
ENTH	060421
GETBA	060711
SIO$	060730
SYSTEM$	062371
ACCNER$	063401
INPUTC$	063414
KODER$	063543
KRAKER$	065156
OUTPTC$	066710
ARS$	067004
INT$	067007
FLOAT$	067012
ALNLOGE	067015
EXP$	067054
EXPE	067116
LEGVAR$	067162

--LABELED---COMMON----ADDRESS-

NANCOM	000100
NANCOM	000100
NANCYMC	001612
NANCOM	000100
NANCYMC	001612
NANCOM	000100
NANCOM	000100
NANCOM	000100
NANCOM	000100
NANCOM	000100
NANCOM	000100
PAR	006260
VECT	006410
X	007351
VECTOR	007563
GOO	007640
SEP	007674
AMNT	010442
INPUT	011062
FNN	011125
DUM	011215
ZO	011227
PRTS	053265
VECTOR	007563
PAR	006260
INPUT	011062
GOO	007640
ZO	011227
ZO	011227
GOO	007640
VECT	006410
DUM	011215
PAR	006260
ZO	011227
PAR	006260
ZO	011227
FNN	011125
SEP	007674
X	007351
ZO	011227

PROGRAM OUTPUT

REMARK$ 067167
SINCOSE 067217
XTCIE 067274
XTOY$ 067311
----UNSATISFIED EXTERNALS-----

REFERENCES

INPUT COMPS

.2369	.0098	.0586	.0021	.0267	.0814	.0000	.0000	17.7484	0.0000
98.4475	7.2890	166.7045	0.0000	-0.0000	-0.0000	-0.0000			
19.6969	.8138	4.7095	.1659	2.1800	.1120	.0000	.0000	5.1237	.0082
0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000			
.1626	.0067	.0348	.0012	.0162	.0008	.0000	.0000	18.3440	0.0000
115.7939	8.5315	225.2497	0.0000	-0.0000	-0.0000	-0.0000			
22.2942	.9181	4.7744	.1684	2.2202	.1135	.0000	.0000	5.2285	.0011
0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000			
.1622	.0066	.0352	.0013	.0162	.0008	.0000	.0000	18.3436	0.0000
115.7934	8.5315	225.2502	0.0000	-0.0000	-0.0000	-0.0000			
22.2942	.9181	4.7744	.1684	2.2202	.1135	.0000	.0000	5.2284	.0011
0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000			
.0155	.0012	.8947	.0316	.5307	.0267	.0000	.0000	32.0027	0.0000
150.1290	11.0790	121.2359	0.0000	-0.0000	-0.0000	-0.0000			
1.1946	.0701	31.1216	1.0958	18.6797	.9397	.0000	.0000	7.4833	.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000			
.0000	.0000	.8592	.0264	.5718	.0123	.0000	.0000	31.9137	0.0000
150.0900	11.1179	121.3574	0.0000	-0.0000	-0.0000	-0.0000			
1.1946	.0701	31.1240	1.0959	18.6813	.9398	.0000	.0000	7.4702	.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000			
.0000	.0000	2.0072	.0495	3.0870	.1621	.0000	.0000	28.0589	0.0000
91.2021	5.5665	0.0000	18.1638	-0.0000	-0.0000	-0.0000			
.0036	.0002	18.8472	.4657	28.9187	1.5179	.0000	.0000	0.0006	.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000			
.0000	.0000	3.2694	.0542	9.0009	.4572	.0000	.0000	37.0926	0.0000
170.9098	13.0381	0.0000	14.4370	-0.0000	-0.0000	-0.0000			
.0000	.0000	14.8901	.2473	40.9146	2.0786	.0000	.0000	0.0000	.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000			
.0000	.0000	1.7454	.0168	10.1950	.5830	.0000	.0000	35.2239	0.0000
172.5596	13.4700	0.0000	12.3552	-0.0000	-0.0000	-0.0000			
.0000	.0000	14.9284	.2476	41.1394	2.0832	.0000	.0000	0.0000	.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000			
.0000	.0000	.8589	.0093	11.1689	.4962	.0000	.0000	64.8087	0.0000
167.3102	7.2422	0.0000	77.5872	-0.0000	-0.0000	-0.0000			
.0000	.0000	3.1125	.0339	40.8936	1.7818	.0000	.0000	0.0000	.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000			
.0000	.0000	.2583	.0018	11.6526	.4999	.0000	.0000	64.0386	0.0000
167.6963	7.4483	0.0000	76.7158	-0.0000	-0.0000	-0.0000			
.0000	.0000	3.1143	.0339	40.1764	1.7854	.0000	.0000	0.0000	.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000			
.0000	.0000	.1298	.0010	8.1521	.3481	.0000	.0000	41.1571	0.0000
94.1930	1.4421	0.0000	63.5643	-0.0000	-0.0000	-0.0000			
.0000	.0000	.6710	.0053	42.1366	1.7993	.0000	.0000	0.0000	.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000			
.0000	.0000	.0208	.0001	8.2398	.3446	.0000	.0000	41.0111	0.0000
94.3154	1.4890	0.0000	63.3951	-0.0000	-0.0000	-0.0000			
.0000	.0000	.6710	.0053	42.1495	1.7999	.0000	.0000	0.0000	.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000			
.0000	.0000	.0171	.0001	6.5581	.2773	.0000	.0000	34.5685	0.0000
72.3983	.2380	0.0000	53.8828	-0.0000	-0.0000	-0.0000			
.0000	.0000	.0789	.0005	29.8754	1.2633	.0000	.0000	0.0000	.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000			
.0000	.0000	.0016	.0000	6.5722	.2774	.0000	.0000	34.5475	0.0000
72.4159	.2448	0.0000	53.8576	-0.0000	-0.0000	-0.0000			
.0000	.0000	.0789	.0005	29.8758	1.2633	.0000	.0000	0.0000	.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000			

*****INPUT DATA*****

RATE CONSTANTS

K12	K3W	K4W	K3S	K4S	K5S	K6S	K7	K8	K10
24,802583330.00	322403.00	671000.00	671000.00	154.50	506.76	.28	1.33	.00	

ACTIVATION ENERGIES

E21	E3W	E4W	E3S	E4S	E5S	E6S	E7	E8	E10
89.	24000.	17462.	17200.	10600.	9300.	6500.	6300.	10000.	1.

CONSTANTS

A	B	C	D	E	G	H	I	J
.44	5000.00	4.27	1.55	2.00	7000.00	4.9560000.00		.36

GAS LAW CONSTANT = .90
REFERENCE TEMPERATURE = 343.30 DEG K
MASS TX. COEFF. = 20000.0
MASS TX. COEFF. (TOL) = 5000.0
CONVENSION OF HWOSO4 DECOMPOSITION REACTION = .5610
OXYGEN COEFFICIENT = .7000

PHYSICAL PROPERTIES

COMPONENT	MOL. WT.	DENSITY	HT. CAP.	REACTION	HT. OF REACTION
1	137.0	.50	33.00	1	15340.
2	137.0	.50	33.00	2	15010.
3	182.0	.46	33.00	3	15080.
4	182.0	.46	33.00	4	14920.
5	227.0	.40	33.00	5	11260.
6	227.0	.40	33.00	6	14520.
7	213.0	.40	31.00	7	237000.
8	258.0	.40	33.00	8	321000.
9	63.0	1.45	10.01	9	16300.
10	42.0	.55	33.00	10	0.
11	98.0	1.15	15.55		
12	126.0	1.15	0.00		
13	18.0	3.39	8.16		
14	80.0	1.15	14.30		

```
STAGE 1
     NITRATOR 1A                    NITRATOR 1B
     VOL. = 52.1                    VOL. = 52.1
     TEMP.= 44.0                    TEMP.= 24.0

     SEPARATOR 1
     VOL. = 20.1
     NOTCH SETTING = 1
     ENTRAINMENT
          ORGANIC IN ACID  .00071
          ACID IN ORGANIC 0.00000

STAGE 2
     NITRATOR 2
     VOL. = 48.1
     TEMP.= 48.0

     SEPARATOR 2
     VOL. = 20.1
     NOTCH SETTING = 2
     ENTRAINMENT
          ORGANIC IN ACID  .02787
          ACID IN ORGANIC  .15615

STAGE 3
     NITRATOR 3A                    NITRATOR 3B
     VOL. = 53.5                    VOL. = 52.1
     TEMP.= 76.0                    TEMP.= 78.0

     SEPARATOR 3
     VOL. = 20.1
     NOTCH SETTING = 3
     ENTRAINMENT
          ORGANIC IN ACID  .09532
          ACID IN ORGANIC  .13910

STAGE 4
     NITRATOR 4
     VOL. = 53.5
     TEMP.= 92.0

     SEPARATOR 4
     VOL. = 20.1
     NOTCH SETTING = 4
     ENTRAINMENT
          ORGANIC IN ACID  .03047
          ACID IN ORGANIC  .02421

STAGE 5
     NITRATOR 5
     VOL. = 60.2
     TEMP.=100.0

     SEPARATOR 5
     VOL. = 20.1
     NOTCH SETTING = 2
     ENTRAINMENT
          ORGANIC IN ACID  .04133
          ACID IN ORGANIC  .01950

STAGE 6
     NITRATOR 6
```

```
     VOL. = 60.2
     TEMP.=195.8

     SEPARATOR 6
     VOL. = 20.1
     NOTCH SETTING = 1
     ENTRAINMENT
          ORGANIC IN ACID  .04715
          ACID IN ORGANIC  .00477
SUM2    1        .1451       .0807       0.0000       1.0000       .9927       0.0000       .0073
PT.AT.OP.OA.FWX.FF.OT    35.7183   369.1415    66.3379   188.0040   410.0000       .0655   188.5698

SUM2    2        .3230       .0287       .1050       .9697       .0550       .0303       .1450
PT.AT.OP.OA.FWX.FF.OT    66.5759   315.9691   126.7222   201.0940   410.0000       .1655   214.1455

SUM2    3        .4301       .1054       .1516       .9783       .5457       .0217       .4343
PT.AT.OP.OA.FWX.FF.OT    58.4837   245.8498   140.2071   227.6231   410.0000       .2918   283.5696

SUM2    4        .5622       .0314       .0248       .9974       .7717       .0026       .2283
PT.AT.OP.OA.FWX.FF.OT    45.1180   328.6110   118.7546   294.7274   410.0000       .4294   319.2423

SUB2    2        .3294       .0431       .0199       .9966       .7989       .0034       .2011
PT.AT.OP.OA.FWX.FF.OT    44.6257   208.8197   110.2655   140.4270   410.0000       .1655   209.9562

SUM2    1        .1595       .0495       .0848       .9993       .7340       .0007       .2660
PT.AT.OP.OA.FWX.FF.OT    31.2185   167.9169    77.2588   151.1140   410.0000       .0655   171.5666
```

TIME OF RUN, HRS 9.0000

INTEGRATION INTERVAL, HRS .009560

TIME BETWEEN PRINTOUT, HRS 4.5000

/////PROCESS CHANGES/////

VARIABLE	VESSEL	CHANGE	TIME	INTERVAL
5	8	1000.00	1.0000	0.0000

ACID STRENGTHS, WT. PCT.

COM.	AMNT	MMNT	ADNT	MDNT	ATNT	NTNT	TNBA	TNB	HNO3	TOL	H2SO4	MHSO4	H2O,	SO3
WEAK NIT.	0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	57.00	-0.00	-0.00	-0.00	43.00	-0.00
FR.	0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	55.00	-0.00	-0.00	-0.00	45.00	-0.00
YELLOW WA.	0.00	-0.00	-0.00	-0.00	.50	-0.00	-0.00	-0.00	5.50	-0.00	10.00	-0.00	84.00	-0.00
STRONG NI.	0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	98.00	-0.00	-0.00	-0.00	2.00	-0.00
OLEUM	0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	5.23	-0.00	57.10	-0.00	-0.00	37.67

INPUT MATRIX

VESSEL	1A	1B	2	3A	3B	4	5	6
WEAK NIT.	2000.	-0.	2000.	-0.	-0.	-0.	-0.	-0.
FR.	600.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
YELLOW WA.	-0.	500.	-0.	-0.	-0.	-0.	-0.	-0.
STRONG NI.	-0.	-0.	-0.	253.	87.	475.	50.	1362.
OLEUM	-0.	-0.	-0.	-0.	-0.	-0.	-0.	10044.
TOLUENE	2089.	223.	-0.	-0.	-0.	-0.	-0.	-0.
WATER	-0.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
TEMPERATURES	44.00	24.00	68.00	76.00	78.00	92.00	100.00	105.00

*****SOLUTION AT TIME = 4.493 HOURS*****

INPUT MATRIX

VESSEL	1A	1B	2	3A	3B	4	5	6
WEAK NIT.	2000.	-0.	2000.	-0.	-0.	-0.	-0.	-0.
FR.	600.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
YELLOW HA.	-0.	500.	-0.	-0.	-0.	-0.	-0.	-0.
STRONG NI.	-0.	-0.	-0.	251.	87.	475.	50.	1362.
[illegible]	-0.	-0.	-0.	-0.	-0.	-0.	-0.	11844.
TOLUENE	2889.	223.	-0.	-0.	-0.	-0.	-0.	-0.
WATER	-0.	-0.	-0.	-0.	-0.	-0.	-0.	-0.

TEMPERATURES 44.00 24.00 60.00 76.00 78.00 92.00 100.00 105.00

NITRATOR 1A

	ANIT	MNIT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	MHOSO4	H2O	SO3	
ACID IN	.000	.000	.787	.019	.547	.033	.000	.000	46.101	0.000	180.413	7.746	140.049	0.000	
ACID OUT	.252	.018	.071	.002	.033	.002	.000	.000	18.771	0.000	180.423	7.692	163.602	0.000	
PCT CHNG	0.376	0.000	0.000	0.000	0.000	0.000	0.000	0.000	5.809	0.000	10.133	5.535	-1.901	0.000	(10.133)
ORG. IN	.097	.005	3.177	.110	2.005	.104	.360	.000	.463	21.837					
ORG. OUT	19.342	.799	5.278	.181	2.516	.134	.000	.000	4.717	.009					
PCT CHNG	-1.002	-1.798	12.077	9.292	15.402	19.790	0.000	0.000	-7.943	0.000	(19.790)				

NITRATOR 1B

	ANIT	MNIT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	MHOSO4	H2O	SO3	
ACID IN	.279	.012	.878	.003	.048	.002	.000	.000	21.907	0.000	126.441	8.920	217.196	0.000	
ACID OUT	.169	.007	.841	.001	.020	.001	.000	.000	19.435	0.000	126.431	8.871	219.662	0.000	
PCT CHNG	3.849	0.000	0.000	0.000	4.000	0.000	0.000	0.000	5.949	0.000	9.187	3.974	-2.481	0.000	(9.187)
ORG. IN	19.505	.804	5.318	.183	2.535	.135	.000	.000	4.753	2.433					
ORG. OUT	21.980	.905	5.316	.183	2.554	.136	.000	.000	4.897	.001					
PCT CHNG	-1.393	-1.403	11.336	8.638	15.238	19.525	0.000	0.000	-6.332	0.000	(19.525)				

SEPARATOR 1

	ANIT	MNIT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	MHOSO4	H2O	SO3	
ACID IN	.169	.007	.041	.001	.020	.001	.000	.000	19.435	0.000	126.431	8.871	219.662	0.000	
ACID OUT	.194	.008	.049	.002	.023	.001	.000	.000	15.447	0.000	126.416	8.853	219.485	0.000	
PCT CHNG	19.483	0.000	0.000	0.000	0.000	0.000	0.000	0.000	6.125	0.000	9.173	3.773	-2.471	0.000	(19.483)
ORG. IN	21.980	.905	5.316	.183	2.554	.136	.000	.000	4.897	.001					
ORG. OUT	21.973	.905	5.295	.182	2.554	.135	.000	.000	4.901	.000					
PCT CHNG	-1.441	-1.464	10.899	8.238	15.026	19.236	0.000	0.000	-6.269	0.000	(19.236)				

NITRATOR 2

	ANIT	MNIT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	MHOSO4	H2O	SO3	
ACID IN	.000	.000	1.663	.023	4.644	.325	.000	.000	56.526	0.000	149.777	11.490	182.456	12.167	
ACID OUT	.014	.001	1.034	.036	.647	.031	.000	.000	32.992	0.000	161.869	11.539	112.313	0.000	
PCT CHNG	0.000	0.000	15.537	0.000	21.874	0.000	0.000	0.000	3.093	0.000	7.820	4.152	-7.368	0.000	(21.874)
ORG. IN	21.954	.908	11.876	.398	14.227	.736	.000	.000	5.161	.000					
ORG. OUT	.993	.049	32.329	1.117	28.484	1.055	.000	.000	6.762	.000					
PCT CHNG	-17.715	0.000	3.871	1.984	9.232	12.230	0.000	0.000	-9.633	0.000	(17.715)				

SEPARATOR 2

	ANIT	MNIT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	MHOSO4	H2O	SO3	
ACID IN	.014	.001	1.034	.036	.647	.033	.000	.000	32.992	0.000	161.869	11.539	112.313	0.000	
ACID OUT	.059	.000	1.054	.029	.017	.049	.000	.000	32.000	0.000	161.828	11.546	112.495	0.000	
PCT CHNG	0.000	0.000	22.454	0.000	42.454	0.000	0.000	0.000	3.004	0.000	7.021	4.030	-7.303	0.000	(42.454)

ORG. IN	.983	.049	32.326	1.117	20.404	1.055	.000	.000	6.762	.000						
ORG. OUT	.981	.048	32.206	1.113	20.330	1.051	.000	.000	6.724	.000						
PCT CHNG	-17.879	0.000	3.475	1.533	4.424	11.790	0.000	0.000	-0.987	0.000	(17.879)					

SEPARATOR 3A

	AMNT	NMNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	MM03	TOL	H2SO4	HNOSO4	H20	SO3	
ACID IN	.000	.000	.242	.003	6.300	.274	.000	.000	32.546	0.000	84.983	4.260	3.756	36.053	
ACID OUT	.000	.000	2.289	.056	1.280	.173	.000	.000	29.447	0.000	98.690	6.057	0.000	23.320	
PCT CHNG	0.000	0.000	9.991	0.000	6.246	6.449	0.000	0.000	2.040	0.000	6.026	0.819	0.000	28.390	(28.390)
ORG. IN	.941	.042	28.022	.959	21.695	1.093	.000	.000	5.765	.000					
ORG. OUT	.895	.040	28.636	.928	30.599	1.009	.000	.000	8.000	.000					
PCT CHNG	0.000	0.000	9.494	11.754	5.809	6.816	0.000	0.000	0.000	0.000	(11.759)				

SEPARATOR 3B

	AMNT	NMNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	MM03	TOL	H2SO4	HNOSO4	H20	SO3	
ACID IN	.000	.000	3.132	.046	7.471	.305	.000	.000	44.953	0.000	166.252	11.568	.047	31.678	
ACID OUT	.000	.000	3.772	.047	9.257	.474	.000	.000	37.486	0.000	172.938	13.346	0.000	23.172	
PCT CHNG	0.000	0.000	15.370	0.000	2.841	4.205	0.000	0.000	1.060	0.000	1.187	2.513	0.000	60.508	(60.508)
ORG. IN	.656	.000	23.657	.574	34.007	1.991	.000	.000	0.000	.000					
ORG. OUT	.000	.000	17.123	.384	41.954	2.169	.000	.000	0.000	.000					
PCT CHNG	5.000	0.000	14.994	22.983	2.540	3.897	0.000	0.000	0.000	0.000	(22.983)				

SEPARATOR 3

	AMNT	NMNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	MM03	TOL	H2SO4	HNOSO4	H20	SO3	
ACID IN	.000	.000	3.772	.047	9.257	.476	.000	.000	37.486	0.000	172.938	13.366	0.000	23.172	
ACID OUT	.000	.000	2.323	.025	11.031	.536	.000	.000	35.538	0.000	174.648	13.843	0.000	20.959	
PCT CHNG	0.000	0.000	33.079	0.000	8.196	10.541	0.000	0.000	.068	0.000	1.222	2.771	0.000	49.636	(49.636)
ORG. IN	.828	.000	17.123	.384	41.954	2.168	.000	.000	0.000	.000					
ORG. OUT	.000	.000	16.989	.382	41.663	2.144	.000	.000	0.000	.000					
PCT CHNG	0.000	0.000	13.885	21.818	1.275	2.638	0.000	0.000	0.000	0.000	(21.818)				

SEPARATOR 4

	AMNT	NMNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	MM03	TOL	H2SO4	HNOSO4	H20	SO3	
ACID IN	.398	.000	.326	.003	14.384	.615	.000	.000	68.026	0.000	167.695	6.225	.520	89.872	
ACID OUT	.000	.000	1.152	.014	17.007	.540	.000	.000	61.119	0.000	173.476	8.222	0.000	81.442	
PCT CHNG	9.000	0.000	34.114	0.000	7.499	8.433	0.000	0.000	-5.693	0.000	3.673	13.523	0.000	4.968	(34.114)
ORG. IN	.000	.000	10.187	.177	34.594	1.696	.000	.000	0.000	.000					
ORG. OUT	.000	.000	4.841	.049	41.827	1.882	.000	.000	0.000	.000					
PCT CHNG	0.000	0.000	29.836	0.000	4.324	5.613	0.000	0.000	0.000	0.000	(29.836)				

SEPARATOR 4

	AMNT	NMNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	MM03	TOL	H2SO4	HNOSO4	H20	SO3	
ACID IN	.000	.000	1.152	.014	17.007	.540	.000	.000	61.119	0.000	173.476	8.222	0.000	81.442	
ACID OUT	.000	.000	.454	.004	19.679	.593	.000	.000	68.125	0.000	174.322	8.510	0.000	80.303	
PCT CHNG	0.000	0.000	76.472	0.000	17.305	10.607	0.000	0.000	-6.111	0.000	3.745	14.250	0.000	4.677	(76.472)
ORG. IN	.000	.000	4.841	.049	41.827	1.882	.000	.000	0.000	.000					
ORG. OUT	.000	.000	3.943	.047	40.876	1.839	.000	.000	0.000	.000					
PCT CHNG	0.000	0.000	26.625	0.000	1.741	2.994	0.000	0.000	0.000	0.000	(26.625)				

SEPARATOR 5

	AMNT	NMNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	MM03	TOL	H2SO4	HNOSO4	H20	SO3	
ACID IN	.000	.000	.018	.000	8.477	.418	.000	.000	42.812	0.000	98.631	.941	.056	70.531	
ACID OUT	.000	.000	.197	.002	8.765	.377	.000	.000	40.168	0.000	100.696	1.092	0.000	67.323	
PCT CHNG	5.000	0.000	52.895	0.000	7.427	8.251	0.000	0.000	-2.452	0.000	4.902	30.516	0.000	5.913	(52.895)

ORG. IN	.000	.000	3.142	.037	41.597	1.067	.000	.000	0.000	.000	
ORG. OUT	.000	.000	1.000	.009	44.253	1.903	.000	.000	0.000	.000	
PCT CHNG	0.000	0.000	49.041	0.000	5.024	5.737	0.000	0.000	0.000	0.000	(49.041)

SEPARATOR 5

	AMNT	MMNT	ADNT	MDNT	ATNT	MTNT	TMB	TMBA	MMB3	TBL	M2SO4	MMBSO4	M2B	SB3	
ACID IN	.000	.000	.197	.002	8.765	.377	.000	.000	40.148	0.000	100.694	1.002	0.000	67.323	
ACID OUT	.000	.000	.045	.000	9.744	.414	.000	.000	39.931	0.000	100.871	1.959	0.000	67.067	
PCT CHNG	0.000	0.000	0.000	0.000	10.250	10.729	0.000	0.000	-2.634	0.000	0.951	31.536	0.000	5.792	(31.536)
ORG. IN	.000	.000	1.000	.009	44.253	1.903	.000	.000	0.000	.000					
ORG. OUT	.000	.000	.979	.009	43.418	1.867	.000	.000	0.000	.000					
PCT CHNG	0.000	0.000	45.947	0.000	1.810	3.783	0.000	0.000	0.000	0.000	(45.947)

NITRATOR 6

	AMNT	MMNT	ADNT	MDNT	ATNT	MTNT	TMB	TMBA	MMB3	TBL	M2SO4	MMBSO4	M2B	SB3	
ACID IN	.000	.000	.001	.000	1.181	.050	.000	.000	35.606	0.000	76.252	.861	1.513	60.814	
ACID OUT	.000	.000	.038	.000	4.965	.205	.000	.000	34.758	0.000	78.462	.358	0.000	58.306	
PCT CHNG	0.000	0.000	0.000	0.000	5.095	6.241	0.000	0.000	.549	0.000	0.376	58.259	0.000	8.218	(58.259)
ORG. IN	.000	.000	.785	.007	35.001	1.539	.000	.000	0.000	.000					
ORG. OUT	.000	.000	.134	.001	34.512	1.295	.000	.000	0.000	.000					
PCT CHNG	0.000	0.000	0.000	0.000	2.131	2.405	0.000	0.000	0.000	0.000	(2.405)

SEPARATOR 6

	AMNT	MMNT	ADNT	MDNT	ATNT	MTNT	TMB	TMBA	MMB3	TBL	M2SO4	MMBSO4	M2B	SB3	
ACID IN	.000	.000	.038	.000	4.965	.205	.000	.000	34.758	0.000	78.462	.358	0.000	58.306	
ACID OUT	.000	.000	.004	.000	7.791	.338	.000	.000	34.723	0.000	78.491	.378	0.000	58.264	
PCT CHNG	0.000	0.000	0.000	0.000	10.561	10.825	0.000	0.000	.507	0.000	0.389	51.158	0.000	8.182	: 51.158)
ORG. IN	.000	.000	.134	.001	34.512	1.295	.000	.000	0.000	.000					
ORG. OUT	.000	.000	.130	.001	29.667	1.259	.000	.000	0.000	.000					
PCT CHNG	0.000	0.000	0.000	0.000	-.699	-.363	0.000	0.000	0.000	0.000	(.699)

CONVERGENCE TESTS

	ACID	ORGANIC
MAXIMUM PERCENT ERROR FROM STEADY STATE EQUATIONS	0.000	0.000
MAXIMUM PERCENT CHANGE FROM PREVIOUS ITERATION	76.672	49.041

PARAMETERS USED IN RECYCLE CALCULATIONS

STAGE	1	2	3	4	5	6
FRACTION ACID PHASE IN ORG. STREAM	0.04008	.03099	.02147	.00265	.00333	.00050
FRACTION ORG. PHASE IN ACID STREAM	.00761	.16269	.43693	.22984	.28433	.28662
FRACTION INTERNAL RECYCLE	.13065	.30873	.48495	.53992	.30029	.14767

SEPARATOR 1

ORGANIC STREAM TO NEXT STAGE

	AMNT	MMNT	ADNT	MDNT	ATNT	MTNT	TMB	TMBA	MMB3	TBL	M2SO4	MMBSO4	M2B	SB3
ACID PH.	0.000	0.000	0.006	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ORG. PH.	21.818	.898	5.256	.101	2.535	.134	.000	.000	4.864	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	0.000	35.678	35.678
MASS	0.000	5012.824	5012.824
VOLUME	0.000	66.996	66.996

EXTERNAL ACID RECYCLE

	AMNT	MMNT	ADNT	MDNT	ATNT	MTNT	TMB	TMBA	MMB3	TBL	M2SO4	MMBSO4	M2B	SB3
ACID PH.	.147	.067	.041	.002	.019	.001	.000	.000	16.768	0.000	100.898	7.626	109.225	0.000
ORG. PH.	.148	.065	.036	.001	.016	.001	.000	.000	.031	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	322.743	.229	322.972
MASS	16130.471	32.219	1414?.689

VOLUME	169.576	.431	170.006										

INTERNAL ACID RECYCLE

	AMNT	HMNT	AOMT	HOMT	ATMT	HTMT	TMB	TMBA	HMB3	TBL	H2SO4	HMBSO4	H2O	SO3
ACID PH.	.027	.001	.067	.000	.003	.000	.000	.000	2.699	0.000	17.528	1.220	30.460	0.000
ORG. PH.	.023	.001	.005	.000	.003	.000	.000	.000	.005	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	51.953	.037	51.990
MASS	2596.571	5.186	2601.757
VOLUME	27.297	.069	27.366

SEPARATOR 2

ORGANIC STREAM TO NEXT STAGE

	AMNT	HMNT	AOMT	HOMT	ATMT	HTMT	TMB	TMBA	HMB3	TBL	H2SO4	HMBSO4	H2O	SO3
ACID PH.	.000	.000	.033	.001	.025	.002	.000	.000	1.016	0.000	4.999	.357	3.475	0.000
ORG. PH.	.043	.042	27.618	.954	17.429	.981	.000	.000	5.765	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	9.987	53.541	63.448
MASS	673.622	9843.627	10517.250
VOLUME	6.536	113.594	120.132

EXTERNAL ACID RECYCLE

	AMNT	HMNT	AOMT	HOMT	ATMT	HTMT	TMB	TMBA	HMB3	TBL	H2SO4	HMBSO4	H2O	SO3
ACID PH.	.000	.000	.787	.019	.548	.033	.000	.000	22.039	0.000	108.412	7.748	75.363	0.000
ORG. PH.	.097	.005	3.177	.119	2.005	.104	.000	.000	.463	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	214.864	6.160	221.029
MASS	14489.958	1132.570	15742.124
VOLUME	141.402	13.070	154.471

INTERNAL ACID RECYCLE

	AMNT	HMNT	AOMT	HOMT	ATMT	HTMT	TMB	TMBA	HMB3	TBL	H2SO4	HMBSO4	H2O	SO3
ACID PH.	.000	.000	.316	.009	.245	.015	.000	.000	9.043	0.000	48.417	3.460	33.857	0.000
ORG. PH.	.043	.002	1.419	.040	.896	.046	.000	.000	.296	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	95.961	2.751	98.712
MASS	6524.698	505.811	7030.509
VOLUME	63.329	5.837	69.166

SEPARATOR 3

ORGANIC STREAM TO NEXT STAGE

	AMNT	HMNT	AOMT	HOMT	ATMT	HTMT	TMB	TMBA	HMB3	TBL	H2SO4	HMBSO4	H2O	SO3
ACID PH.	.000	.000	.050	.001	.237	.011	.000	.000	.763	0.000	3.750	.297	0.000	.450
ORG. PH.	.000	.000	9.566	.170	23.459	1.207	.000	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	5.558	34.403	39.961
MASS	554.583	7371.300	7925.883
VOLUME	5.173	82.360	87.534

EXTERNAL ACID RECYCLE

	AMNT	HMNT	AOMT	HOMT	ATMT	HTMT	TMB	TMBA	HMB3	TBL	H2SO4	HMBSO4	H2O	SO3
ACID PH.	.000	.000	1.348	.015	6.401	.310	.000	.000	20.618	0.000	101.383	8.034	0.000	12.163
ORG. PH.	.000	.000	4.482	.078	10.796	.556	.000	.000	5.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	150.251	15.832	166.083
MASS	14909.283	3392.205	18301.488
VOLUME	139.047	37.902	177.948

INTERNAL ACID RECYCLE

	AMNT	HMNT	AOMT	HOMT	ATMT	HTMT	TMB	TMBA	HMB3	TBL	H2SO4	HMBSO4	H2O	SO3
ACID PH.	.000	.000	.925	.018	4.393	.213	.000	.000	14.148	0.000	69.595	5.513	0.000	8.346
ORG. PH.	.000	.000	3.021	.054	7.404	.381	.000	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	103.102	10.864	113.966
MASS	10295.573	2327.727	12613.300
VOLUME	95.963	26.008	121.971

SEPARATOR 4

ORGANIC STREAM TO NEXT STAGE

	AMNT	MNT	ADNT	MDNT	ATNT	MTNT	THB	THBA	MeB3	TOL	H2SO4	MMBSO4	H2O	SO3
ACID PH.	.000	.000	.001	.000	.036	.002	.000	.000	.150	0.000	.442	.023	0.000	.213
ORG. PH.	.000	.000	3.049	.017	31.604	1.422	.000	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	.096	36.111	37.007
MASS	84.000	8058.307	8142.306
VOLUME	.815	88.497	99.312

EXTERNAL ACID RECYCLE

	AMNT	MNT	ADNT	MDNT	ATNT	MTNT	THB	THBA	MeB3	TOL	H2SO4	MMBSO4	H2O	SO3
ACID PH.	.000	.000	.289	.002	6.277	.272	.000	.000	27.589	0.000	70.999	3.985	0.000	36.048
ORG. PH.	.000	.000	.412	.005	4.286	.192	.000	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	155.090	4.874	159.965
MASS	14541.829	1047.762	15429.591
VOLUME	141.805	11.946	152.951

INTERNAL ACID RECYCLE

	AMNT	MNT	ADNT	MDNT	ATNT	MTNT	THB	THBA	MeB3	TOL	H2SO4	MMBSO4	H2O	SO3
ACID PH.	.000	.000	.246	.002	7.366	.319	.000	.000	32.377	0.000	93.871	4.583	0.000	43.242
ORG. PH.	.000	.000	.483	.004	5.006	.225	.000	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	182.005	5.720	187.726
MASS	17065.447	1276.536	18342.082
VOLUME	165.476	14.019	179.495

SEPARATOR 5

ORGANIC STREAM TO NEXT STAGE

	AMNT	MNT	ADNT	MDNT	ATNT	MTNT	THB	THBA	MeB3	TOL	H2SO4	MMBSO4	H2O	SO3
ACID PH.	.000	.000	.000	.000	.032	.001	.000	.000	.113	0.000	.336	.007	0.000	.223
ORG. PH.	.000	.000	.779	.007	36.567	1.405	.000	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	.732	36.818	37.550
MASS	67.641	8322.291	8389.932
VOLUME	.669	90.909	91.576

EXTERNAL ACID RECYCLE

	AMNT	MNT	ADNT	MDNT	ATNT	MTNT	THB	THBA	MeB3	TOL	H2SO4	MMBSO4	H2O	SO3
ACID PH.	.000	.000	.031	.000	6.784	.295	.000	.000	27.609	0.000	69.441	1.348	0.000	44.178
ORG. PH.	.000	.000	.139	.001	6.129	.263	.000	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	151.471	6.531	158.002
MASS	13993.425	1478.188	15469.613
VOLUME	139.340	16.125	155.465

INTERNAL ACID RECYCLE

	AMNT	MNT	ADNT	MDNT	ATNT	MTNT	THB	THBA	MeB3	TOL	H2SO4	MMBSO4	H2O	SO3
ACID PH.	.000	.000	.014	.000	3.004	.129	.000	.000	12.309	0.000	31.095	.604	0.000	20.674
ORG. PH.	.000	.000	.062	.001	2.744	.119	.000	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	67.426	2.924	70.751
MASS	6226.826	661.813	6927.038
VOLUME	61.946	7.221	69.167

SEPARATOR 6

ORGANIC STREAM TO NEXT STAGE

	AMNT	MNT	ADNT	MDNT	ATNT	MTNT	THB	THBA	MeB3	TOL	H2SO4	MMBSO4	H2O	SO3
ACID PH.	.000	.000	.006	.000	.005	.000	.000	.000	.020	0.000	.046	.000	0.000	.034
ORG. PH.	.000	.000	.043	.001	21.161	.[illegible]	.000	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	.104	23.152	23.256
MASS	9.653	5027.121	5036.816
VOLUME	.097	54.405	54.502

EXTERNAL ACID RECYCLE

	AMNT	MMNT	ABNT	MBNT	ATNT	MTNT	TNH	THBA	MMB3	TBL	N2SO4	MMBSO4	H2O	SO3
ACID PH.	.000	.000	.003	.000	6.638	.201	.000	.000	29.585	0.000	66.875	.385	0.000	49.643
ORG. PH.	.000	.000	.032	.009	7.248	.300	.000	.040	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	153.348	7.580	160.928
MASS	13999.983	1720.906	15720.889
VOLUME	139.429	14.772	154.201

INTERNAL ACID RECYCLE

	AMNT	MMNT	ABNT	MBNT	ATNT	MTNT	TNH	THBA	MMB3	TBL	N2SO4	MMBSO4	H2O	SO3
ACID PH.	.000	.000	.001	.000	1.148	.049	.000	.000	5.118	0.000	11.568	.055	0.000	8.587
ORG. PH.	.000	.000	.005	.004	1.254	.053	.000	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	26.526	1.313	27.838
MASS	2421.776	297.705	2719.481
VOLUME	24.119	3.247	27.366

*****SOLUTION AT TIME = 8.986 HOURS*****

INPUT MATRIX

VESSEL	1A	1B	2	3A	3B	4	5	6
HEAVY NIT.	2000.	-0.	2000.	-0.	-0.	-0.	-0.	-0.
FE.	600.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
YELLOW HA.	-0.	500.	-0.	-0.	-0.	-0.	-0.	-0.
STRONG NI.	-0.	-0.	-0.	253.	87.	475.	50.	1362.
OLEUM	-0.	-0.	-0.	-0.	-0.	-0.	-0.	11044.
TOLUENE	2009.	223.	-0.	-0.	-0.	-0.	-0.	-0.
WATER	-0.	-0.	-0.	-0.	-0.	-0.	-0.	-0.

TEMPERATURES	44.00	24.00	60.00	76.00	78.00	92.00	100.00	105.00

NITRATOR 1A

	AMMT	WMMT	ADMT	WDMT	ATMT	WTMT	TMA	TMBA	HNO3	TOL	H2SO4	HNO3SO4	H2O	SO3	
ACID IN	.000	.202	.742	.071	.953	.032	.000	.000	41.901	0.000	100.192	8.066	144.320	0.000	
ACID OUT	.278	.012	.094	.093	.038	.002	.000	.000	16.748	0.000	100.197	8.060	147.051	0.000	
PCT CHNG	18.419	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-18.700	0.000	-.209	4.782	2.723	0.000	(18.700)
ORG. IN	.095	.005	3.225	.111	2.950	.106	.000	.000	.632	21.837					
ORG. OUT	19.109	.791	5.550	.192	2.563	.136	.000	.050	4.244	.009					
PCT CHNG	-1.282	-1.079	5.291	5.729	1.484	1.678	0.000	0.000	-9.987	0.000	(9.987)				

NITRATOR 1B

	AMMT	WMMT	ADMT	WDMT	ATMT	WTMT	TMA	TMBA	HNO3	TOL	H2SO4	HNO3SO4	H2O	SO3	
ACID IN	.305	.013	.091	.003	.052	.002	.000	.000	19.557	0.000	120.194	9.355	222.315	0.000	
ACID OUT	.144	.000	.048	.002	.022	.001	.000	.000	17.100	0.000	120.199	9.349	224.693	0.000	
PCT CHNG	9.250	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-11.977	0.000	-.184	5.391	2.290	0.000	(11.977)
ORG. IN	19.273	.797	5.600	.193	2.583	.137	.000	.000	4.278	2.433					
ORG. OUT	21.735	.896	5.639	.195	2.612	.138	.000	.000	4.330	.001					
PCT CHNG	-1.142	-1.027	6.885	6.643	2.098	2.045	0.000	0.000	-11.594	0.000	(11.594)				

SEPARATOR 1

	AMMT	WMMT	ADMT	WDMT	ATMT	WTMT	TMA	TMBA	HNO3	TOL	H2SO4	HNO3SO4	H2O	SO3	
ACID IN	.144	.000	.048	.002	.022	.001	.000	.000	17.100	0.000	120.199	9.349	224.693	0.000	
ACID OUT	.196	.000	.052	.002	.024	.001	.000	.000	17.120	0.000	120.201	9.346	224.672	0.000	
PCT CHNG	1.203	0.000	0.000	0.000	9.300	0.000	0.000	0.000	-12.050	0.000	-.170	5.569	2.270	0.000	(12.050)
ORG. IN	21.735	.896	5.639	.195	2.612	.138	.000	.000	4.330	.001					
ORG. OUT	21.726	.896	5.634	.195	2.610	.139	.000	.000	4.330	.000					
PCT CHNG	-1.136	-1.015	6.486	6.783	7.213	2.222	0.000	0.000	-11.649	0.000	(11.649)				

NITRATOR 2

	AMMT	WMMT	ADMT	WDMT	ATMT	WTMT	TMA	TMBA	HNO3	TOL	H2SO4	HNO3SO4	H2O	SO3	
ACID IN	.000	.000	1.431	.020	7.237	.356	.000	.000	53.297	0.000	154.164	11.987	100.334	7.420	
ACID OUT	.016	.001	1.157	.044	.729	.039	.000	.000	29.728	0.000	161.581	11.995	118.674	0.000	
PCT CHNG	0.000	0.000	11.982	0.000	17.770	0.000	0.000	0.000	-9.996	0.000	-.227	3.950	5.664	0.000	(12.778)
ORG. IN	21.682	.891	11.485	.323	14.116	.733	.000	.000	4.579	.000					
ORG. OUT	.961	.050	32.700	1.125	28.705	1.075	.000	.000	6.429	.000					
PCT CHNG	-2.203	0.000	1.154	.787	1.046	1.950	0.000	0.000	-4.929	0.000	(4.929)				

SEPARATOR 2

	AMMT	WMMT	ADMT	WDMT	ATMT	WTMT	TMA	TMBA	HNO3	TOL	H2SO4	HNO3SO4	H2O	SO3	
ACID IN	.016	.001	1.157	.044	.729	.039	.000	.000	29.728	0.000	161.581	11.995	118.674	0.000	
ACID OUT	.000	.000	1.144	.032	.626	.044	.000	.000	29.611	0.000	161.457	12.030	118.837	0.000	
PCT CHNG	0.060	0.000	4.951	0.000	.906	0.000	0.000	0.000	-9.992	0.000	-.229	4.001	5.638	0.000	(9.992)

ORG. IN	.961	.050	32.700	1.125	28.785	1.075	.000	.000	6.429	.000					
ORG. OUT	.961	.050	32.676	1.125	28.760	1.074	.000	.000	6.406	.000					
PCT CHNG	-2.057	0.000	1.462	1.075	2.161	2.264	0.000	0.000	-4.726	0.000	(	4.726)			
NITRATOR 3A															
	AMMT	NMMT	ADMT	MDMT	ATMT	MTMT	THB	THBA	MM83	TDL	M2SO4	MNBSO4	M2B	SO3	
ACID IN	.000	.000	.272	.303	6.763	.291	.000	.000	30.572	0.000	89.800	4.536	4.372	32.654	
ACID OUT	.000	.000	2.326	.059	3.440	.101	.000	.000	27.276	0.000	101.335	6.307	0.000	18.606	
PCT CHNG	0.000	0.000	5.370	0.000	4.096	4.042	0.000	0.000	-7.375	0.000	4.795	4.123	0.000	-20.218	(20.218)
ORG. IN	.024	.043	28.429	.304	22.033	1.112	.000	.000	5.492	.000					
ORG. OUT	.000	.000	21.191	.535	31.154	1.630	.000	.000	0.000	.000					
PCT CHNG	0.000	0.000	2.252	2.441	1.415	1.764	0.000	0.000	0.000	0.000	(	2.891)			
NITRATOR 3B															
	AMMT	NMMT	ADMT	MDMT	ATMT	MTMT	THB	THBA	MM83	TDL	M2SO4	MNBSO4	M2B	SO3	
ACID IN	.000	.000	3.422	.071	8.231	.415	.000	.000	41.185	0.000	173.886	11.999	.242	23.695	
ACID OUT	.000	.000	4.084	.076	9.745	.503	.000	.000	33.779	0.000	140.629	13.794	0.000	15.157	
PCT CHNG	0.000	0.000	8.338	0.000	5.276	5.611	0.000	0.000	-9.296	0.000	4.447	3.287	0.000	-34.591	(34.591)
ORG. IN	.000	.000	24.154	.501	38.425	2.013	.000	.000	0.000	.000					
ORG. OUT	.000	.000	17.775	.321	42.338	2.148	.000	.000	0.000	.000					
PCT CHNG	0.000	0.000	3.006	5.726	.915	1.235	0.000	0.000	0.000	0.000	(	5.726)			
SEPARATOR 3															
	AMMT	NMMT	ADMT	MDMT	ATMT	MTMT	THB	THBA	MM83	TDL	M2SO4	MNBSO4	M2B	SO3	
ACID IN	.000	.000	4.084	.076	9.745	.503	.000	.000	33.779	0.000	140.629	13.794	0.000	15.157	
ACID OUT	.000	.000	2.756	.031	12.047	.586	.000	.000	31.449	0.000	162.465	14.316	0.000	12.799	
PCT CHNG	0.000	0.000	18.640	0.000	9.219	13.227	0.000	0.000	-16.834	0.000	4.444	3.417	0.000	-38.935	(38.935)
ORG. IN	.000	.000	17.775	.321	42.338	2.148	.000	.000	0.000	.000					
ORG. OUT	.000	.000	17.461	.316	41.592	2.148	.000	.000	0.000	.000					
PCT CHNG	0.000	0.000	2.778	4.496	-.179	.161	0.000	0.000	0.000	0.000	(	4.496)			
NITRATOR 4															
	AMMT	NMMT	ADMT	MDMT	ATMT	MTMT	THB	THBA	MM83	TDL	M2SO4	MNBSO4	M2B	SO3	
ACID IN	.000	.000	.272	.303	6.763	.291	.000	.000	30.572	0.000	89.800	4.536	4.372	32.654	
ACID OUT	.000	.000	1.272	.015	12.041	.595	.000	.000	57.411	0.000	182.273	8.705	0.000	72.411	
PCT CHNG	0.000	0.000	18.489	0.000	8.199	8.369	0.000	0.000	-6.047	0.000	5.071	5.040	0.000	-11.089	(11.089)
ORG. IN	.000	.000	10.592	.197	36.768	1.710	.000	.000	0.000	.000					
ORG. OUT	.000	.000	4.149	.051	42.095	1.897	.000	.000	0.000	.000					
PCT CHNG	0.000	0.000	2.447	0.000	.646	.797	0.000	0.000	0.000	0.000	(	2.447)			
SEPARATOR 4															
	AMMT	NMMT	ADMT	MDMT	ATMT	MTMT	THB	THBA	MM83	TDL	M2SO4	MNBSO4	M2B	SO3	
ACID IN	.000	.000	1.272	.015	12.041	.595	.000	.000	57.411	0.000	182.273	8.705	0.000	72.411	
ACID OUT	.062	.038	.517	.004	14.679	.038	.000	.000	56.382	0.000	183.217	9.029	0.000	71.141	
PCT CHNG	0.000	0.000	13.392	0.000	7.314	7.527	0.000	0.000	-6.350	0.000	5.103	4.095	0.000	-11.409	(13.392)
ORG. IN	.000	.000	4.149	.051	42.095	1.897	.000	.000	0.000	.000					
ORG. OUT	.000	.000	4.061	.050	41.196	1.856	.000	.000	0.000	.000					
PCT CHNG	0.000	0.000	2.978	0.000	.782	.951	0.000	0.000	0.000	0.000	(	2.978)			
NITRATOR 5															
	AMMT	NMMT	ADMT	MDMT	ATMT	MTMT	THB	THBA	MM83	TDL	M2SO4	MNBSO4	M2B	SO3	
ACID IN	.000	.000	.828	.000	9.975	.623	.000	.000	41.648	0.000	181.974	.000	.139	66.993	
ACID OUT	.000	.000	.799	.000	9.171	.583	.000	.000	39.844	0.000	184.661	1.972	0.000	63.522	
PCT CHNG	0.000	0.000	6.634	0.000	4.056	4.010	0.000	0.000	-3.240	0.000	3.741	4.795	0.000	-5.646	(6.634)

ORG. IN	.000	.000	3.249	.039	41.966	1.867	.000	.000	0.000	.000					
ORG. OUT	.000	.000	1.022	.009	44.644	1.922	.000	.000	0.000	.000					
PCT CHNG	0.000	0.000	2.288	0.000	.882	1.004	0.000	0.000	0.000	0.000	(	2.288)			

SEPARATOR 5

	ANNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	MN03	TOL	M2S04	MN0S04	M20	S03	
ACID IN	.000	.000	.209	.002	9.173	.395	.000	.000	38.844	0.000	184.461	1.972	0.000	63.522	
ACID OUT	.000	.000	.048	.000	10.184	.429	.000	.000	38.595	0.000	184.666	2.059	0.000	63.230	
PCT CHNG	0.000	0.000	0.000	0.000	3.696	3.812	0.000	0.000	-.345	0.000	3.762	5.146	0.000	-5.722	(5.722)
ORG. IN	.000	.000	1.022	.009	44.644	1.922	.000	.000	0.000	.000					
ORG. OUT	.000	.000	1.005	.009	43.877	1.889	.000	.000	0.000	.000					
PCT CHNG	0.000	0.000	2.591	0.000	1.055	1.145	0.000	0.000	0.000	0.000	(	2.591)			

NITRATOR 6

	ANNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	MN03	TOL	M2S04	MN0S04	M20	S03	
ACID IN	.000	.000	.091	.000	1.214	.051	.000	.000	34.836	0.000	76.680	.064	3.793	68.405	
ACID OUT	.000	.000	.032	.000	7.296	.318	.000	.000	33.944	0.000	81.201	.371	0.000	55.576	
PCT CHNG	0.000	0.000	0.000	0.000	5.066	5.198	0.000	0.000	-2.744	0.000	3.490	3.834	0.000	-4.681	(5.198)
ORG. IN	.000	.000	.008	.007	36.296	1.562	.000	.000	0.000	.000					
ORG. OUT	.000	.000	.134	.001	30.796	1.309	.000	.000	0.000	.000					
PCT CHNG	0.000	0.000	.375	0.000	.933	1.060	0.000	0.000	0.000	0.000	(	1.060)			

SEPARATOR 6

	ANNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	MN03	TOL	M2S04	MN0S04	M20	S03	
ACID IN	.000	.000	.032	.000	7.296	.318	.000	.000	33.944	0.000	81.201	.371	0.000	55.576	
ACID OUT	.000	.000	.004	.000	8.005	.339	.000	.000	33.901	0.000	81.235	.386	0.000	55.527	
PCT CHNG	0.000	0.000	0.000	0.000	2.748	2.880	0.000	0.000	-2.366	0.000	3.497	4.319	0.000	-4.698	(4.698)
ORG. IN	.000	.000	.134	.001	30.796	1.308	.000	.000	0.000	.000					
ORG. OUT	.000	.000	.132	.001	30.113	1.279	.000	.000	0.000	.000					
PCT CHNG	0.000	0.000	1.295	0.000	1.504	1.640	0.000	0.000	0.000	0.000	(	1.640)			

CONVERGENCE TESTS

	ACID	ORGANICS
MAXIMUM PERCENT ERROR FROM STEADY STATE EQUATIONS	0.000	0.000
MAXIMUM PERCENT CHANGE FROM PREVIOUS ITERATION	38.935	11.649

PARAMETERS USED IN RECYCLE CALCULATIONS

STAGE	1	2	3	4	5	6
FRACTION ACID PHASE IN ORG. STREAM	0.00000	.03048	.02287	.00271	.00339	.00061
FRACTION ORG. PHASE IN ACID STREAM	.00755	.14273	.42993	.22298	.20127	.28143
FRACTION INTERNAL RECYCLE	.13956	.30955	.40668	.53976	.30935	.14753

SEPARATOR 1

ORGANIC STREAM TO NEXT STAGE

	ANNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	MN03	TOL	M2S04	MN0S04	M20	S03
ACID PH.	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ORG. PH.	21.569	.889	5.591	.193	2.591	.137	.000	.000	4.297	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	0.000	35.258	35.258
MASS	0.000	5018.189	5018.189
VOLUME	0.000	66.995	66.995

EXTERNAL ACID RECYCLE

	ANNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	MN03	TOL	M2S04	MN0S04	M20	S03
ACID PH.	.169	.007	.045	.002	.020	.001	.000	.000	14.748	0.000	108.714	8.051	193.541	0.000
ORG. PH.	.141	.006	.037	.001	.017	.001	.000	.000	.028	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	325.297	.231	325.529
MASS	16118.641	32.895	16151.536

VOLUME	169.695		.439		170.134									

INTERNAL ACID RECYCLE

	AMNT	MMNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	MNOSO4	H2O	SO3
ACID PH.	.027	.001	.007	.000	.003	.000	.000	.000	2.372	0.000	17.487	1.295	31.131	0.000
ORG. PH.	.023	.001	.006	.000	.003	.000	.000	.000	.095	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	52.325	.037	52.362
MASS	2592.713	5.291	2598.004
VOLUME	27.296	.071	27.366

SEPARATOR 2

ORGANIC STREAM TO NEXT STAGE

	AMNT	MMNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	MNOSO4	H2O	SO3
ACID PH.	.000	.000	.634	.001	.025	.001	.000	.000	.914	0.000	4.986	.372	3.670	0.000
ORG. PH.	.824	.043	28..	[illegible]	17.805	.921	.000	.000	5.492	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	10.004	54.062	64.065
MASS	671.633	9989.337	10660.970
VOLUME	6.531	115.259	121.790

EXTERNAL ACID RECYCLE

	AMNT	MMNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	MNOSO4	H2O	SO3
ACID PH.	.000	.000	.742	.021	.553	.032	.000	.000	19.842	0.000	108.192	8.067	79.632	0.000
ORG. PH.	.895	.005	3.225	.111	2.050	.106	.000	.000	.632	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	217.081	6.224	223.305
MASS	14574.374	1149.963	15724.337
VOLUME	141.731	13.268	154.999

INTERNAL ACID RECYCLE

	AMNT	MMNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	MNOSO4	H2O	SO3
ACID PH.	.000	.000	.331	.009	.247	.014	.000	.000	8.854	0.000	48.279	3.600	35.535	0.000
ORG. PH.	.042	.002	1.439	.050	.915	.047	.000	.000	.282	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	96.870	2.777	99.647
MASS	6503.632	513.157	7016.789
VOLUME	63.245	5.921	69.166

SEPARATOR 3

ORGANIC STREAM TO NEXT STAGE

	AMNT	MMNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	MNOSO4	H2O	SO3
ACID PH.	.000	.000	.001	.001	.266	.013	.000	.000	.699	0.000	4.028	.316	0.000	.283
ORG. PH.	.000	.000	9.954	.180	23.710	1.224	.000	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	5.666	35.069	40.735
MASS	575.727	7504.602	8080.330
VOLUME	5.343	83.895	89.238

EXTERNAL ACID RECYCLE

	AMNT	MMNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	MNOSO4	H2O	SO3
ACID PH.	.000	.000	1.599	.018	6.991	.342	.000	.000	18.384	0.000	105.885	8.308	0.000	7.427
ORG. PH.	.000	.000	4.455	.081	10.611	.548	.000	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	148.955	15.695	164.649
MASS	15134.882	3358.561	18493.442
VOLUME	140.468	37.546	178.086

INTERNAL ACID RECYCLE

	AMNT	MMNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	MNOSO4	H2O	SO3
ACID PH.	.000	.000	1.096	.012	4.790	.234	.000	.000	12.597	0.000	72.552	5.693	0.000	5.089
ORG. PH.	.000	.000	3.052	.055	7.271	.375	.000	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	102.063	10.754	112.817
MASS	10370.335	2301.267	12671.602
VOLUME	96.242	25.726	121.969

SEPARATOR 4

ORGANIC STREAM TO NEXT STAGE

	AMNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PH.	.000	.000	.001	.000	.040	.002	.000	.000	.153	0.000	.496	.024	0.000	.193
ORG. PH.	.000	.000	3.155	.039	32.018	1.442	.009	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	.000	36.646	37.555
MASS	86.449	8174.874	8261.323
VOLUME	.836	89.791	90.624

EXTERNAL ACID RECYCLE

	AMNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PH.	.000	.000	.238	.002	6.737	.293	.000	.000	25.842	0.000	84.095	4.164	0.000	32.653
ORG. PH.	.000	.000	.417	.005	6.228	.191	.000	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	154.004	4.840	158.844
MASS	14643.199	1079.783	15722.981
VOLUME	141.189	11.859	153.048

INTERNAL ACID RECYCLE

	AMNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PH.	.000	.000	.279	.002	7.902	.343	.000	.000	30.307	0.000	98.626	4.860	0.000	38.295
ORG. PH.	.000	.000	.489	.006	6.958	.223	.000	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	180.615	5.676	186.291
MASS	17173.415	1266.266	18439.681
VOLUME	165.585	13.908	179.494

SEPARATOR 5

ORGANIC STREAM TO NEXT STAGE

	AMNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PH.	.000	.000	.000	.000	.034	.001	.000	.000	.131	0.000	.355	.007	0.000	.214
ORG. PH.	.000	.000	.002	.007	35.046	1.508	.000	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	.743	37.364	38.107
MASS	69.198	8445.131	8514.329
VOLUME	.682	92.252	92.934

EXTERNAL ACID RECYCLE

	AMNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PH.	.000	.000	.833	.030	6.955	.296	.000	.000	25.565	0.000	72.042	1.417	0.000	43.522
ORG. PH.	.000	.000	.148	.001	6.899	.263	.000	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	150.830	6.503	157.333
MASS	14845.984	1469.751	15515.634
VOLUME	133.367	16.055	154.422

INTERNAL ACID RECYCLE

	AMNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PH.	.000	.000	.015	.000	3.115	.132	.000	.000	11.899	0.000	32.268	.635	0.000	19.494
ORG. PH.	.000	.000	.063	.001	2.732	.118	.000	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	67.558	2.913	70.470
MASS	6291.246	658.311	6949.557
VOLUME	61.975	7.191	69.167

SEPARATOR 6

ORGANIC STREAM TO NEXT STAGE

	AMNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PH.	.000	.000	.000	.000	.005	.000	.000	.000	.021	0.000	.049	.000	0.000	.034
ORG. PH.	.000	.000	.895	.001	21.639	.919	.000	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	.105	22.653	22.761
MASS	9.975	5137.469	5147.446
VOLUME	.099	56.044	56.143

EXTERNAL ACID RECYCLE

	AMNT	MMNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PH.	.000	.000	.003	.000	4.820	.245	.000	.000	28.882	0.000	69.289	.329	0.000	47.307
ORG. PH.	.000	.000	.032	.000	7.224	.307	.000	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	152.839	7.563	160.402
MASS	14642.362	1715.364	15757.726
VOLUME	139.426	18.711	158.137

INTERNAL ACID RECYCLE

	AMNT	MMNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PH.	.000	.000	.001	.000	1.189	.050	.000	.000	4.990	0.000	11.977	.057	0.000	8.187
ORG. PH.	.000	.000	.005	.000	1.250	.053	.000	.000	0.000	.000				

	ACID PH.	ORG. PH.	TOTAL
MOLES	24.458	1.309	27.768
MASS	2430.102	296.852	2726.955
VOLUME	24.128	3.238	27.366

CONT	CRUDE	CWASA	CUSA	CONTSA	TTCOX	TTROX	SPENT
.20396	5209.8	.19844	22.951	19.778	0.0347	1.0725	15102.02
.20348	5208.9	.19847	22.954	19.762	0.0377	1.0728	15101.56
.20384	5208.8	.19849	22.956	19.752	0.0394	1.0730	15101.73
.20390	5209.8	.19851	22.976	19.739	0.0389	1.0731	15102.30
.20397	5209.9	.19851	22.958	19.728	0.0393	1.0732	15103.05
.20405	5209.8	.19849	21.881	19.712	0.0396	1.0732	15103.83
.20413	5208.8	.19847	21.814	19.698	0.0399	1.0733	15104.55
.20421	5208.7	.19844	21.825	19.686	0.0402	1.0734	15105.13
.20429	5209.7	.19840	21.836	19.674	0.0406	1.0735	15105.54
.20437	5209.5	.19837	21.846	19.663	0.0410	1.0736	15105.77
.20446	5209.4	.19835	21.854	19.653	0.0415	1.0737	15105.81
.20502	5196.3	.19832	21.861	19.644	0.0410	1.0736	15105.68
.20911	5134.1	.19831	21.867	19.637	0.0429	1.0740	15105.43
.21105	5042.2	.19829	21.8	19.631	0.0457	1.0747	15105.07
.22103	5055.1	.19829	21.877	19.625	0.0480	1.0754	15104.66
.22654	4952.6	.19824	21.881	19.621	0.0529	1.0764	15104.21
.23175	4918.5	.19828	21.885	19.617	0.0583	1.0776	15103.90
.23673	4894.8	.19829	21.887	19.614	0.6466	1.0791	15103.56
.24153	4878.9	.19830	21.889	19.612	0.0723	1.0809	15103.77
.24613	4868.4	.19834	21.888	19.612	0.0816	1.0831	15105.15
.25051	4861.7	.19842	21.885	19.614	0.0930	1.0858	15104.75
.25465	4857.4	.19856	21.875	19.619	0.1049	1.0890	15116.84
.25852	4854.5	.19881	21.858	19.630	0.1235	1.0929	15128.71
.26211	4852.1	.19919	21.829	19.648	0.1431	1.0975	15148.45
.26543	4849.4	.19975	21.787	19.676	0.1650	1.1028	15176.61
.26856	4846.4	.20051	21.731	19.708	0.1910	1.1087	15213.95
.27150	4843.2	.20148	21.658	19.752	0.2191	1.1153	15260.51
.27437	4839.5	.20267	21.771	19.805	0.2495	1.1226	15315.54
.27721	4835.7	.20406	21.670	19.866	0.2818	1.1308	15377.65
.28009	4832.4	.20563	21.558	19.934	0.3156	1.1379	15444.87
.28304	4830.1	.20733	21.439	20.006	0.3504	1.1466	15514.99
.28607	4829.1	.20914	21.315	20.080	0.3857	1.1542	15585.79
.28919	4829.9	.21099	21.199	20.156	0.4212	1.1625	15656.17
.29233	4832.7	.21284	21.097	20.232	0.4564	1.1708	15721.36
.29542	4837.5	.21468	21.008	20.306	0.4908	1.1788	15783.81
.29847	4844.4	.21649	21.837	20.378	0.5243	1.1866	15839.18
.30219	4853.2	.21819	21.733	20.448	0.5566	1.1941	15889.35
.30523	4863.6	.21979	21.639	20.516	0.5875	2.0016	15933.36
.30839	4875.3	.22129	21.553	20.578	0.6170	2.0082	15971.33
.31148	4888.0	.22266	21.477	20.640	0.6449	2.0148	16003.58
.31450	4901.5	.22392	21.411	20.700	0.6714	2.0210	16030.61
.31737	4915.3	.22507	21.354	20.759	0.6964	2.0268	16052.95
.31971	4929.2	.22612	21.304	20.817	0.7200	2.0323	16071.18
.32221	4943.8	.22707	21.262	20.875	0.7421	2.0375	16085.89
.32458	4956.5	.22794	21.227	20.933	0.7629	2.0423	16097.60
.32680	4969.4	.22873	21.199	20.991	0.7825	2.0469	16106.82
.32889	4981.8	.22945	21.175	21.050	0.8009	2.0512	16113.97
.33085	4993.5	.23010	21.156	21.110	0.8183	2.0553	16119.45
.33268	5004.5	.23071	21.142	21.171	0.8346	2.0591	16123.56
.33432	5014.7	.23126	21.133	21.233	0.8501	2.0627	16126.58
.33579	5024.1	.23178	21.127	21.295	0.8647	2.0661	16128.76
.33713	5032.9	.23225	21.117	21.359	0.8786	2.0693	16130.22
.33842	5040.8	.23270	21.113	21.423	0.8917	2.0724	16131.16
.34016	5048.2	.23312	21.111	21.487	0.9043	2.0753	16131.69
.34137	5054.9	.23351	21.111	21.552	0.9162	2.0781	16131.98
.34253	5059.9	.23388	21.112	21.617	0.9239	2.0799	16131.86
.34341	5059.5	.23421	21.114	21.681	0.9256	2.0803	16131.64
.34363	5057.9	.23454	21.117	21.746	0.9253	2.0803	16131.28
.34336	5054.3	.23484	21.121	21.809	0.9233	2.0799	16130.82
.34316	5049.2	.23511	21.125	21.872	0.9201	2.0790	16130.31
.34267	5043.4	.23537	21.131	21.934	0.9160	2.0781	16129.78
.34204	5036.8	.23559	21.137	21.993	0.9112	2.0770	16129.26
.34094	5029.8	.23581	21.145	22.051	0.9060	2.0759	16128.79

.34170	5053.9	.22824	21.153	22.184	8.9006	2.0745	16128.37
.34134	5054.2	.22849	21.163	22.150	8.8951	2.0732	16128.82
.34101	5054.9	.22871	21.176	22.787	8.8897	2.0719	16127.72
.34071	5055.9	.22892	21.186	22.252	8.8845	2.0707	16127.48
.34044	5057.3	.22910	21.199	22.294	8.8797	2.0694	16127.27
.34020	5059.0	.22924	21.213	22.331	8.8753	2.0686	16127.18
.33999	5061.0	.22944	21.228	22.365	8.8715	2.0677	16126.97
.33981	5063.3	.22959	21.244	22.394	8.8682	2.0669	16126.86
.33966	5065.8	.22971	21.260	22.420	8.8655	2.0663	16126.79
.33952	5068.6	.22983	21.278	22.441	8.8634	2.0658	16126.76
.33941	5071.6	.22994	21.293	22.459	8.8619	2.0655	16126.75
.33932	5074.7	.23003	21.311	22.473	8.8611	2.0653	16126.78
.33926	5077.9	.23012	21.329	22.483	8.8608	2.0652	16126.82
.33918	5081.3	.23020	21.346	22.490	8.8610	2.0652	16126.88
.33913	5084.7	.23027	21.363	22.495	8.8617	2.0654	16126.95
.33910	5088.1	.23033	21.385	22.497	8.8629	2.0657	16127.01
.33907	5091.6	.23039	21.397	22.496	8.8644	2.0660	16127.05
.33905	5095.1	.23044	21.413	22.494	8.8663	2.0665	16127.06
.33903	5098.5	.23049	21.429	22.490	8.8686	2.0670	16127.04
.33901	5101.9	.23054	21.444	22.485	8.8708	2.0675	16126.98
.33900	5105.3	.23059	21.459	22.478	8.8736	2.0681	16126.87
.33899	5108.5	.23063	21.473	22.474	8.8761	2.0688	16126.71
.33895	5111.7	.23068	21.486	22.468	8.8791	2.0694	16126.50
.33893	5114.8	.23073	21.499	22.462	8.8819	2.0701	16126.25
.33890	5117.7	.23077	21.509	22.457	8.8849	2.0708	16125.95
.33886	5120.5	.23082	21.520	22.452	8.8880	2.0715	16125.61
.33881	5123.2	.23088	21.530	22.448	8.8910	2.0722	16125.24
.33875	5125.7	.23093	21.539	22.445	8.8941	2.0730	16124.84
.33869	5128.1	.23099	21.548	22.443	8.8971	2.0737	16124.41
.33861	5130.4	.23104	21.556	22.441	8.9002	2.0744	16123.96
.33853	5132.5	.23110	21.563	22.441	8.9032	2.0751	16123.49
.33844	5134.5	.23117	21.570	22.442	8.9061	2.0758	16123.01
.33833	5136.4	.23123	21.576	22.443	8.9090	2.0764	16122.53
.33822	5138.1	.23129	21.582	22.446	8.9118	2.0771	16122.05
.33810	5139.8	.23136	21.587	22.450	8.9146	2.0778	16121.56
.33797	5141.3	.23142	21.592	22.454	8.9173	2.0784	16121.09
.33784	5142.7	.23149	21.597	22.459	8.9199	2.0790	16120.61
.33769	5144.0	.23155	21.601	22.465	8.9225	2.0796	16120.15
.33754	5145.2	.23162	21.605	22.472	8.9250	2.0802	16119.70
.33737	5146.4	.23168	21.608	22.479	8.9274	2.0807	16119.25
.33720	5147.5	.23175	21.612	22.487	8.9297	2.0813	16118.83

HEAT LOADS

1	2	3	4	5	6	7	8
1803454.6	589895.5	2060892.4	1209727.2	888842.3	975116.4	321188.9	111171.7
1803517.6	589538.1	2061070.1	1209265.8	891053.6	976403.8	321245.9	111149.3
1803731.3	589288.5	2061675.3	1209282.8	891140.1	976777.7	321354.9	111157.7
1803941.6	589247.7	2062193.1	1209148.8	891181.5	976999.7	321461.2	111181.8
1803978.6	589336.2	2062608.8	1209114.6	891264.3	977028.6	321555.1	111207.5
1803945.3	589582.5	2062979.2	1209058.3	891231.6	977126.9	321668.8	111232.1
1803932.8	589788.4	2063314.3	1209048.1	891253.6	977232.6	321722.2	111254.3
1803913.4	589926.3	2063627.9	1208980.8	891274.6	977343.4	321486.6	111275.4
1803883.3	589937.2	2063989.9	1208814.9	891296.3	977461.9	321805.6	111297.2
1803854.8	589929.3	2064177.1	1208715.9	891313.5	977547.3	321889.9	111320.8
1803[illegible].9	589844.8	2064476.6	1208616.6	891330.6	977719.6	322089.6	111347.8
1803831.8	589838.8	2064652.2	1208586.9	891346.7	977916.6	324346.3	105856.6
1803[illegible].3	589754.1	2064[illegible].2	1208[illegible]	891355.2	978044.8	349181.7	155458.2
1803[illegible].4	589647.5	2065057.4	1209144.1	891461.9	985237.8	345472.3	131744.4
1803709.8	589521.6	2065314.2	1211494.9	891254.7	992567.8	374055.8	114417.1
1803676.2	589477.8	2065551.9	1215119.5	892779.9	1008241.8	375961.8	102448.2
1803644.5	589811.2	2065757.1	1219548.8	894283.7	1389843.8	374688.9	96577.5
1803717.2	590007.2	2065939.6	1223525.9	895284.1	1009489.5	378262.8	89921.8
1803912.3	589963.8	2067219.3	1229145.6	894256.7	1011188.2	366112.3	85179.7
1803[illegible].2	589786.8	2237717.2	1227877.8	898175.2	1011673.8	342381.9	82797.7
1803[illegible].8	589534.2	2065724.8	1226143.9	898414.8	1010749.7	359167.9	81763.8
1803644.6	589159.2	2066129.8	1223448.1	892569.8	1009422.8	356422.8	80547.3
1803612.8	588922.7	2103311.7	1219698.8	892871.8	1009123.4	355276.5	80138.4
1811144.5	588699.6	2112434.6	1215477.7	892795.6	1008971.8	354499.6	80114.5
1815978.2	588293.5	2122755.9	1218498.1	892331.4	1009558.1	354449.7	80247.1
1813965.8	588[illegible].7	2131[illegible].1	1205384.6	891667.8	1010324.9	355876.7	80542.3
1[illegible].9	588588.8	2133372.8	1209145.8	893374.8	1013842.9	356321.1	81053.8
1439178.3	589498.1	2144651.7	1195164.1	888138.2	1015948.1	358111.8	81728.8
1435[illegible].8	589957.4	215[illegible].9	1196415.5	887476.8	1019384.6	360366.9	82545.6
1[illegible].6	590954.8	2154329.1	1195883.8	888582.7	1023297.2	362997.6	83578.1
1[illegible].9	592184.8	2162488.3	1181935.8	885285.9	1027547.7	365912.3	84748.2
1451114.3	593518.3	2166671.1	1174716.5	883967.5	1032824.6	369824.3	86023.9
1455473.8	594862.7	2164655.7	1174832.6	882813.8	1034631.6	372753.9	87195.6
1453365.7	594175.6	2171496.8	1171754.5	881748.8	1041257.4	375529.1	88419.6
1462774.3	597348.7	2173427.3	1168367.5	880816.2	1045439.9	378782.9	90758.2
1[illegible].9	594492.2	2175368.2	1166429.8	879958.3	1050341.1	381475.8	91682.6
1[illegible].1	594636.9	2176583.5	1164113.6	879189.7	1054731.9	385075.3	93044.1
1[illegible].8	600218.6	2177536.9	1161991.8	878596.6	1058995.8	388844.1	94395.3
1[illegible].8	600865.6	2178272.8	1160834.8	878096.8	1063848.9	390428.3	95634.1
1[illegible].2	601326.7	2178833.1	1159229.9	877354.8	1067827.6	393668.3	96803.7
1[illegible].6	601477.3	2179267.3	1156564.6	876472.9	1070797.9	396256.7	97891.3
1[illegible].3	602000.9	2179537.1	1156977.8	876665.8	1076399.9	398717.7	98897.6
1[illegible].9	602469.5	2179718.9	1153584.9	876845.9	1077832.9	401845.6	99825.6
1[illegible].1	602769.2	2179[illegible].8	1152113.7	875728.1	1081134.9	403744.6	100479.6
1[illegible].3	602927.5	2179484.5	1150414.3	875427.5	1084221.2	405328.8	101465.4
1[illegible].8	603080.5	2179725.3	1149541.5	875161.4	1087189.6	407277.9	102148.7
1[illegible].7	603813.4	2179574.8	1142416.8	874825.6	1090818.2	409124.9	102855.5
1[illegible].6	602959.9	2179355.5	1147319.9	874717.8	1092715.7	410467.6	103471.8
1[illegible].1	602863.1	2179975.3	1146275.6	874535.9	1095298.3	412512.6	104042.8
1[illegible].7	602734.9	2178739.1	1145292.3	874377.7	1097758.2	414044.6	104573.6
1[illegible].6	602585.3	2178349.2	1144343.9	874242.3	1100102.9	415535.2	105060.7
1[illegible].6	602621.7	2177913.2	1143484.3	874127.1	1102355.6	416926.7	105532.1
1[illegible].3	602258.2	2177435.2	1142662.7	874031.3	1104514.8	418268.2	105967.1
1[illegible].7	602075.2	2176929.8	1141895.2	873952.7	1106594.6	419446.8	106376.7
1[illegible].5	601988.2	2176372.3	1141154.2	873891.5	1108571.7	420449.7	106763.5
1[illegible].1	601727.6	2175641.5	1140381.8	873814.6	1112499.6	421183.9	110617.3
1[illegible].5	601555.1	2174681.7	1139688.2	872431.1	1115286.5	419672.8	115317.1
1[illegible].6	601[illegible].8	2173[illegible].2	1137[illegible].8	872696.6	1116765.1	418687.9	119427.5
1[illegible].1	601147.9	2171309.6	1136[illegible].1	872[illegible].9	1117578.2	417968.6	120805.2
1[illegible].6	601[illegible].8	2169[illegible].9	1135[illegible].8	871786.8	1114877.1	414882.2	122454.1
1[illegible].5	600[illegible].1	2167[illegible].8	1133[illegible].8	871[illegible].5	1114691.8	414484.3	123461.8
1[illegible].2	600[illegible].9	2166[illegible].6	1132[illegible].6	871148.8	1119[illegible].7	419919.9	124541.7

1893093.7	608696.2	2164419.3	1130399.8	870792.6	1119587.1	419733.4	125236.4
1893169.5	608580.7	2162636.3	1129759.9	870627.3	1120182.2	420490.6	125751.2
1893172.8	608479.8	2160830.7	1127193.8	870850.9	1120974.5	421220.1	126158.8
1893103.8	608398.2	2159813.8	1126764.6	869712.7	1122582.5	421933.8	126467.8
1892959.9	608317.8	2157203.1	1125757.3	869399.7	1124453.8	422588.3	126722.2
1892745.3	608268.8	2155521.1	1125330.5	869135.6	1125375.2	423189.2	126932.2
1892483.6	608216.4	2153892.3	1124978.3	868927.7	1125483.2	423737.8	127108.2
1892121.9	608184.4	2152033.9	1124691.8	868780.1	1126311.7	424236.3	127258.4
1891772.5	608171.5	2150685.4	1124442.3	868692.4	1126945.8	424693.8	127398.9
1891247.1	608171.5	2149044.4	1124274.1	868659.8	1127514.3	425113.4	127534.4
1890735.9	608187.9	2147734.8	1124152.1	868677.7	1127845.2	425504.4	127648.5
1890357.6	608221.5	2146567.9	1124015.4	868739.4	1128434.2	425878.7	127784.8
1890072.8	608274.8	2145531.1	1123921.6	868837.8	1128923.9	426217.8	127793.8
1889839.5	608342.3	2144648.8	1123864.4	868964.8	1130360.1	426546.7	127877.1
1889718.8	608424.8	2143944.8	1123748.	869113.4	1131143.3	426862.3	127957.2
1889564.6	608530.9	2143269.3	1123724.5	869288.1	1131913.2	427165.5	128033.7
1889436.9	608647.8	2142776.4	1123676.6	869459.3	1132645.1	427457.6	128107.8
1889333.1	608774.6	2142345.8	1123632.	869648.2	1133454.8	427734.5	128176.9
1889282.4	608911.2	2142100.1	1123591.	869837.5	1134213.2	428009.2	128243.1
1889224.8	609056.8	2141803.4	1123554.5	870031.3	1134975.4	428269.4	128305.4
1889121.5	609208.8	2141742.4	1123519.6	870226.8	1135721.1	428519.2	128363.5
1889053.8	609368.3	2141725.5	1123487.8	870419.3	1136456.5	428758.5	128417.2
1889018.9	609494.9	2141729.4	1123457.3	870618.6	1137174.2	428987.1	128466.1
1889014.7	609634.5	2141756.4	1123430.3	870749.8	1137879.8	429205.1	128510.3
1889051.1	609777.5	2141823.4	1123405.6	870945.1	1138558.1	429412.5	128549.6
1889141.8	609919.5	2141912.6	1123386.8	871168.1	1139246.7	429609.2	128584.2
1889284.1	610036.7	2142015.9	1123369.7	871349.2	1139897.3	429795.4	128614.8
1889424.4	610155.3	2142126.7	1123354.3	871525.3	1140534.7	429971.2	128639.4
1889576.7	610224.8	2142218.8	1123341.3	871696.9	1141155.5	430136.6	128660.5
1889744.1	610276.6	2142347.9	1123329.5	871872.2	1141758.6	430291.9	128677.5
1889931.8	610343.0	2142449.8	1123352.8	872052.3	1142347.9	430437.3	128688.6
1890155.7	610369.4	2142541.7	1123342.5	872218.8	1142911.2	430572.8	128788.1
1890374.1	610423.1	2142671.8	1123327.9	872377.6	1143468.7	430699.7	128784.2
1890537.2	610454.5	2142746.1	1123320.8	872541.3	1143997.3	430815.1	128789.1
1890691.2	610476.8	2142774.2	1123324.1	872717.6	1144584.8	430922.1	128789.8
1890817.4	610522.8	2142770.6	1123442.6	872878.7	1145082.8	431020.8	128786.8
1890947.5	610567.3	2142748.4	1123527.2	873033.7	1145580.4	431104.9	128788.2
1891075.4	610629.8	2142791.3	1123550.9	873194.8	1145941.3	431189.9	128791.8
1891205.2	610701.3	2142778.4	1123564.5	873357.3	1146386.8	431260.2	128788.8
1891291.3	610794.7	2142750.5	1123564.6	873518.8	1146811.1	431323.8	128467.4
1891413.9	610831.5	2142704.6	1123730.5	873679.5	1147228.5	431377.4	128651.6
1891e242.1	610868.4	2142653.6	1123803.2	873838.6	1147613.8	431423.5	128633.5

ACTUAL NITRIC

1	2	3	4	5	6
6.5523	9.8476	10.1739	14.6319	15.1218	15.9087
6.5463	9.8479	10.1752	14.6322	15.1214	15.9087
6.5371	9.8528	10.1768	14.6322	15.1217	15.9097
6.5262	9.8491	10.1762	14.6320	15.1215	15.9087
6.5153	9.8389	10.1757	14.6317	15.1213	15.9097
6.5143	9.8272	10.1749	14.6313	15.1218	15.9626
6.5046	9.8196	10.1735	14.6309	15.1207	15.9446
6.4956	9.8184	10.1723	14.6304	15.1206	15.9885
6.4779	9.8055	10.1704	14.6298	15.1201	15.9446
6.4711	9.8004	10.1693	14.6292	15.1197	15.9883
6.4651	9.7962	10.1679	14.6285	15.1193	15.9442
6.4594	9.7921	10.1663	14.6277	15.1186	15.9539
6.4552	9.7943	10.1648	14.6267	15.1108	15.9224
6.4519	9.7868	10.1633	14.6237	15.0428	15.6777
6.4472	9.7815	10.1621	14.6162	15.0133	15.5515
6.4413	9.7724	10.1613	14.6031	14.9695	15.4108
6.4424	9.7748	10.1623	14.5461	14.8978	15.1786
6.4348	9.7740	10.1658	14.5187	14.8263	15.3991
6.4356	9.7738	10.1733	14.5158	14.7538	15.2614
6.4337	9.7735	10.1463	14.6749	14.6846	15.2262
6.4336	9.7756	10.1391	14.6329	14.6257	15.1349
6.4183	9.7417	10.2167	14.3479	14.5718	15.1716
6.4347	9.7699	10.2357	14.3435	14.5224	15.1524
6.4371	9.8309	10.2565	14.2996	14.4796	15.1375
6.4439	9.8162	10.2719	14.2567	14.4416	15.1258
6.4515	9.8291	10.2647	14.2164	14.4077	15.1165
6.4628	9.8453	10.2449	14.1739	14.3777	15.1057
6.4778	9.8415	10.2356	14.1339	14.3587	15.0992
6.4935	9.8771	10.4849	14.0945	14.3264	15.0916
6.5113	9.8912	10.3841	14.0559	14.3035	15.0857
6.5315	9.9035	10.3635	14.0176	14.2424	15.0804
6.5514	9.9136	10.2954	13.9795	14.2624	15.0754
6.5714	9.9236	10.2734	13.9419	14.2433	15.0707
6.5913	9.9291	10.2495	13.9044	14.2249	15.0661
6.6103	9.9267	10.2526	13.8675	14.2069	15.0615
6.6256	9.9255	10.2331	13.8389	14.1933	15.0571
6.6376	9.9215	10.2119	13.7949	14.1721	15.0527
6.6501	9.9158	10.1991	13.7595	14.1554	15.0493
6.6625	9.9062	10.1901	13.7267	14.1344	15.0448
6.6747	9.8992	10.1607	13.6987	14.1227	15.0397
6.6863	9.8926	10.1145	13.6575	14.1071	15.0354
6.6977	9.8870	10.0443	13.6251	14.0916	15.0312
6.7084	9.8828	10.0018	13.5937	14.0779	15.0271
6.7185	9.8756	14.8351	13.5633	14.0427	15.0232
6.7279	9.8192	10.0045	13.5339	14.0409	15.0193
6.7365	9.7999	9.9421	13.5055	14.0357	15.0156
6.7443	9.7795	9.9559	13.4742	14.0239	15.0121
6.7513	9.7492	9.9102	13.4528	14.0108	15.0087
6.7577	9.7497	9.9369	13.4249	13.9992	15.0054
6.7637	9.7212	9.8952	13.4027	13.9442	15.0024
6.7693	9.7013	9.8568	13.3794	13.9776	14.9995
6.7743	9.6928	9.8325	13.3575	13.9477	14.9967
6.7787	9.6661	9.8091	13.3364	13.9582	14.9941
6.7829	9.6457	9.7876	13.3162	13.9492	14.9916
6.7865	9.6279	9.7643	13.2978	13.9487	14.9893
6.7898	9.6195	9.7434	13.2798	13.9312	14.9872
6.7927	9.5979	9.7156	13.2613	13.9162	14.9852
6.7954	9.5763	9.6939	13.2461	13.8967	14.9834
6.7977	9.5568	9.6505	13.2348	13.8852	14.9819
6.7998	9.5371	9.6265	13.2[illegible]	13.[illegible]	14.9805
6.8017	9.5263	9.6021	13.[illegible]	13.[illegible]	14.9793
6.8034	9.4967	9.5781	13.[illegible]	13.[illegible]	14.9784

SPECIFIC GRAVITY

1	2	3	4	5	6
1.19313	1.39424	1.43728	1.46117	1.46784	1.46837
1.19311	1.39422	1.43727	1.46117	1.46784	1.46837
1.19307	1.39421	1.43726	1.46116	1.46784	1.46837
1.19303	1.39419	1.43725	1.46116	1.46784	1.46837
1.19299	1.39418	1.43725	1.46116	1.46784	1.46837
1.19295	1.39417	1.43724	1.46115	1.46784	1.46837
1.19290	1.39416	1.43723	1.46115	1.46784	1.46837
1.19286	1.39416	1.43722	1.46115	1.46784	1.46837
1.19283	1.39415	1.43722	1.46114	1.46784	1.46837
1.19279	1.39414	1.43721	1.46114	1.46784	1.46837
1.19276	1.39414	1.43720	1.46114	1.46784	1.46837
1.19273	1.39413	1.43719	1.46114	1.46784	1.46837
1.19271	1.39413	1.43719	1.46113	1.46784	1.46936
1.19268	1.39412	1.43718	1.46113	1.46783	1.46934
1.19266	1.39412	1.43717	1.46112	1.46782	1.46935
1.19265	1.39411	1.43716	1.46111	1.46781	1.46934
1.19263	1.39412	1.43716	1.46109	1.46779	1.46933
1.19262	1.39413	1.43714	1.46107	1.46776	1.46932
1.19261	1.39416	1.43713	1.46104	1.46774	1.46932
1.19260	1.39421	1.43710	1.46100	1.46771	1.46931
1.19261	1.39438	1.43704	1.46096	1.46769	1.46930
1.19263	1.39461	1.43700	1.46091	1.46766	1.46930
1.19268	1.39466	1.43693	1.46085	1.46764	1.46929
1.19276	1.39473	1.43695	1.46898	1.46762	1.46928
1.19288	1.39491	1.43675	1.46874	1.46760	1.46928
1.19305	1.39710	1.43665	1.46867	1.46757	1.46927
1.19326	1.39728	1.43656	1.46861	1.46755	1.46927
1.19351	1.39746	1.43643	1.46856	1.46753	1.46927
1.19381	1.39763	1.43631	1.46847	1.46751	1.46926
1.19416	1.39778	1.43620	1.46839	1.46749	1.46926
1.19450	1.39791	1.43608	1.46832	1.46746	1.46925
1.19484	1.39803	1.43596	1.46825	1.46744	1.46925
1.19526	1.39813	1.43585	1.46818	1.46742	1.46924
1.19548	1.39822	1.43574	1.46811	1.46739	1.46924
1.19595	1.39838	1.43563	1.46804	1.46737	1.46923
1.19629	1.39836	1.43553	1.46997	1.46735	1.46923
1.19668	1.39842	1.43543	1.46991	1.46732	1.46922
1.19699	1.39847	1.43533	1.46985	1.46730	1.46922
1.19715	1.39851	1.43529	1.46979	1.46728	1.46921
1.19738	1.39854	1.43515	1.46973	1.46726	1.46921
1.19748	1.39857	1.43506	1.46968	1.46724	1.46921
1.19779	1.39860	1.43497	1.46963	1.46723	1.46920
1.19797	1.39862	1.43490	1.46958	1.46721	1.46920
1.19813	1.39864	1.43482	1.46953	1.46719	1.46919
1.19827	1.39866	1.43474	1.46949	1.46718	1.46919
1.19841	1.39867	1.43467	1.46945	1.46716	1.46919
1.19856	1.39868	1.43461	1.46941	1.46715	1.46918
1.19866	1.39869	1.43456	1.46939	1.46714	1.46918
1.19877	1.39870	1.43448	1.46934	1.46713	1.46918
1.19888	1.39871	1.43442	1.46931	1.46711	1.46918
1.19899	1.39872	1.43437	1.46928	1.46710	1.46917
1.19909	1.39872	1.43431	1.46925	1.46709	1.46917
1.19920	1.39873	1.43426	1.46922	1.46708	1.46917
1.19930	1.39874	1.43421	1.46920	1.46708	1.46917
1.19940	1.39874	1.43417	1.46918	1.46707	1.46916
1.19950	1.39875	1.43412	1.46915	1.46706	1.46916
1.19958	1.39875	1.43408	1.46913	1.46705	1.46916
1.19969	1.39876	1.43404	1.46912	1.46705	1.46916
1.19979	1.39876	1.43401	1.46910	1.46705	1.46916
1.19988	1.39877	1.43397	1.46909	1.46704	1.46916
1.19996	1.39878	1.43394	1.46908	1.46704	1.46916
1.20007	1.39879	1.43391	1.46908	1.46704	1.46916

6.3754	9.4509	9.5138	13.0121	13.7219	14.7025		1.20816	1.38879	1.43389	1.45987	1.46784	1.46916
6.3566	9.4364	9.4795	12.9744	13.6912	14.6899		1.20826	1.38880	1.43387	1.45987	1.46785	1.46916
6.3372	9.4895	9.4449	12.9375	13.6642	14.6796		1.20831	1.38881	1.43384	1.45986	1.46785	1.46916
6.3175	9.3921	9.4101	12.9022	13.6408	14.6707		1.20839	1.38882	1.43383	1.45986	1.46785	1.46917
6.2975	9.3552	9.3754	12.8648	13.6208	14.6648		1.20845	1.38882	1.43381	1.45986	1.46785	1.46917
6.2772	9.3208	9.3408	12.8377	13.6039	14.6603		1.20851	1.38883	1.43379	1.45986	1.46785	1.46917
6.2566	9.3035	9.3054	12.8031	13.5898	14.6566		1.20856	1.38884	1.43378	1.45986	1.46785	1.46917
6.2362	9.2729	9.2731	12.7829	13.5798	14.6543		1.20860	1.38885	1.43377	1.45986	1.46785	1.46917
6.2156	9.2451	9.2484	12.7592	13.5681	14.6523		1.20864	1.38886	1.43376	1.45986	1.46785	1.46917
6.1950	9.2175	9.2093	12.7379	13.5488	14.6507		1.20867	1.38886	1.43374	1.45985	1.46785	1.46917
6.1744	9.1982	9.1794	12.7186	13.5532	14.6495		1.20869	1.38887	1.43373	1.45985	1.46785	1.46917
6.1540	9.1636	9.1511	12.7013	13.5475	14.6485		1.20871	1.38887	1.43372	1.45985	1.46785	1.46917
6.1337	9.1372	9.1263	12.6859	13.5428	14.6478		1.20872	1.38888	1.43372	1.45985	1.46785	1.46917
6.1139	9.1117	9.0992	12.6729	13.5399	14.6472		1.20872	1.38888	1.43371	1.45985	1.46785	1.46917
6.0942	9.0871	9.0757	12.6595	13.5356	14.6466		1.20872	1.38889	1.43370	1.45985	1.46785	1.46917
6.0751	9.0636	9.0538	12.6483	13.5325	14.6462		1.20872	1.38889	1.43369	1.45985	1.46785	1.46917
6.0565	9.0408	9.0334	12.6381	13.5299	14.6458		1.20870	1.38890	1.43368	1.45985	1.46785	1.46917
6.0385	9.0191	9.0144	12.6299	13.5277	14.6456		1.20869	1.38890	1.43367	1.45985	1.46785	1.46917
6.0213	8.9986	8.9970	12.6228	13.5257	14.6451		1.20867	1.38890	1.43367	1.45984	1.46785	1.46917
6.0049	8.9798	8.9804	12.6127	13.5238	14.6448		1.20865	1.38890	1.43366	1.45984	1.46785	1.46917
5.9891	8.9605	8.9657	12.6055	13.5222	14.6445		1.20862	1.38890	1.43365	1.45984	1.46785	1.46917
5.9727	8.9438	8.9517	12.5999	13.5205	14.6442		1.20860	1.38890	1.43364	1.45984	1.46785	1.46917
5.9568	8.9254	8.9367	12.5927	13.5192	14.6439		1.20858	1.38890	1.43363	1.45984	1.46785	1.46917
5.9439	8.9109	8.9245	12.5869	13.5178	14.6436		1.20855	1.38890	1.43363	1.45984	1.46785	1.46917
5.9305	8.8968	8.9151	12.5816	13.5165	14.6434		1.20853	1.38890	1.43362	1.45984	1.46785	1.46917
5.9177	8.8821	8.9044	12.5763	13.5153	14.6431		1.20850	1.38890	1.43361	1.45983	1.46785	1.46917
5.9056	8.8678	8.8944	12.5716	13.5142	14.6429		1.20848	1.38890	1.43360	1.45983	1.46785	1.46917
5.8940	8.8547	8.8858	12.5668	13.5131	14.6427		1.20846	1.38891	1.43360	1.45983	1.46785	1.46917
5.8831	8.8458	8.8761	12.5626	13.5121	14.6425		1.20844	1.38891	1.43359	1.45983	1.46785	1.46917
5.8726	8.8341	8.8675	12.5582	13.5111	14.6423		1.20842	1.38891	1.43358	1.45983	1.46785	1.46917
5.8627	8.8237	8.8587	12.5542	13.5102	14.6421		1.20841	1.38891	1.43358	1.45983	1.46785	1.46917
5.8532	8.8148	8.8521	12.5504	13.5093	14.6419		1.20839	1.38891	1.43357	1.45983	1.46785	1.46917
5.8443	8.8048	8.8448	12.5468	13.5085	14.6418		1.20838	1.38891	1.43357	1.45983	1.46785	1.46917
5.8357	8.7951	8.8379	12.5433	13.5077	14.6416		1.20838	1.38891	1.43356	1.45983	1.46785	1.46917
5.8275	8.7870	8.8313	12.5400	13.5070	14.6415		1.20837	1.38891	1.43355	1.45983	1.46785	1.46917
5.8197	8.7892	8.8250	12.5369	13.5064	14.6414		1.20837	1.38891	1.43355	1.45983	1.46785	1.46917
5.8121	8.7730	8.8190	12.5339	13.5057	14.6413		1.20837	1.38891	1.43355	1.45983	1.46785	1.46917
5.8052	8.7661	8.8133	12.5309	13.5052	14.6412		1.20837	1.38892	1.43354	1.45983	1.46785	1.46917
5.7985	8.7595	8.8077	12.5282	13.5047	14.6411		1.20837	1.38892	1.43354	1.45983	1.46785	1.46917
5.7928	8.7535	8.8024	12.5256	13.5042	14.6411		1.20837	1.38892	1.43354	1.45983	1.46784	1.46917
5.7869	8.7478	8.7973	12.5231	13.5038	14.6411		1.20836	1.38892	1.43353	1.45983	1.46785	1.46917
5.7960	8.7423	8.7925	12.5208	13.5035	14.6410		1.20839	1.38892	1.43353	1.45983	1.46785	1.46917

NITRIC/SULFURIC RATIO IN EXTERNAL ACID RECYCLE FROM EACH SEPARATOR

1	2	3	4	5	6
.15837	.21232	.19852	.24178	.26004	.27359
.15823	.21198	.19855	.24171	.26004	.27359
.15[illegible]0	.21156	.19854	.24171	.26004	.27359
.15774	.21132	.19854	.24170	.26004	.27359
.15768	.21111	.19855	.24170	.26003	.27359
.15772	.21094	.19854	.24169	.26003	.27359
.15800	.21079	.19851	.24169	.26002	.27359
.15674	.21066	.19849	.24168	.26002	.27359
.15644	.21054	.19846	.24167	.26001	.27359
.15[illegible]6	.21043	.19843	.24166	.26000	.27359
.15630	.21033	.19840	.24166	.26000	.27359
.15619	.21024	.19838	.24165	.25998	.27358
.15607	.21015	.19833	.24165	.25998	.27359
.15597	.21007	.19838	.24164	.25972	.26723
.15588	.20999	.19828	.24135	.25928	.26466
.15578	.20992	.19826	.24182	.25697	.26760
.15573	.20986	.19824	.24068	.25538	.26100
.15564	.20979	.19819	.25077	.25395	.25977
.15548	.20973	.19818	.25491	.25239	.25841
.15555	.20967	.19791	.25255	.25183	.25787
.15551	.20961	.19849	.25436	.24980	.25760
.15548	.20957	.19848	.25592	.24878	.25706
.15547	.20953	.19818	.24498	.24773	.25648
.15569	.20951	.19838	.25392	.24689	.25638
.15551	.20948	.19845	.25297	.24615	.25614
.15541	.20953	.19855	.25206	.24558	.25595
.15572	.20955	.19858	.25119	.24692	.25578
.15547	.20957	.19857	.25034	.24642	.25565
.15536	.20959	.19847	.24956	.24596	.25553
.15523	.20959	.19832	.24879	.24555	.25542
.15542	.20958	.19838	.24804	.24516	.25533
.15542	.20956	.19883	.24731	.24481	.25526
.15481	.20947	.19851	.24659	.24447	.25516
.15604	.20936	.19815	.24598	.24415	.25508
.15713	.20923	.19875	.24521	.24383	.25498
.15725	.20905	.19893	.24455	.24353	.25493
.15733	.20894	.19898	.24389	.24324	.25485
.15737	.20848	.19841	.24324	.24295	.25479
.15737	.20833	.19793	.24263	.24267	.25478
.15733	.20882	.19766	.24203	.24240	.25463
.15725	.20778	.19696	.24144	.24214	.25456
.15712	.20735	.19644	.24087	.23988	.25449
.15695	.20678	.19593	.24032	.23963	.25442
.15674	.20659	.19563	.23979	.23939	.25434
.15649	.20628	.19496	.23924	.23916	.25429
.15622	.20598	.19445	.23878	.23894	.25423
.15591	.20539	.19397	.23831	.23873	.25417
.15558	.20498	.19369	.23785	.23852	.25411
.15523	.20457	.19383	.23741	.23833	.25405
.15486	.20417	.19258	.23700	.23815	.25401
.15448	.20377	.19214	.23660	.23797	.25396
.15409	.20338	.19171	.23622	.23781	.25392
.15369	.20299	.19138	.23585	.23765	.25387
.15327	.20262	.19098	.23551	.23750	.25383
.15[illegible]6	.20225	.19061	.23517	.23736	.25379
.15[illegible]5	.20189	.19011	.23482	.23721	.25352
.15485	.20155	.17949	.23482	.23498	.25262
.15185	.20117	.17981	.23337	.23468	.25166
.15125	.20076	.17948	.23275	.23404	.25082
.15045	.20031	.17779	.23213	.23547	.25015
.15044	.19964	.17715	.23149	.23484	.24963
.15003	.19934	.17652	.23043	.23421	.24923

.14961	.19083	.17509	.23015	.23363	.26893
.14917	.19030	.17525	.22968	.23310	.26878
.14873	.18976	.17461	.22903	.23264	.26852
.14828	.18922	.17396	.22819	.23224	.26839
.14782	.18866	.17332	.22760	.23189	.26829
.14735	.18809	.17267	.22704	.23160	.26821
.14688	.18751	.17203	.22652	.23136	.26815
.14641	.18692	.17140	.22605	.23115	.26811
.14594	.18633	.17079	.22563	.23098	.26807
.14546	.18575	.17020	.22526	.23084	.26805
.14499	.18516	.16963	.22489	.23072	.26803
.14452	.18457	.16910	.22458	.23063	.26801
.14405	.18398	.16859	.22430	.23056	.26800
.14359	.18340	.16811	.22405	.23047	.26799
.14313	.18285	.16766	.22383	.23042	.26798
.14269	.18234	.16725	.22362	.23037	.26797
.14225	.18184	.16684	.22344	.23032	.26796
.14183	.18137	.16648	.22327	.23028	.26796
.14142	.18093	.16616	.22312	.23025	.26795
.14103	.18052	.16585	.22298	.23022	.26795
.14065	.18012	.16557	.22285	.23019	.26794
.14029	.17974	.16530	.22274	.23016	.26794
.13994	.17935	.16505	.22263	.23014	.26793
.13960	.17897	.16482	.22252	.23012	.26793
.13929	.17859	.16460	.22243	.23009	.26792
.13898	.17822	.16440	.22233	.23007	.26792
.13870	.17786	.16420	.22225	.23005	.26791
.13842	.17752	.16403	.22217	.23004	.26791
.13816	.17717	.16386	.22209	.23002	.26791
.13791	.17683	.16370	.22202	.23000	.26790
.13764	.17650	.16354	.22195	.22998	.26790
.13745	.17619	.16340	.22188	.22997	.26790
.13724	.17589	.16326	.22182	.22996	.26790
.13703	.17560	.16313	.22176	.22995	.26789
.13686	.17533	.16301	.22170	.22994	.26789
.13666	.17506	.16289	.22164	.22993	.26789
.13648	.17480	.16278	.22159	.22992	.26789
.13631	.17456	.16267	.22154	.22991	.26789
.13615	.17432	.16257	.22149	.22990	.26789
.13600	.17409	.16247	.22145	.22989	.26789
.13585	.17386	.16237	.22141	.22988	.26789
.13571	.17365	.16229	.22137	.22988	.26788

NITRIC/SULPHURIC RATIO IN EACH NITRATOR

1	2	3	4	5	6	7	8
.17976	.15832	.21255	.26396	.20816	.26463	.26889	.27374
.17933	.15811	.21216	.26396	.20819	.26463	.26889	.27374
.17894	.15765	.21184	.26393	.20820	.26463	.26888	.27374
.17868	.15757	.21164	.26390	.20819	.26463	.26888	.27374
.17863	.15731	.21151	.26387	.20817	.26462	.26888	.27374
.17823	.15704	.21136	.26383	.20815	.26462	.26887	.27374
.17866	.15685	.21122	.26380	.20813	.26461	.26887	.27374
.17792	.15666	.21110	.26376	.20810	.26460	.26886	.27374
.17780	.15649	.21099	.26373	.20807	.26459	.26886	.27374
.17769	.15635	.21088	.26370	.20804	.26458	.26885	.27374
.17759	.15622	.21079	.26367	.20801	.26457	.26884	.27374
.17751	.15611	.21070	.26364	.19998	.26455	.26881	.27102
.17743	.15600	.21061	.26361	.19995	.26452	.26834	.26728
.17735	.15591	.21054	.26358	.19993	.26462	.25962	.26455
.17728	.15583	.21047	.26352	.19990	.26417	.25810	.26251
.17722	.15575	.21040	.26342	.19989	.26373	.25659	.26097
.17715	.15569	.21034	.26326	.19988	.26311	.25585	.25979
.17711	.15562	.21028	.26303	.19985	.26233	.25357	.25889
.17707	.15557	.21023	.26274	.20004	.26163	.25210	.25818
.17706	.15552	.21020	.26239	.20018	.26066	.25095	.25763
.17703	.15549	.21017	.26197	.20036	.25945	.24996	.25720
.17704	.15547	.21014	.26151	.20052	.25845	.24867	.25685
.17699	.15549	.21017	.26102	.20049	.25787	.24782	.25657
.17715	.15552	.21019	.26049	.20046	.25763	.24727	.25634
.17726	.15559	.21023	.25996	.20034	.25762	.24642	.25615
.17737	.15570	.21027	.25937	.20018	.25776	.24485	.25599
.17751	.15583	.21031	.25878	.20006	.25795	.24555	.25586
.17766	.15600	.21035	.25819	.20000	.25816	.24510	.25576
.17781	.15619	.21037	.25753	.20016	.25761	.24669	.25566
.17796	.15639	.21037	.25699	.20055	.25149	.24432	.25555
.17810	.15659	.21034	.25639	.20030	.25087	.24397	.25547
.17813	.15678	.21024	.25578	.20048	.25029	.24345	.25539
.17826	.15696	.21019	.25518	.19947	.24941	.24333	.25532
.17838	.15712	.21004	.25458	.19934	.24845	.24303	.25526
.17830	.15725	.20998	.25399	.19976	.24831	.24274	.25517
.17826	.15734	.20971	.25358	.19958	.24768	.24266	.25510
.17818	.15748	.20947	.25282	.19896	.24706	.24219	.25503
.17806	.15761	.20921	.25225	.19758	.24646	.24192	.25496
.17794	.15738	.20892	.25168	.19712	.24587	.24165	.25488
.17784	.15730	.20869	.25117	.19666	.24538	.24149	.25482
.17776	.15719	.20825	.25058	.19617	.24475	.24115	.25475
.17716	.15783	.20749	.25006	.19569	.24421	.24091	.25469
.17695	.15803	.20751	.24957	.19521	.24369	.24068	.25462
.17651	.15659	.20712	.24901	.19473	.24319	.24046	.25456
.17615	.15632	.20672	.24851	.19427	.24271	.24026	.25450
.17577	.15603	.20631	.24803	.19380	.24225	.24006	.25444
.17536	.15570	.20590	.24756	.19335	.24180	.23986	.25438
.17495	.15535	.20549	.24710	.19290	.24137	.23965	.25433
.17453	.15499	.20509	.24667	.19247	.24096	.23947	.25428
.17409	.15461	.20469	.24624	.19204	.24057	.23930	.25424
.17366	.15421	.20429	.24584	.19163	.24019	.23914	.25419
.17322	.15381	.20391	.24546	.19123	.23984	.23898	.25415
.17279	.15341	.20353	.24507	.19085	.23949	.23886	.25411
.17236	.15300	.20316	.24470	.19047	.23917	.23870	.25407
.17193	.15259	.20281	.24436	.19011	.23886	.23857	.25404
.17152	.15218	.20247	.24379	.18967	.23926	.23940	.25314
.17111	.15178	.20218	.24304	.18912	.23758	.23904	.25195
.17078	.15139	.20178	.24239	.18856	.23696	.23750	.25105
.17024	.15098	.20126	.24173	.18796	.23634	.23698	.25037
.16985	.15058	.20079	.24109	.18733	.23575	.23633	.24986
.16948	.15017	.20038	.24045	.18672	.23511	.23569	.24947
.16896	.14975	.19979	.23981	.18611	.23445	.23509	.24918

.16847	.14932	.19927	.23916	.18550	.23379	.23495	.24895
.16799	.14888	.19873	.23851	.18488	.23313	.23407	.24879
.16758	.14843	.19818	.23784	.19426	.23250	.23366	.24866
.16701	.14797	.19762	.23718	.18363	.23189	.23331	.24854
.16652	.14751	.19705	.23653	.18309	.23132	.23301	.24849
.16602	.14704	.19648	.23590	.18237	.23079	.23275	.24843
.16552	.14657	.19589	.23530	.18175	.23038	.23256	.24839
.16502	.14609	.19530	.23472	.18115	.22986	.23237	.24835
.16452	.14562	.19471	.23418	.18057	.22946	.23222	.24833
.16403	.14514	.19412	.23367	.18001	.22910	.23210	.24831
.16354	.14467	.19354	.23319	.17947	.22877	.23200	.24829
.16305	.14420	.19297	.23275	.17897	.22848	.23192	.24828
.16258	.14373	.19242	.23235	.17849	.22822	.23185	.24827
.16212	.14328	.19190	.23197	.17805	.22799	.23179	.24826
.16167	.14283	.19136	.23163	.17763	.22778	.23174	.24825
.16123	.14239	.19086	.23131	.17724	.22759	.23169	.24825
.16082	.14196	.19038	.23101	.17690	.22742	.23165	.24826
.16041	.14155	.18992	.23076	.17654	.22726	.23162	.24826
.16003	.14115	.18949	.23049	.17623	.22712	.23159	.24823
.15966	.14076	.18907	.23026	.17594	.22699	.23156	.24822
.15931	.14040	.18868	.23004	.17567	.22687	.23153	.24822
.15894	.14004	.18831	.22984	.17542	.22675	.23151	.24822
.15866	.13971	.18797	.22965	.17519	.22665	.23149	.24821
.15835	.13939	.18766	.22947	.17497	.22655	.23147	.24821
.15807	.13908	.18733	.22930	.17477	.22646	.23145	.24820
.15779	.13878	.18703	.22914	.17458	.22637	.23143	.24820
.15753	.13850	.18676	.22899	.17448	.22629	.23141	.24820
.15729	.13824	.18650	.22885	.17423	.22621	.23139	.24819
.15705	.13799	.18625	.22872	.17407	.22614	.23139	.24819
.15683	.13775	.18602	.22859	.17392	.22607	.23136	.24819
.15662	.13752	.18581	.22847	.17377	.22600	.23135	.24819
.15641	.13730	.18560	.22835	.17364	.22594	.23133	.24818
.15622	.13709	.18541	.22824	.17351	.22587	.23132	.24818
.15604	.13690	.18523	.22814	.17338	.22582	.23131	.24818
.15586	.13671	.18506	.22803	.17327	.22576	.23130	.24817
.15569	.13653	.18490	.22794	.17315	.22571	.23129	.24817
.15553	.13635	.18475	.22785	.17304	.22566	.23128	.24817
.15539	.13620	.18461	.22776	.17294	.22561	.23127	.24817
.15524	.13604	.18447	.22767	.17284	.22556	.23126	.24817
.15510	.13589	.18435	.22759	.17275	.22552	.23125	.24817
.15497	.13575	.18423	.22752	.17266	.22548	.23125	.24817
.15484	.13562	.18412	.22746	.17257	.22544	.23124	.24817

A-NITRATION IN EACH NITRATOR

1	2	3	4	5	6	7	8
22.10341	2.33833	21.04568	7.92066	5.93827	4.88153	1.56143	.41338
22.09874	2.33833	21.04516	7.92626	5.94016	4.88309	1.56168	.41328
22.09813	2.33833	21.04596	7.92569	5.94114	4.88421	1.56223	.41334
22.09770	2.33833	21.04791	7.92624	5.94156	4.88499	1.56288	.41348
22.09624	2.33833	21.05068	7.92634	5.94160	4.88559	1.56333	.41364
22.09315	2.33833	21.05394	7.92615	5.94147	4.88611	1.56382	.41381
22.08681	2.33832	21.05745	7.92577	5.94126	4.88664	1.56428	.41397
22.07851	2.33832	21.06101	7.92526	5.94095	4.88720	1.56474	.41412
22.07479	2.33832	21.06448	7.92466	5.94062	4.88780	1.56521	.41427
22.07536	2.33832	21.06776	7.92394	5.94038	4.88845	1.56578	.41443
22.07418	2.33832	21.07079	7.92327	5.93997	4.88912	1.56621	.41458
22.07320	2.33831	21.07355	7.92250	5.93965	4.88982	1.56647	.40749
22.07232	2.33831	21.07601	7.92168	5.93933	4.88995	1.56150	.40193
22.07170	2.33831	21.07820	7.92016	5.93897	4.89449	1.55071	.40091
22.07113	2.33831	21.08017	7.91550	5.93830	4.87450	1.53308	.40172
22.07068	2.33831	21.08216	7.90394	5.93675	4.85946	1.52653	.40397
22.07036	2.33831	21.08436	7.88233	5.93367	4.83869	1.51741	.40744
22.07031	2.33831	21.08829	7.86937	5.92961	4.81013	1.51094	.41181
22.07076	2.33831	21.09381	7.86582	5.92141	4.78177	1.50719	.41677
22.07219	2.33831	21.10169	7.75370	5.91219	4.75345	1.50585	.42206
22.07478	2.33832	21.11207	7.69566	5.90124	4.72678	1.50648	.42747
22.07832	2.33832	21.12468	7.63424	5.88491	4.70312	1.50868	.43281
22.08273	2.3383	21.13898	7.57163	5.87551	4.68356	1.51218	.43797
22.08443	2.33836	21.15390	7.50452	5.86131	4.66883	1.51685	.44289
22.10522	2.33839	21.16975	7.44915	5.84651	4.65931	1.52267	.44757
22.11781	2.33842	21.18260	7.39139	5.83128	4.65503	1.52968	.45210
22.13175	2.33845	21.19472	7.33681	5.81580	4.65572	1.53791	.45654
22.14656	2.33849	21.20461	7.28574	5.80021	4.66088	1.54738	.46101
22.16173	2.33852	21.21197	7.23833	5.78469	4.66987	1.55800	.46560
22.17685	2.33856	21.21672	7.19457	5.76936	4.68196	1.56967	.47036
22.19163	2.33860	21.21897	7.15437	5.75438	4.69843	1.58221	.47534
22.20587	2.33864	21.21895	7.11751	5.73984	4.71262	1.59542	.48054
22.21951	2.33867	21.21696	7.08377	5.72585	4.72990	1.60907	.48593
22.23257	2.33870	21.21337	7.05286	5.71245	4.74757	1.62295	.49148
22.24516	2.33873	21.20851	7.02449	5.69965	4.76527	1.63681	.49713
22.25742	2.33875	21.20270	6.99837	5.68746	4.78276	1.65048	.50280
22.26951	2.33878	21.19618	6.97425	5.67536	4.79945	1.66383	.50844
22.28158	2.33880	21.18916	6.95189	5.66483	4.81636	1.67677	.51401
22.29376	2.33881	21.18177	6.93104	5.65432	4.83218	1.68922	.51944
22.30618	2.33883	21.17409	6.91154	5.64472	4.84725	1.70113	.52472
22.31889	2.33885	21.16614	6.89322	5.63477	4.86153	1.71246	.52981
22.33196	2.33886	21.15794	6.87595	5.62564	4.87502	1.72321	.53468
22.34540	2.33888	21.14946	6.85963	5.61690	4.88774	1.73337	.53933
22.35921	2.33889	21.14068	6.84416	5.60852	4.89972	1.74294	.54375
22.37335	2.33890	21.13157	6.82948	5.60049	4.91099	1.75196	.54793
22.38746	2.33892	21.12239	6.81553	5.59280	4.92161	1.76043	.55187
22.40269	2.33893	21.11223	6.80227	5.58542	4.93162	1.76838	.55558
22.41757	2.33894	21.10198	6.78967	5.57836	4.94109	1.77585	.55907
22.43269	2.33895	21.09134	6.77768	5.57160	4.95005	1.78287	.56234
22.44792	2.33897	21.08032	6.76629	5.56514	4.95856	1.78946	.56541
22.46318	2.33898	21.06896	6.75547	5.55898	4.96666	1.79565	.56829
22.47844	2.33900	21.05727	6.74520	5.55311	4.97438	1.80148	.57098
22.49364	2.33901	21.04529	6.73545	5.54753	4.98176	1.80697	.57351
22.50874	2.33902	21.03308	6.72620	5.54222	4.98883	1.81215	.57587
22.52369	2.33904	21.02067	6.71745	5.53718	4.99562	1.81703	.57809
22.53845	2.33905	21.00807	6.70972	5.53230	5.00391	1.82176	.58115
22.55294	2.33906	20.99547	6.70287	5.52752	5.01201	1.82623	.58397
22.56712	2.33908	20.98311	6.69631	5.52289	5.01867	1.83037	.58581
22.58047	2.33909	20.96692	6.69017	5.51840	5.02482	1.83422	.58702
22.59342	2.33910	20.95247	6.68449	5.51405	5.03045	1.83775	.58776
22.60522	2.33912	20.93790	6.67930	5.56987	5.03692	1.84093	.58819
22.61594	2.33913	20.92338	6.67459	5.50585	5.04307	1.84375	.58840

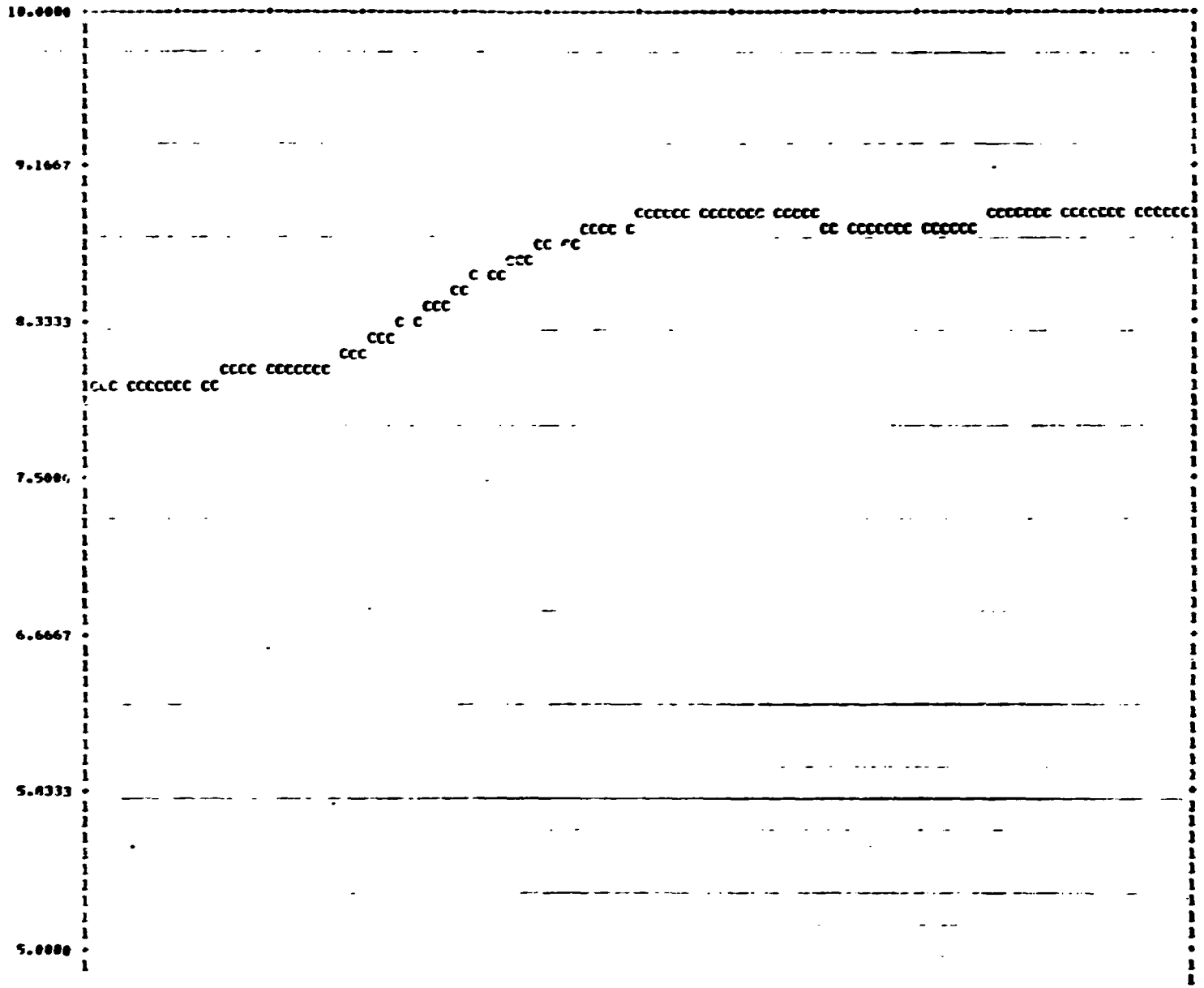
22.62564	2.33916	20.98904	6.67031	5.58198	5.84926	1.84625	.58848
22.63421	2.33915	20.89502	6.66644	5.49826	5.85543	1.84845	.58850
22.64169	2.33916	20.88142	6.66296	5.49468	5.86156	1.85041	.58849
22.64806	2.33917	20.86835	6.65983	5.49124	5.86753	1.85216	.58848
22.65337	2.33918	20.85591	6.65704	5.48793	5.87337	1.85375	.58849
22.65761	2.33918	20.84416	6.65456	5.48477	5.87905	1.85521	.58852
22.66081	2.33919	20.83321	6.65237	5.48177	5.88456	1.85657	.58859
22.66299	2.33920	20.82311	6.65044	5.47892	5.88990	1.85786	.58868
22.66422	2.33920	20.81392	6.64875	5.47625	5.89510	1.85908	.58881
22.66455	2.33920	20.80570	6.64725	5.47373	5.90014	1.86027	.58898
22.66409	2.33921	20.79848	6.64592	5.47137	5.90506	1.86144	.58917
22.66298	2.33921	20.79228	6.64474	5.46918	5.90984	1.86258	.58938
22.66114	2.33921	20.78710	6.64367	5.46712	5.91454	1.86373	.58962
22.65893	2.33921	20.78293	6.64269	5.46521	5.91910	1.86486	.58989
22.65630	2.33921	20.77972	6.64178	5.46343	5.92356	1.86599	.59017
22.65347	2.33921	20.77743	6.64092	5.46177	5.92791	1.86712	.59047
22.65051	2.33921	20.77597	6.64010	5.46022	5.93214	1.86823	.59078
22.64753	2.33920	20.77528	6.63929	5.45877	5.93626	1.86934	.59109
22.64461	2.33920	20.77525	6.63850	5.45740	5.94027	1.87042	.59141
22.64183	2.33920	20.77579	6.63772	5.45612	5.94416	1.87148	.59173
22.63925	2.33920	20.77676	6.63696	5.45492	5.94793	1.87252	.59205
22.63692	2.33920	20.77815	6.63615	5.45380	5.95159	1.87352	.59236
22.63488	2.33920	20.77978	6.63538	5.45273	5.95514	1.87448	.59265
22.63315	2.33919	20.78160	6.63461	5.45172	5.95857	1.87541	.59294
22.63176	2.33919	20.78350	6.63384	5.45078	5.96189	1.87630	.59320
22.63071	2.33919	20.78543	6.63308	5.44989	5.96510	1.87716	.59346
22.62999	2.33919	20.78731	6.63234	5.44906	5.96820	1.87796	.59369
22.62961	2.33919	20.78909	6.63162	5.44827	5.97120	1.87869	.59390
22.62955	2.33919	20.79073	6.63092	5.44754	5.97410	1.87940	.59409
22.62979	2.33919	20.79218	6.63025	5.44686	5.97690	1.88006	.59426
22.63033	2.33919	20.79343	6.62960	5.44623	5.97960	1.88068	.59441
22.63113	2.33919	20.79445	6.62900	5.44564	5.98221	1.88125	.59454
22.63218	2.33919	20.79522	6.62844	5.44511	5.98473	1.88178	.59465
22.63345	2.33919	20.79576	6.62792	5.44462	5.98717	1.88226	.59474
22.63492	2.33919	20.79604	6.62745	5.44419	5.98951	1.88270	.59481
22.63658	2.33919	20.79609	6.62704	5.44379	5.99178	1.88310	.59486
22.63840	2.33919	20.79590	6.62666	5.44345	5.99396	1.88346	.59489
22.64036	2.33919	20.79548	6.62636	5.44315	5.99606	1.88378	.59491
22.64244	2.33919	20.79484	6.62610	5.44289	5.99809	1.88407	.59490
22.64463	2.33920	20.79403	6.62590	5.44268	6.00004	1.88431	.59488
22.64690	2.33920	20.79302	6.62575	5.44251	6.00191	1.88452	.59485
22.64924	2.33920	20.79184	6.62567	5.44238	6.00371	1.88469	.59479

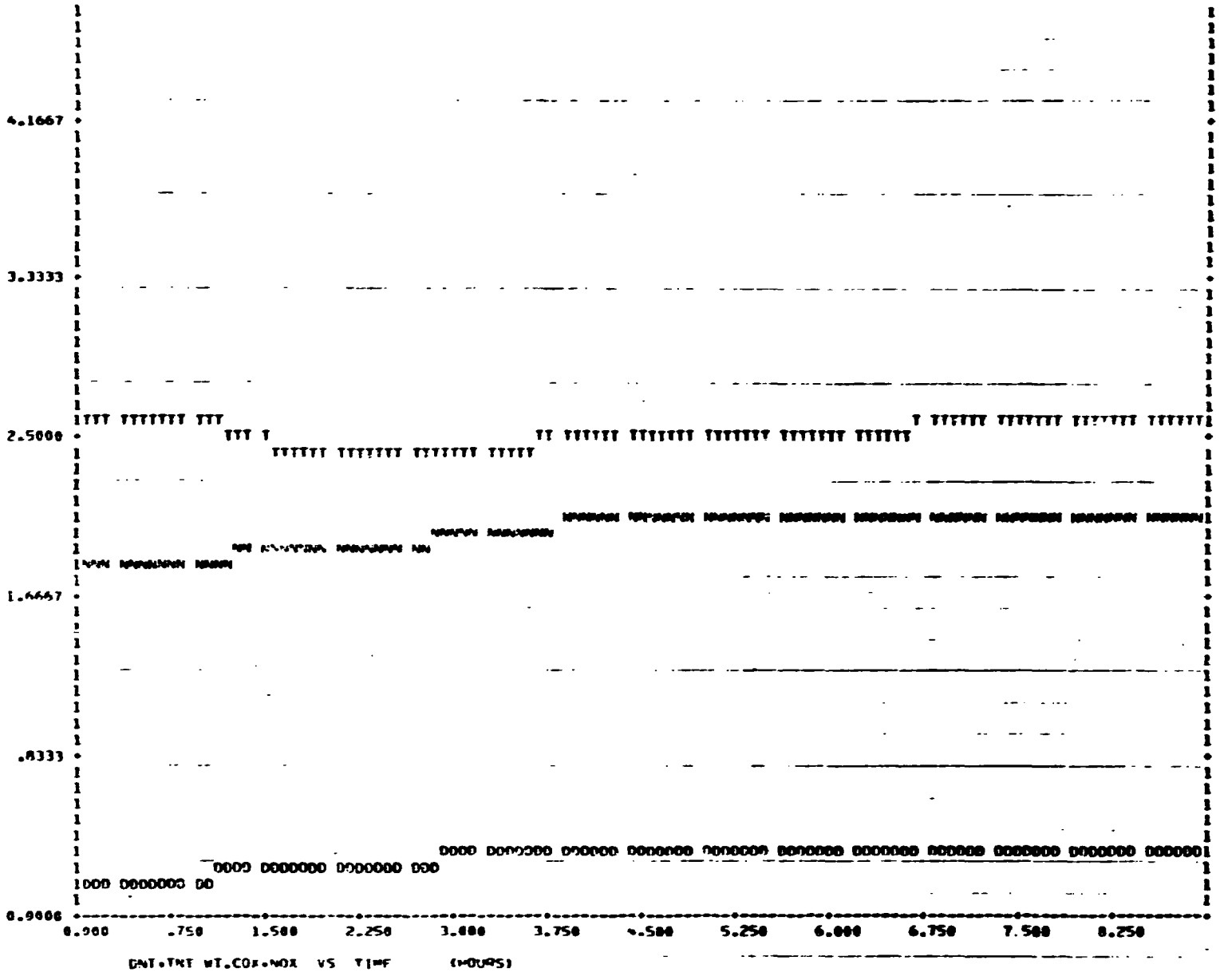
N-NITRATION IN EACH NITRATOR

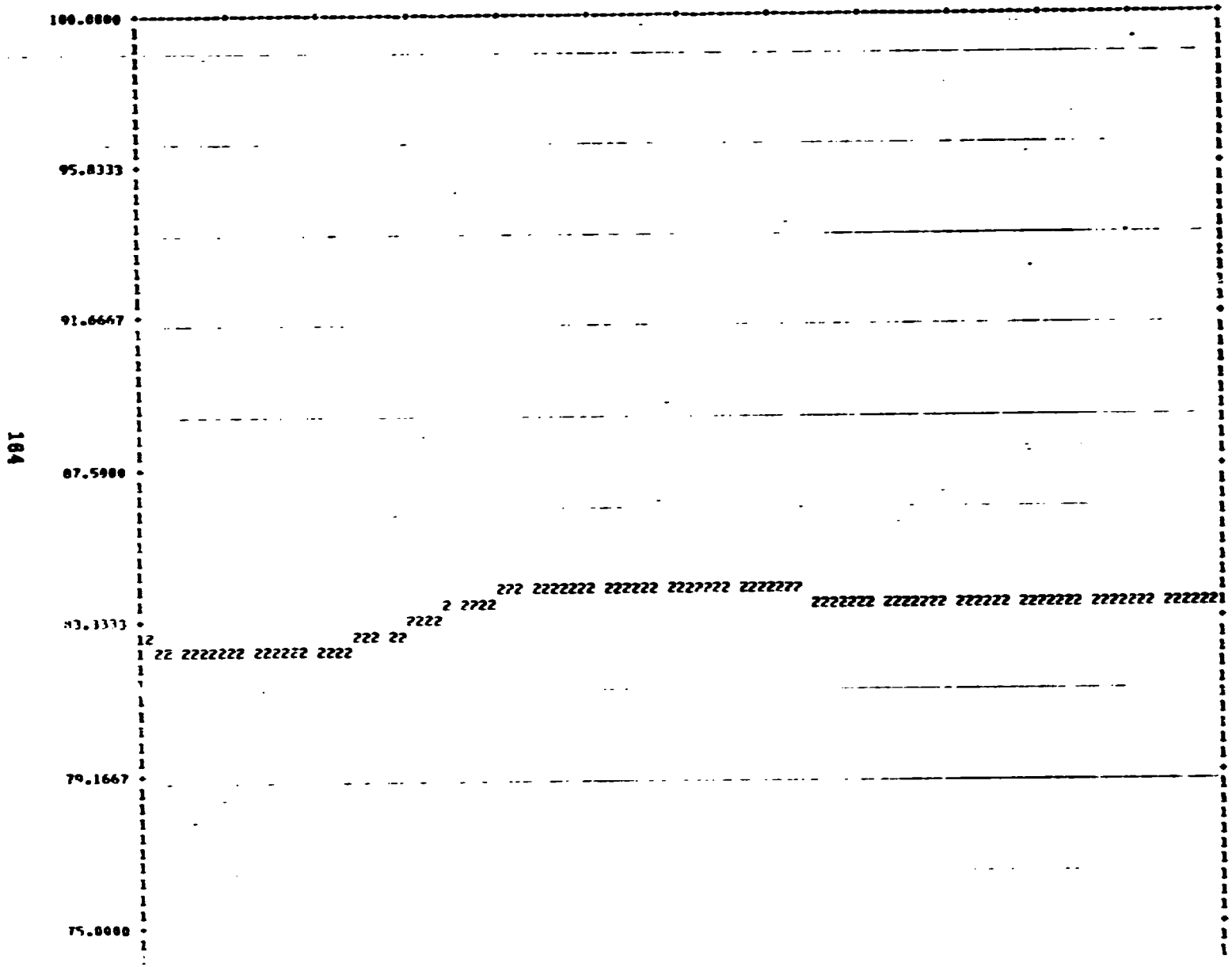
1	2	3	4	5	6	7	8
.90196	.09398	.85445	.53785	.26281	.10039	.01947	.00350
.90179	.09398	.85424	.53839	.26300	.10047	.01948	.00350
.90161	.09397	.85412	.53872	.26310	.10052	.01949	.00350
.90146	.09397	.85408	.53896	.26317	.10057	.01951	.00351
.90132	.09397	.85410	.53910	.26323	.10060	.01952	.00351
.90121	.09397	.85416	.53921	.26327	.10063	.01953	.00351
.90111	.09397	.85424	.53929	.26331	.10067	.01954	.00351
.90103	.09397	.85433	.53935	.26335	.10070	.01955	.00351
.90097	.09397	.85442	.53940	.26338	.10074	.01956	.00352
.90091	.09397	.85452	.53943	.26341	.10077	.01957	.00352
.90087	.09397	.85461	.53946	.26345	.10081	.01958	.00352
.90083	.09397	.85469	.53947	.26348	.10084	.01959	.00347
.90080	.09397	.85474	.53948	.26350	.10087	.01954	.00344
.90078	.09397	.85483	.53943	.26353	.10083	.01946	.00344
.90076	.09397	.85490	.53939	.26355	.10070	.01933	.00346
.90074	.09397	.85500	.53932	.26356	.10067	.01926	.00349
.90073	.09397	.85523	.53926	.26356	.10017	.01920	.00353
.90073	.09397	.85569	.53534	.26359	.09966	.01918	.00358
.90074	.09397	.85650	.53280	.26367	.09953	.01921	.00364
.90079	.09397	.85775	.52971	.26382	.09927	.01927	.00370
.90083	.09397	.85962	.52620	.26404	.09910	.01937	.00376
.90105	.09397	.86147	.52235	.26432	.09906	.01949	.00383
.90130	.09397	.86379	.51830	.26463	.09910	.01963	.00389
.90142	.09397	.86626	.51412	.26496	.09928	.01980	.00395
.90202	.09397	.86870	.50993	.26522	.09958	.01998	.00401
.90268	.09398	.87107	.50598	.26546	.09998	.02015	.00408
.90360	.09398	.87328	.50151	.26563	.10047	.02040	.00414
.90455	.09398	.87526	.49800	.26574	.10104	.02063	.00420
.90611	.09399	.87699	.49442	.26579	.10166	.02087	.00426
.90667	.09399	.87847	.49109	.26577	.10232	.02112	.00433
.90822	.09400	.87971	.48801	.26571	.10301	.02138	.00439
.90975	.09400	.88071	.48518	.26561	.10370	.02165	.00446
.91126	.09400	.88151	.48259	.26548	.10439	.02191	.00453
.91274	.09401	.88212	.48022	.26533	.10506	.02217	.00460
.91421	.09401	.88257	.47807	.26516	.10571	.02242	.00467
.91567	.09401	.88288	.47609	.26499	.10633	.02267	.00473
.91712	.09402	.88310	.47429	.26481	.10693	.02291	.00480
.91857	.09402	.88321	.47264	.26463	.10750	.02314	.00486
.92002	.09402	.88324	.47112	.26445	.10806	.02336	.00493
.92149	.09403	.88321	.46973	.26427	.10860	.02357	.00499
.92296	.09403	.88312	.46846	.26410	.10914	.02377	.00506
.92445	.09403	.88298	.46725	.26393	.10970	.02395	.00510
.92595	.09403	.88280	.46614	.26378	.10993	.02413	.00515
.92747	.09404	.88259	.46511	.26362	.11034	.02430	.00520
.92900	.09404	.88233	.46415	.26348	.11073	.02446	.00525
.93055	.09404	.88204	.46326	.26334	.11110	.02460	.00529
.93210	.09404	.88172	.46243	.26321	.11145	.02475	.00534
.93366	.09405	.88137	.46165	.26309	.11178	.02488	.00537
.93523	.09405	.88101	.46092	.26297	.11210	.02500	.00541
.93680	.09405	.88061	.46024	.26287	.11240	.02512	.00545
.93837	.09405	.88021	.45960	.26277	.11269	.02524	.00548
.93994	.09406	.87978	.45901	.26268	.11297	.02534	.00551
.94152	.09406	.87934	.45845	.26259	.11324	.02544	.00554
.94308	.09406	.87890	.45793	.26252	.11349	.02554	.00557
.94464	.09407	.87844	.45744	.26244	.11374	.02563	.00560
.94620	.09407	.87797	.45701	.26237	.11401	.02572	.00563
.94775	.09407	.87745	.45664	.26238	.11426	.02579	.00566
.94928	.09407	.87686	.45629	.26222	.11447	.02586	.00568
.95079	.09408	.87623	.45597	.26215	.11467	.02593	.00569
.95227	.09408	.87556	.45569	.26207	.11487	.02598	.00570
.95371	.09408	.87486	.45544	.26200	.11506	.02604	.00570
.95512	.09408	.87415	.45524	.26194	.11525	.02608	.00571

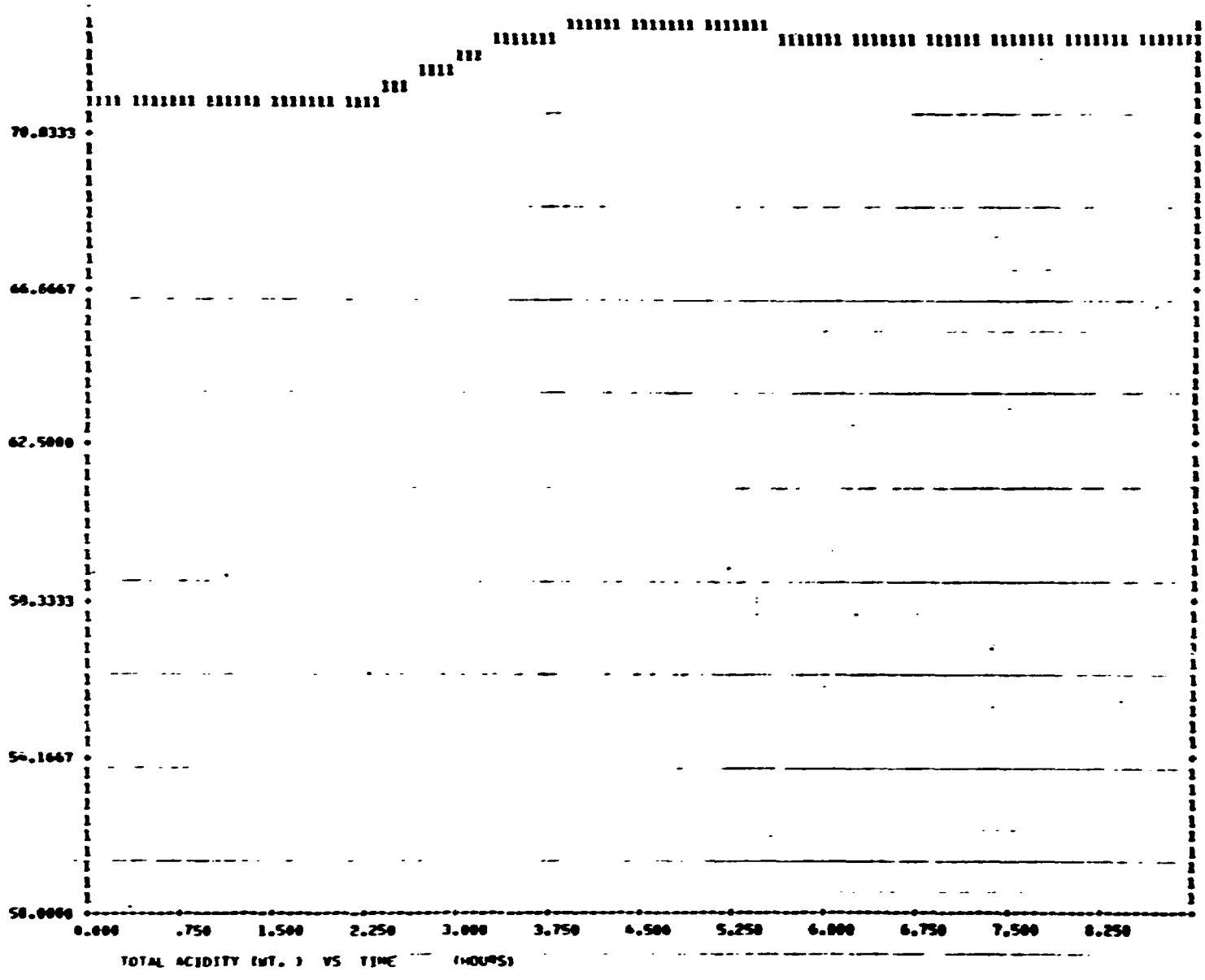
.92148	.09409	.87343	.45507	.26188	.11545	.02613	.00571
.92180	.09409	.87271	.45493	.26193	.11563	.02616	.00571
.92209	.09409	.87199	.45483	.26178	.11582	.02620	.00571
.92233	.09409	.87128	.45475	.26174	.11601	.02623	.00571
.92253	.09409	.87059	.45470	.26171	.11619	.02626	.00571
.92269	.09410	.86991	.45468	.26168	.11636	.02629	.00572
.92281	.09410	.86925	.45468	.26166	.11653	.02632	.00572
.92290	.09410	.86863	.45470	.26165	.11670	.02635	.00572
.92296	.09410	.86803	.45474	.26164	.11687	.02637	.00572
.92298	.09410	.86747	.45479	.26164	.11703	.02640	.00573
.92298	.09410	.86696	.45486	.26164	.11719	.02642	.00573
.92298	.09410	.86649	.45493	.26166	.11734	.02645	.00573
.92293	.09410	.86608	.45502	.26167	.11749	.02648	.00574
.92285	.09410	.86571	.45510	.26170	.11764	.02650	.00574
.92265	.09410	.86539	.45519	.26172	.11779	.02653	.00575
.92255	.09410	.86511	.45528	.26175	.11793	.02655	.00575
.92244	.09410	.86489	.45536	.26178	.11807	.02658	.00576
.92233	.09410	.86471	.45544	.26182	.11821	.02660	.00576
.92222	.09410	.86456	.45552	.26185	.11834	.02663	.00577
.92211	.09410	.86445	.45559	.26189	.11847	.02665	.00577
.92202	.09410	.86437	.45566	.26192	.11860	.02667	.00578
.92193	.09410	.86432	.45571	.26196	.11872	.02670	.00578
.92185	.09409	.86429	.45577	.26199	.11883	.02672	.00579
.92179	.09409	.86427	.45581	.26202	.11894	.02674	.00579
.92174	.09409	.86427	.45585	.26205	.11905	.02676	.00580
.92170	.09409	.86428	.45588	.26208	.11915	.02678	.00580
.92167	.09409	.86430	.45591	.26211	.11925	.02680	.00580
.92166	.09409	.86431	.45594	.26213	.11935	.02681	.00581
.92165	.09409	.86433	.45596	.26216	.11943	.02683	.00581
.92164	.09409	.86435	.45597	.26218	.11952	.02684	.00581
.92164	.09409	.86436	.45599	.26220	.11960	.02685	.00582
.92171	.09409	.86437	.45600	.26221	.11968	.02687	.00582
.92175	.09409	.86438	.45601	.26223	.11975	.02688	.00582
.92180	.09409	.86438	.45601	.26224	.11982	.02689	.00582
.92186	.09409	.86437	.45602	.26225	.11988	.02689	.00582
.92192	.09409	.86436	.45603	.26227	.11995	.02690	.00582
.92199	.09409	.86434	.45603	.26228	.12000	.02691	.00582
.92206	.09409	.86431	.45604	.26228	.12006	.02691	.00582
.92214	.09409	.86428	.45604	.26229	.12011	.02692	.00582
.92222	.09409	.86424	.45605	.26230	.12015	.02692	.00582
.92231	.09409	.86420	.45606	.26230	.12020	.02693	.00582
.92239	.09409	.86415	.45607	.26231	.12024	.02693	.00582

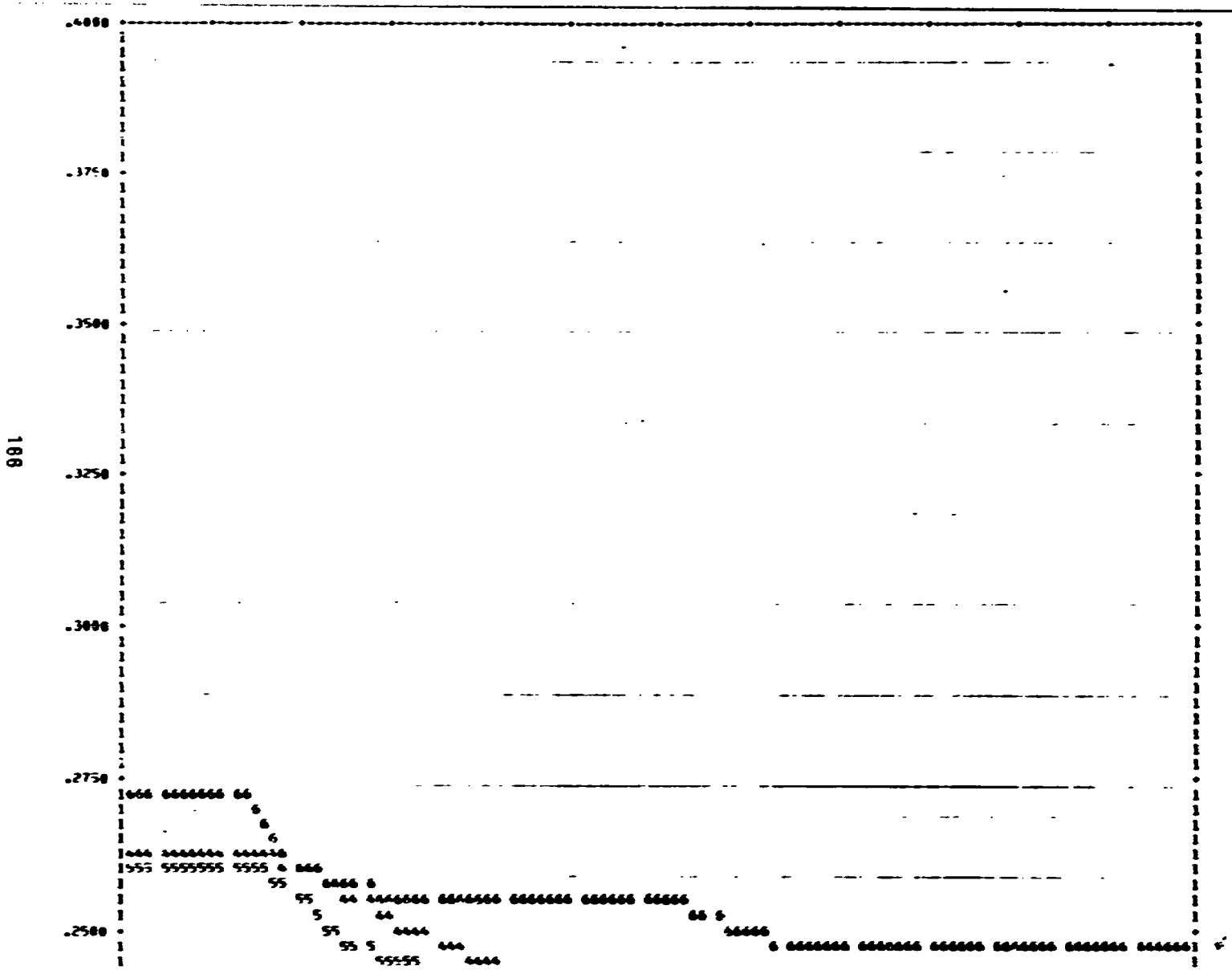
TIME BETWEEN POINTS = 5.16240 MINUTES

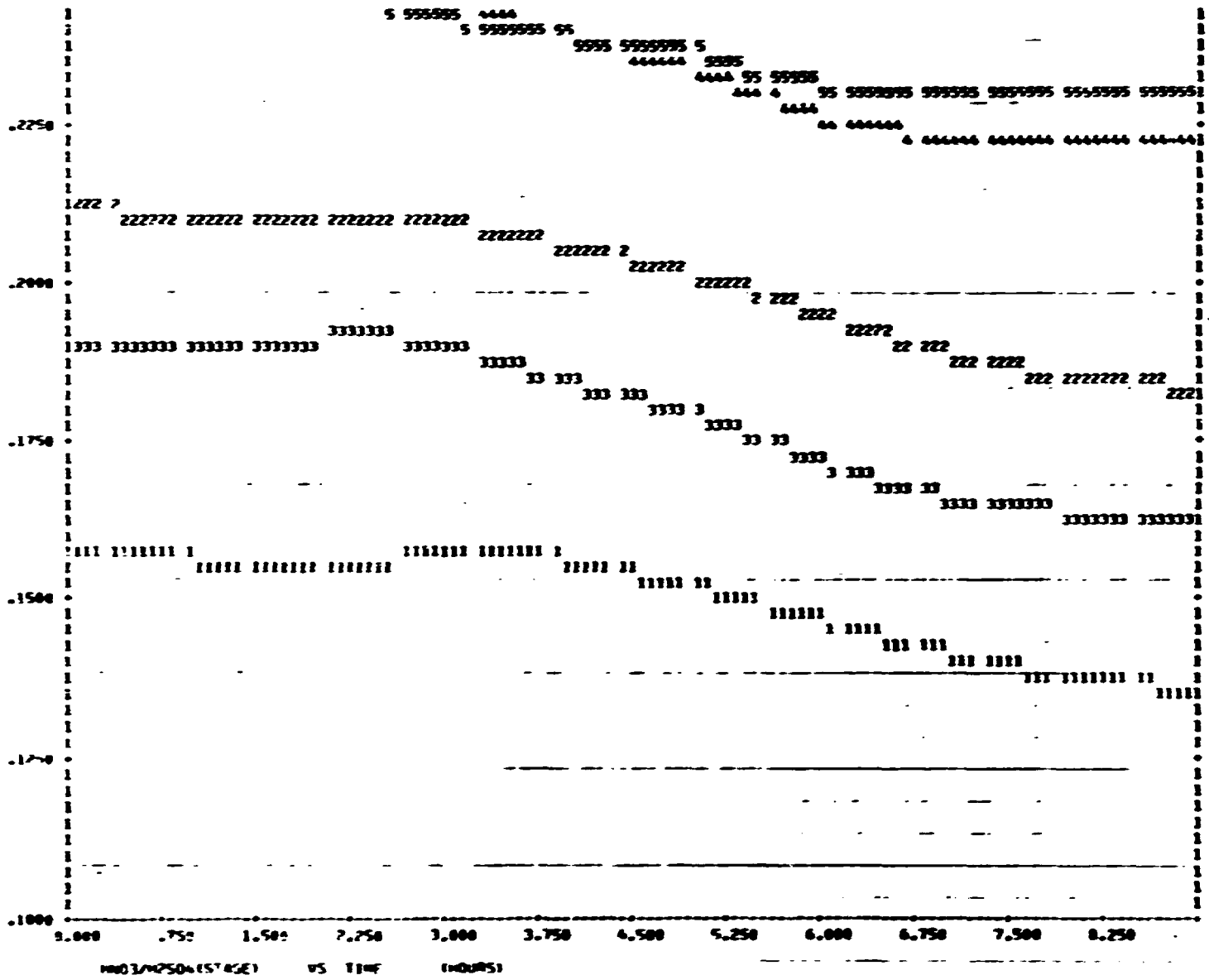

10.0000
9.1667
8.3333
7.5000
6.6667
5.8333
5.0000


4.1667
3.3333
2.5000
1.6667
.8333
0.0000
0.000
.750
1.500
2.250
3.000
3.750
4.500
5.250
6.000
6.750
7.500
8.250
DNT.TNT WT.COx.NOX VS TIME (HOURS)

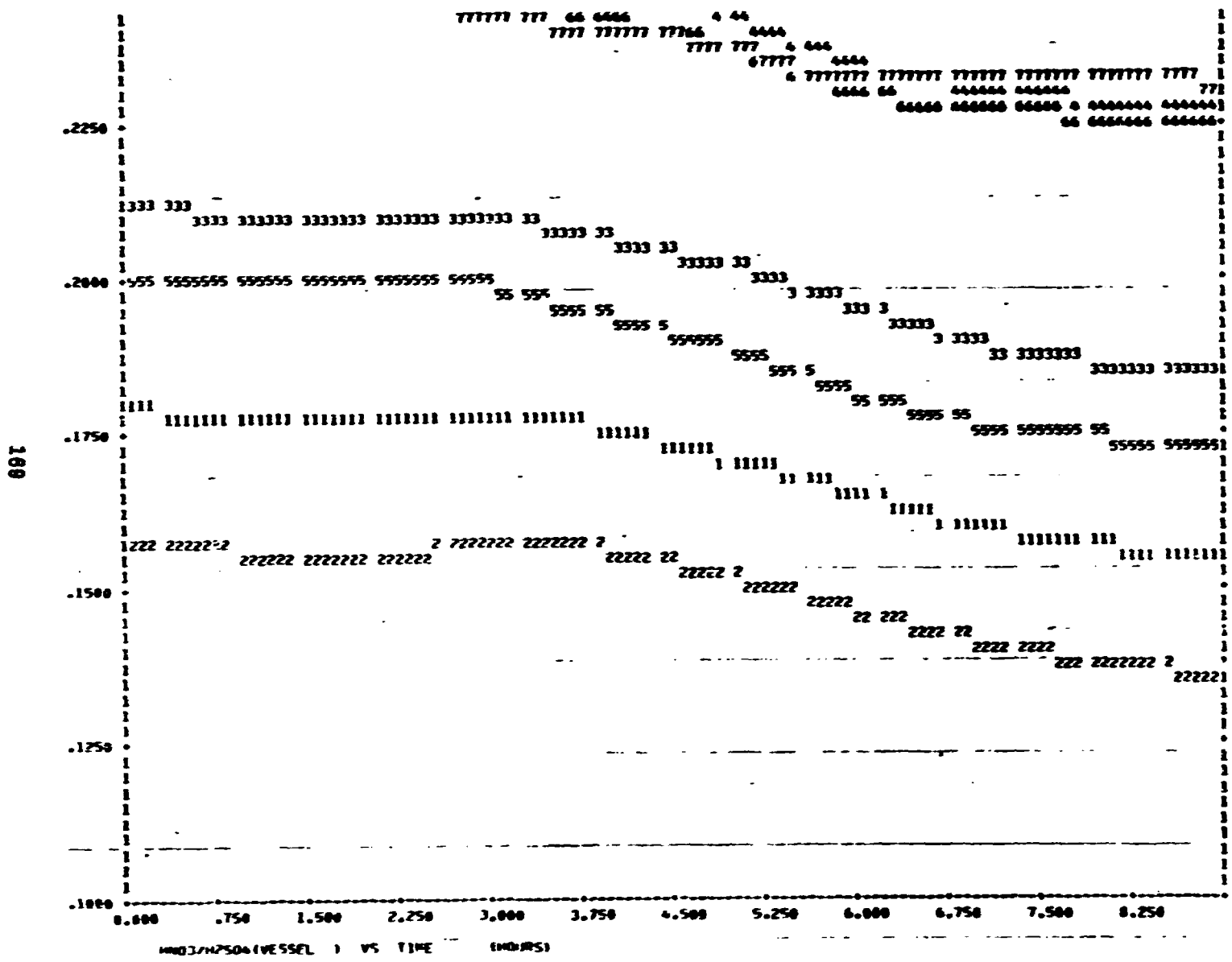

100.0000
95.8333
91.6667
87.5000
83.3333
79.1667
75.0000

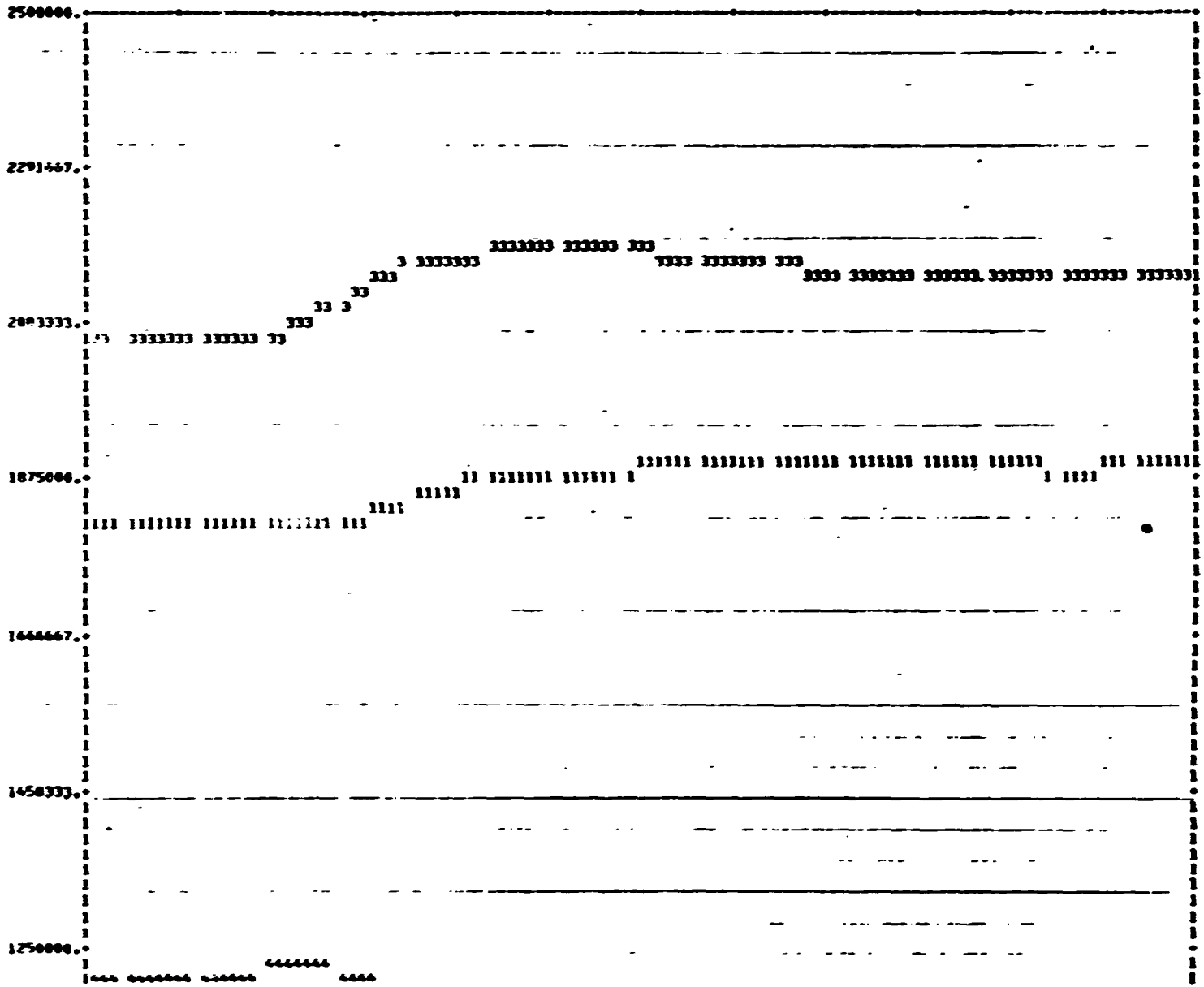

70.8333
66.6667
62.5000
58.3333
54.1667
50.0000
0.000
.750
1.500
2.250
3.000
3.750
4.500
5.250
6.000
6.750
7.500
8.250
TOTAL ACIDITY (MT.) VS TIME (HOURS)


.4000
.3750
.3500
.3250
.3000
.2750
.2500

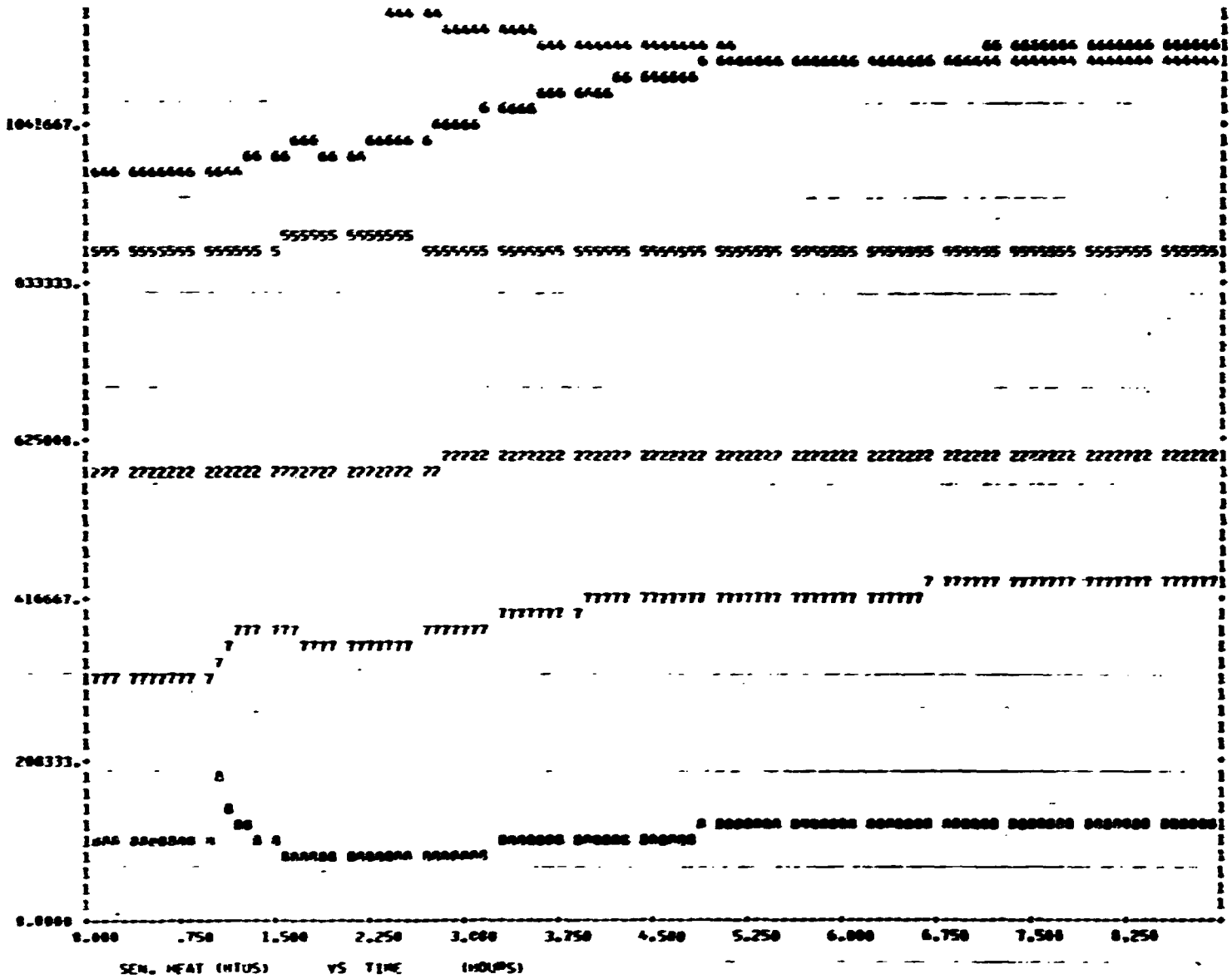

.2250
.2000
.1750
.1500
.1250
.1000
1.000
.750
1.500
2.250
3.000
3.750
4.500
5.250
6.000
6.750
7.500
8.250
HN03/H2SO4(STAGE) VS TIME (HOURS)

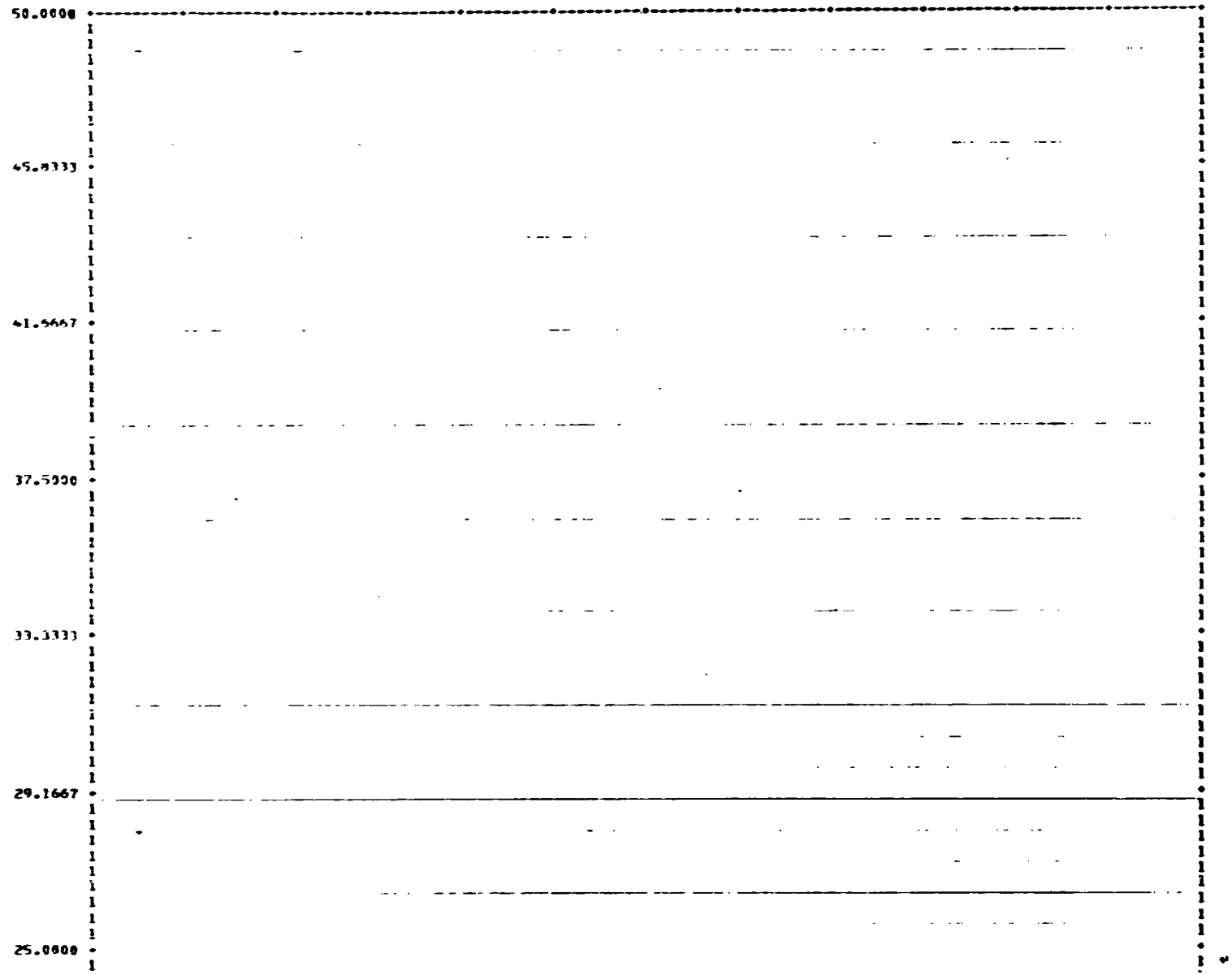
.4000
.3750
.3500
.3250
.3000
.2750
.2500

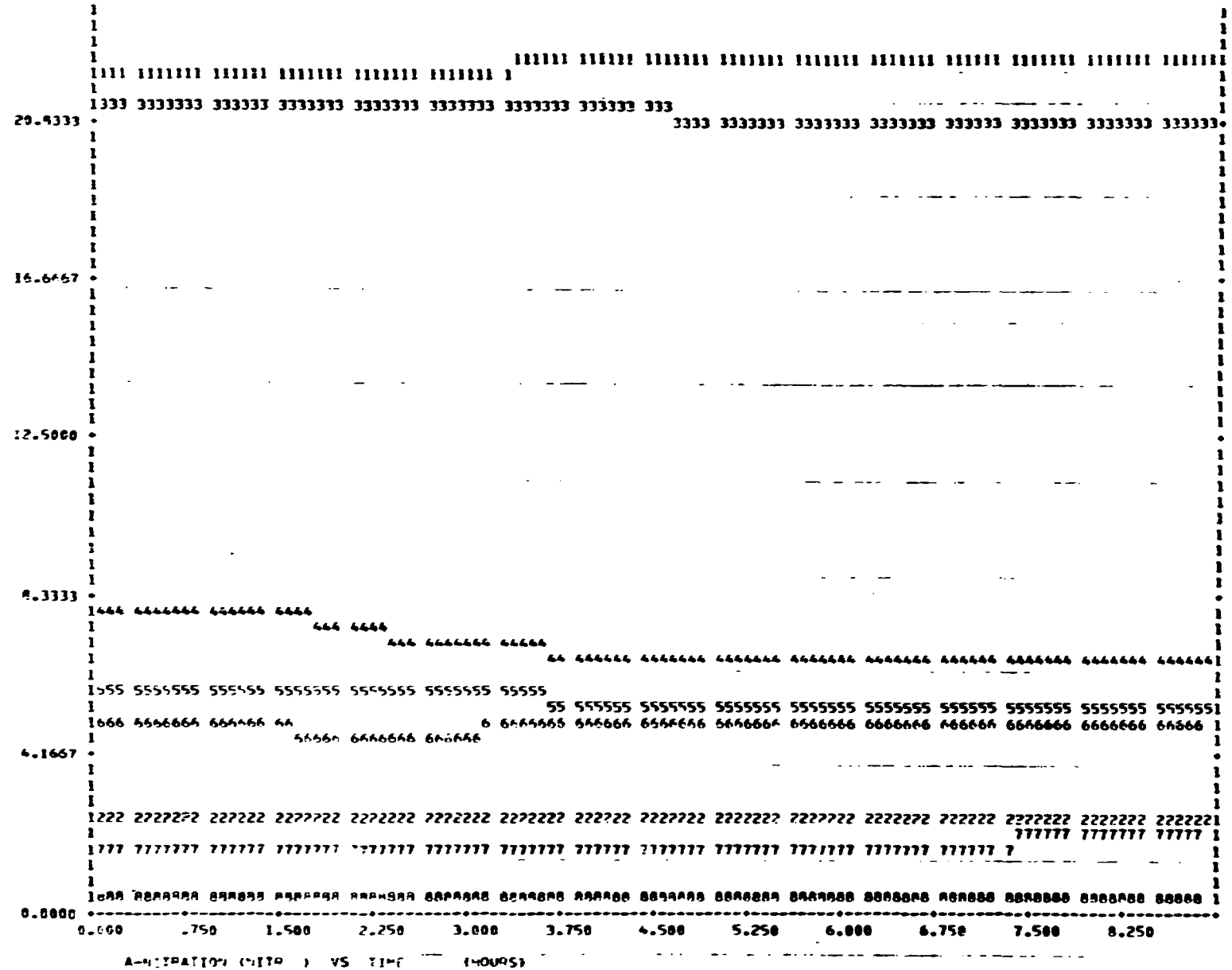

.2250
.2000
.1750
.1500
.1250
.1000
0.000
.750
1.500
2.250
3.000
3.750
4.500
5.250
6.000
6.750
7.500
8.250
HHDI/HPSOA(VESSEL) VS TIME (HOURS)

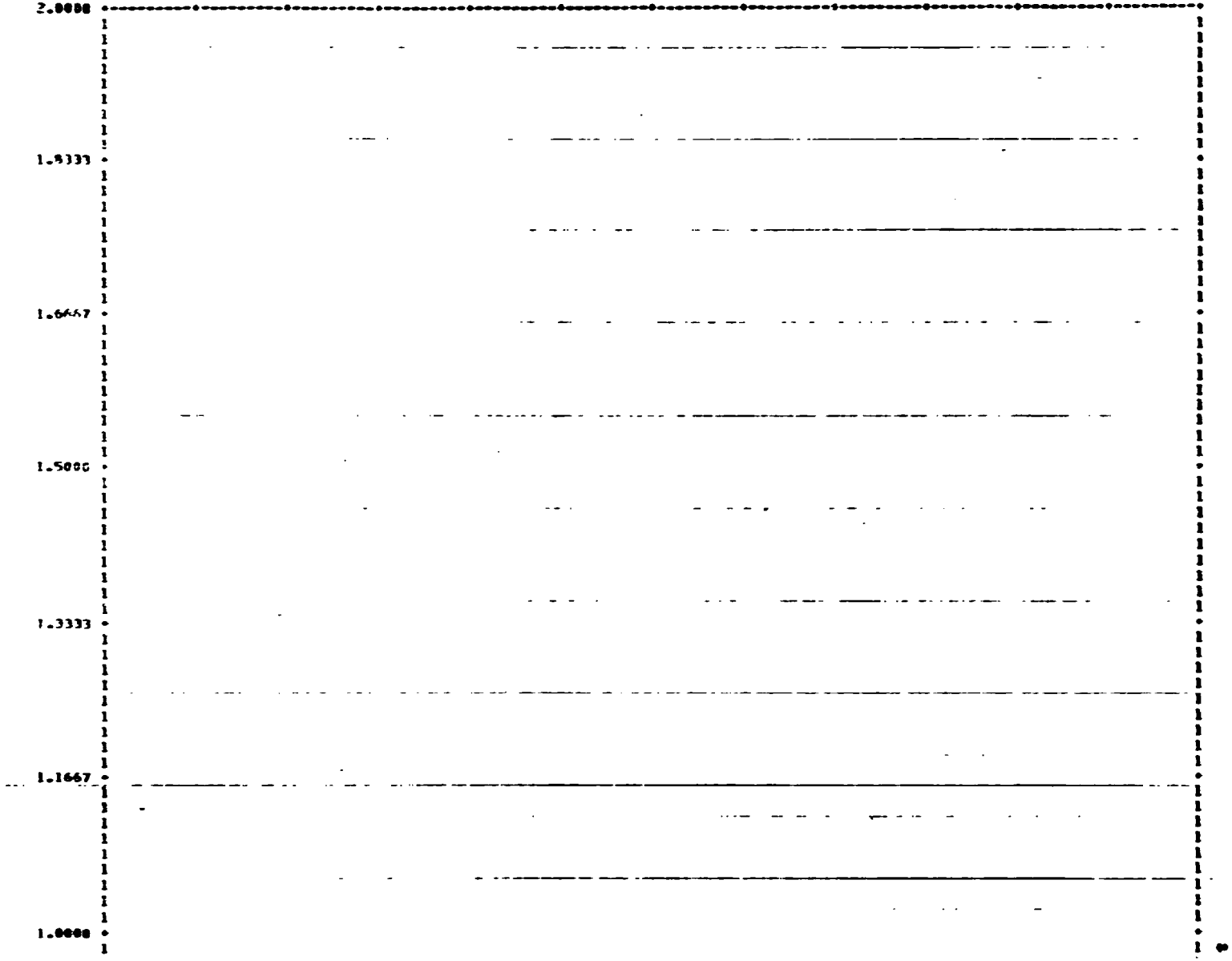


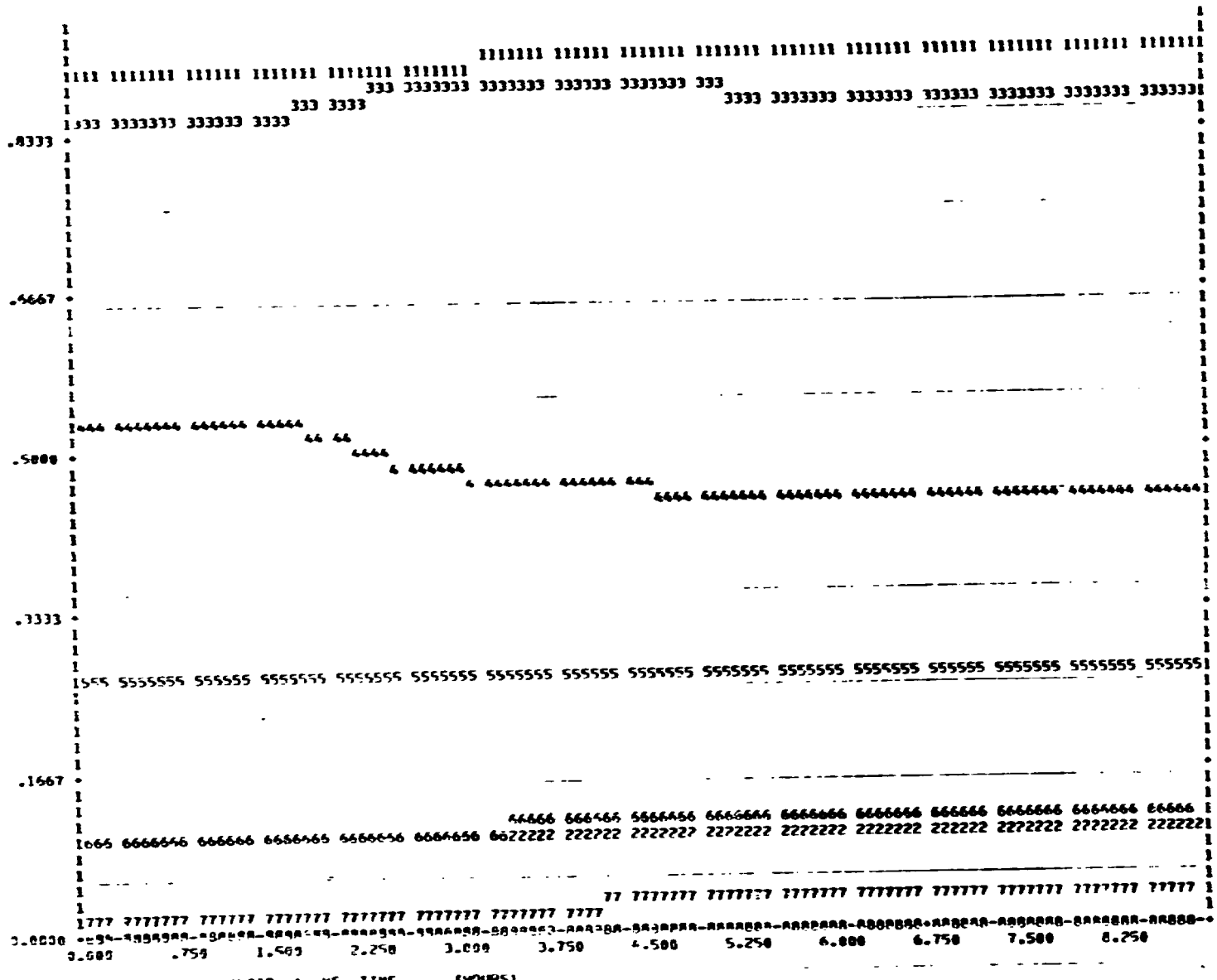
170

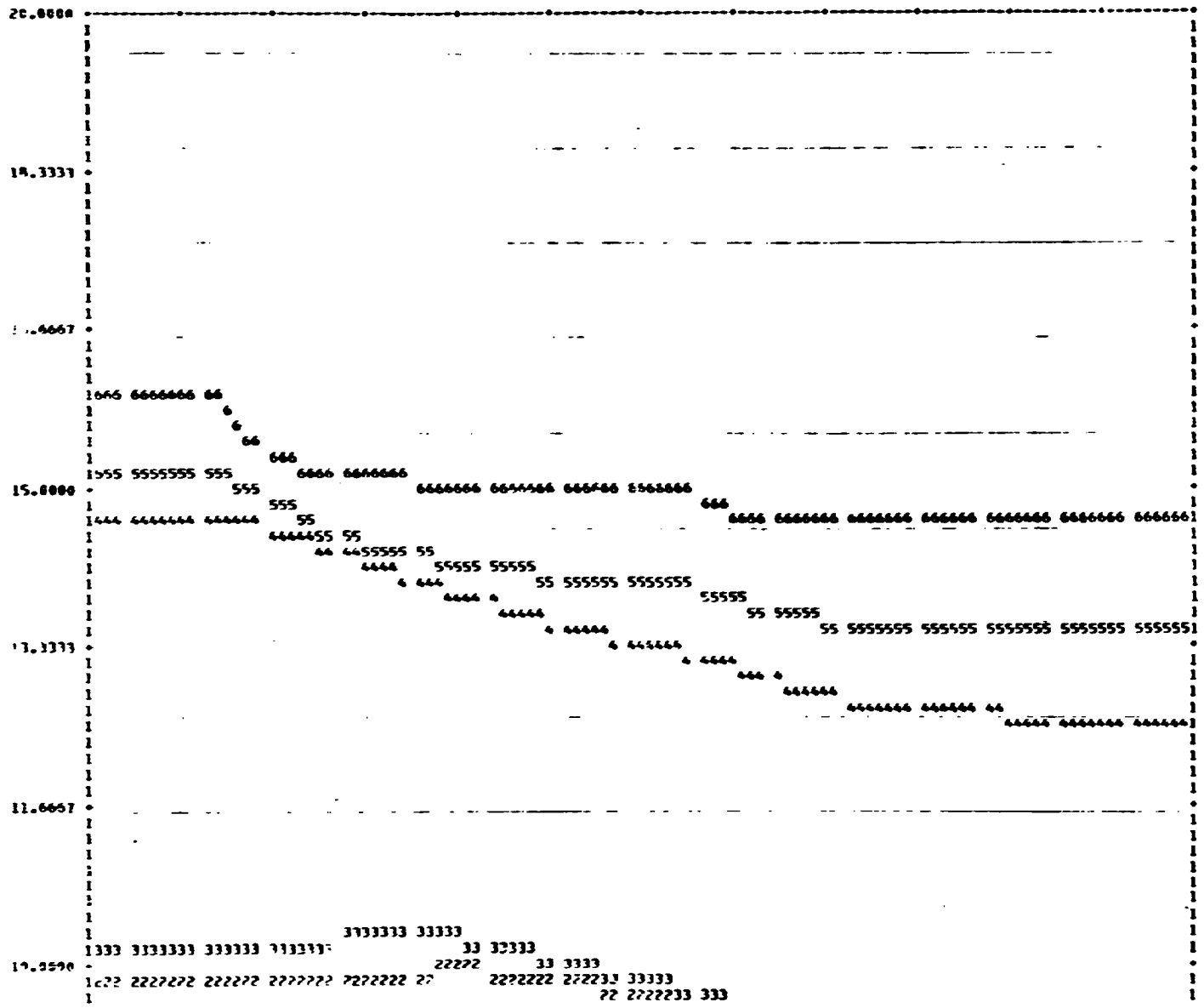

1041667.
833333.
625000.
416667.
208333.
0.0000
0.000
.750
1.500
2.250
3.000
3.750
4.500
5.250
6.000
6.750
7.500
8.250
SEN. HEAT (BTUS) VS TIME (HOURS)

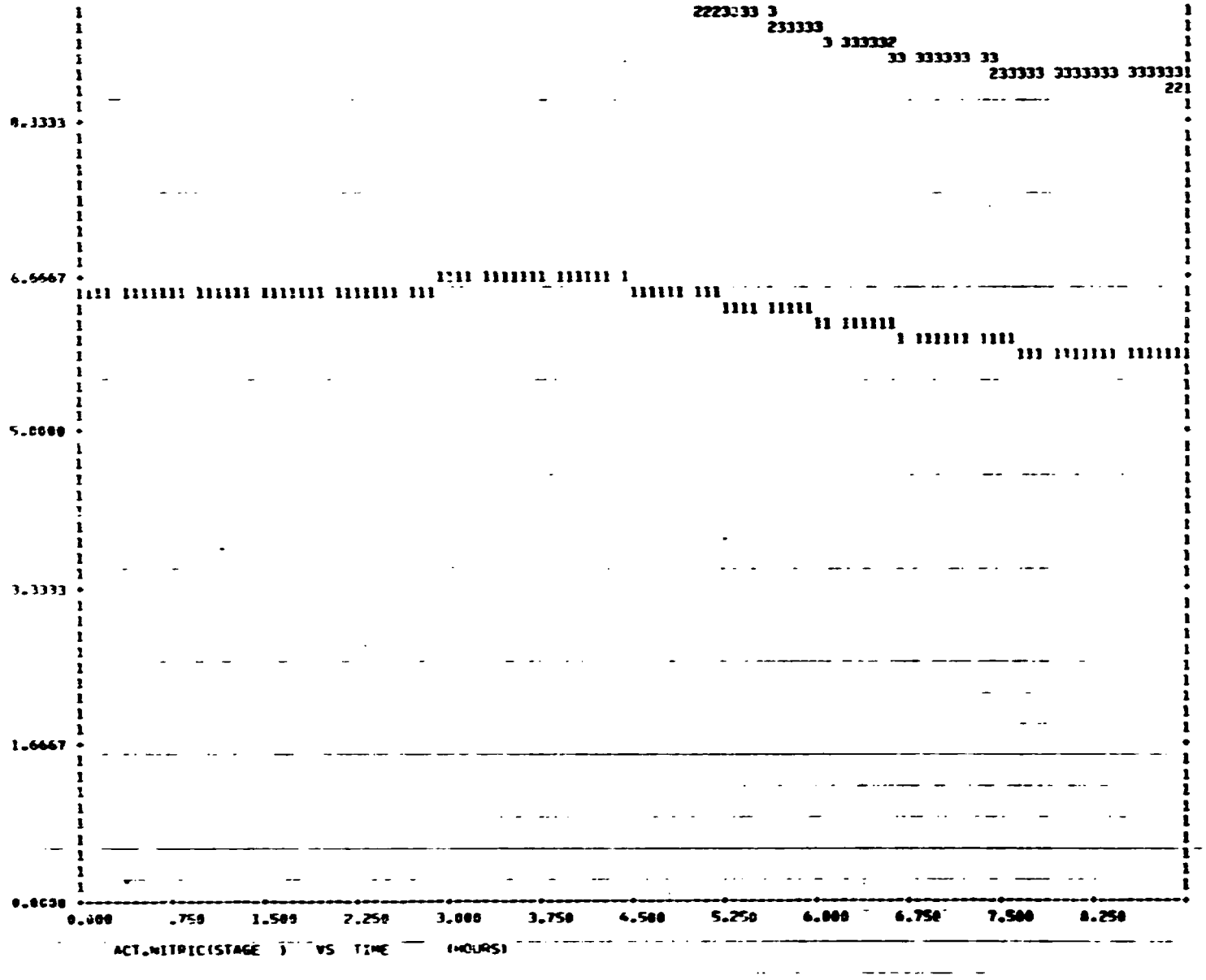

50.0000
45.8333
41.6667
37.5000
33.3333
29.1667
25.0000

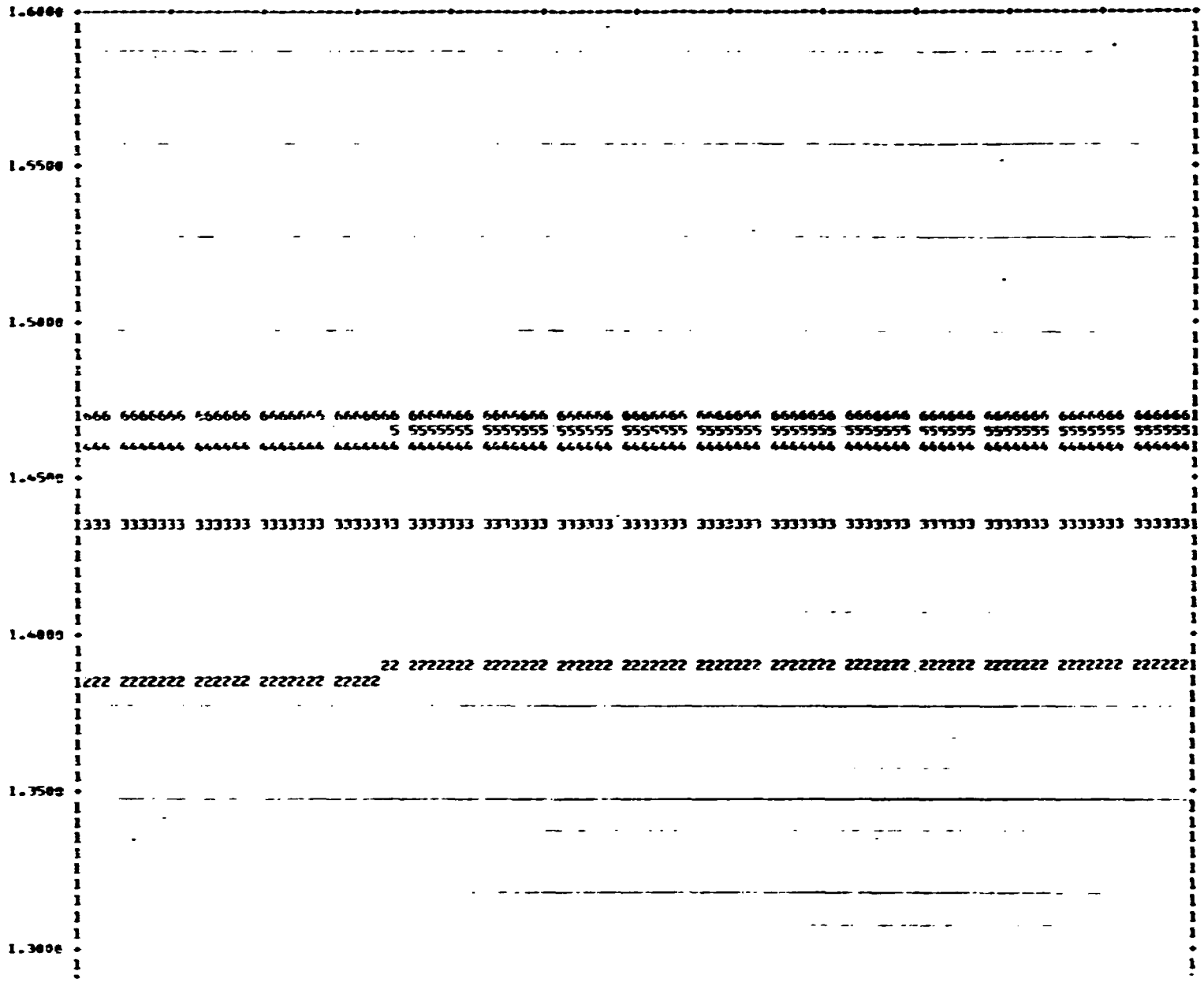

20.8333
16.6667
12.5000
8.3333
4.1667
0.0000
0.000
.750
1.500
2.250
3.000
3.750
4.500
5.250
6.000
6.750
7.500
8.250
(HOURS)

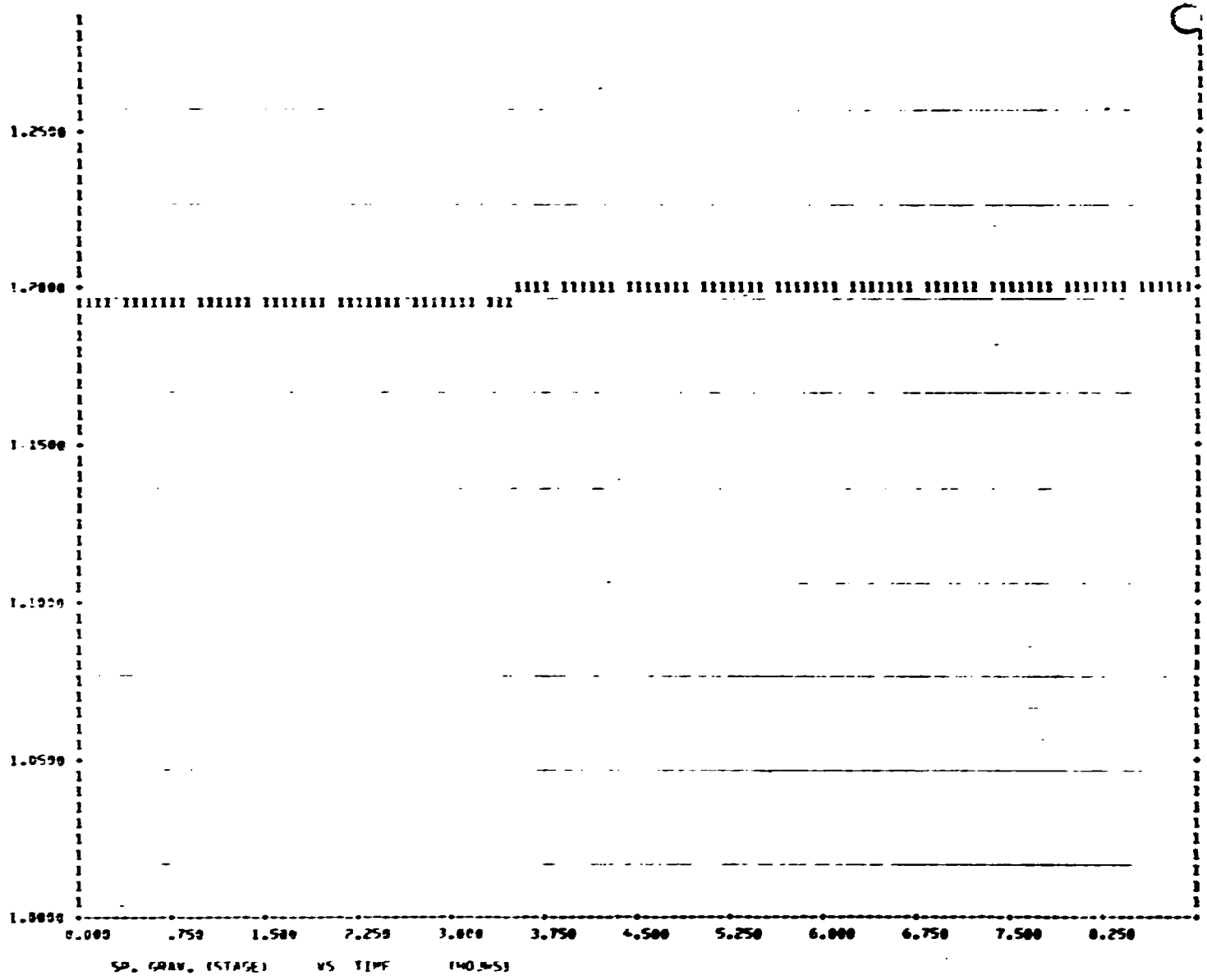

2.0000
1.8333
1.6667
1.5000
1.3333
1.1667
1.0000

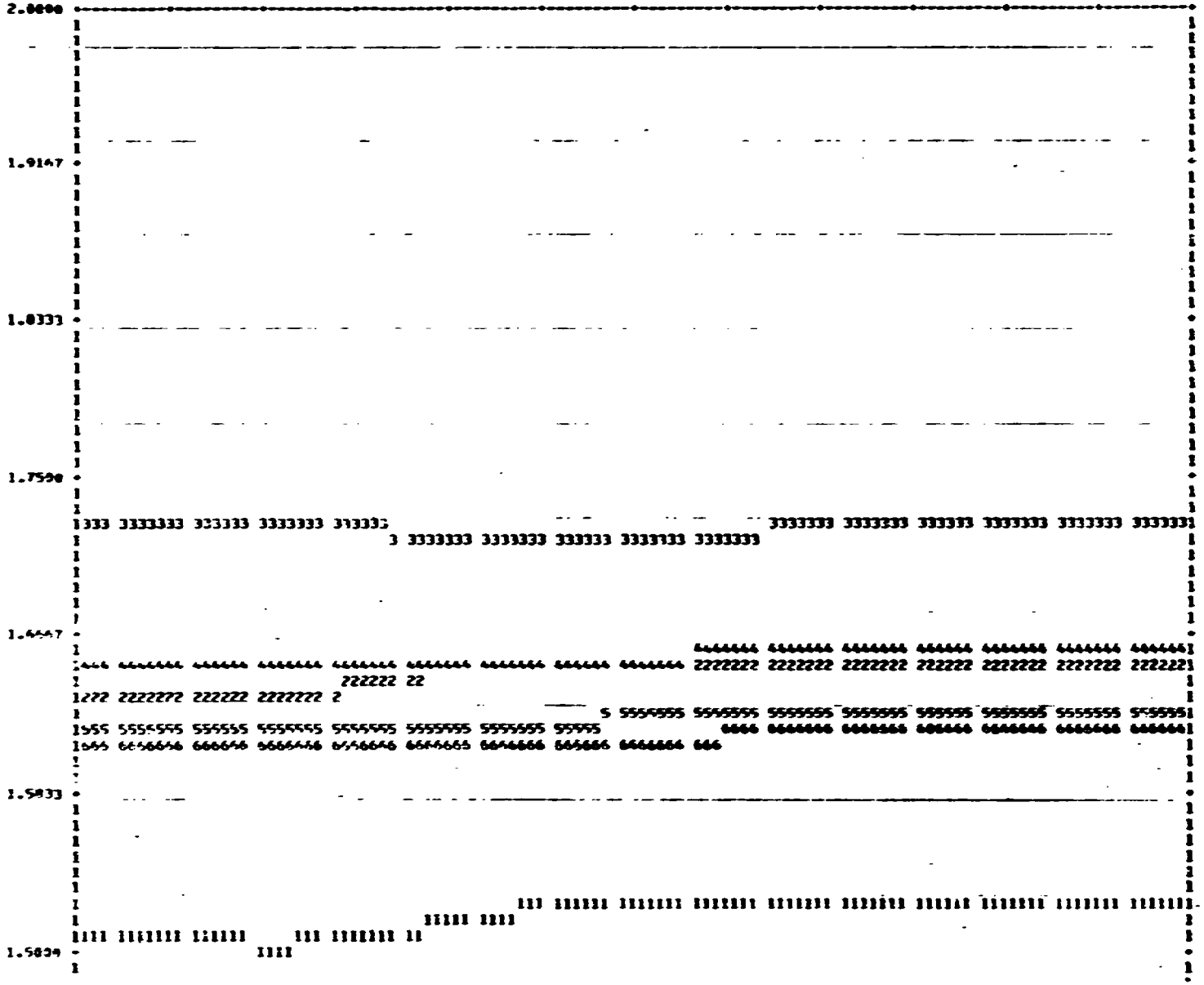

.8333
.4667
.5000
.3333
.1667
0.0000
0.000
.750
1.500
2.250
3.000
3.750
4.500
5.250
6.000
6.750
7.500
8.250
M-NITRATION (NIT2) VS TIME (HOURS)

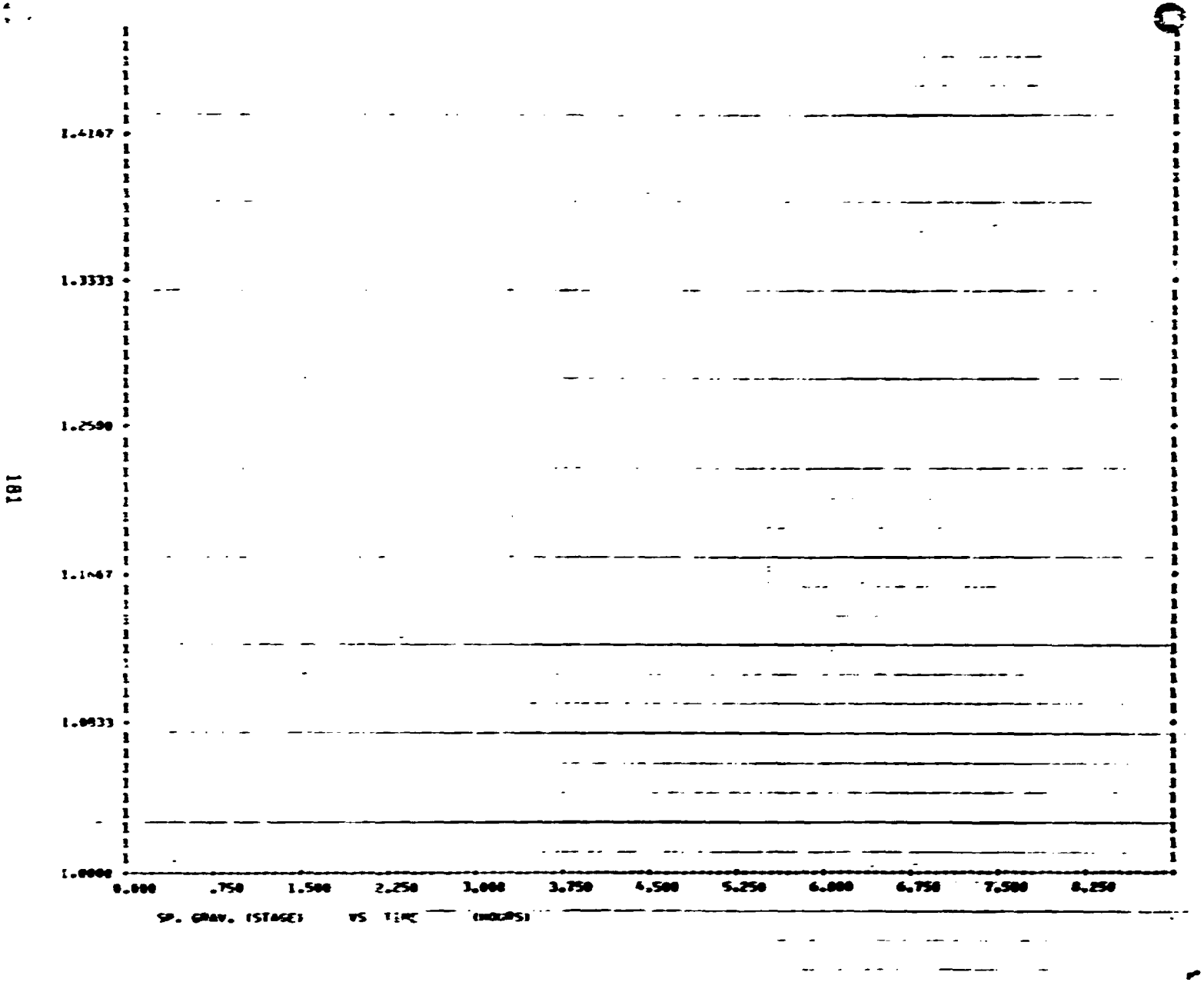

20.0000
18.3333
16.6667
15.0000
13.3333
11.6667
10.0000

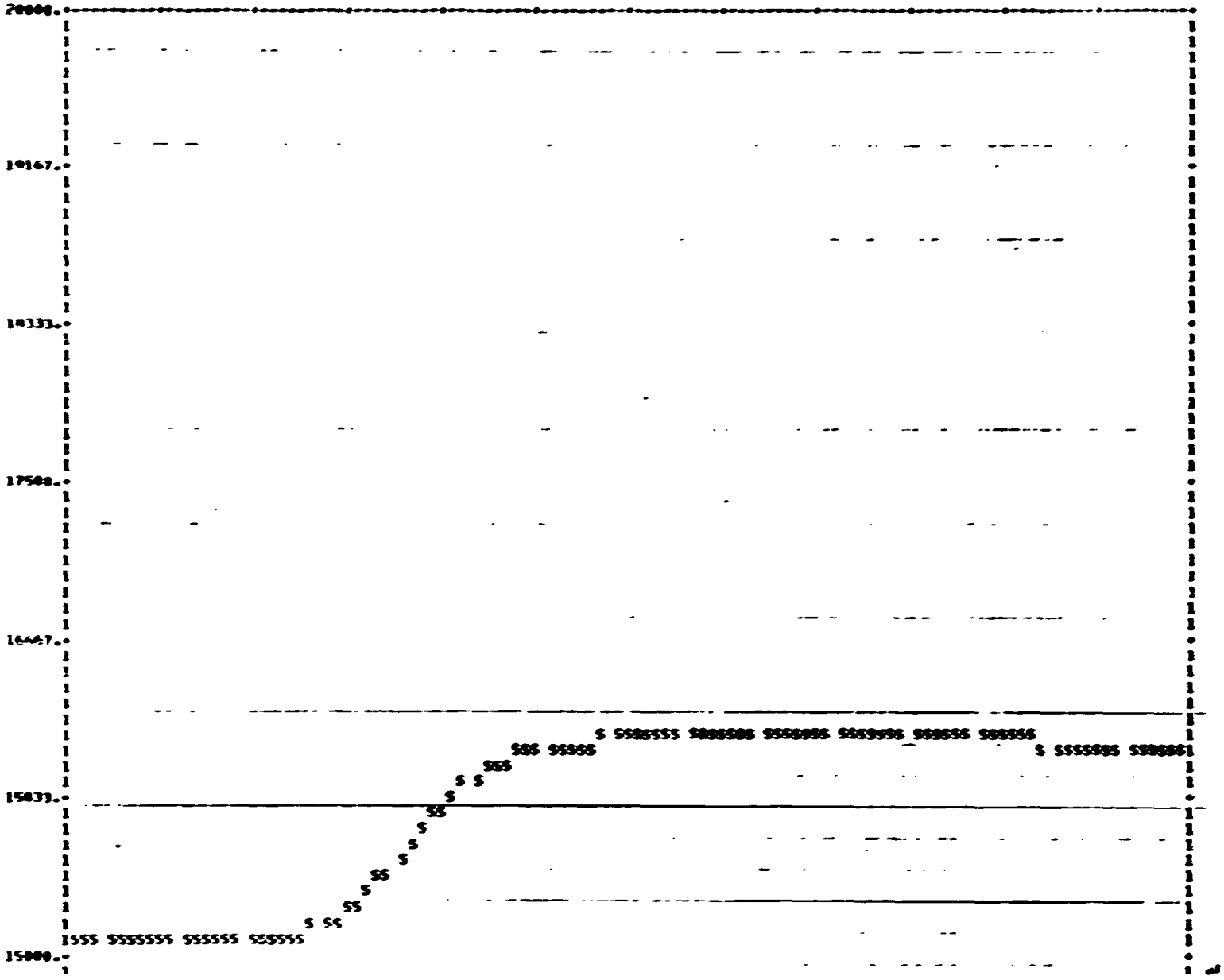

8.3333
6.6667
5.0000
3.3333
1.6667
0.0000
0.000
.750
1.500
2.250
3.000
3.750
4.500
5.250
6.000
6.750
7.500
8.250
ACT.NITRIC(STAGE) VS TIME (HOURS)

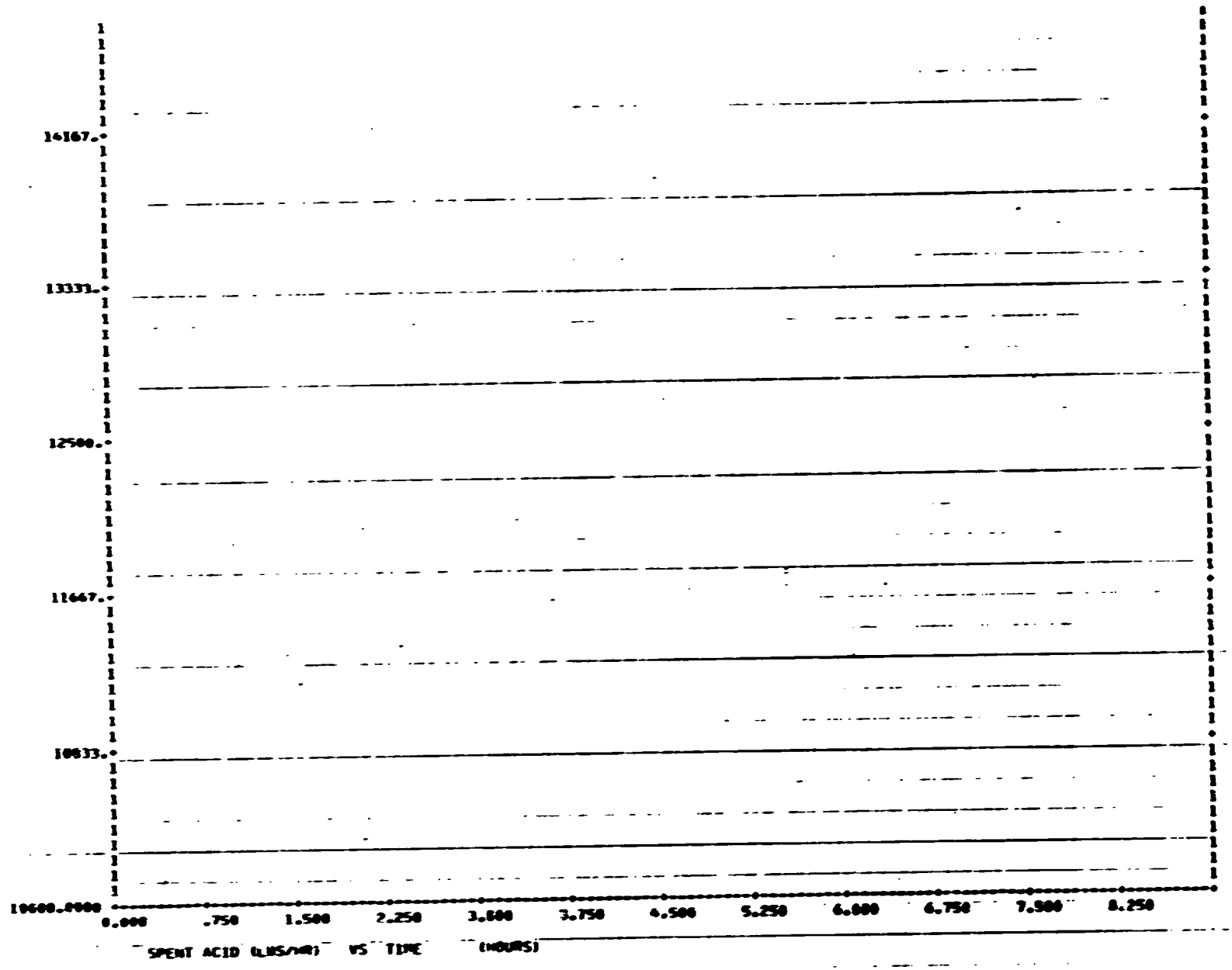

1.6000
1.5500
1.5000
1.4500
1.4000
1.3500
1.3000

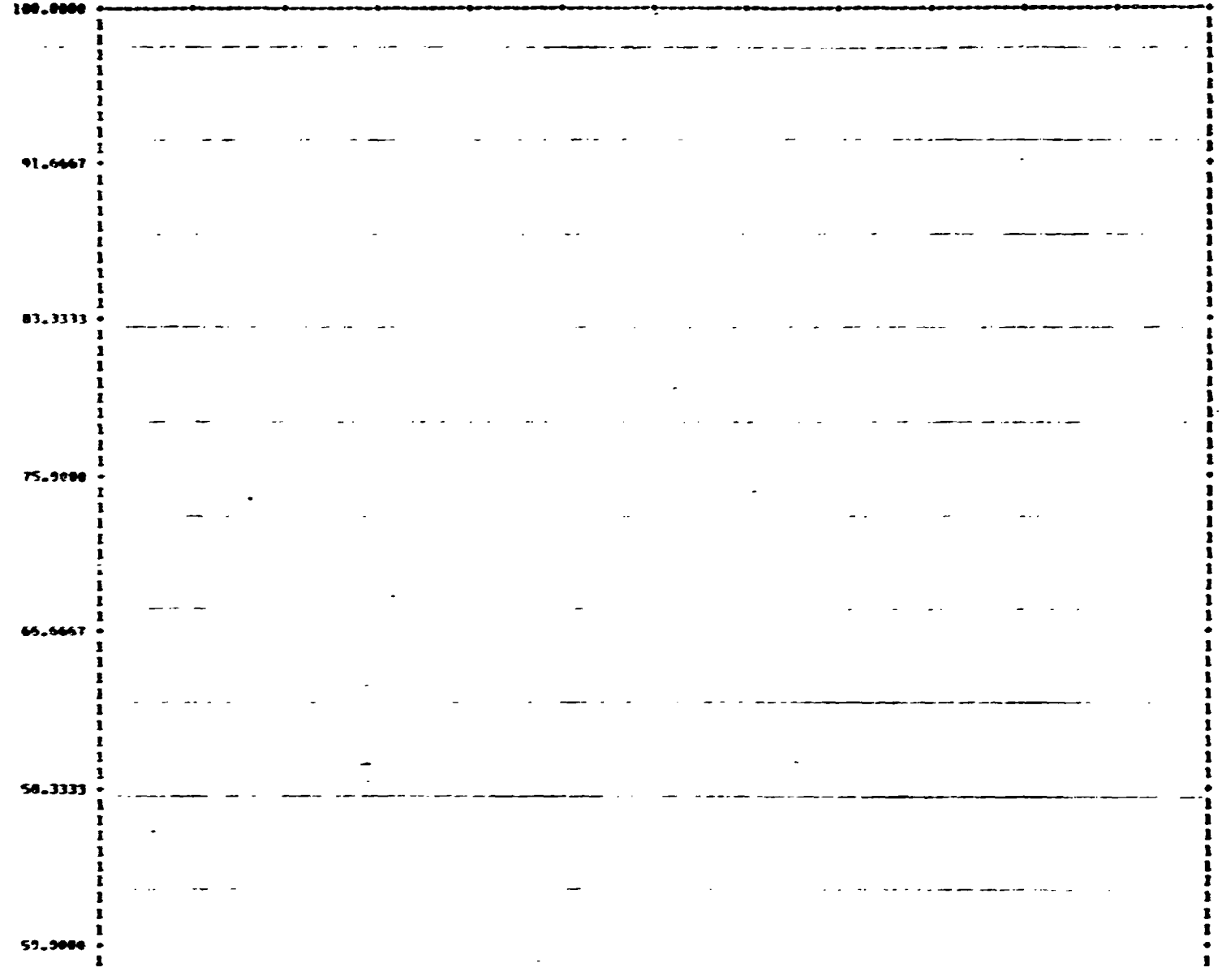

1.2500
1.2000
1.1500
1.1000
1.0500
1.0000
0.000
.750
1.500
2.250
3.000
3.750
4.500
5.250
6.000
6.750
7.500
8.250
SP. GRAV. (STAGE) VS TIME (HOURS)


2.0000
1.9167
1.8333
1.7500
1.6667
1.5833
1.5000


1.4167
1.3333
1.2500
1.1667
1.0833
1.0000
0.000
.750
1.500
2.250
3.000
3.750
4.500
5.250
6.000
6.750
7.500
8.250
SP. GRAV. (STAGE) VS TIME (HOURS)


20000.
19167.
18333.
17500.
16667.
15833.
15000.


14167.
13333.
12500.
11667.
10833.
10000.0000
0.000
.750
1.500
2.250
3.000
3.750
4.500
5.250
6.000
6.750
7.500
8.250
SPENT ACID (LBS/HR) VS TIME (HOURS)

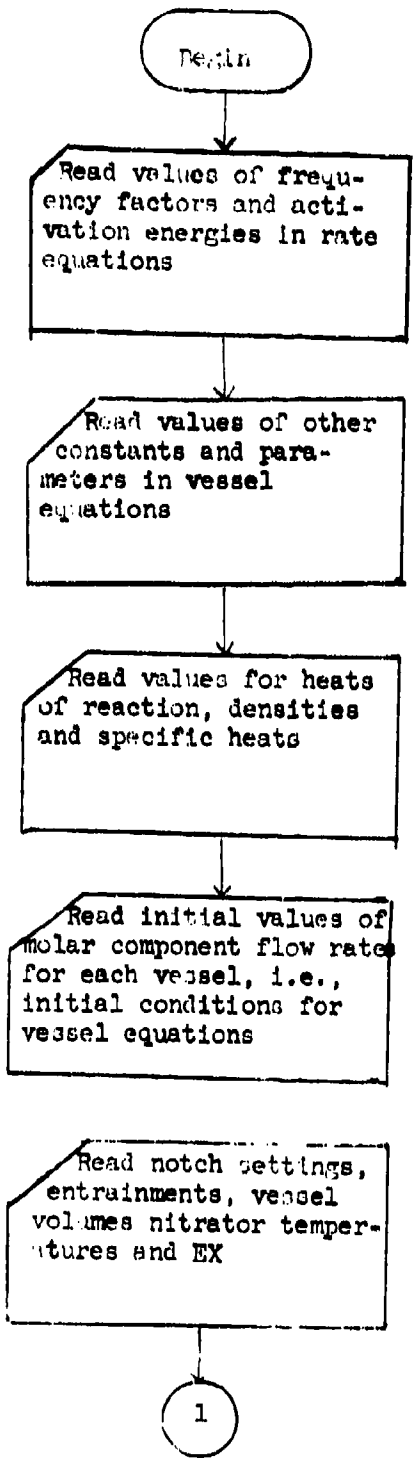

100.0000
91.6667
83.3333
75.0000
66.6667
50.3333
59.0000

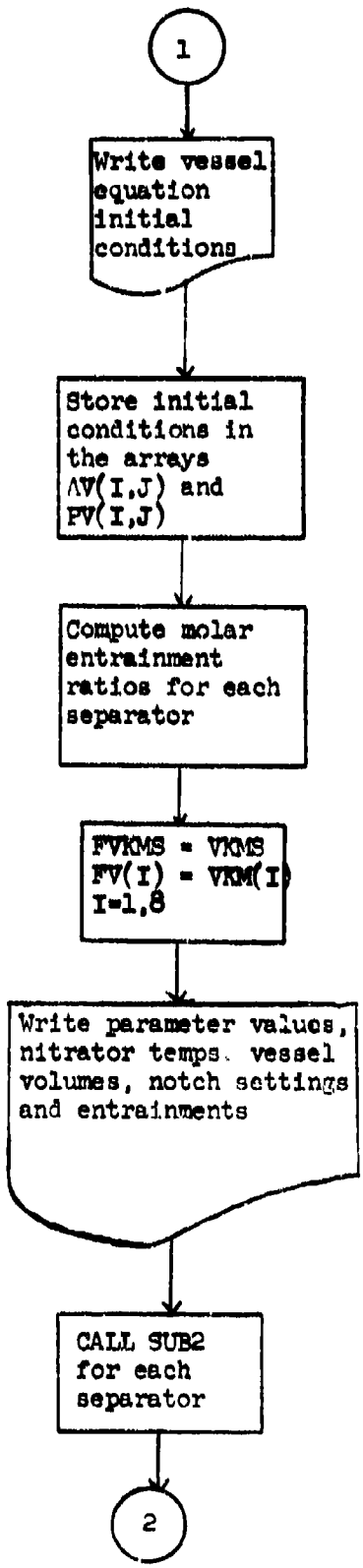
APPENDIX C

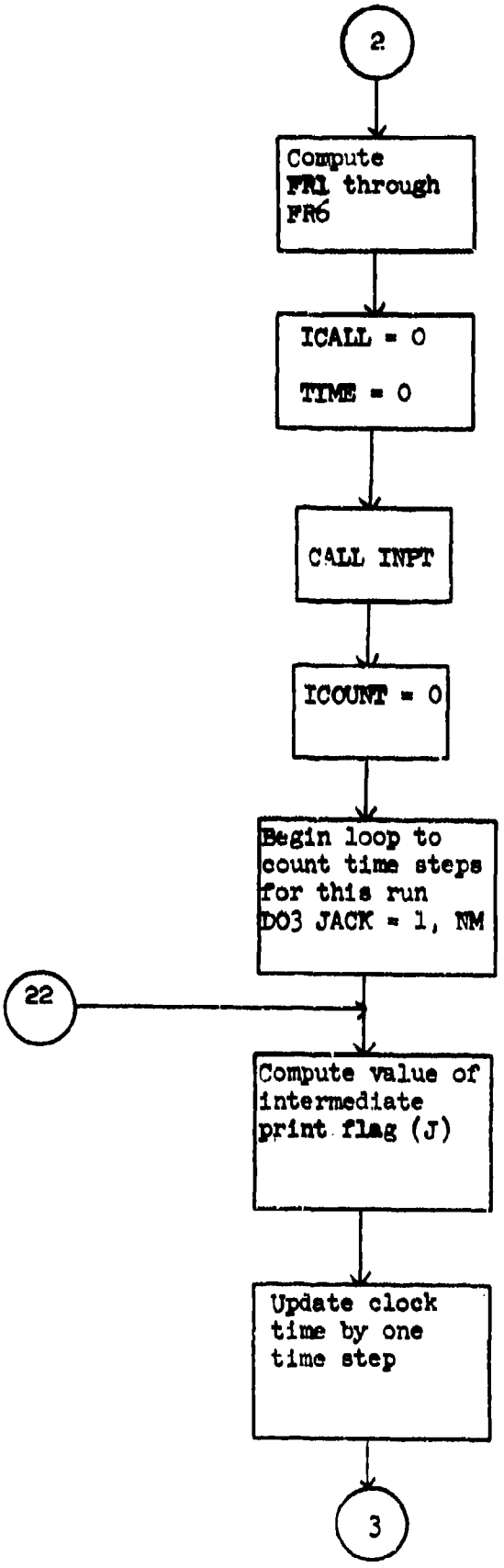
Dynamic Simulation--Program Flowchart

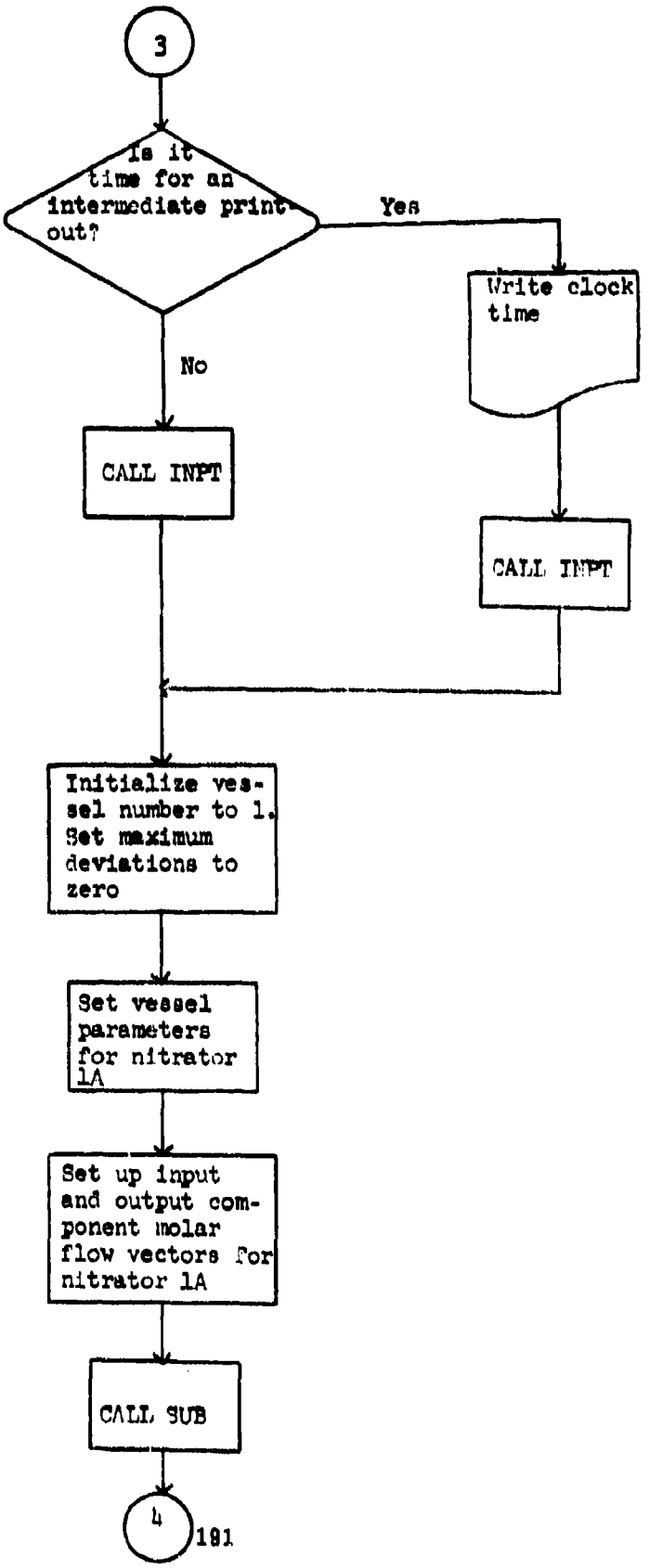
Preceding page blank

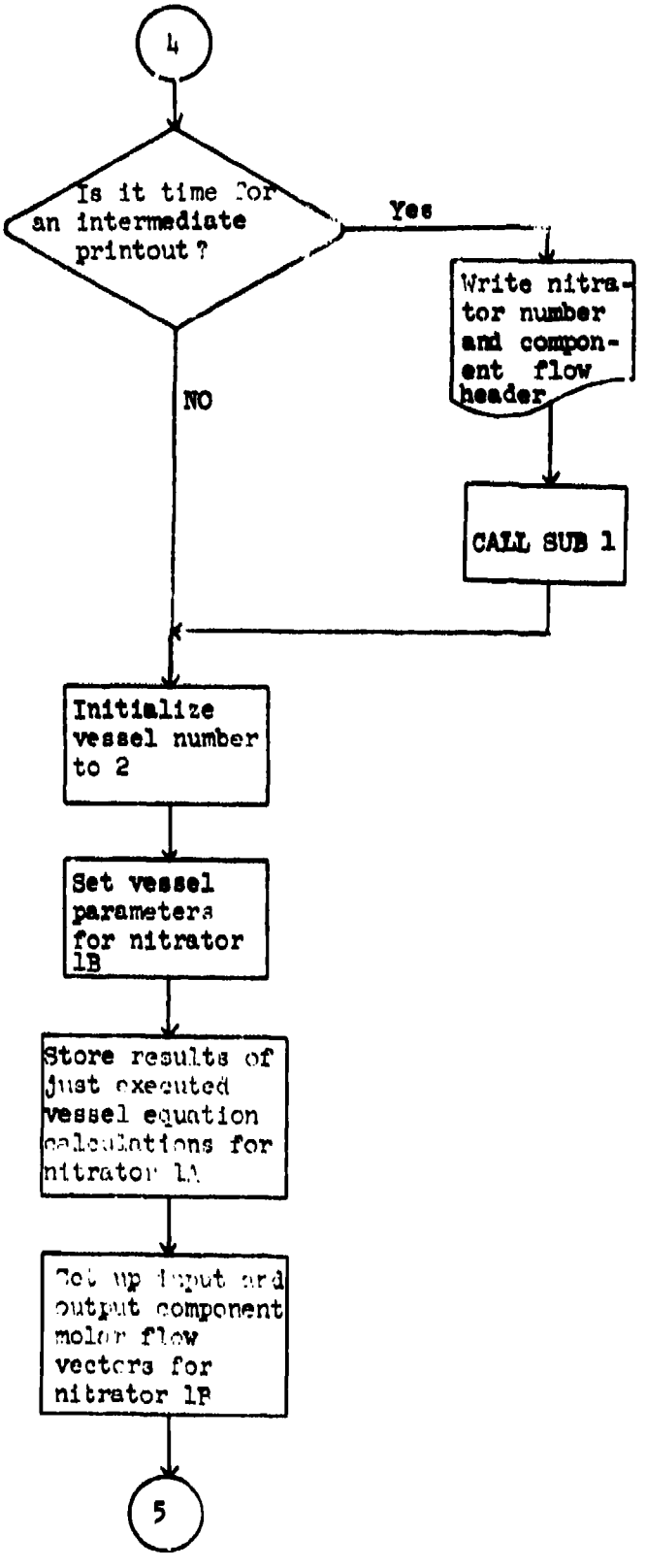
Main Program

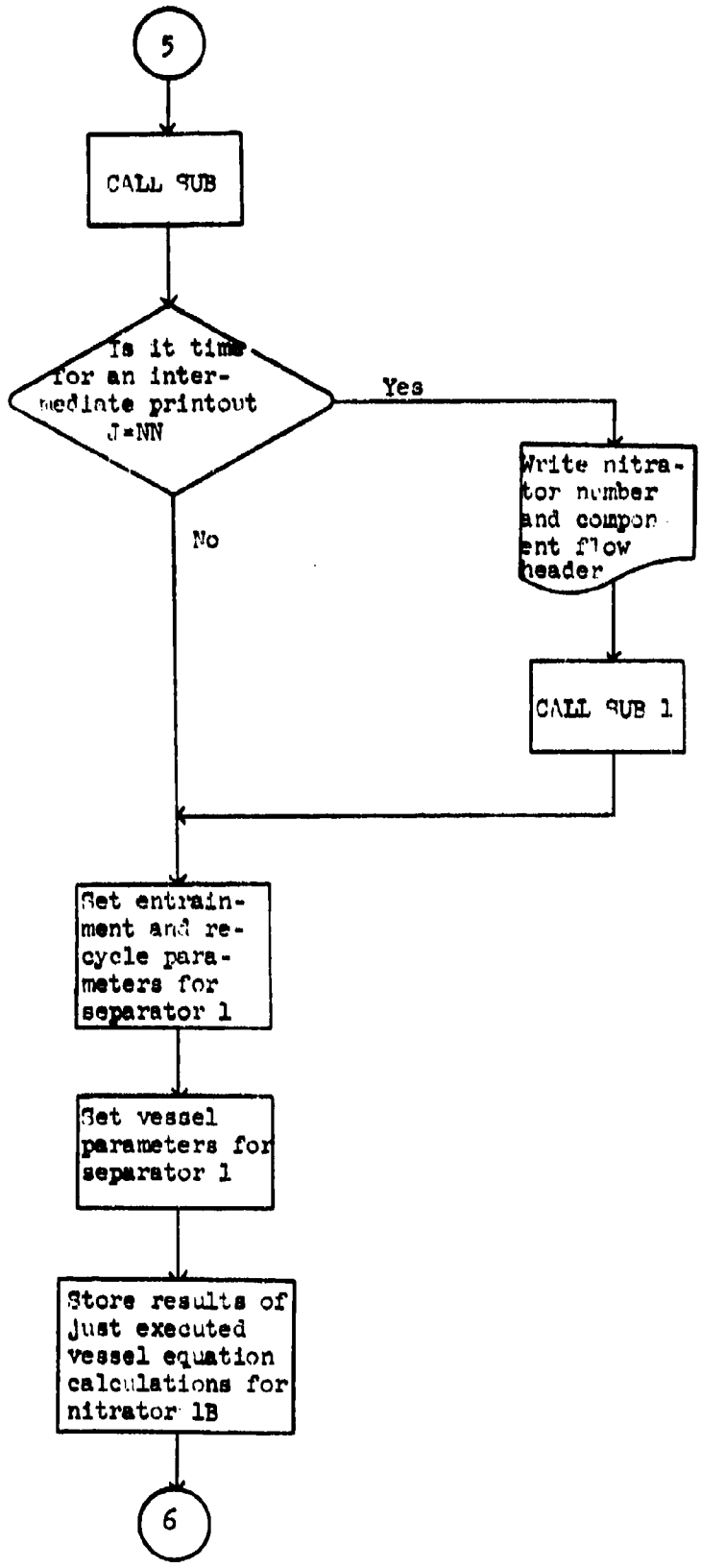


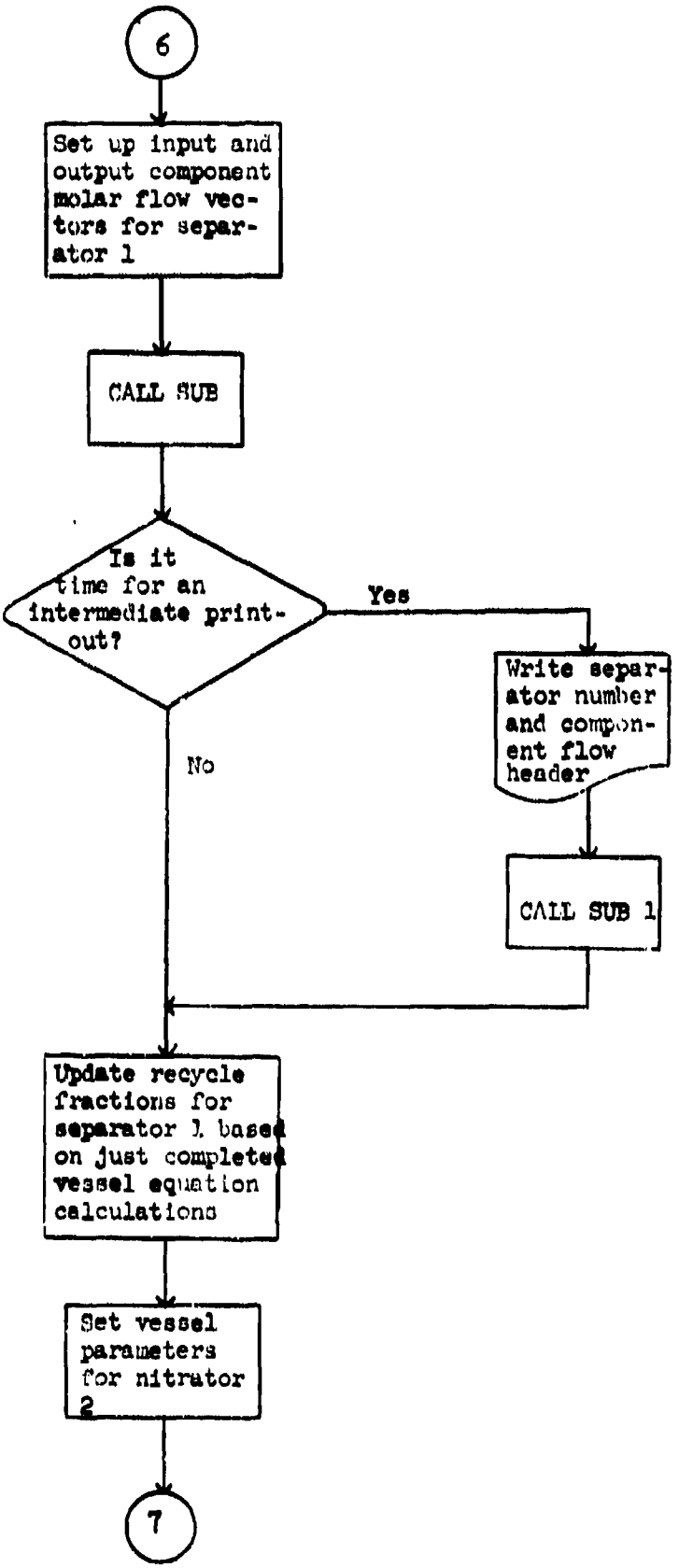

1
Write vessel equation initial conditions
Store initial conditions in the arrays AV(I,J) and PV(I,J)
Compute molar entrainment ratios for each separator
FVKMS = VKMS
FV(I) = VKM(I)
I=1,8
Write parameter values, nitrator temps. vessel volumes, notch settings and entrainments
CALL SUB2 for each separator
2

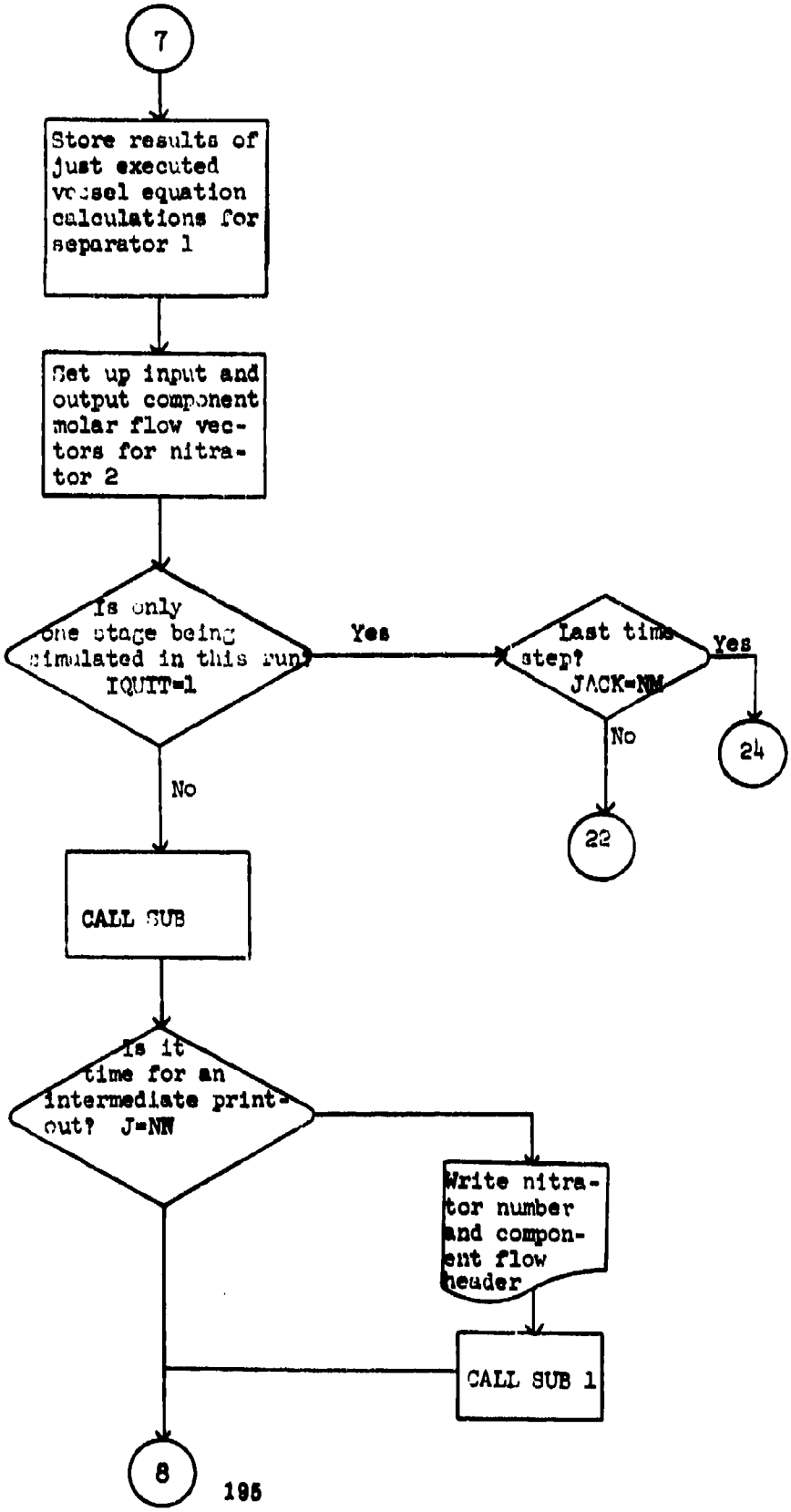

2
Compute FR1 through FR6
ICALL = 0
TIME = 0
CALL INPT
ICOUNT = 0
Begin loop to count time steps for this run
DO3 JACK = 1, NM
22
Compute value of intermediate print flag (J)
Update clock time by one time step
3

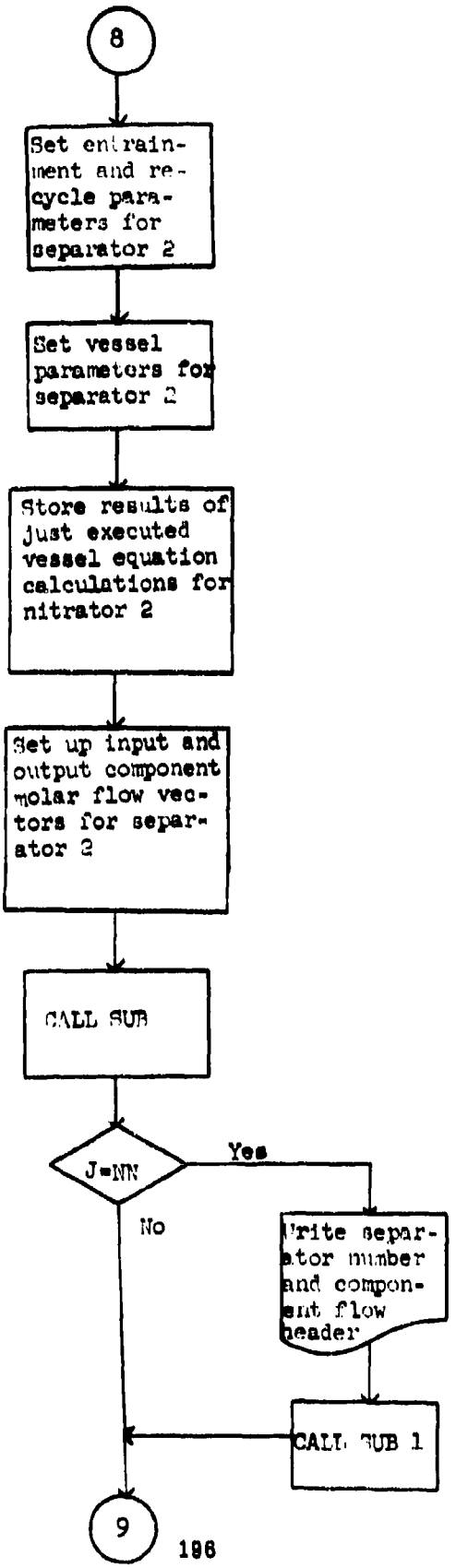

3
Is it time for an intermediate print-out?
Yes
No
Write clock time
CALL INPT
CALL INPT
Initialize vessel number to 1. Set maximum deviations to zero
Set vessel parameters for nitrator 1A
Set up input and output component molar flow vectors for nitrator 1A
CALL SUB
4

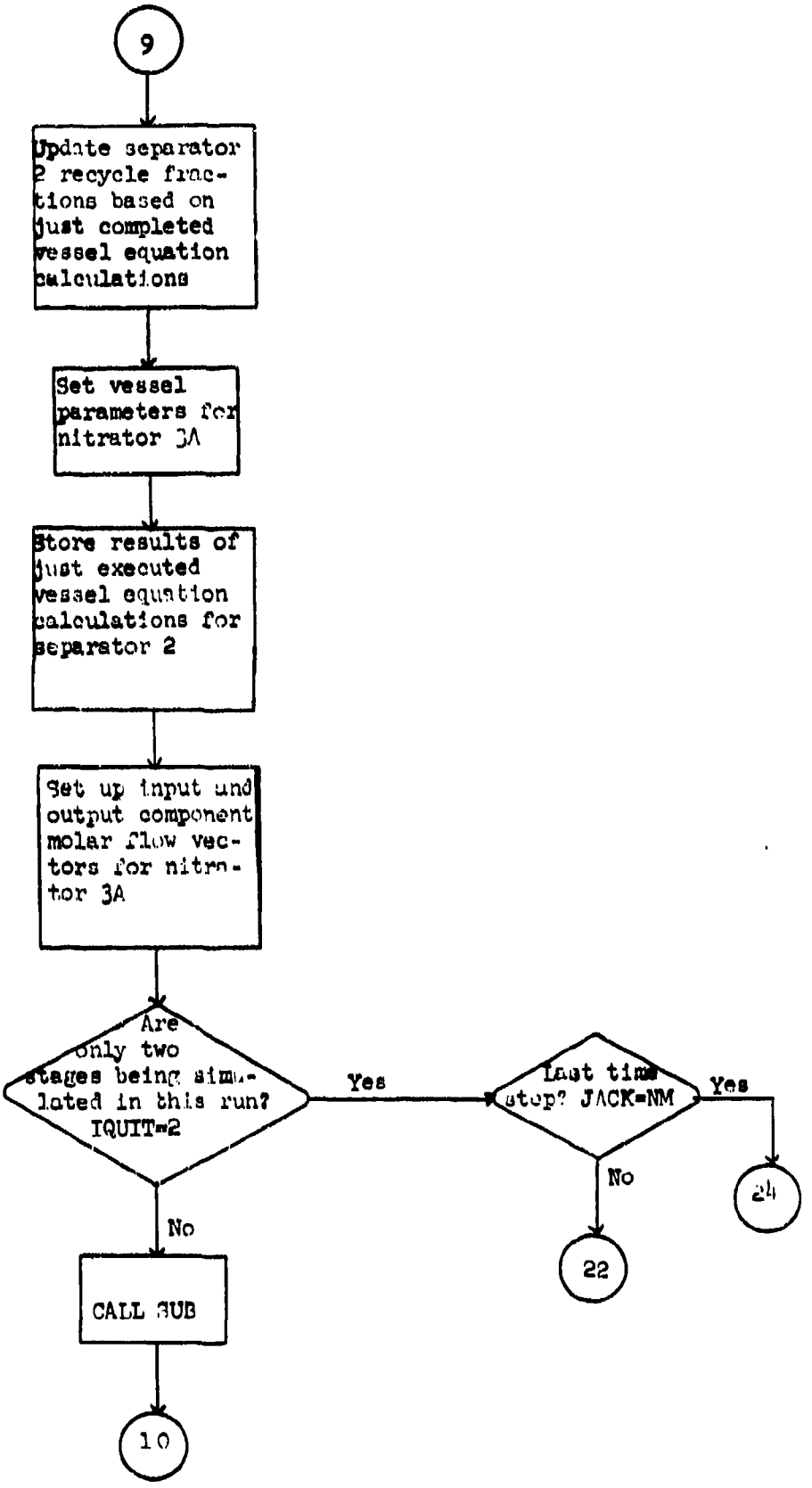

4
Is it time for an intermediate printout ?
Yes
NO
Write nitrator number and component flow header
CALL SUB 1
Initialize vessel number to 2
Set vessel parameters for nitrator 1B
Store results of just executed vessel equation calculations for nitrator 1A
Set up input and output component molar flow vectors for nitrator 1B
5

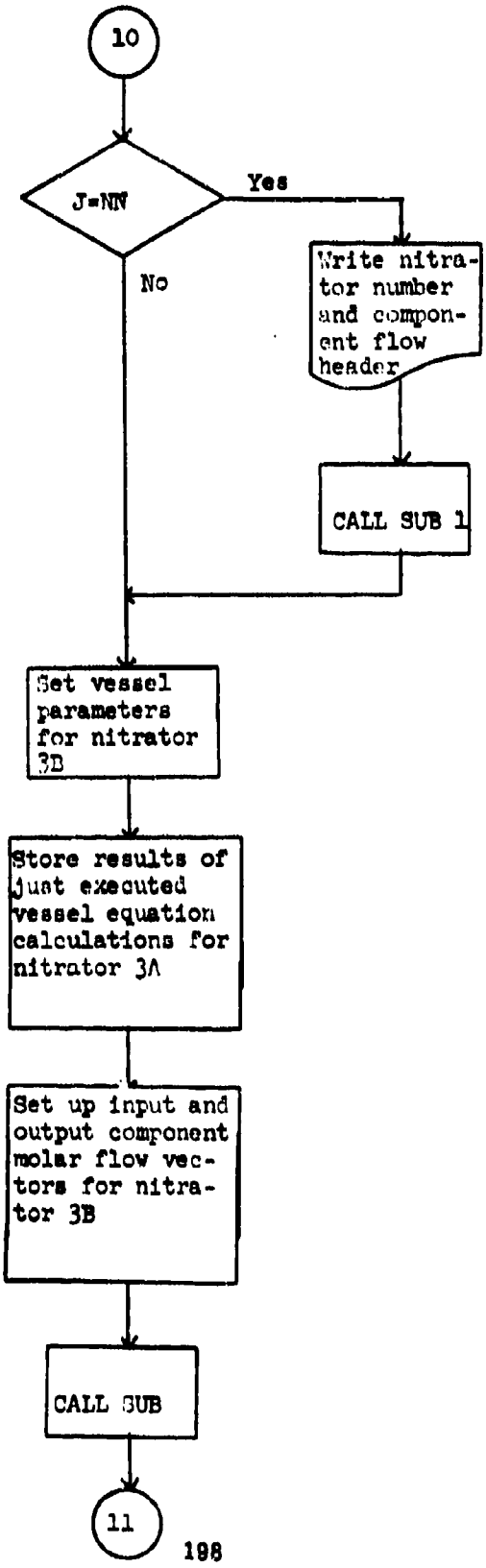

5
CALL SUB
Is it time for an intermediate printout J=NN
Yes
No
Write nitrator number and component flow header
CALL SUB 1
Get entrainment and recycle parameters for separator 1
Get vessel parameters for separator 1
Store results of just executed vessel equation calculations for nitrator 1B
6

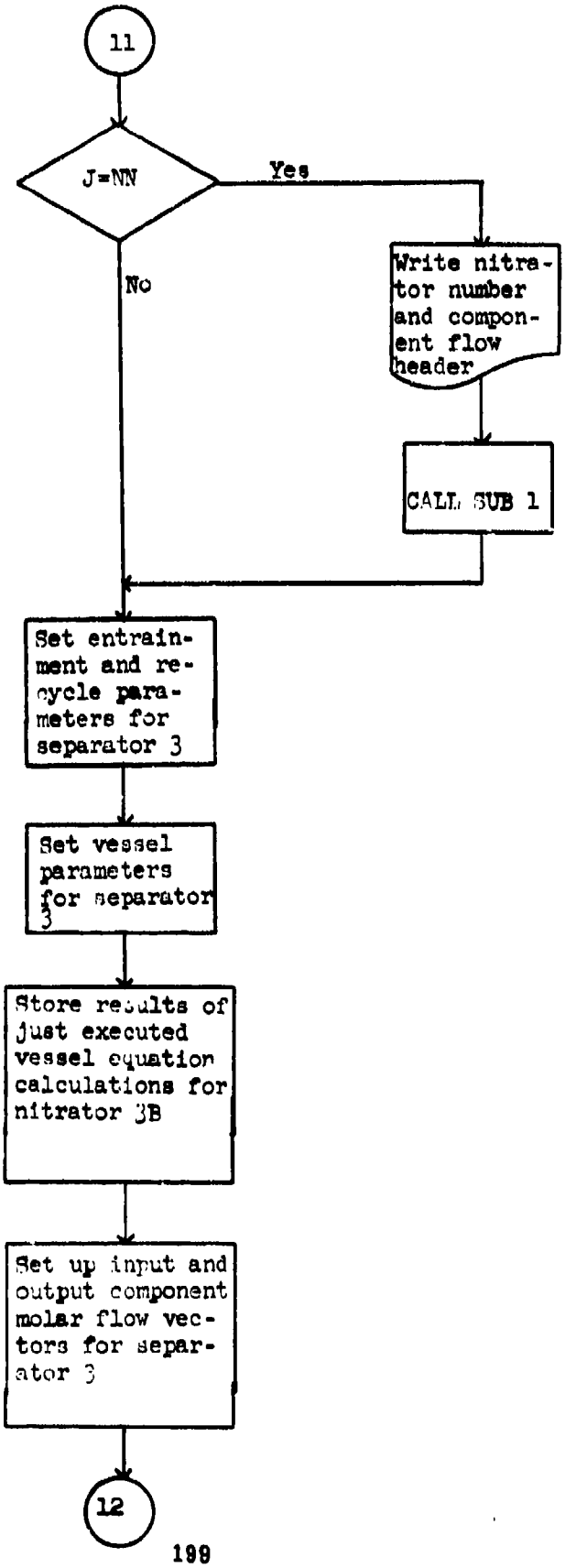

6
Set up input and output component molar flow vectors for separator 1
CALL SUB
Is it time for an intermediate print-out?
Yes
No
Write separator number and component flow header
CALL SUB 1
Update recycle fractions for separator 1 based on just completed vessel equation calculations
Set vessel parameters for nitrator 2
7

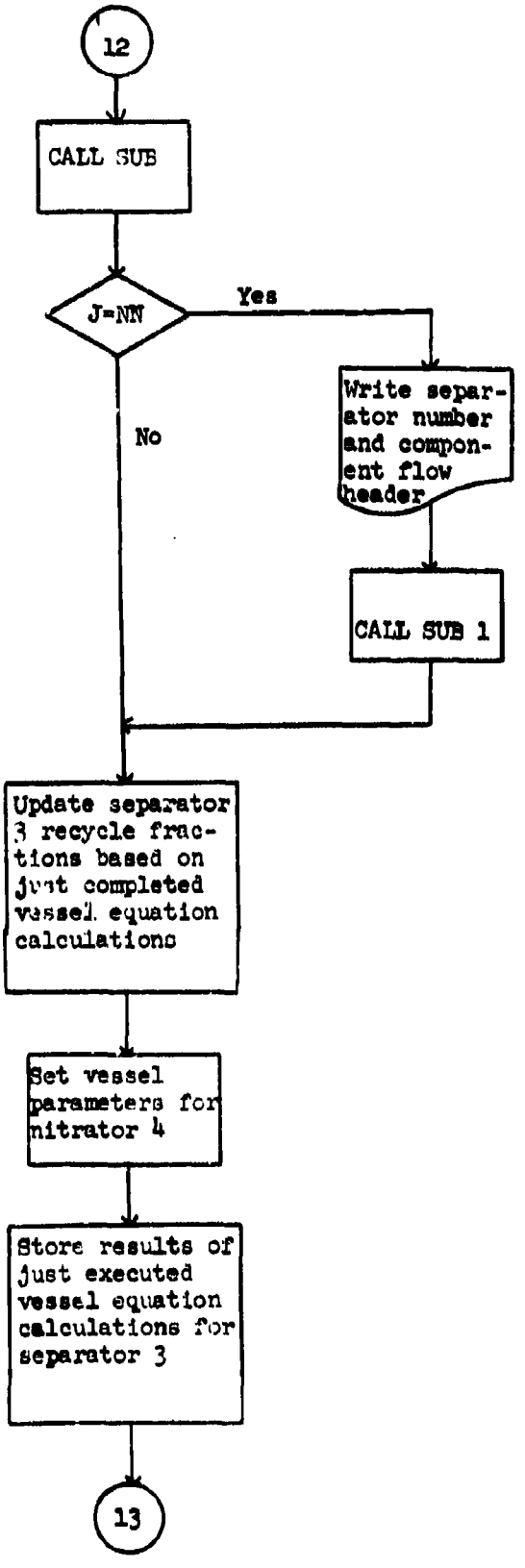

7
Store results of just executed vessel equation calculations for separator 1
Set up input and output component molar flow vectors for nitrator 2
Is only one stage being simulated in this run? IQUIT=1
Yes
Last time step? JACK=NM
Yes
No
24
22
No
CALL SUB
Is it time for an intermediate print-out? J=NN
Write nitrator number and component flow header
CALL SUB 1
8

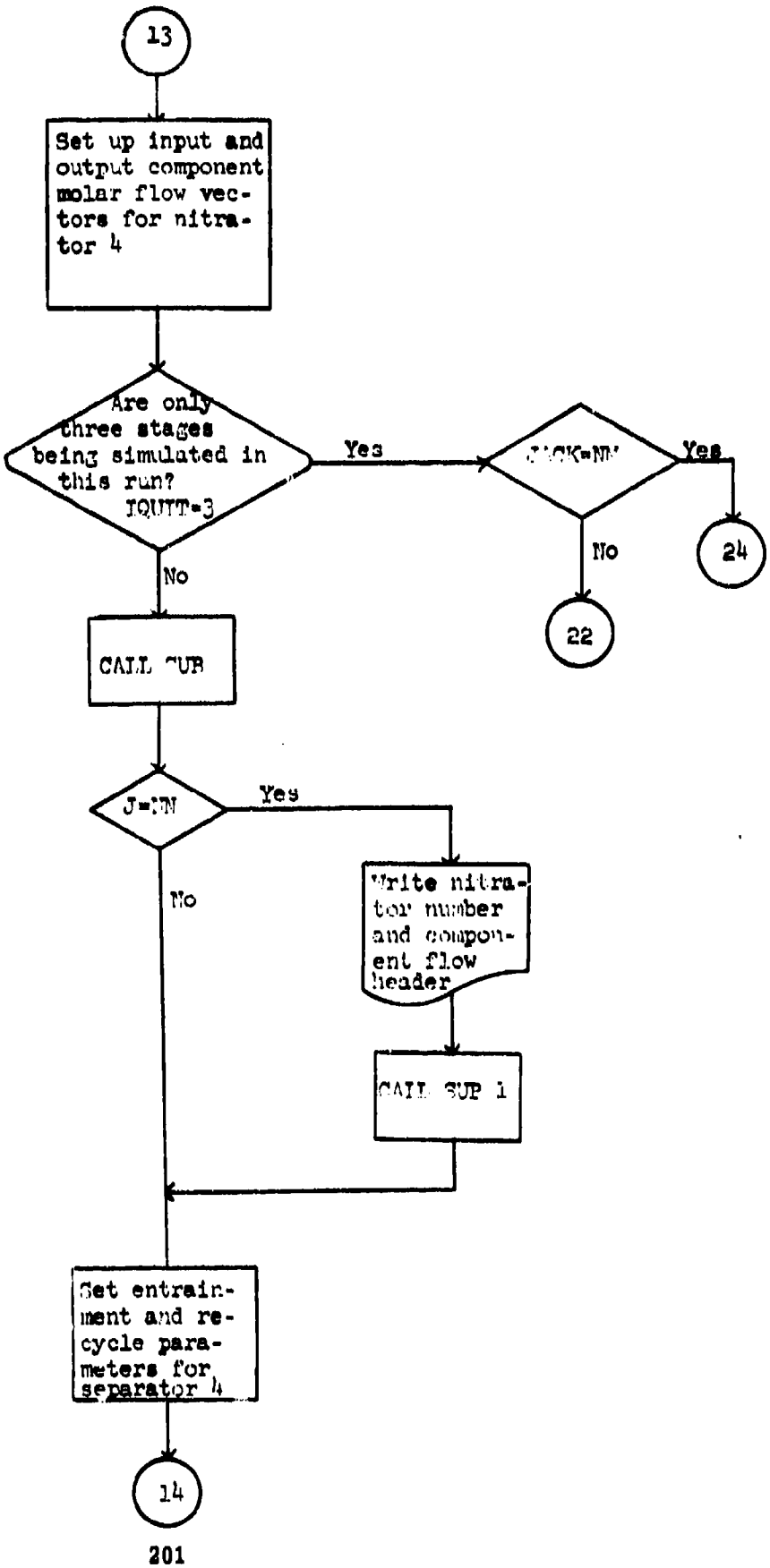

8
Set entrainment and recycle parameters for separator 2
Set vessel parameters for separator 2
Store results of just executed vessel equation calculations for nitrator 2
Set up input and output component molar flow vectors for separator 2
CALL SUB
J=NN
Yes
No
Write separator number and component flow header
CALL SUB 1
9

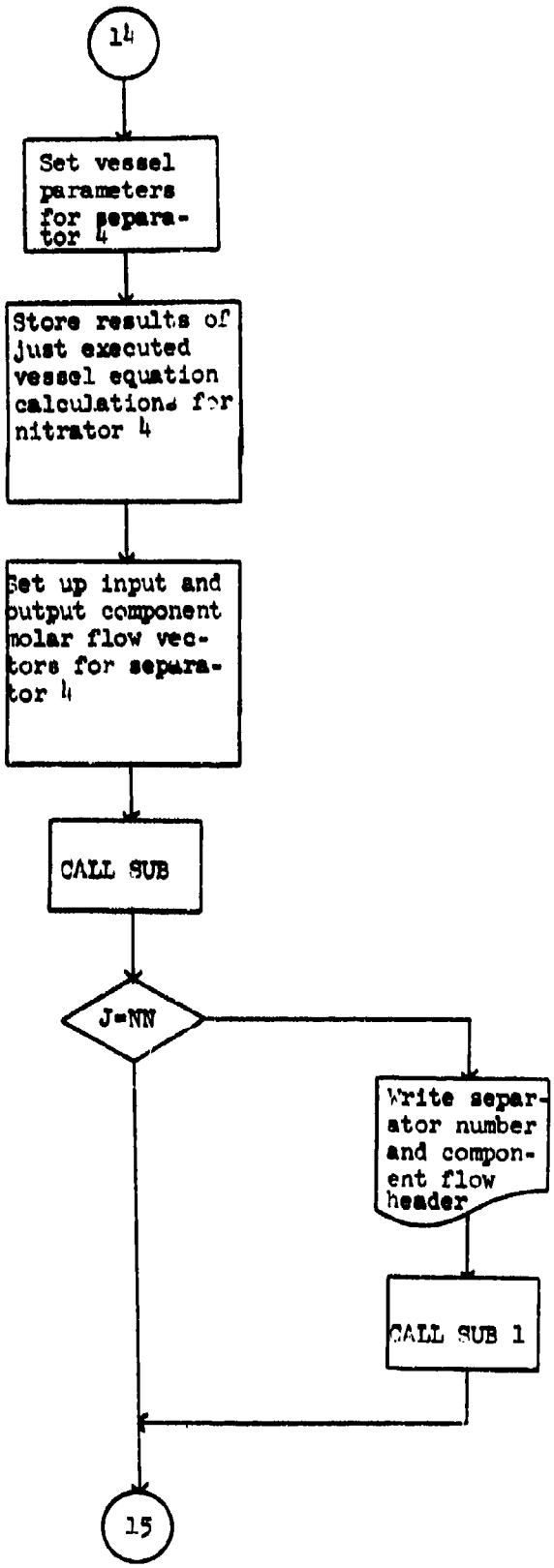

9
Update separator 2 recycle fractions based on just completed vessel equation calculations
Set vessel parameters for nitrator 3A
Store results of just executed vessel equation calculations for separator 2
Set up input and output component molar flow vectors for nitrator 3A
Are only two stages being simulated in this run? IQUIT=2
Yes
Last time step? JACK=NM
Yes
No
24
No
22
CALL SUB
10

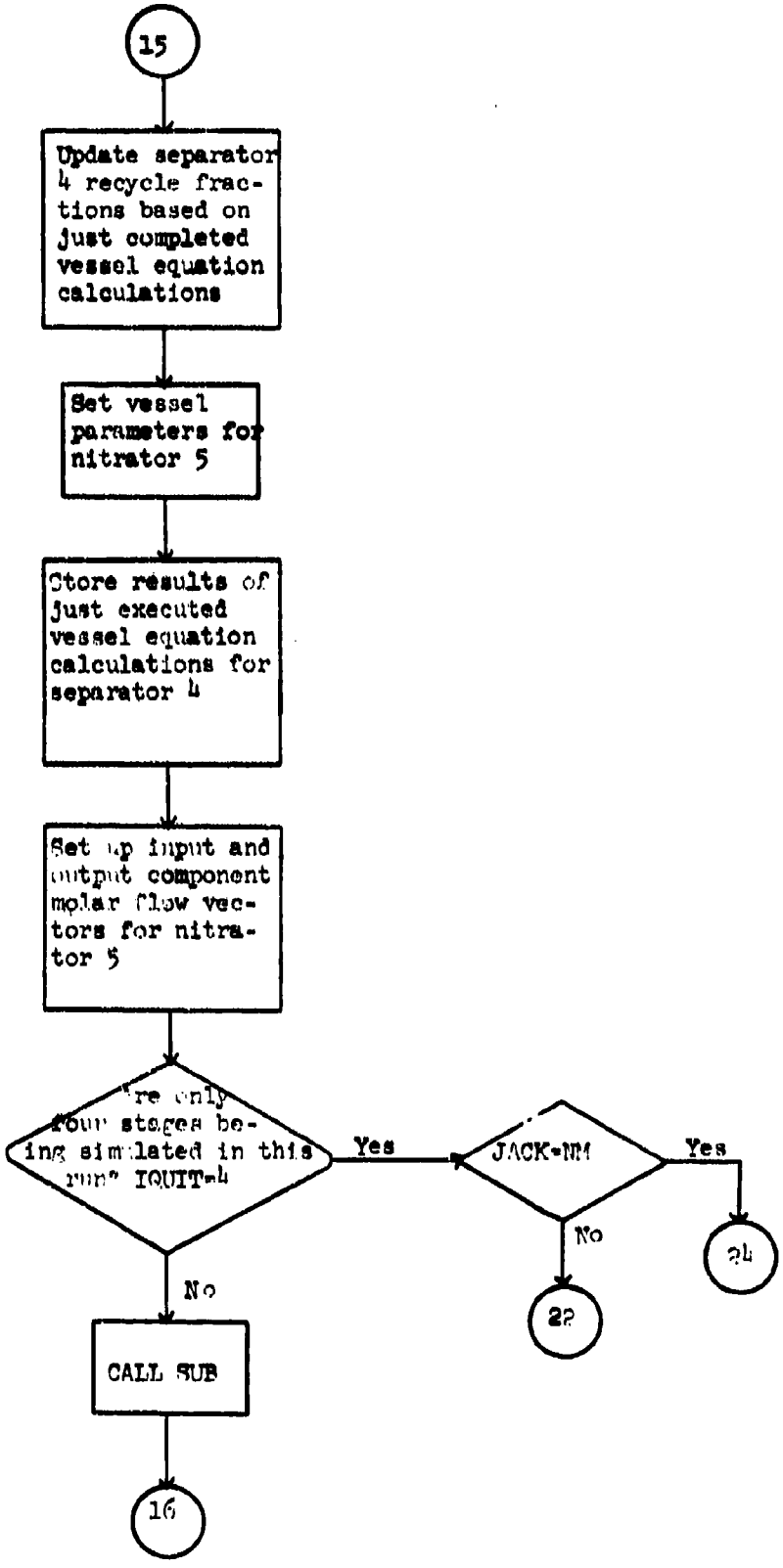

10
J=NN
Yes
No
Write nitrator number and component flow header
CALL SUB 1
Set vessel parameters for nitrator 3B
Store results of just executed vessel equation calculations for nitrator 3A
Set up input and output component molar flow vectors for nitrator 3B
CALL SUB
11

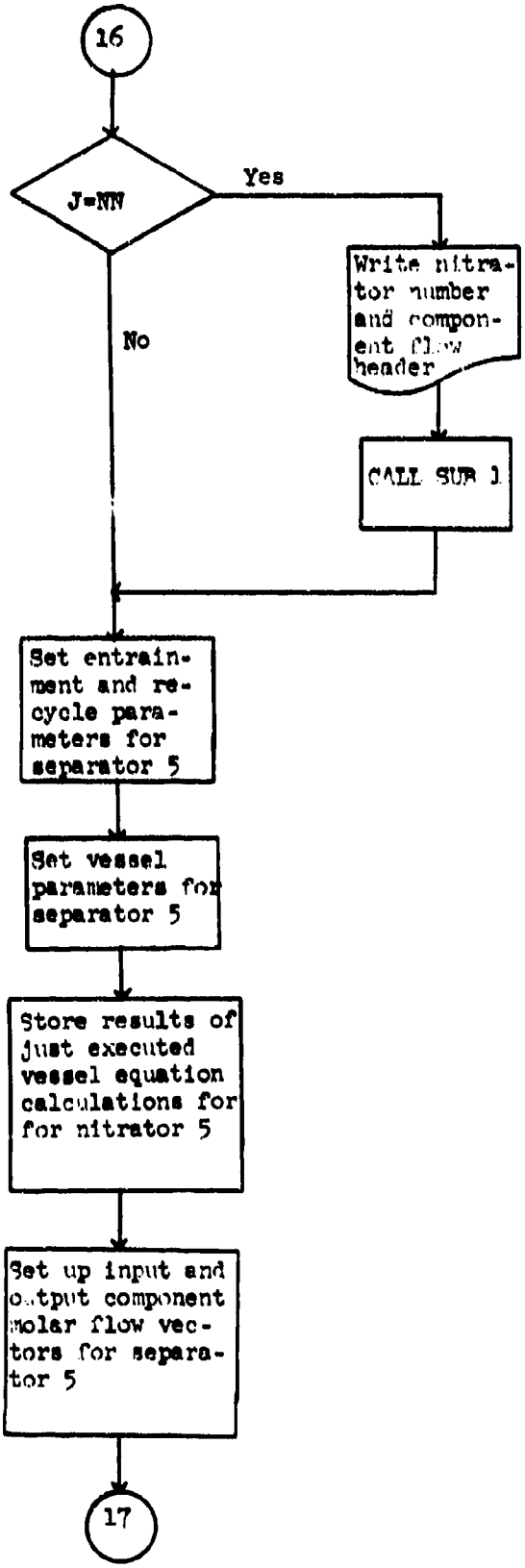

11
J=NN
Yes
No
Write nitrator number and component flow header
CALL SUB 1
Set entrainment and recycle parameters for separator 3
Set vessel parameters for separator 3
Store results of just executed vessel equation calculations for nitrator 3B
Set up input and output component molar flow vectors for separator 3
12

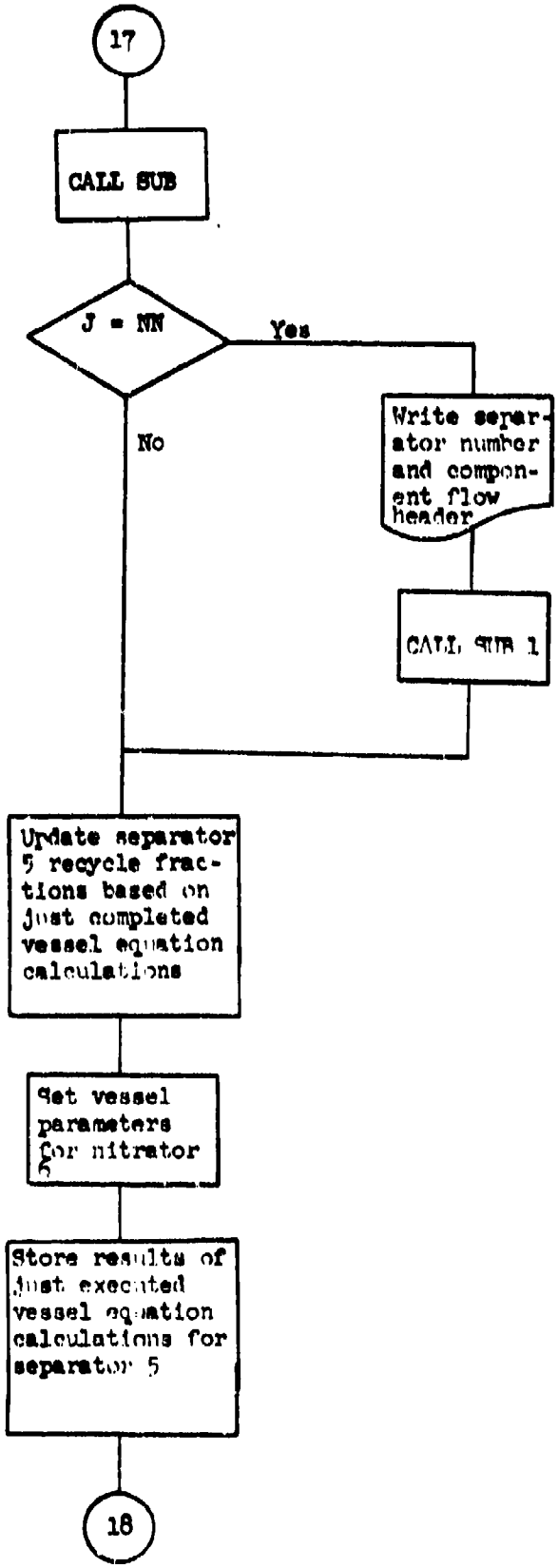

12
CALL SUB
J=NN
Yes
No
Write separator number and component flow header
CALL SUB 1
Update separator 3 recycle fractions based on just completed vessel equation calculations
Set vessel parameters for nitrator 4
Store results of just executed vessel equation calculations for separator 3
13

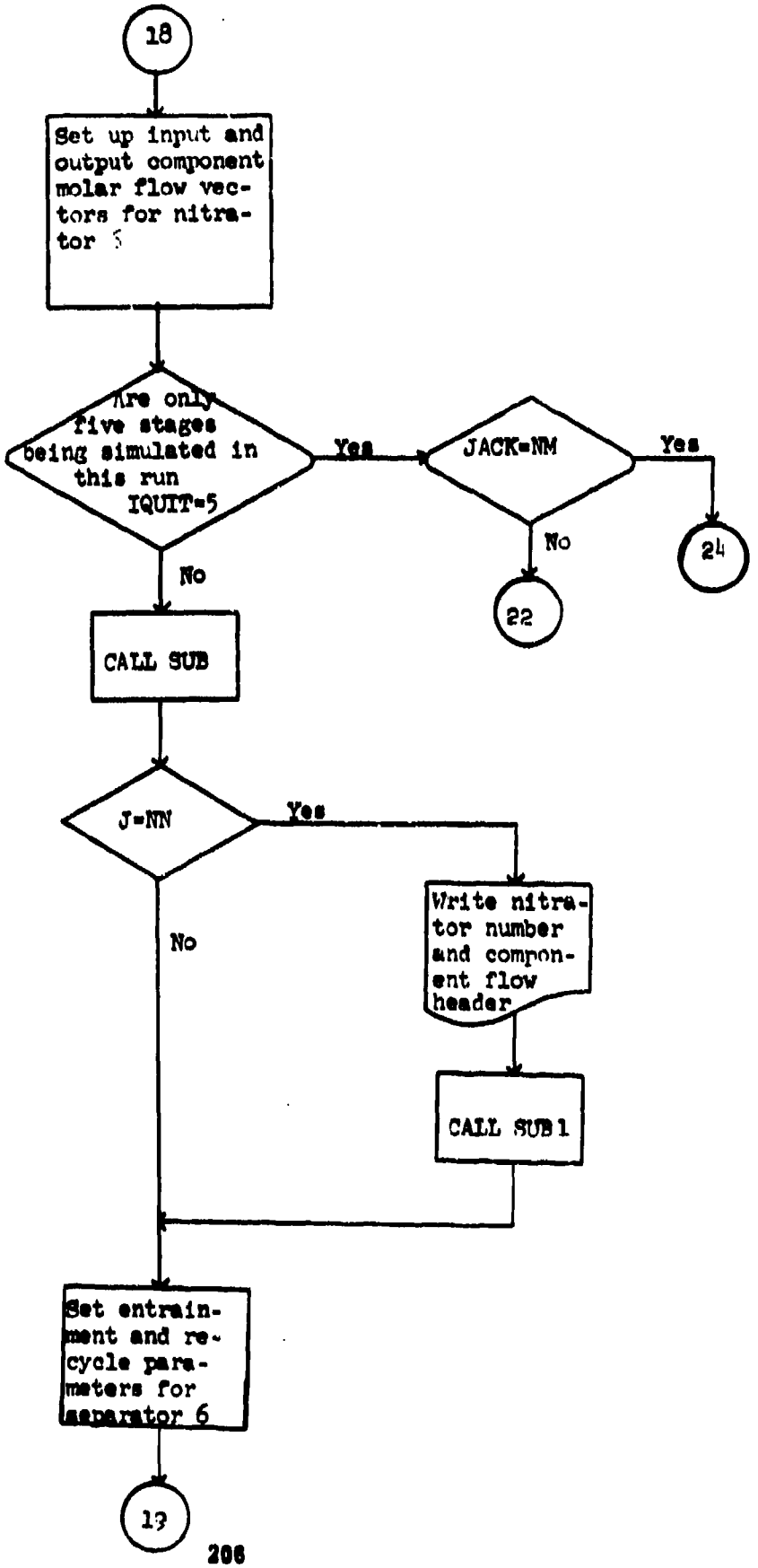

13
Set up input and output component molar flow vectors for nitrator 4
Are only three stages being simulated in this run? IQUIT=3
Yes
No
Yes
No
24
22
CALL SUB
J=JN
Yes
No
Write nitrator number and component flow header
CALL SUP 1
Set entrainment and recycle parameters for separator 4
14

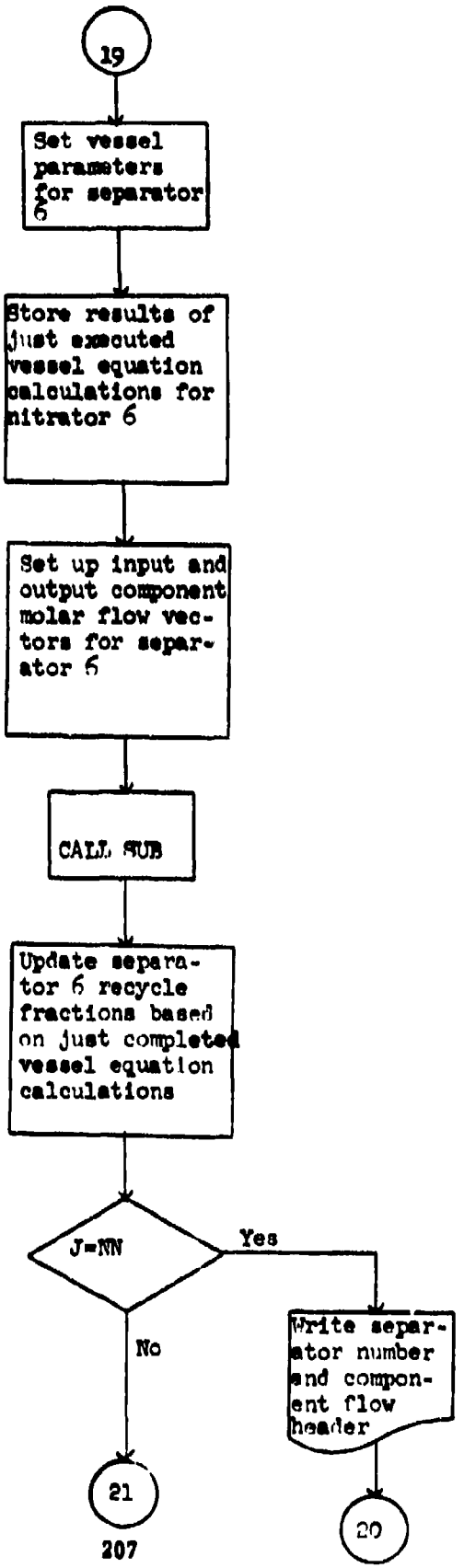

14
Set vessel parameters for separator 4
Store results of just executed vessel equation calculations for nitrator 4
Set up input and output component molar flow vectors for separator 4
CALL SUB
J=NN
Write separator number and component flow header
CALL SUB 1
15

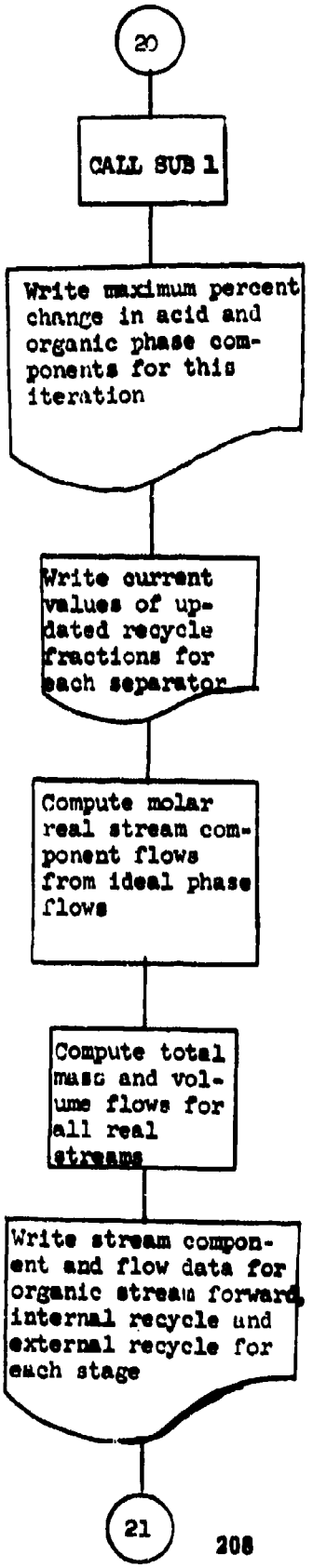

15
Update separator 4 recycle fractions based on just completed vessel equation calculations
Set vessel parameters for nitrator 5
Store results of just executed vessel equation calculations for separator 4
Set up input and output component molar flow vectors for nitrator 5
Are only four stages being simulated in this run? IQUIT=4
Yes
JACK=NN
Yes
No
24
22
No
CALL SUB
16

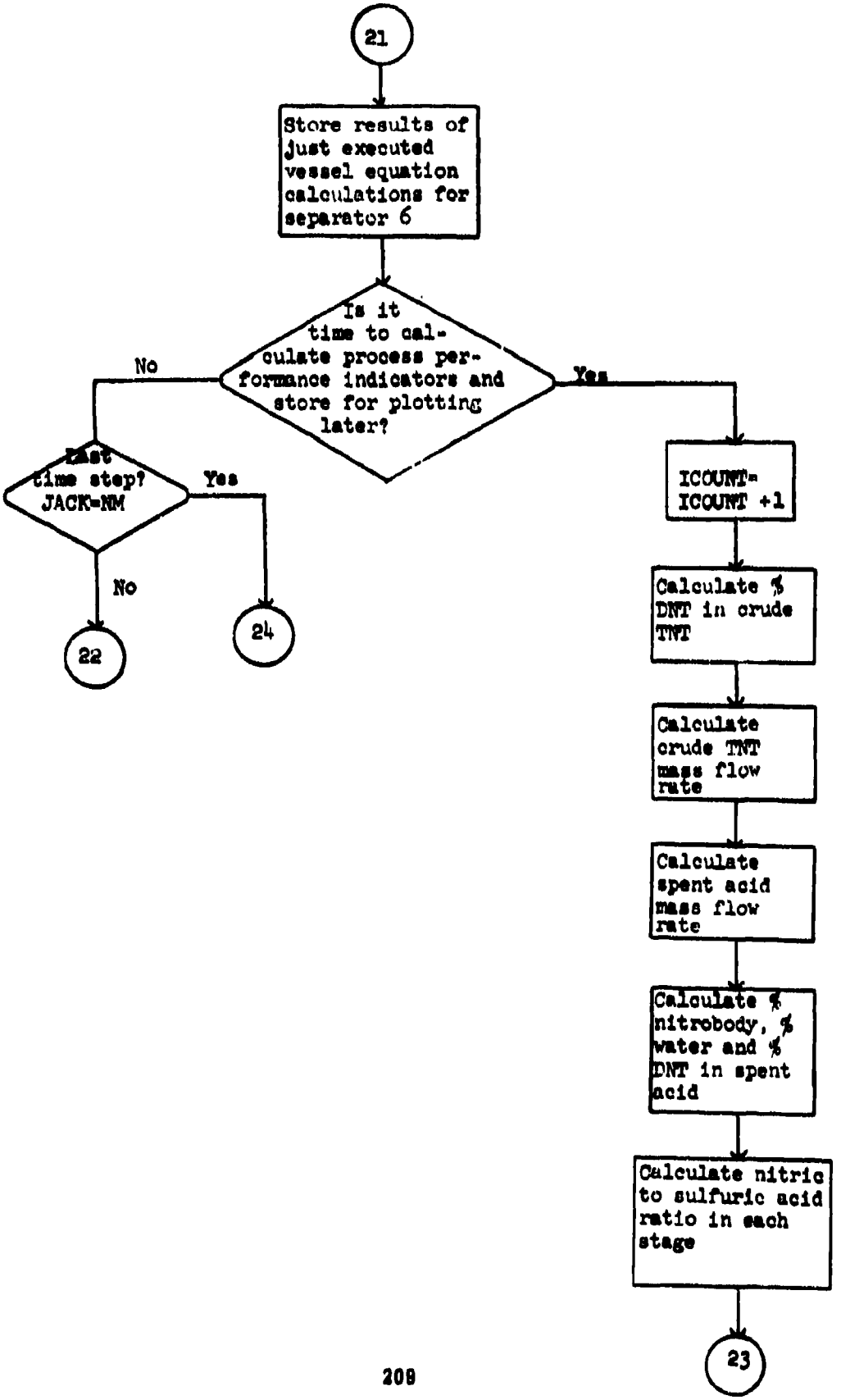

16
J=NN
Yes
No
Write nitrator number and component flow header
CALL SUB 1
Set entrainment and recycle parameters for separator 5
Set vessel parameters for separator 5
Store results of just executed vessel equation calculations for for nitrator 5
Set up input and output component molar flow vectors for separator 5
17

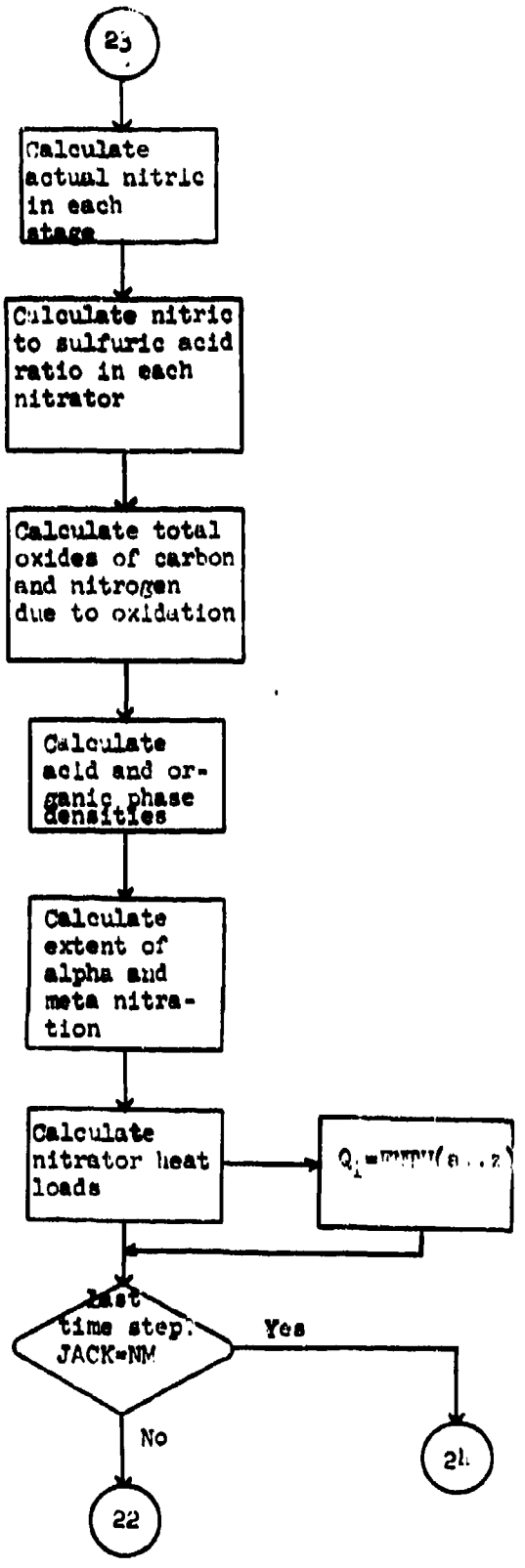

17
CALL SUB
J = NN
Yes
No
Write separator number and component flow header
CALL SUB 1
Update separator 5 recycle fractions based on just completed vessel equation calculations
Set vessel parameters for nitrator 5
Store results of just executed vessel equation calculations for separator 5
18

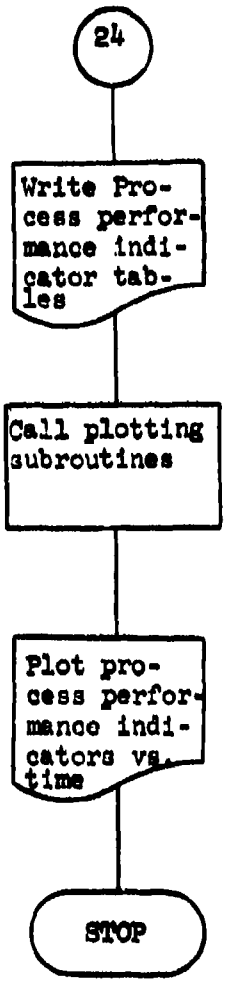

18
Set up input and output component molar flow vectors for nitrator 5
Are only five stages being simulated in this run IQUIT=5
Yes
JACK=NM
Yes
No
24
22
No
CALL SUB
J=NN
Yes
Write nitrator number and component flow header
No
CALL SUB1
Set entrainment and recycle parameters for separator 6
13


19
Set vessel parameters for separator 6
Store results of just executed vessel equation calculations for nitrator 6
Set up input and output component molar flow vectors for separator 6
CALL SUB
Update separator 6 recycle fractions based on just completed vessel equation calculations
J=NN
Yes
No
Write separator number and component flow header
21
20

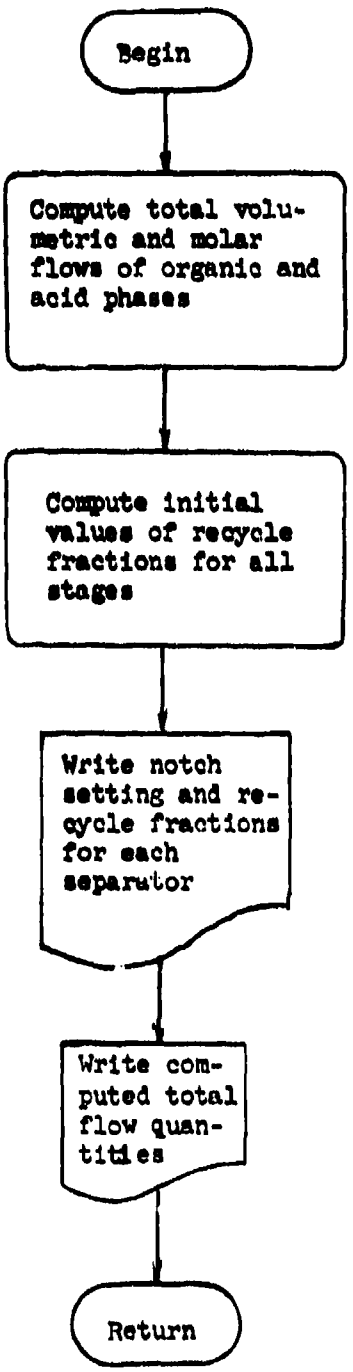

20
CALL SUB 1
Write maximum percent change in acid and organic phase components for this iteration
Write current values of updated recycle fractions for each separator
Compute molar real stream component flows from ideal phase flows
Compute total mass and volume flows for all real streams
Write stream component and flow data for organic stream forward, internal recycle and external recycle for each stage
21


21
Store results of just executed vessel equation calculations for separator 6
Is it time to calculate process performance indicators and store for plotting later?
No
Yes
Last time step? JACK=NM
Yes
No
22
24
ICOUNT= ICOUNT +1
Calculate % DNT in crude TNT
Calculate crude TNT mass flow rate
Calculate spent acid mass flow rate
Calculate % nitrobody, % water and % DNT in spent acid
Calculate nitric to sulfuric acid ratio in each stage
23

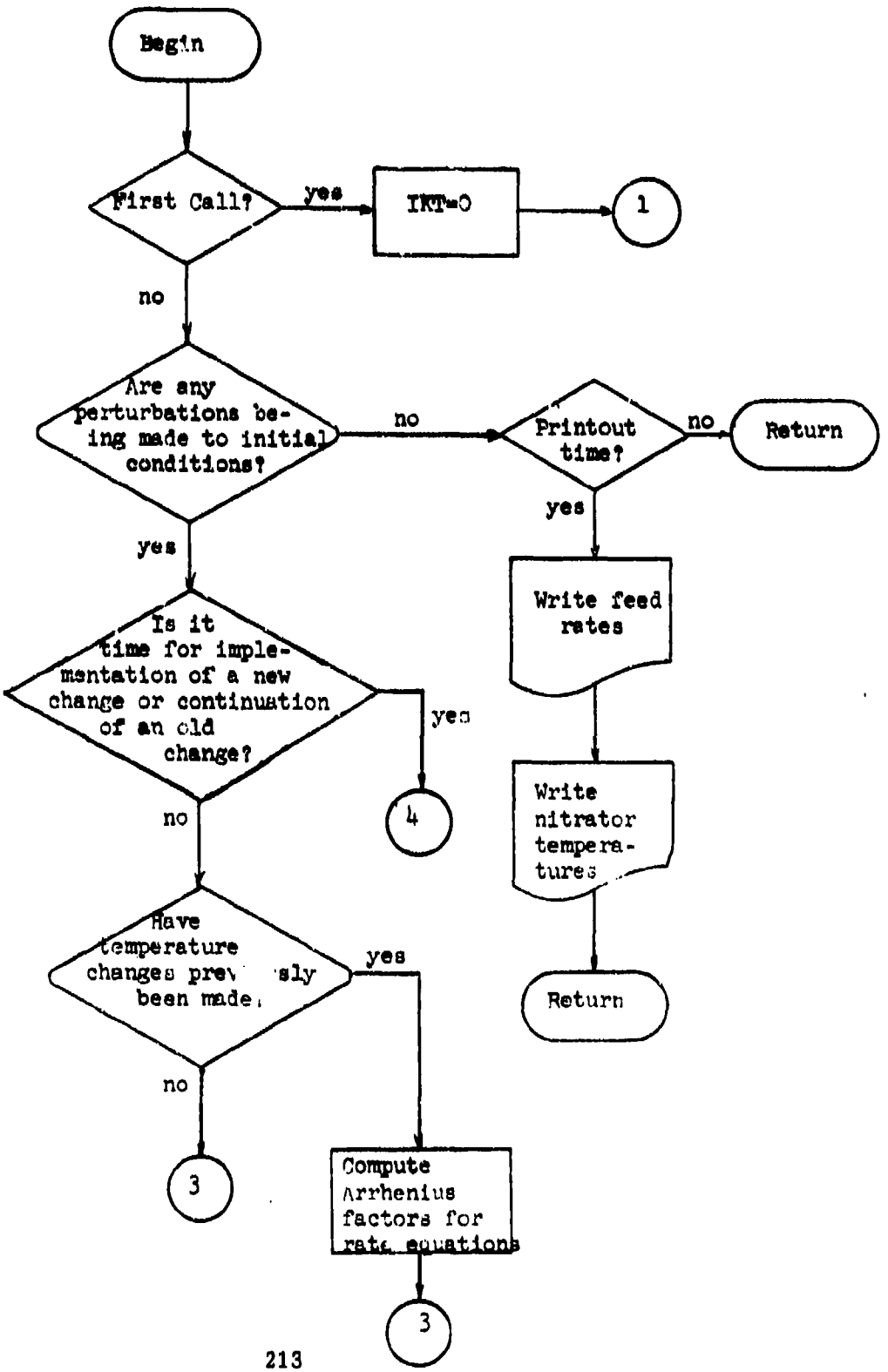

23
Calculate actual nitric in each stage
Calculate nitric to sulfuric acid ratio in each nitrator
Calculate total oxides of carbon and nitrogen due to oxidation
Calculate acid and organic phase densities
Calculate extent of alpha and meta nitration
Calculate nitrator heat loads
Last time step: JACK=NM
Yes
No
21
22

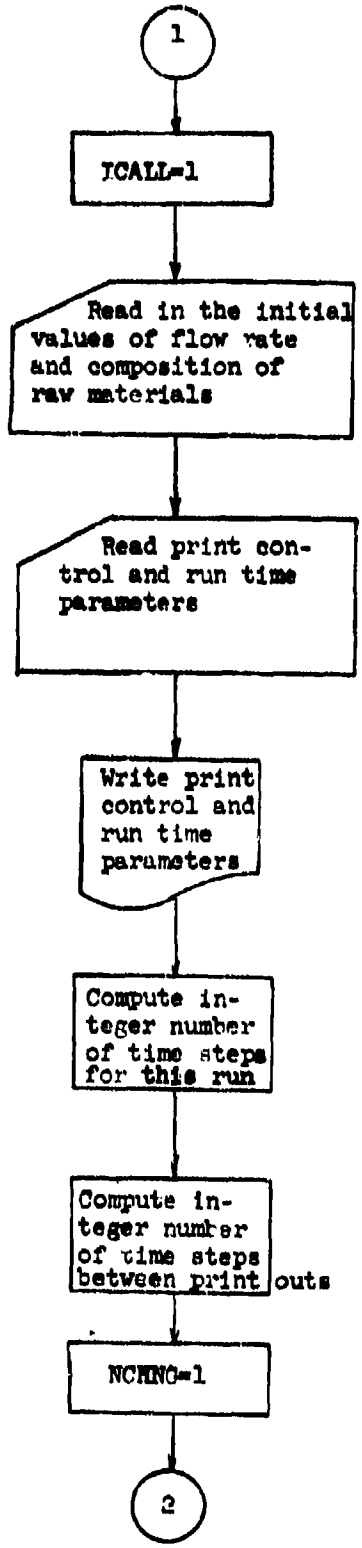

24
Write Process performance indicator tables
Call plotting subroutines
Plot process performance indicators vs. time
STOP

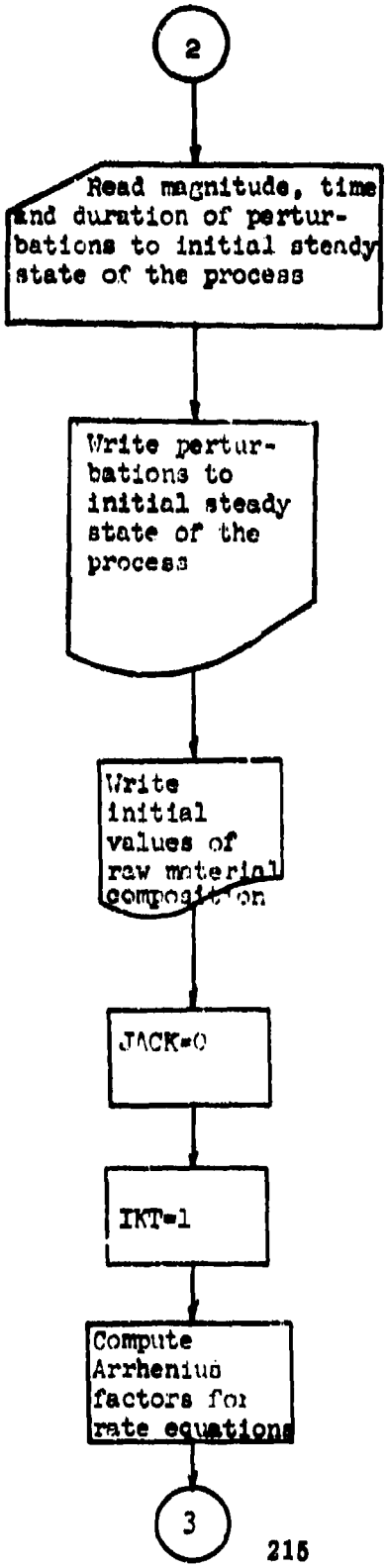
Subroutine SUB2

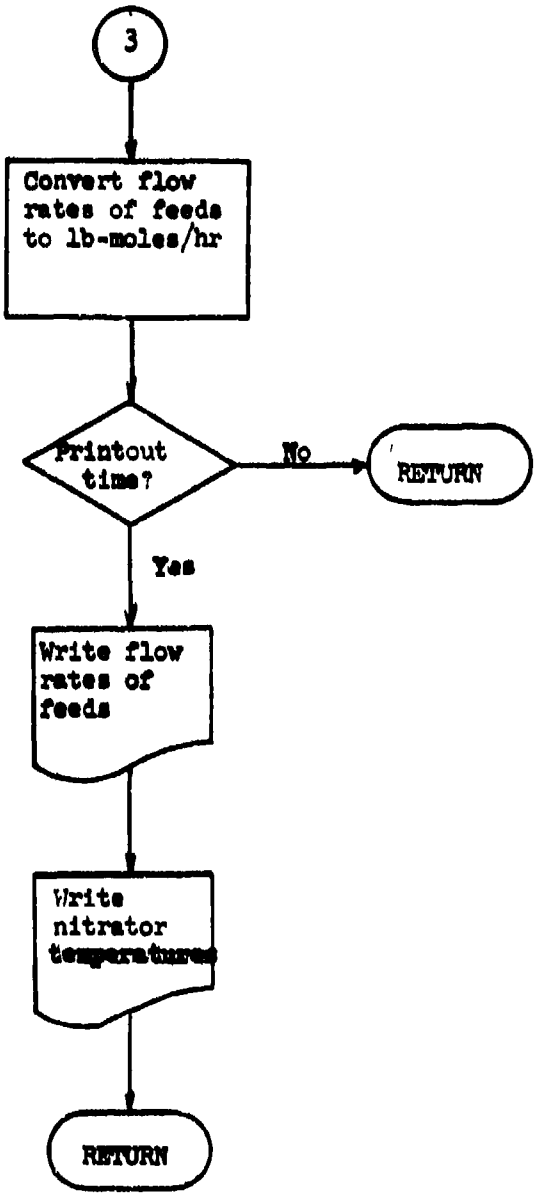


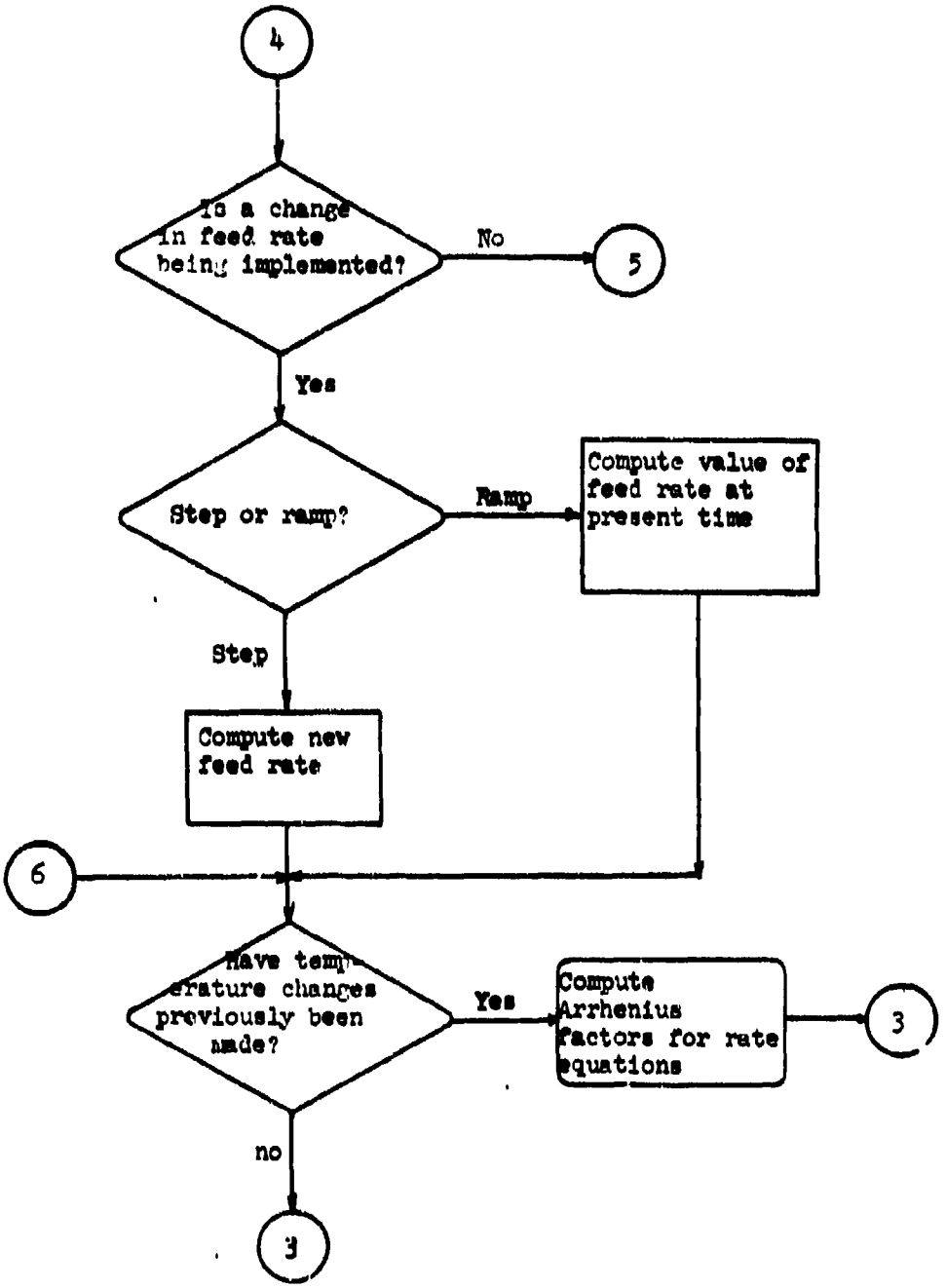
Subroutine **INPT**

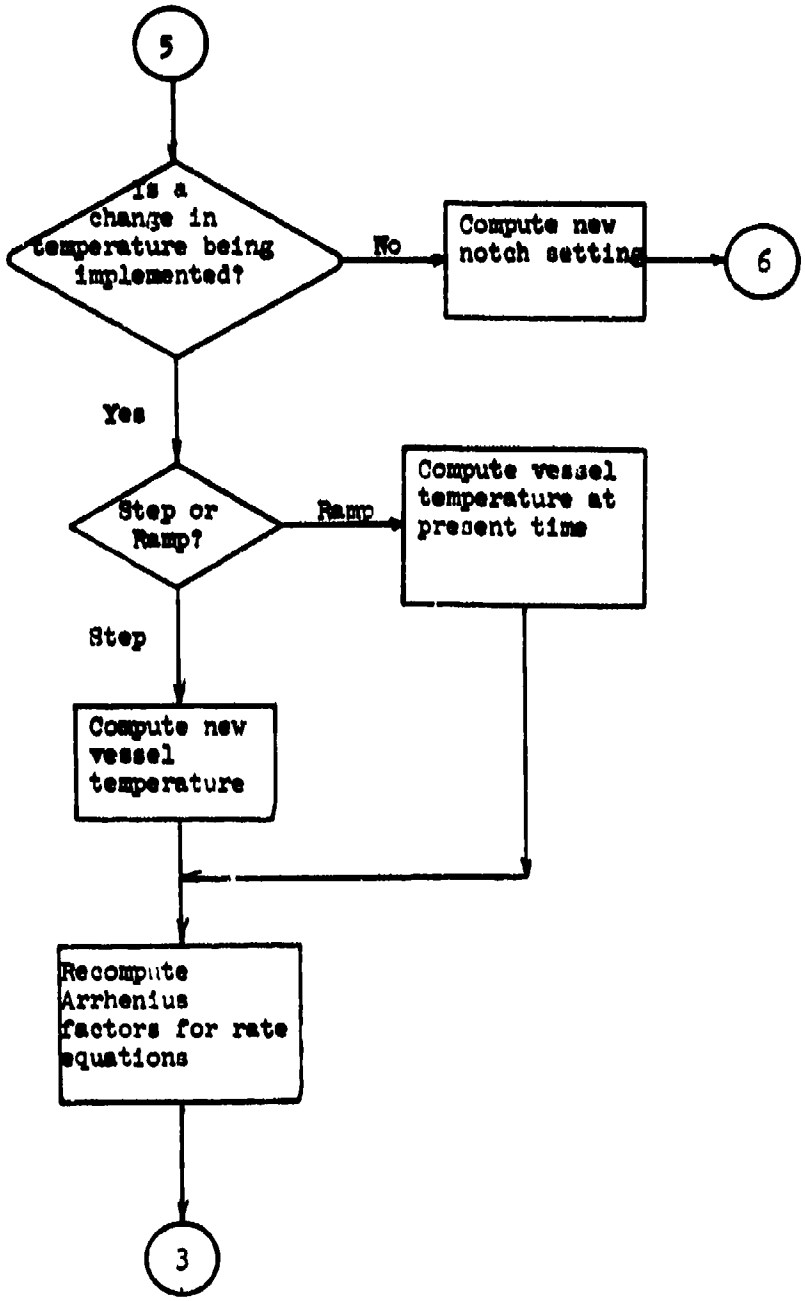



1
ICALL=1
Read in the initial values of flow rate and composition of raw materials
Read print control and run time parameters
Write print control and run time parameters
Compute integer number of time steps for this run
Compute integer number of time steps between print outs
NCHNG=1
2

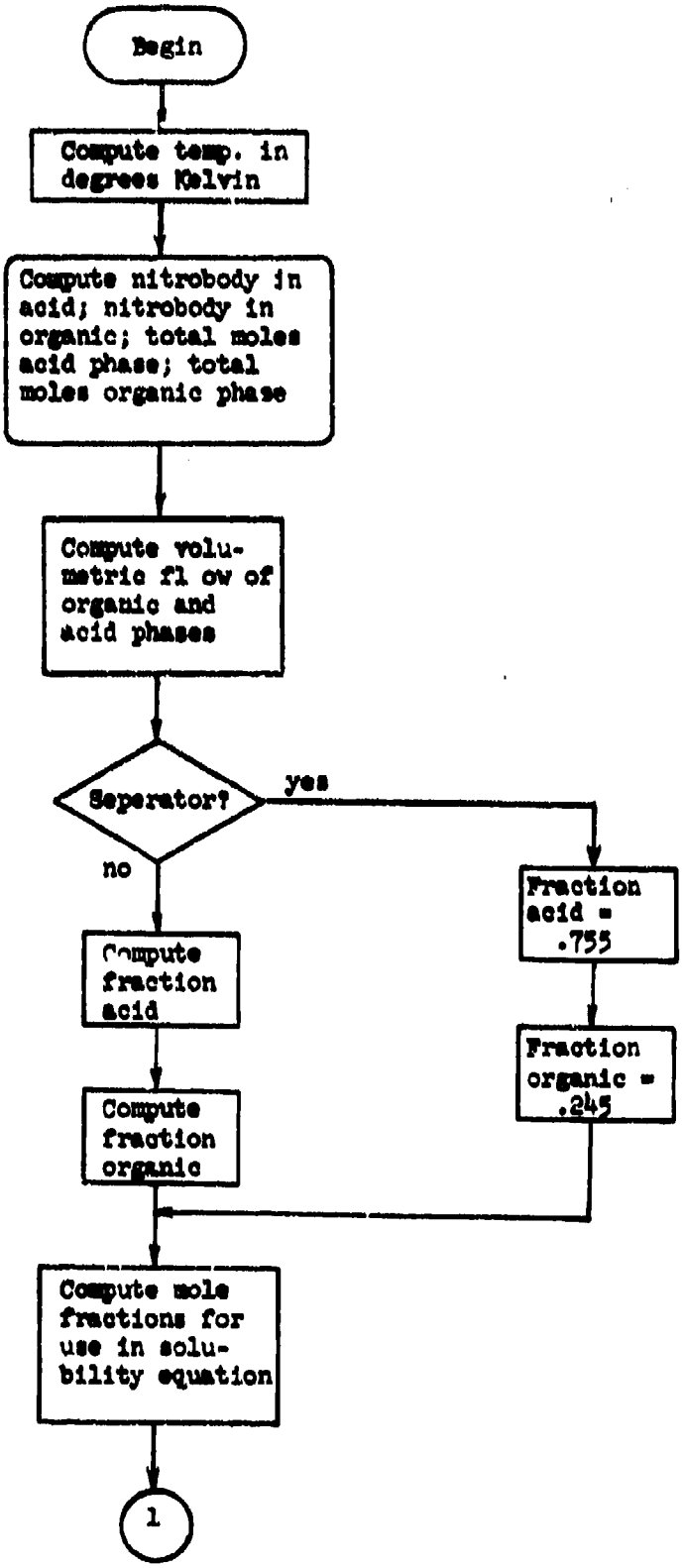

2
Read magnitude, time and duration of perturbations to initial steady state of the process
Write perturbations to initial steady state of the process
Write initial values of raw material
JACK=0
IKT=1
Compute Arrhenius factors for rate equations
3

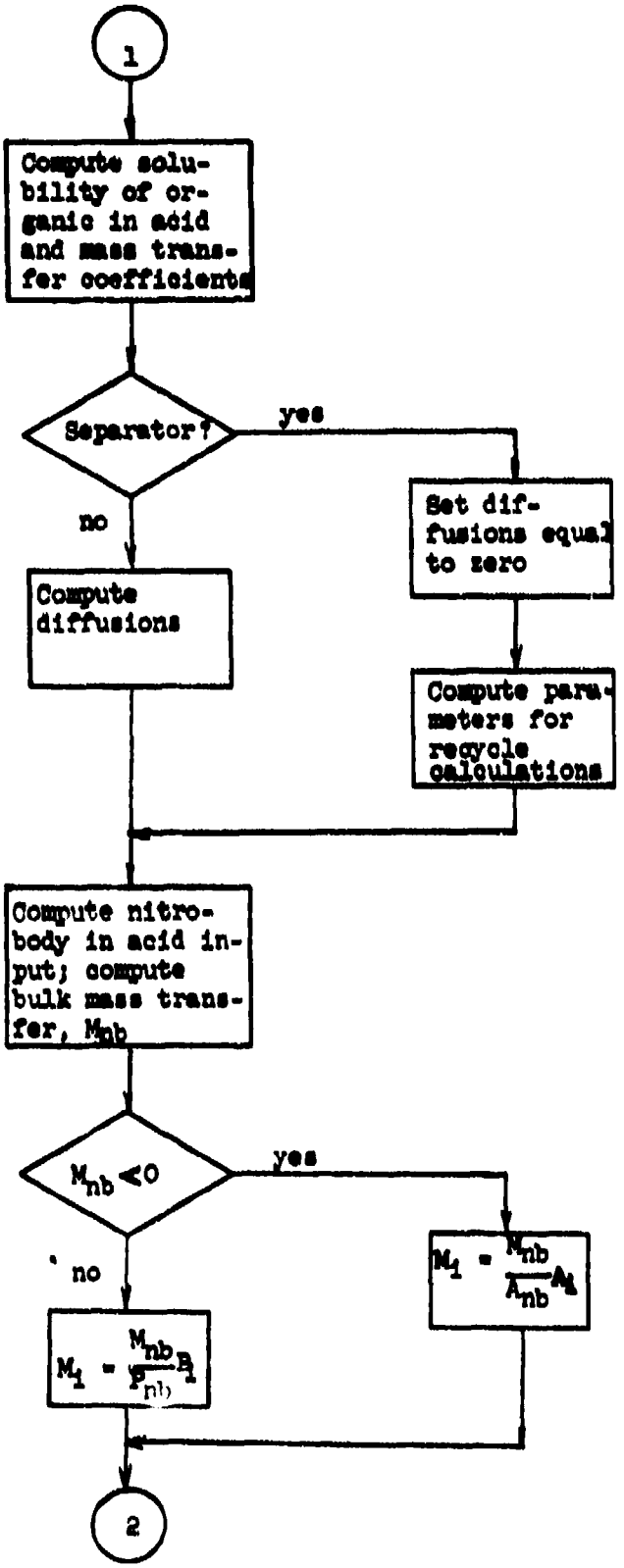

3
Convert flow rates of feeds to lb-moles/hr
Printout time?
No
RETURN
Yes
Write flow rates of feeds
Write nitrator temperatures
RETURN

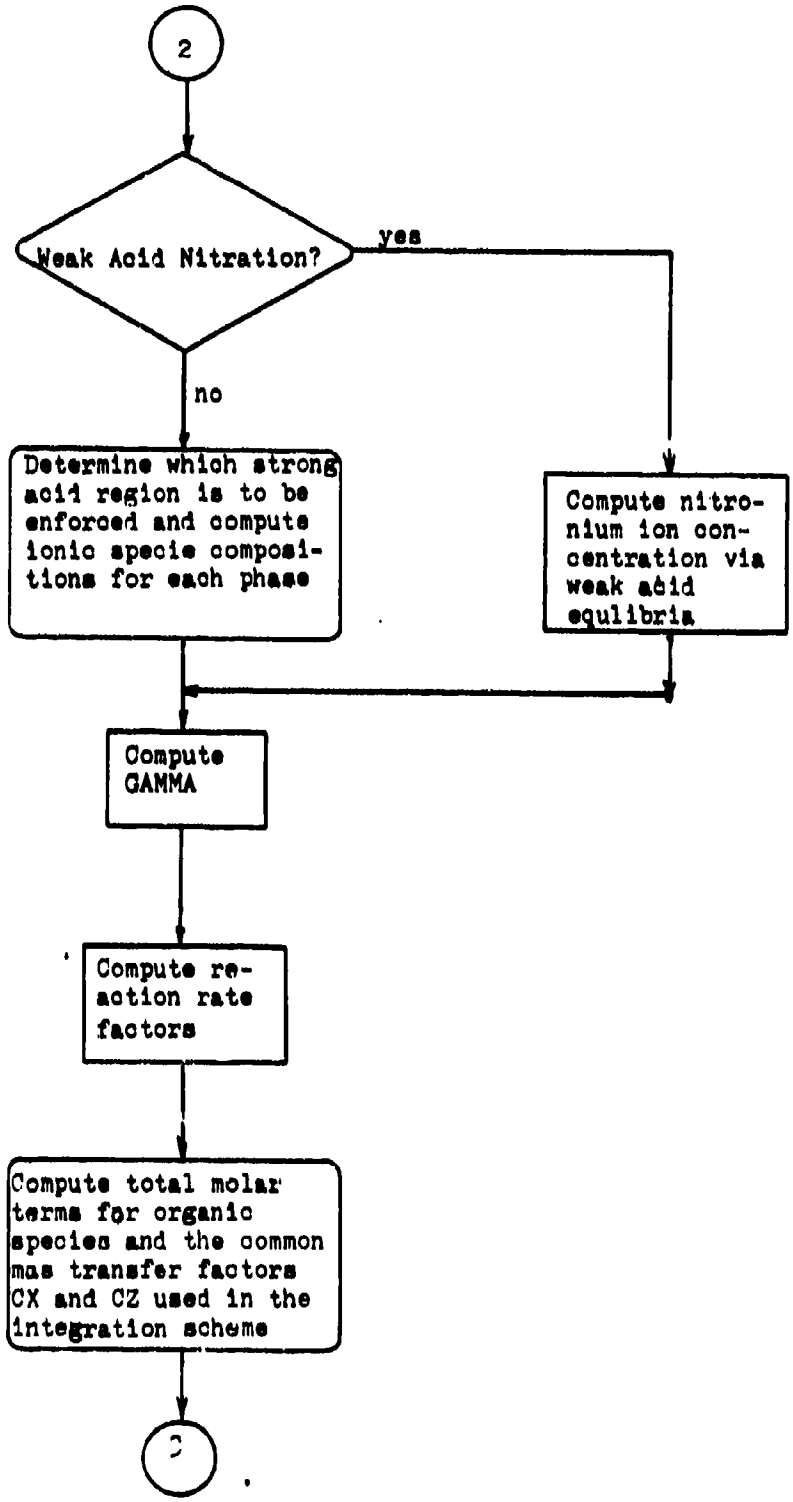

4
Is a change in feed rate being implemented?
No
5
Yes
Step or ramp?
Ramp
Compute value of feed rate at present time
Step
Compute new feed rate
6
Have temperature changes previously been made?
Yes
Compute Arrhenius factors for rate equations
3
no
3

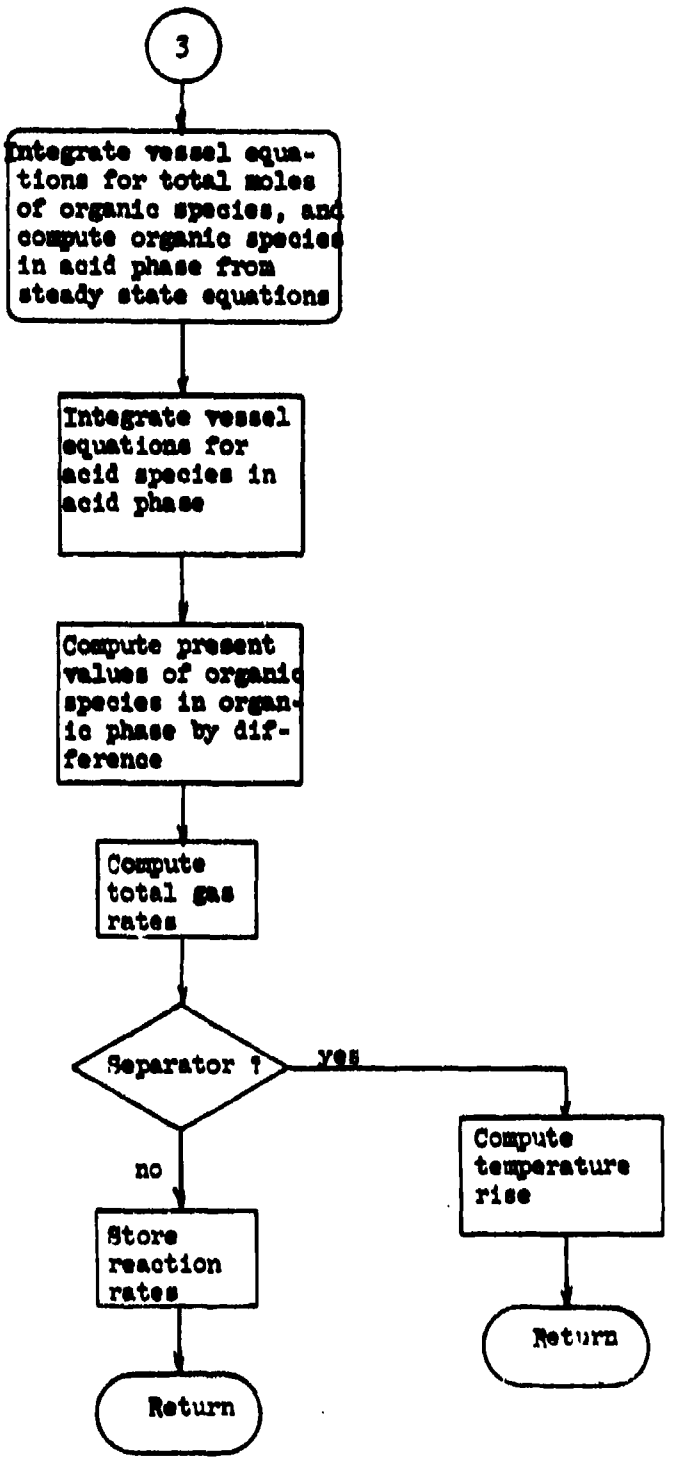

5
Is a change in temperature being implemented?
No
Compute new notch setting
6
Yes
Step or Ramp?
Ramp
Compute vessel temperature at present time
Step
Compute new vessel temperature
Recompute Arrhenius factors for rate equations
3

Subroutine SUB

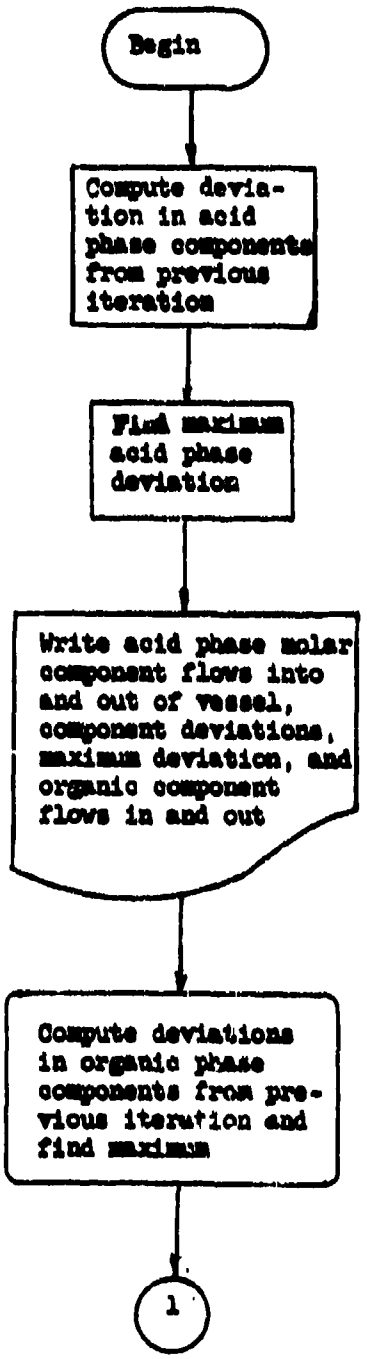


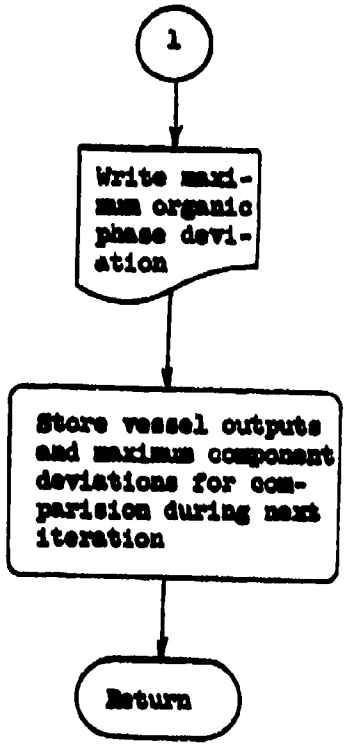

1
Compute solubility of organic in acid and mass transfer coefficients
Separator?
yes
no
Set diffusions equal to zero
Compute diffusions
Compute parameters for recycle calculations
Compute nitrobody in acid input; compute bulk mass transfer, M_{nb}
$M_{nb} < 0$
yes
no
$M_i = \frac{M_{nb}}{A_{nb}} A_i$
$M_i = \frac{M_{nb}}{p_{nb}} B_i$
2


2
Weak Acid Nitration?
yes
no
Determine which strong acid region is to be enforced and compute ionic specie compositions for each phase
Compute nitronium ion concentration via weak acid equilibria
Compute GAMMA
Compute reaction rate factors
Compute total molar terms for organic species and the common mas transfer factors CX and CZ used in the integration scheme
3

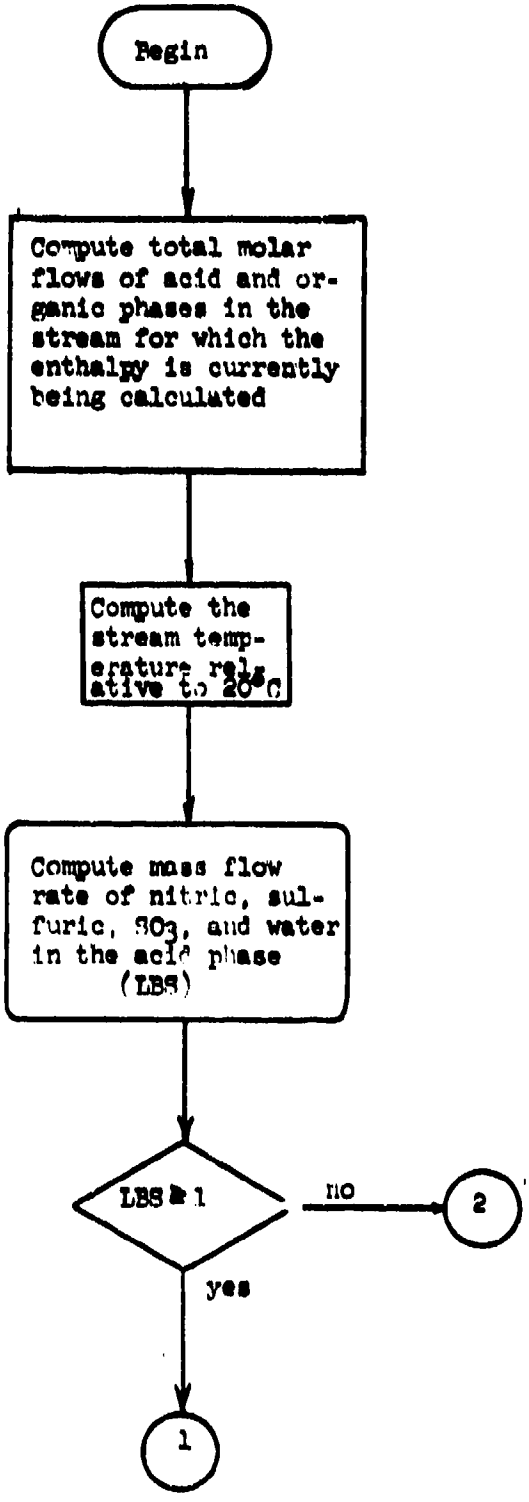

3
Integrate vessel equations for total moles of organic species, and compute organic species in acid phase from steady state equations
Integrate vessel equations for acid species in acid phase
Compute present values of organic species in organic phase by difference
Compute total gas rates
Separator ?
yes
no
Compute temperature rise
Store reaction rates
Return
Return

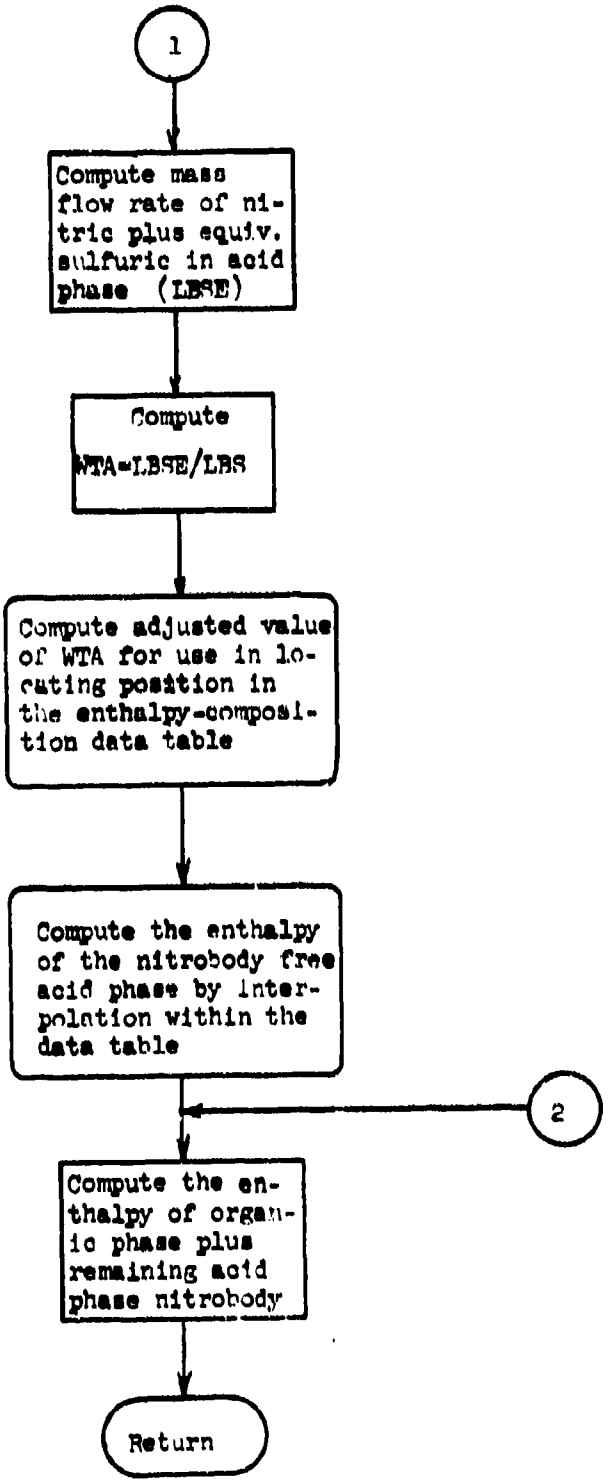
Subroutine SUB1




1
Write maximum organic phase deviation
Store vessel outputs and maximum component deviations for comparision during next iteration
Return

Function ENTH




1
Compute mass flow rate of nitric plus equiv. sulfuric in acid phase (LBSE)
Compute WTA=LBSE/LBS
Compute adjusted value of WTA for use in locating position in the enthalpy-composition data table
Compute the enthalpy of the nitrobody free acid phase by interpolation within the data table
2
Compute the enthalpy of organic phase plus remaining acid phase nitrobody
Return

APPENDIX D

Dynamic Simulation--Program Nomemclature

Main Program

A (I)	moles/hr of component i in the total acid phase leaving the vessel currently being calculated
AA (I,J)	moles/hr of component i in the stream phase j of the separator currently being calculated
AF (I)	moles/hr of component i in the acid phase of the organic stream leaving a separator
AI (I)	moles/hr of component i in the total acid phase input to the vessel currently being calculated
AIR (I)	moles/hr of component i in the acid phase of the internal recycle leaving a separator
AKMA	acid phase mass transfer coefficient
AK10	rate constant for reaction 10
AK12	ratio of rate constants for reactions 1 and 2
AK3S	rate constant for reaction 3 in strong acid
AK3W	rate constant for reaction 3 in weak acid. NOT USED
AK4S	rate constant for reaction 4 in strong acid
AK4W	rate constant for reaction 4 in weak acid. NOT USED
AK5S	rate constant for reaction 5 in strong acid
AK6S	rate constant for reaction 6 in strong acid
AK7	rate constant for reaction 7
AK8	rate constant for reaction 8

AK9	NOT USED
AN(I,J)	percent actual nitric acid in the acid phase of the external recycle leaving separator j at the end of the ith plot interval
ANA(I,J)	amount of α - nitration taking place in nitrator j at the end of the ith plot interval
ANAC	running sum used in computation of ANA(I,J)
ANM(I,J)	amount of m-nitration taking place in nitrator j at the end of the ith plot interval
ANMC	running sum used in computation of ANM(I,J)
ANT(I,J)	moles/hr component i in the total acid phase leaving nitrator j
ARRAY(I,J)	moles/hr of component i from fresh acid feeds to nitrator j
AS(I,J)	moles/hr of component i in the total acid phase leaving separator j
ATM(I)	total moles/hr of stream phase i leaving the separator currently being calculated
ATW(I)	total lb/hr of stream phase i leaving the separator currently being calculated
AV(I,J)	initial value of moles/hr component j in the total acid phase leaving vessel i
AVL(I)	total cu ft/hr of stream phase i leaving the separator currently being calculated
AXR(I)	moles/hr of component i in the acid phase of the external recycle leaving a separator
A1A(I)	moles/hr of component i in the acid phase leaving nitrator 1A

A1AI (I)	moles/hr of component i in the fresh acid feeds to nitrator 1A
A1B (I)	moles/hr of component i in the acid phase leaving nitrator 1B
A1BI (I)	moles/hr of component i to nitrator 1B from fresh acid feeds
A1S (I)	moles/hr of component i in the total acid phase leaving separator 1
A2 (I)	moles/hr of component i in the acid phase leaving nitrator 2
A2I (I)	moles/hr of component i to nitrator 2 from fresh acid feeds
A2S (I)	moles/hr of component i in the total acid phase leaving separator 2
A3A (I)	moles/hr of component i in the acid phase leaving nitrator 3A
A3AI (I)	moles/hr of component i to nitrator 3A from fresh acid feeds
A3B (I)	moles/hr of component i in the acid phase leaving nitrator 3B
A3BI (I)	moles/hr of component i to nitrator 3B from fresh acid feeds
A3S (I)	moles/hr of component i in total acid phase leaving separator 3
A4 (I)	moles/hr of component i in acid phase leaving nitrator 4
A4S (I)	moles/hr of component i in total acid phase leaving separator 4
A4I (I)	moles/hr of component i to nitrator 4 from fresh acid feeds

A5(I)	moles/hr of component i in acid phase leaving nitrator 5
A5I(I)	moles/hr of component i to nitrator 5 from fresh acid feeds
A5S(I)	moles/hr of component i in the total acid phase leaving separator 5
A6(I)	moles/hr of component i in the acid phase leaving nitrator 6
A6I(I)	moles/hr of component i to nitrator 6 from fresh acid feeds
A6S(I)	moles/hr of component i in the total acid phase from separator 6
BASIS	NOT USED
CDNT	weight % DNT in crude TNT leaving separator 6
CDNTSA	weight % DNT in the nitrobody dissolved in the spent acid
CHAMXØ	NOT USED
CHPMXØ	NOT USED
CNBSA	weight % nitrobody dissolved in the acid phase of the spent acid leaving separator 1
CP(I)	specific heat of component i
CRUDE	lb/hr crude TNT leaving separator 6 (i.e., the mass flow of the total organic stream leaving separator 6)
CWSA	weight % water in the acid phase of the spent acid leaving separator 1

DENS (I,J)	specific gravity of the organic phase of any of the streams leaving the jth separator at the end of the ith plot interval
DENSA (I,J)	specific gravity of the acid phase in any of the streams leaving the jth separator at the end of the ith plot interval
DFAMXØ	maximum % change in an acid phase component between two successive iterations of the nitration section
DFPMXØ	maximum % change in an organic phase component between two successive iterations of the nitration section
DH (I)	heat of reaction for the ith reaction in BTU/lb-mole of reactant
DLT	estimated temperature of entrained organic phase that would be returned to nitrator 1B from the after separator
DT	itegration time step (hrs)
DTPR	time between plotted points (mins)
EAØ (I)	molar ratio of acid phase in the organic stream to total organic stream leaving the ith separator
EAØP (I)	molar ratio of acid to organic phase in the organic stream leaving the ith separator
EAØP1	equivalent to EAOP (1)
EAØP2	equivalent to EAOP (2)
EAØP3	equivalent to EAOP (3)
EAØP4	equivalent to EAOP (4)
EAØP5	equivalent to EAOP (5)

EAØP6	equivalent to EAOP (6)
EAP	value of EAOP (I) for the separator currently being calculated
EFR	enthalpy of mixing for fume recovery acid
EØA (I)	molar ratio of organic phase in the external recycle to total external recycle leaving the separator i
EØAP (I)	molar ratio of organic to acid phase in either of the acid recycle streams leaving the ith separator
EØAP1	equivalent to EOAP (1)
EØAP2	equivalent to EOAP (2)
EØAP3	equivalent to EOAP (3)
EØAP4	equivalent to EOAP (4)
EØAP5	equivalent to EOAP (5)
EØAP6	equivalent to EOAP (6)
EØL	enthalpy of mixing for 40% oleum
EØP	value of EOAP (I) for the separator currently being calculated
EWN	enthalpy of mixing for weak nitric acid
EX	imposed upper bound on the Arrhenius coefficient in the reaction rate expressions for reactions 3 and 4 (MNT to DNT)
EYW	enthalpy of mixing for yellow water
E10	activation energy for reaction 10
E21	ratio of activation energies for reactions 2 and 1

E3S	activation energy for reaction 3 in a strong acid medium
E3W	NOT USED
E4S	activation energy for reaction 4 in a strong acid medium
E4W	NOT USED
E5S	activation energy for reaction 5 in a strong acid medium
E6S	activation energy for reaction 6 in a strong acid medium
E7	activation energy for reaction 7
E8	activation energy for reaction 8
E9	NOT USED
FA(I)	ratio of acid phase leaving i^{th} separator that is recycled to total acid phase leaving the ith separator (fraction of acid phase recycled)
FACID(I)	ratio of acid phase leaving the ith separator in the organic stream forward to total acid phase leaving the ith separator (fraction of acid phase sent forward)
FACID1	equivalent to FACID(1)
FACID2	equivalent to FACID(2)
FACID3	equivalent to FACID(3)
FACID4	equivalent to FACID(4)
FACID5	equivalent to FACID(5)
FACID6	equivalent to FACID(6)

FAFR	fraction of total acid phase leaving separator 1 that appears in the external recycle from that separator
FAR	fraction of total acid phase leaving the separator that is recycled for the separator currently being calculated
FA1	equivalent to FA(1)
FA2	equivalent to FA(2)
FA3	equivalent to FA(3)
FA4	equivalent to FA(4)
FA5	equivalent to FA(5)
FA6	equivalent to FA(6)
FD	extent of reaction for nitrosylsulfuric decomposition
FIN(I,J)	lb/hr of feed i to nitration vessel j
FMAX	maximum allowable volumetric flow of internal acid recycle
FMX	equivalent to FMAX
FØ(I)	ratio of organic phase leaving the ith separator with the organic stream forward to total organic phase leaving the ith separator (fraction organic phase forward)
FØRG(I)	ratio of organic phase leaving the ith separator with the acid recycle streams to total organic phase leaving the ith separator
FØRG1	equivalent to FØRG(1)

FØRG2	equivalent to FØRG(2)
FØRG3	equivalent to FØRG(3)
FØRG4	equivalent to FØRG(4)
FØRG5	equivalent to FØRG(5)
FØRG6	equivalent to FØRG(6)
FØ1	equivalent to FØ(1)
FØ2	equivalent to FØ(2)
FØ3	equivalent to FØ(3)
FØ4	equivalent to FØ(4)
FØ5	equivalent to FØ(5)
FØ6	equivalent to FØ(6)
FPØ	fraction of organic phase leaving a separator that appears in the organic stream forward for the separator currently being calculated
FR(I)	ratio of external recycle stream to total recycle leaving the ith separator
FRAC	ratio of internal recycle stream to total recycle leaving the separator currently being calculated
FRAC1	equivalent to FRC(1)
FRAC2	equivalent to FRC(2)
FRAC3	equivalent to FRC(3)
FRAC4	equivalent to FRC(4)
FRAC5	equivalent to FRC(5)

FRAC6	equivalent to FRC (6)
FRC (I)	ratio of internal recycle stream to total recycle stream leaving the ith separator
FR1	equivalent to FR (1)
FR2	equivalent to FR (2)
FR3	equivalent to FR (3)
FR4	equivalent to FR (4)
FR5	equivalent to FR (5)
FR6	equivalent to FR (6)
FV (I)	volume of the ith nitrator (cu ft)
FVKM	volume of the vessel currently being calculated
FVKMS	volume of a separator (all separators have the same volume)
FVKM1A	volume of nitrator 1A; equivalent to FV (1)
FVKM1B	volume of nitrator 1B; equivalent to FV (2)
FVKM2	volume of nitrator 2; equivalent to FV (3)
FVKM3A	volume of nitrator 3A; equivalent to FV (4)
FVKM3B	volume of nitrator 3B; equivalent to FV (5)
FVKM4	volume of nitrator 4; equivalent to FV (6)
FVKM5	volume of nitrator 5; equivalent to FV (7)
FVKM6	volume of nitrator 6; equivalent to FV (8)
G1 (I)	ratio of Arrhenius coefficients in the kinetic rate expressions for reaction 1 and 2 in the ith nitrator

G10(I)	value of the Arrhenius coefficient in the kinetic rate expression for reaction 10 in the ith nitrator
G3(I)	NOT USED
G3S(I)	value of the Arrhenius coefficient in the kinetic rate expression for reaction 3 in the ith nitrator under strong acid conditions
G4S(I)	NOT USED
G4S(I)	same as G3S(I) but for reaction 5
G5(I)	value of Arrhenius coefficient in the kinetic rate expression for reaction 5 in the ith nitrator
G6(I)	same as G5(I) but for reaction 6
G7(I)	same as G5(I) bur for reaction 7
G8(I)	same as G5(I) bur for reaction 8
G9(I)	NOT USED
I	DØ LØØP index
IC	counter for plotting intervals
ICALL	flag for first call to SUBRØUTINE INPT
ICØUNT	equivalent to IC
IN	DØ LØØP index for certain loops pertaining to nitrators
IPNCH	I/O device numbe.. for punched cards
IPRNT	print control flag: 0 summary printout only 1 debug printout of internal calculations during each integration step

IQUIT	number of stages being simulated
IS	DØ LØØP index for certain loops pertaining to separators
ISTGE	stage number
ITYPE	vessel type flag: ITYPE=0 for nitrator ITYPE=1 for separator
IV	nitration vessel number
IVSL	general vessel number
J	DØ LØØP counter and generally used integer operator
JACK	counter for integration time steps
K	DØ LØØP counter and generally used integer operator
MW(I)	molecular weight of component i
NM	integer number of integration passes through the process (or iterations) required for a particular run. Also the integer number of integration time steps required for the run
NN	integer number of iterations between summary printouts
NØ(I)	notch setting on internal recycle gate valve for separator i
NOTCH	notch setting for the separator currently being calculated
NP	integer number of iterations between computations of process performance indicators and other data for plotting

N1	equivalent to NØ(1)
N2	equivalent to NØ(2)
N3	equivalent to NØ(3)
N4	equivalent to NØ(4)
N5	equivalent to NØ(5)
N6	equivalent to NØ(6)
P(I)	moles/hr of component i in the total organic phase leaving the vessel currently being calculated
PA	lb/hr of total acid phase leaving a separator for which acid phase specific gravity is being calculated
PF(I)	moles/hr component i in the organic phase of the organic stream leaving a separator
PI(I)	moles/hr component i in the total organic phase input to the vessel currently being calculated
PIR(I)	moles/hr of component i in the organic phase of the internal recycle leaving a separator
PNT(I,J)	moles/hr of component i in the total organic phase leaving nitrator j
PP	lb/hr of total organic phase leaving a separator for which organic phase specific gravity is being calculated
PS(I,J)	moles/hr of component i in the total organic phase leaving the jth separator
PV(I,J)	initial value of moles/hr component j in the total organic phase leaving vessel i

PXR (I)	moles/hr of component i in the organic phase of the external recycle leaving a separator
P1A (I)	moles/hr of component i in the organic phase leaving nitrator 1A
P1AI (I)	moles/hr of component i in the organic feed stream to nitrator 1A (moles/hr toluene to 1A)
P1B (I)	moles/hr of component i in the organic phase leaving nitrator 1B
P1BI (I)	moles/hr of component i in the organic feed stream to nitrator 1B (moles/hr toluene to 1B)
P1S (I)	moles/hr component i in the total organic phase leaving separator 1
P2 (I)	moles/hr component i in the organic phase leaving nitrator 2
P2S (I)	moles/hr component i in the total organic phase leaving separator 2
P3A (I)	moles/hr component i in the organic phase leaving nitrator 3A
P3B (I)	moles/hr component i in the organic phase leaving nitrator 3B
P3S (I)	moles/hr component i in the total organic phase leaving separator 3
P4 (I)	moles/hr component i in the organic phase leaving nitrator 4
P4S (I)	moles/hr component i in the total organic phase leaving separator 4
P5 (I)	moles/hr component i in the organic phase leaving nitrator 5

P5S (I)	moles/hr component i in the total organic phase leaving separator 5
P6 (I)	moles/hr component i in the organic phase leaving nitrator 6
P6S (I)	moles/hr component i in the total organic phase leaving separator 6
Q	accumulation term used in calculation of nitrator heat loads
QA	volumetric flow of total acid phase leaving a separator for which acid phase specific gravity is being calculated
QN (I,J)	heat load in nitrator j calculated at the end of the ith plotting interval
QP	volument flow of total organic phase leaving a separator for which organic phase specific gravity is being calculated
QY (I)	fraction of nitric acid converted to nitronium ions in nitration vessel i
R (I)	NOT USED
RATES (I,J)	rate of reaction j in nitration vessel i
RHØ (I)	molar density of component i
RHØ1	equivalent to RHØ (1)
RHØ10	equivalent to PHØ (10)
RHØ11	equivalent to RHØ (11)
RHØ12	equivalent to RHØ (12)
RHØ13	equivalent to RHØ (13)
RHØ14	equivalent to RHØ (14)

RHØ2	equivalent to RHØ(2)
RHØ3	equivalent to RHØ(3)
RHØ4	equivalent to RHØ(4)
RHØ5	equivalent to RHØ5
RHØ6	equivalent to RHØ(6)
RHØ7	equivalent to RHØ(7)
RHØ8	equivalent to RHØ(8)
RHØ9	equivalent to RHØ(9)
RNS(I,J)	nitric to sulfuric acid ratio in nitration vessel j calculated at the end of the ith plotting interval (for acid phase only)
RNSS(I,J)	nitric to sulfuric acid ratio in separator j calculated at the end of the ith plotting interval (for acid phase only)
RP	coefficient on the molecular oxygen term in reaction 9
RR	ideal gas law constant
SA	adjustable constant. NOT USED
SB	equivalent to organic phase mass transfer coefficient (KMAP)
SC	equivalent to AKEQ4 in SUBRØUTINE SUB
SD	NOT USED
SE	equivalent to AK9. NOT USED
SG	equivalent to E9. NOT USED

SH	equivalent to AKEQ1 in SUBRØUTINE SUB
SI	NOT USED
SJ	equivalent to AKEQ3 in SUBRØUTINE SUB
SPA	accumulator term used in calculation of spent acid mass flow rate
SPENT (I)	spent acid mass flow rate at the end of the ith plotting interval (flow rate of acid phase of the external recycle stream leaving separator 1)
SPØ	mass flow rate of dissolved organic in the spent acid
SUM	accumulator term used in calculation of the mass flow rate of crude TNT leaving separator 8
T	temperature of nitration vessel currently being calculated
TDNT	mass flow rate of DNT in the total organic stream leaving separator 8
TCOX	cumulative total moles/hr oxides of carbon (gas) leaving all vessels in the nitration section during a given iteration
TEMP (I)	temperature of the ith nitration vessel
TI	NOT USED
TIME	simulated elapsed time since beginning of run
TLBS	total lb/hr of acid phase leaving a separator on a nitrobody free basis. Used in computation of acid concentration indicators
TM (I)	total moles/hr of stream i leaving a separator currently being calculated

TNOX	total moles/hr oxides of nitrogen (gas) leaving all vessels in the nitration section during a given iteration
TR	reference temperature
TSEP(I)	computed temperature of the separator currently being calculated
TTCOX(I)	same as TCOX except that value is particular value at the end of the ith plotting interval
TTME	total time of process operation to be simulated
TTNOX(I)	same as TNOX except that value is particular value at the end of the ith plotting interval
TVL(I)	volumetric flow (cu ft/hr) of the ith stream leaving the separator currently being calculated
TW(I)	mass flow (lb/hr) of the ith stream leaving the separator currently being calculated
T1A	temperature of nitrator 1A (equivalent to TEMP(1))
T1B	temperature of nitrator 1B (equivalent to TEMP(2))
T2	temperature of nitrator 2 (equivalent to TEMP(3))
T3A	temperature of nitrator 3A (equivalent to TEMP(4))
T3B	temperature of nitrator 3B (equivalent to TEMP(5))
T4	temperature of nitrator 4 (equivalent to TEMP(6))
T5	temperature of nitrator 5 (equivalent to TEMP(7))
T6	temperature of nitrator 6 (equivalent to TEMP(8))
VKM(I)	volume of the ith nitrator
VKMS	volume of a separator (same for all separators)

X(I)	elapsed simulated time at the end of the ith plotting interval (nomenclature is specific to plotting routine for plotting one dimensional variables as a function of time)
XX(I,J)	elapsed simulated time at the end of the ith plotting interval (this form of elapsed time is used for plotting variables of up to j dimension)
XYY(I)	moles/hr nitric acid in the acid phase converted to nitronium ions in nitration vessel i

Subroutine INPT

The definitions of the following variables are identical to those in the main program: AF(I), AIR(I), AKMA, AKMATL, AK10, AK12, AK3S, AK3W, AK4S, AK4W, AK5S, AK6S, AK7, AK8, AK9, ARRAY(I,J), AXR(I), A1S(I), A2S(I), A3S(I), A4S(I), A5S(I), A6S(I), CP(I), DH(I), DT, EAØP1, EAØP2, EAØP EAØP3, EAØP4, EAØP5, EAØP6, EØAP1, EØAP2, EØAP3, EØAP4, EØAP5, EØAP6, EX, E10, E21, E3S, E3W, E4S, E4W, E5S, E6S, E7, E8, E9, FAC1D1, FAC1D2, FAC1D3, FAC1D4, FACID5, FACID6, FA1, FA2, FA3, FA4, FA5, FA6, FIN(I,J), FMX, FØRG1, FØRG2, FØRG3, FØRG4, FØRG5, FØRG6, FØ1, FØ2, FØ3, FØ4, FØ5, FØ6, FRAC1, FRAC2, FRAC3, FRAC4, FRAC5, FRAC6, FR1, FR2, FR3, FR4, FR5, FR6, FVKM1A, FVKM1B, FVKM2, FVKM3A, FVKM3B, FVKM4, FVKM5, FVKM6, G1(I), G10(I), G3(I), G3S(I), G4(I), G4S(I), G5(I), G6(I), G7(I), G8(I), G9(I), ICALL, IPRNT, JACK, MW(I), NM, NN, NP, N1, N2, N3, N4, N5, N6, PF(I), PIR(I), PXR(I), P1AI(I), P1BI(I), P1S(I), P2S(I), P3S(I), P4S(I), P5S(I), P6S(I), RATES(I,J), RHØ1, RHØ10, RHØ11, RHØ12, RHØ13, RHØ14, RHØ2, RHØ3, RHØ4, RHØ5, RHØ6, RHØ7, RHØ8, RHØ9, RP, RR, SA, SB, SC, SD, SE, SG, SH, SI, SJ, TCOX, TEMP(I), TNOX, TR, TSEP(I), TTME, T1A, T1B, T2, T3, T4, T5, T6,

Remaining variables are defined as follows:

CØMP(I,J)	weight % component i in feedstock type j
DDL	fractional part of a change in feed rate or nitrator temperature which is applied to the process during a given iteration
DL(I)	magnitude of the ith change in an indepenent variable

ICH(J)	integer code number for the independent variable type to which the jth change is being made
IKT	flag to indicate whether or not temperature changes have been made to the initial conditions
IPRNT	simulated time between summary printouts
IVS(J)	integer code number for the vessel to which the jth change in one of the independent variable types is made
NCHNG	number of given change which is to be made during the run
NOTCH(I)	notch setting on internal recycle gate value for the ith separator
NTME(I)	number of iterations between the beginning of a run the initiation of the ith change in an independent variable
NTVL(I)	number of iterations over which the magnitude of the ith change is to be equally distributed (used for ramping an independent variable)
TME	simulated time at which a given change is to be initiated
TVL	simulated time interval over which a given change is to be made
ZA	temperature coefficient in the exponent of the Arrhenius rate expression

Subroutine SUB

The definitions of the following variables are identical to those in the main program: A(I), AI(I), AKMA, AKMATL, AK10, AK12, AK3S, AK3W, AK4S, AK4W, AK5S, AK6S, AK7, AK8, CP(I), DH(I), DT, EX, E10, E21, E3W, E3S, E4W, E4S, E6S, E7, E8, FAIL, FD, FMX, FPØ, E5S, FRAC, FVKM, G1(I), G10(I), G3(I), G3S(I), G4(I), G4S(I), G5(I), G3(I), G7(I), G8(I), G9(I), ICALL, IPRNT, ISTGE, ITYPE, IV, JACK, NM, NN, NOTCH, NP, P(I), PI(I), QY(I), RATES(I,J), RHØ1, RHØ11, RHØ12, RHØ13, RHØ14, RHØ2, RHØ3, RHØ4, RHØ5, RHØ6, RHØ7, RHØ8, RHØ9, RR, RP, SA, SB, SC, SD, SE, SG, SH, SI, SJ, T, TCOX, TI, TNOX, TR, TSEP(I), TTME, XYY(I)

The definitions of the following variables are identical to other variables defined for the main program:

Variable in SUB	Variable in main program
AI1 thru AI17	AI(1) thru AI(17)
A1 thru A17	A(1) thru A(17)
EAØP	EAP
EØAP	EØP
PI1 thru PI17	PI(1) thru PI(17)
P1 thru P17	P(1) thru P(17)

Remaining variables are defined as follows:

AINB	moles/hr nitrobody in the aggragate acid phase input to the vessel currently being calculated
AKA	general rate factor for all nitration reactions. Also if Bennett's strong acid rate expression is used, the coefficient of the besulfate ion concentration
AKB	coefficient of the sulfuric acid concentration in Bennett's rate expression
AKC	coefficient of the pyrosulfate ion concentration in Bennett's rate expression

AKEQ	equilibrium constant for the dissociation of sulfuric acid in an aqueous medium
AKEQOV	equilibrium constant for the dissociation of a mixture of sulfuric and pyrosulfuric acids to ionic species. NOT USED
AKEQ1	equilibrium constant for the dissociation of nitric acid in aqueous sulfuric acid
AKEQ2	equivalent to AKEQ
AKEQ3	equilibrium constant for the dissociation of nitric acid in anhydrous sulfuric acid
AKEQ4	equilibrium constant for the recombination of nitronium and bisulfate ions in anhydrous acid mixtrues
AKMAP	organic phase mass transfer coefficient
AK1	computed value of AKEQ1 obtained from interval halving procedure
AK3	computed value of AKEQ3 obtained from interval halving procedure
AK4	computed value of AKEQ4 obtained from interval halving procedure
AL	moles/hr water in the total acid phase of the vessel current being calculated; can have negative value which then represents moles/hr SO_3
AMNB	moles/hr nitrobody transferred from organic to acid phase by bulk mass transfer; negative value means transfer from acid to organic phase
AM1	moles/hr αMNT transferred by bulk mass transfer
AM2	same as AM1 but for mMNT

AM3	same as AM1 but for αDNT
AM4	same as AM1 but for mDNT
AM5	same as AM1 but for αTNT
AM6	same as AM1 but for mTNT
aM7	same as AM1 but for TNP
AM8	same as AM1 but for TNBX
ANB	total moles/hr of nitrobody dissolved in the acid phase leaving the vessel currently being calculated
ASO4	combined moles/hr of SO_3 and H_2SO_4 in the acid phase leaving the vessel currently being calculated
AT	total moles/hr of acid phase leaving the vessel currently being calculated
A11QA	concentration (moles/ft^3) of sulfuric acid in the acid phase of the vessel currently being calculated
B	initial concentration (moles/ft^3) of free sulfuric acid in the acid phase of the vessel currently being calculated
BC	3 + (3 x C)
C	initial concentration (moles/ft^3) of pyrosulfuric acid in the acid phase of the vessel currently being calculated
CB	(.5 x B) + (1.5 x C)
CF	C-F
CHNO3	equilibrium concentration of nitric acid in the acid phase of the vessel currently being calculated

CHSO4	equilibrium concentration of bisulfate ions in the acid phase of the vessel currently being calculated
CHS2O7	equilibrium concentration of pyrosulfate ions in the acid phase of the vessel currently being calculated
CH2O	same as CHNO3 but for water
CH2SO4	equilibrium concentration of sulfuric acid in the acid phase of the vessel currently being calculated
CH3O	equilibrium concentration of hydronium ions in the acid phase of the vessel currently being calculated
CNO2	equilibrium concentration of nitronium ions in the acid phase of the vessel currently being calculated
CX	consolidation term for (ZA + YP)
CZ	consolidation term for (ZB - YA + 1 + CX)
C5	moles/hr nitrosylfulfuric acid produced by oxidation reactions in the vessel currently being calculated
CP5	moles/hr nitrosylsulfuric acid which remain undecomposed in the vessel currently being calculated
D	initial acid phase concentration of combined sulfuric acid plus pyrosulfuric acid in the vessel currently being calculated
DAL	rate of change of AL with respect to time in the vessel currently being calculated
DASO4	rate of change of ASO4 with respect to time in the vessel currently being calculated
DA1	rate of change of A1 with respect to time in the vessel currently being calculated

DA12	rate of change of A12 with respect to time in the vessel currently being calculated
DA2	rate of change of A2 with respect to time in vessel currently being calculated
DA3	rate of change of A3 with respect to time in the vessel currently being calculated
DA4	same as DA3 but for A4
DA5	same as DA3 but for A5
DA6	same as DA3 but for A6
DA7	same as DA3 but for A7
DA8	same as DA3 but for A8
DA9	same as DA3 but for A9
DELTA	acid concentration term in the weak acid nitration rate expression. NOT USED
DP1	rate of change of P1 with respect to time in the vessel currently being calculated
DP10	same as DP1 but for P10
DP2	same as DP1 but for P2
DP3	same as DP1 but for P3
DP4	same as DP1 but for P4
DP5	same as DP1 but for P5
DP6	same as DP1 but for P6
DP7	same as DP1 but for P7
DP8	same as DP1 but for P8

DTA	acid phase adjusted integration time step
DTP	organic phase adjusted integration time step
D1	moles/hr of α -MNT that diffuse into the acid phase in the vessel currently being calculated
D10	moles/hr of toluene which diffuse from the bulk organic phase to the acid-organic interface
D2	same as D1 but for m-MNT
D3	same as D1 but for α -DNT
D4	same as D1 but for m-DNT
D5	same as D1 but for α -TNT
D6	same as D1 but for m-TNT
D7	same as D1 but for TNB
D8	same as D1 but for TNBX
ETA	overall mass transfer coefficient in the vessel currently being calculated
ETAA	acid phase mass transfer coefficient in the vessel currently being calculated
ETAP	organic phase mass transfer coefficient in the vessel currently being calculated
ETATL	mass transfer coefficient for toluene
F	initial acid phase concentration of nitric acid in the vessel currently being calculated
FA	volumetric fraction of acid phase in the vessel currently being calculated

FF(I)	cross sectional area fraction corresponding to the ith notch setting on the gate valve in the internal recycle line of the separator currently being calculated
FOV	constant set equal to one
FP	volumetric fraction of organic phase in the vessel currently being calculated
F10A	reaction rate factor for reaction 10 where α -TNT is the reactant for the vessel currently being calculated
F10M	same as F10A but for m-TNT
F3	reaction rate factor for reaction 3 in the vessel currently being calculated
F4	same as F3 but for reaction 4
F5	same as F3 but for reaction 5
F6	same as F3 but for reaction 6
F7A	reaction rate factor for reaction 7 in the vessel currently being calculated where α -DNT is the reactant
F7M	same as F7A but for m-DNT
F8A	reaction rate factor for reaction 8 in the vessel currently being calculated where α -DNT is the reactant
F8M	same as F8A but for m-DNT
F9A	Zero
F9M	Zero

GAMMA	acid concentration term used in all nitration rate expressions
KLM	flag to indicate which nitration region exists in the vessel being calculated
PNB	total flow (moles/hr) of organic phase nitrobody components leaving the vessel currently being calculated
PP	exponent of nitrobody-in-acid- solubility correlation
Q	fraction nitric acid converted to nitronium ions for the vessel currently being calculated
QA	volumetric flow of the acid phase leaving the vessel currently being calculated
QP	volumetric flow of the organic phase leaving the vessel currently being calculated
QT	total volumetric flow of combined internal and external recycle leaving the separator currently being calculated
RATE(I)	rate of the ith reaction in the vessel currently being calculated
R1	rate of reaction 1 in the vessel currently being calculated; equivalent to RATE(1) (moles/hr)
R10	same as R1 but for reaction 10; equivalent to RATE(10); also R10A + R10M
R10A	rate of reaction 10 in the vessel currently being calculated where α -TNT is the reactant
R10M	same as R10A but for m-TNT
R2	same as R1 but for reaction 2; equivalent to RATE(2)

R3	same as R1 but for reaction 3; equivalent to RATE(3)
R4	same as R1 but for reaction 4; equivalent to RATE(4)
R5	same as R1 but for reaction 5; equivalent to RATE(5)
R6	same as R1 but for reaction 6; equivalent to RATE(6)
R7	same as R1 but for the combined reaction 7; equivalent to RATE(7); also R7A + R7M
R7A	rate of reaction 7 in the vessel currently being calculated where α -DNT is the reactant
R7M	same as R7A but for m-DNT
R8	same as R1 but for the combined reaction 8; equivalent to RATE(8); also R8A + R8M
R8A	same as R7A but for reaction 8
R8M	same as R8A but for m-DNT
R9	same as R1 but for reaction 9; equivalent to RATE(9)
R9A	Zero
R9G	Zero
R9M	Zero
TKEL	temperature of the vessel currently being calculated (°K)
T1	A1 + P1
T2	A2 + P2

T3	A3 + P3
T4	A4 + P4
T5	A5 + P5
T6	A6 + P6
T7	A7 + P7
T8	A8 + P8
W	initial acid phase concentration of water in the vessel currently being calculated (moles/ft^3)
X	consolidation term used in the integration sequence of organic species in the acid phase of the vessel currently being calculated
XEQA	equilibrium solubility of nitrobody in the acid phase of the vessel currently being calculated (moles/hr)
XL	lower limit of an ionic species concentration which is applied during internal halving procedure
XU	upper limit of an ionic species concentration which is applied during internal halving procedure
XUP	upper limit of $HS_2O_7^-$ concentration (resulting from dissociation according to equation 19) which is applied during internal halving procedure
X1	mole fraction α -MNT in the acid phase of the vessel currently being calculated
X13	mole fraction water in acid phase of the vessel currently being calculated
X14	mole fraction sulfur trioxide in the acid phase of the vessel currently being calculated

X2	mole fraction m-MNT in the acid phase of the vessel currently being calculated
X5	mole fraction α -TNT in the acid phase of the vessel currently being calculated
X6	mole fraction m-TNT in the acid phase of the vessel currently being calculated
X9	mole fraction nitric acid in the acid phase of the vessel currently being calculated
Y	consolidation term used in the integration sequence for organic species in the acid phase of the vessel currently being calculated; also used for initial concentration (moles/ft^3) of free sulfuric in the acid phase of the vessel currently being calculated
YA	ratio of AMNB to ANB
YP	ratio of AMNB to PNB
Z	initial acid phase concentration of nitric acid which is used under strong acid nitrating conditions for which water is present; also used as a consolidation term in the integration sequence for organic species in the acid phase
ZA	enthalpy of the contents of a separator (BTU/hr - °C)
ZB	rate of heat generated in a separator due to reaction (BTU/Hr)
ZD	A8-A17; undissociated acid phase nitric acid remaining at equilibrium in the vessel currently being calculated (moles/hr)

Subroutine SUB2

The definitions of the following variables are identical to those in the main program: AKMA, AKMATL, AK10, AK12, AK3S, AK3W, AK4S, AK4W, AK5S, AK6S, AK7, AK8, CP(I), DH(I), E10, E21, E3S, E3W, E4S, E4W, E5S, E6S, E7, E8, FD, DMX, QA, QP, RHO(I), RP, RR, SA, SB, SC, SD, SE, SG, SH, SI, SJ, TR

Remaining variables are defined as follows:

AØ(I)	moles/hr component i in the total acid phase leaving the separator for which recycle parameters are currently being calculated
AT	total moles/hr of acid phase leaving the separator for which recycle parameters are currently being calculated
EAØP	molar ratio of acid to organic phase in the organic stream leaving the separator for which recycle parameters are currently being calculated
EØAP	molar ratio of organic to acid phase in either of the recycle streams leaving the separator for which recycle parameters are currently being calculated
FAR	fraction of acid phase that is recycled in the separator for which recycle parameters are currently being calculated
FAR1	fraction of acid phase sent forward from the separator for which recycle parameters are currently being calculated
FF(I)	identical to definitions given in subroutine SUB
FFØ	fraction of organic phase sent forward from the separator for which recycle parameters are currently being calculated

FPØ1	fraction of organic phase which is recycled in the separator for which recycle parameters are currently being calculated
FRAC	ratio of internal recycle stream to total recycle streams leaving the separator for which recycle parameters are currently being calculated
NOTCH	notch setting on the internal recycle gate valve for the separator for which recycle parameters are being calculated
PØ	moles/hr component i the total organic phase leaving the separator for which recycle parameters are currently being calculated
PT	moles/hr total organic phase leaving the separator for which recycle parameters are currently being calculated
QT	volumetric flow (ft^3/hr) of combined recycle streams leaving the separator for which recycle parameters are currently being calculated

Subroutine SUB1

The definitions of the following variables are identical to those in the main program: AI(J), AKMA, AKMATL, AK10, AK12, AK3S, AK3W, AK4S, AK4W, AK5S, AK6S, AK7, AK8, AV(1,J), CHAMXØ, CP(I), DFAMXØ, DH(I), DT, EX, E10, E21, E3S, E3W, E4S, E4W, E5S, E6S, E7, E8, FD, FMX, G1(I), G10(I), G3(I), G3S(I), G4(I), G4S(I), G5(I), G6(I), G7(I), G8(I), G9(I), ICALL, IPRNT, IVSL, JACK, NM, NN, NP, PI(I), PV(I,J), QY(I), RATES(I,J), RHØ1, RHØ10, RHØ11, RHØ12, RHØ13, RHØ14, RHØ2, RHØ3, RHØ4, RHØ5, RHØ6, RHØ7, RHØ8, RHØ9, RP, RR, SA, SB, SC, SD, SE, SG, SH, SI, SJ, TCOX, TNOX, TR, TSEP(I), TTME, XYY(I)

Remaining variables are defined as follows:

AØ(I)	moles/hr component i in the acid phase of the vessel for which component % changes are currently being calculated

DFA(I)	acid phase component i % change during NN iterations in the vessel currently being calculated
DFAMX	maximum % change in an acid phase component in the vessel currently being calculated
DFP(I)	same as DFA(I) but for organic phase
DFPMX	same as DFAMX but for organic phase
PØ(I)	moles/hr component i in the organic phase of the vessel for which component % changes are currently being calculated
R1-R10	NOT USED

Function ENTH

The definitions of the following variables are identical to those in the main program: AKMA, AKMATL, AK10, AK3S, AK3W, AK4S, AK4W, AK5S, AK6S, AK7, AK8, CP(I), DH(I), E10, E12, E3S, E3W, E4S, E4W, E5S, E6S, E7, E8, FD, FMAX, RHØ1, RHØ10, RHØ11, RHØ12, RHØ13, RHØ14, RHØ2, RHØ3, RHØ4, RHØ5, RHØ6, RHØ7, RHØ8, RHØ9, RR, SA, SB, SC, SD, SE, SG, SH, SI, SJ, TR

Remaining variables are defined as follows:

A(I)	moles/hr component i in the acid phase of the stream for which the enthalpy is currently being calculated
AX(I)	moles/hr component i in the total acid phase leaving a vessel for which the enthalpy of a particular leaving stream is currently being calculated
CP11	equivalent to CP(11)
CP12	equivalent to CP(12)
CP13	equivalent to CP(13)
CP14	equivalent to CP(14)

DLT	temperature of the vessel (relative to 20°C) for which the enthalpy of a particular exiting stream is currently being calculated
ENTH	enthalpy of the stream currently being calculated (kcal/hr)
ENTHØ	enthalpy of mixing of the acid components in the acid phase of the stream currently being calculated based on the zero nitric curve of the McKinley and Brown data (kcal/lb)
ENTH2	enthalpy of mixing of the acid components in the acid phase of the stream currently being calculated based on the 20% nitric curve of the McKinley and Brown data (kcal/lb)
F	adjusted weight fraction of nitric acid plus sulfuric acid in the acid phase of the stream currently being calculated on a nitrobody free basis
LBS	lb/hr of nitric acid, sulfuric acid, water (or sulfur trioxide) in the acid phase of the stream currently being calculated
LBSE	lb/hr of nitric acid and equivalent sulfuric acid in the acid phase of the stream currently being calculated
P(I)	moles/hr component i in the organic phase of the stream for which the enthalpy is currently being calculated
PX(I)	moles/hr component i in the total organic phase leaving a vessel for which the enthalpy of a particular leaving stream is currently being calculated
T	moles/hr combined organic and acid phase nitrobody component in the stream for which enthalpy is currently being calculated

TP	temperature of the vessel for which the enthalpy of an exiting stream is being calculated (°C)
WTA	LBSE/LBS; nitrobody free weight fraction of equivalent sulfuric plus nitric acid in the acid phase of the stream for which the enthalpy is currently being calculated
WTN	weight fraction of nitric acid in the equivalent sulfuric plus nitric acid of the acid phase of the stream for which the enthalpy is currently being calculated
X(I)	the ith data point on the zero % nitric curve from the enthalpy concentration data of McKinley and Brown
XA1	FACID, FA or 1 dependent on the origination point of the stream for which the enthalpy is currently being calculated
XA2	FR, FRAC or 1 dependent on the origination point of the stream for which the enthalpy is currently being calculated
XP1	FØ, FØRG or 1 dependent on the origination point of the stream for which the enthalpy is currently being calculated
XP2	FR, FRAC or 1 dependent on the origination point of the stream for which the enthalpy is currently being calculated
Y(I)	the ith data point on the 20% nitric curve from the enthalpy concentration data of McKinley and Brown

APPENDIX E

Dynamic Simulation--Input Data Format

Preceding page blank

Card	Data Read	Format
1	AK12, AK3W, AK4W, AK5S, AK6S, AK7, AK8, AK10	8F10.0
2	AK3S, AK4S, E3S, E4S	8F10.0
3	EK1, E3W, E4W, E5S, E6S, E7, E8, E10	8F10.0
4	SA, SB, SC, SD, SE, SG, SH, SI	8F10.0
5	TS, RR, TR, AKMA, AKMATL, FD, RP	8F10.0
6, 7	DH (I), I=1, 10	8F10.0
8, 9	RHØ (I), I=1, 14	8F10.0
10, 11	CP (I), I=1, 14	8F10.0
12 - 14	A1A (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
14 - 16	P1A (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
17 - 19	A1B (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
20 - 22	P1B (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
23 - 25	A1S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
26 - 28	P1S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
29 - 31	A2 (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
32 - 34	P2 (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
35 - 37	A2T (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
38 - 40	P2T (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
41 - 43	A3 (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
44 - 46	P3A (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
47 - 49	A3B (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
50 - 52	P3B (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
53 - 55	A3S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0

Card	Data Read	Format
56 - 58	P3S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
59 - 61	A4 (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
62 - 64	P4 (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
65 - 67	A4S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
68 - 70	P4S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
71 - 73	A5 (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
74 - 76	P5 (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
77 - 79	A5S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
80 - 82	P5S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
83 - 85	A6 (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
86 - 88	P6 (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
89 - 91	A6S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
92 - 94	P6S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
95	N1, N2, N3, N4, N5, N6	6I1
96	EAØ (I), I=1,6	8F10.0
97	EØA (I), I=1, 6	8F10.0
98	VKM (I), I=1, 8	8F10.0
99	VKMS	8F10.0
100	TEMP (I), I=1, 8	8F10.0
101	FX	8F10.0
102 - 108	(FIN(I,J), J= 1, 8), I= 1, 7	8F10.0
109 - 118	(CØMP(J,I), I=1, 14), J=1, 5	8F10.0/6F10.0
119	IPRNT, TIME, DT, DPRNT	I5, 3F10.0
120-(120+NCHNG)	ICH(NCHNG), IVS(NCHNG), DL(NCHNG), TME, TVL	2I5, 3F10.0
120+NCHNG+1	Blank	

APPENDIX F

Steady State Simulation--Program Listing and Output

Preceding page blank

SOURCE PROGRAM LISTING

```
      PROGRAM TNTSI*(INPUT,TAPE5=INPUT,OUTPUT,TAPE6=OUTPUT,PUNCH,TAPE7      TNTSS     2
     C=PUNCH)                                                               TNTSS     3
      REAL NTOS(4),NTOS1A,NTOS3A                                            TNTSS     4
      DIMENSION TEMP(8)                                                     TNTSS     5
      DIMENSION IMIT(14)                                                    TNTSS     6
      DIMENSION ATU(8)                                                      TNTSS     7
      DIMENSION AIRLBS(14,6),PIRLBS(14,6),AXRLBS(14,6),PIPLBS(14,6),        TNTSS6    1
     C AFLBS(14,6),PFLBS(14,6),AWS(6)                                       TNTSS6    2
      REAL MW(17)                                                           TNTSS     8
      INTEGER TITLE(20)                                                     TNTSS     9
      INTEGER MDD(2,5)                                                      TNTSS    10
      REAL CA(5,4)                                                          TNTSS    11
      REAL ATOM(5,14)                                                       TNTSS    12
      DIMENSION AV(14,15),PV(14,15)                                         TNTSS    13
      DIMENSION GGS(14,4)                                                   TNTSS    14
      DIMENSION PTHO(8)                                                     TNTSS    15
      DIMENSION AXP2O(14),AXP3O(14),AXP4O(14),AXP5O(14),AXP6O(14),          TNTSS    16
     C PIP2O(14),PIP3O(14),PIP4O(14),PIP5O(14),PIP6O(14)                    TNTSS    17
      DIMENSION FIN(7,8)                                                    TNTSS    18
      DIMENSION AF(14,6),AIP(14,6),AXR(14,6),PF(14,6),PIR(14,6),            TNTSS    19
     C PIP(14,6)                                                            TNTSS    20
      DIMENSION ARRAY(14,8),PV(14,15),AV(14,15)                             TNTSS    21
      DIMENSION CHA(4),AN(6),AS(6),TAS(6),TN(6),TS(6),SWN(6),WHOWDS(6)      TNTSS    22
      DIMENSION DWO(14),COMP(5,14)                                          TNTSS    23
      DIMENSION YOL(14),XP(12,14),POUNDS(10,14),TTLBS(14)                   TNTSS4    1
      DIMENSION IPA(10,14),PACID(10,14),TTLMSA(14)                          TNTSS4    2
      REAL MWOLD                                                            TNTSS4    3
      COMMON/FLAG/IFLG(6)                                                   TNTSS    24
      COMMON/PARA/T1A,T1B,T2,T3A,T3B,T4,T5,T6,WOW(8),VWMS                   TNTSS    25
      COMMON/INPUT/AI(17),PI(17)                                            TNTSS    26
      COMMON/MTSP/AII(14),PII(14)                                           TNTSS    27
      COMMON/OOO/OO(14)                                                     TNTSS    28
      COMMON/FO/V(22)                                                       TNTSS    29
      COMMON/X/A1A(14),A1B(14),A2(14),A3A(14),A3B(14),                      TNTSS    30
     C A4(14),A5(14),A6(14)                                                 TNTSS    31
      EQUIVALENCE (ARRAY(1,1),A1A(1)),(PV(1,1),P1A(1)),                     TNTSS    32
     C (AV(1,1),A1A(1))                                                     TNTSS    33
      COMMON/PC/P1A(14),P1B(14),P15(14),P2(14),P2S(14),P3A(14),              TNTSS    34
     C P3B(14),P3S(14),P4(14),P4S(14),P5(14),P5S(14),P6(14),P6S(14)         TNTSS    35
     C ,PES(14)                                                             TNTSS    36
      COMMON/AC/A1A(14),A1B(14),A1S(14),A2(14),A2S(14),A3A(14),              TNTSS    37
     C A3B(14),A3S(14),A4(14),A4S(14),A5(14),A5S(14),A6(14),A6S(14)         TNTSS    38
     C ,A8S(14)                                                             TNTSS    39
      COMMON/SOLV/AF1(14),AF2(14),AF3(14),AF4(14),AF5(14),AF6(14),          TNTSS    40
     C AIP1(14),AIP2(14),AIP3(14),AIP4(14),AIP5(14),AIP6(14),               TNTSS    41
     C AXP1(14),AXP2(14), AXP3(14),AXP4(14),AXP5(14),AXP6(14),              TNTSS    42
     C PF1(14),PF2(14),PF3(14),PF4(14),PF5(14),PF6(14),                     TNTSS    43
     C PIP1(14),PIP2(14),PIP3(14),PIP4(14),PIP5(14),PIP6(14),               TNTSS    44
     C PIR1(14),PIR2(14),PIR3(14),PIR4(14),PIR5(14),PIR6(14)                TNTSS    45
     C ,TCEP(4),        MO(6),EAMP(4),FOMP(6)                               TNTSS    46
     C ,G1S(14),G1A(14),G1B(14),G1O(14),COL(14)                             TNTSS4    4
     C ,EAO(4),ENA(4),RATES(9,10),FACD(6),YELLOW(14)                        TNTSS    48
      COMMON/DUM/D(16),III                                                  TNTSS    49
      COMMON/VECTOR/ITYPE,IPOINT,NC,ISTGE,IW,IV,DEL,IE,IAFT,ICHECK          TNTSS    50
      COMMON/7/ RW01,RW02,RW03,RW04,RW05,RW06,RW07,RW08,RW09,RW010,         TNTSS    51
     C RW11,RW12,RW013,RW014,CP(14),DW(10),AX12,AX3B,AX4B,AXSS,AXGS,        TNTSS    52
     C AX7S,AX8S,E3S,E4S,                                                   TNTSS    53
```

```
                C AK7,AK8,AK10,E21,F3W,F4W,F5S,F6S,E7,E8,E10,FD,AKKA,AKMATL,SA,SB,    TNTSS      54
                C SC,SD,SE,SG,SH,SI,SJ,RR,TR,FMAX,PP,AKA,AKEC                        TNTSS4      5
     40         COMMON/PAR/G1(8),G3(8),G4(8),G5S(8),G4S(8),G5(8),G6(8),G7(8),         TNTSS      56
                C GR(8),G1C(8),G9(8)                                                 TNTSS      57
                 EQUIVALENCE (AF1(1),AF(1,1)),(AIR1(1),AIR(I,1)),(AXR1(1),           TNTSS      58
                C AXR(I,1)),(PF1(1),PF(1,1)),(PIR1(1),PIR(I,1)),(PXR1(1),           TNTSS      59
                C PXR(1,1))                                                          TNTSS      60
     45          EQUIVALENCE (TEMP(1),T1A)                                           TNTSS      61
                 EQUIVALENCE (AK9,SE),(FG,SG)                                        TNTSS      62
                 E  IVALENCE (RHO1,RHO(1))                                           TNTSS      63
                 EQUIVALENCE(GGS(1,1),G1S(1))                                        TNTSS      64
                 EQUIVALENCE (TSEP1(1),TSEP1),(TSEP2(2),TSEP2),(TSEP3(3),TSEP3),     TNTSS      65
     70          C (TSEP4(4),TSEP4),(TSEP5(5),TSEP5),(TSEP6(6),TSEP6)                TNTSS      66
                 DATA ATOM/7.,7.,2.,1.,  .,7.,7.,2.,1.,0.,7.,6.,4.,2.,0.,            TNTSS      67
                C 7.,6.,4.,2.,0.,7.,5.,4.,3.,0.,7.,5.,6.,3.,0.,                     TNTSS      68
                C 6.,7.,5.,7.,6.,7.,3,67,7.,33,3.,0.,0.,1.,3.,1.,0.,7.,8.,0.,0.,0.,0.,  TNTSS  69
                C  5.,2.,6.,7.,1.,0.,7.,5.,1.,1.,0.,2.,1.,0.,0.,0.,0.,3.,0.,1. /    TNTSS      70
     75          DATA CTL,CSL,CWN,CSN/.2293,.81192,.81063,.81714/                    TNTSS      71
                 DATA III/0/                                                         TNTSS      72
                 DATA IMIT/1,1,0,1,0,1,1,0,1,0,1,0,1,0/                              TNTSS      73
                 DATA HOR/4HCARB,4HON  ,4HHYDR,4HOGEN,4HOXYG,4HEN  ,4HNITR,          TNTSS      74
                C 4HOGEN,4HSULP,4HHING /                                             TNTSS      75
     80          DATA DH/13978.,17120.,11756.,9800.,11760.,14520.,237000.,           TNTSS2      1
                C 921000.,0.,0./                                                     TNTSS      77
                 DATA CP/2*27.6,2*28.9,6*33.8,10.01,18.9,2*15.55,8.16,14.30/         TNTSS2      2
                 DATA RHO/2*.5,2*.46,4*.4,1.45,.55,2*1.15,3.3,1.15/                  TNTSS      79
                 DATA G4      /1,.8,.1,5 .8,.8,.8,.8,.1,.8,1,.8,.1,.8,.8,.4,.8,.     TNTSS      80
     85          C 1,.8,.2,.8,.8,/                                                   TNTSS      81
                 DATA4H/2*197,.2*182,.2*227,.213,.258,.63,.92,.98,.127,.18,.80,      TNTSS      82
                C 791,/                                                              TNTSS      83
                 DATA FWN,EFP,FYW,EOL/-68,.-87,.-45,.104,/                           TNTSS      84
                 READ(5,1)AK12,AK3W,AK4W,AK5S,AK6S,AK7,AK8,AK10                      TNTSS      90
     90          READ(5,1)AK3S,AK4S,AK5S,F4S                                         TNTSS      91
               1  FORMAT(8F10.6)                                                     TNTSS      92
                 READ(5,1) E21,F3W,F4W,F5S,E6S,E7,E8,E10                             TNTSS      93
                 READ(5,1)SA,SB,SC,SD,SE,SG,SH,SI                                   TNTSS      94
                 READ(5,1) SJ,RR,TR,AKMA,AKMATL,FMAX,FD,PP                          TNTSS4      6
     95          READ(5,1) AKA,AKB,AKC,AKEQ,AKEQOV,FOV                              TNTSS4      7
                 DH(9)=71490.,EE=5400.                                              TNTSS4      8
                 PPP=7.,EEP/12.,-2.,PP)                                             TNTSS4      9
                 WRITE(6,780)AK12,AK3W,AK4W,AK3S,AK4S,AK5S,AK6S,AK7,AK8,AK10,       TNTSS      96
                C AKA,AKB,AKC,AKEQ,AKEQOV,                                           TNTSS      97
    100          C E21,                                                              TNTSS      98
                 C F3W,F4W,F3S,F4S,F5S,E4S,E7,E8,E10,SA,SB,SC,SD,SE,SG,SH,SI,SJ,RR,  TNTSS      99
                 C TR,AKMA,AKMATL,FD                                                 TNTSS     100
                  WRITE(6,785) PP                                                    TNTSS     101
    105         785  FORMAT(6X,*OXYGEN COEFFICIENT =*,F8.3)                         TNTSS     102
                  WRITE(6,790) (I,RW(I),DHO(I),CP(I),I=1,10)                         TNTSS     103
                  WRITE(6,792) (I,RW(I),DHO(I),CP(I),I=11,14)                        T TSS     104
    110         790  FORMAT(  1HI,20X 20H**********INPUT DATA******/ 15H0RATE CONSTANTS/12X  TNTSS  105
                C 3HK12,9X,3HK3W,9X,3HK4W,9X,3HK3S,9X,3HK4S,9X,3HK5S,9X,3HK6S,9X,    TNTSS     106
                C 2HK7,9X,2HK8,9X,3HK10/6X10F12.2//12X,*KA*,7X,*KB*,7X,*KC*,7X,      TNTSS     107
    115         C *KEQ*,7X,*KEQOV*/6X,5F10.6/20H0ACTIVATION ENERGIES/12X,3HE21       TNTSS     108
                C,7X,3HF3W,7X,3HE4W,7X,3HF3S,7X,3HE4S,7X,3HE5S,7X,3HE6S,7X,2HE7,8X,  TNTSS     109
                C 2HE8,8X,3HF10/6X10F1                                               TNTSS     110
                C9,0/ 10H0CONSTANTS/11X  1HA,7X  1HB,7X  1HC,     7X  1HD,7X  1HE,7  TNTSS     111
                CX  1HG,7X  1HH,7X  1HI,7X  1HJ/6X9F8.2/6X 18HGAS LAW CONSTANT =,    TNTSS     112
```

```
      C  FS.2/6X 23HREFERENCE TEMPERATURE =.F8.2.    6H DEG K/                TNTSS   113
      C  6X 17HPASS TX. COEFF. =.F10.1/6X 23HMASS TX. COEFF. (TOL) =.F10.     TNTSS   114
     C1/6X.9HEXTENT OF REACTION FOR HN4OSO4 DECOMPOSITION =.F8.4)              TNTSS   115
     701  FORMAT( 29H0PHYSICAL PROPERTIES/6X  9HCOMPONENT.5X  8HMOL. WT..     TNTSS   116
     C         5X  7HDENSITY.5X  8HHT. CAP..10X  6HREACTION.5X 15HHT. OF      TNTSS   117
      CREACTION/      (6X15.F14.1.F12.2.F13.2.110.F20.8))                      TNTSS   118
     702  FORMAT(6X15.F14.1.F12.2.F13.2)                                       TNTSS   119
          READ(5.1429) ((AVI(I.J).I=1.14).(PVI(I.J).I=1.14).J=1.14)            TNTSS2    3
          READ(5.1412) FACT6.FACT5.FACT4.FACT3.FACT2                           TNTSS   121
          READ(5.66) NDS                                                       TNTSS   122
       66 FORMAT(I2)                                                           TNTSS   123
          ISTOP=NDS+1                                                          TNTSS   124
          NSET=0                                                               TNTSS   125
          GO TO 65                                                             TNTSS   126
     1001 WRITE(6.39) III                                                      TNTSS   127
       39 FORMAT(///1X.*NUMBER OF VESSEL EQUATION ITERATIONS FOR THIS DATA S   TNTSS   128
         1ET=.I3)                                                            TNTSS   129
       65 NSET=NSET+1                                                        TNTSS   130
          IF(NSET.EQ.ISTOP) STOP                                               TNTSS   131
          III=9                                                                TNTSS   132
          READ(5.7) TITLE                                                      TNTSS   133
          READ(5.4) IPRNT.IF.ILIST.IWRAL.IPI.IAFT.IPNCH .ICHECK                TNTSS6    3
     7    FORMAT(20A4)                                                         TNTSS   135
          WRITE(6.701)  NSET.TITLE                                             TNTSS   136
     701  FORMAT(1HI.***DATA SET.I2.5H*****.10X20A4)                           TNTSS   137
          READ(5.1)((FIN(I.J).J=1.8).I=1.7)                                    TNTSS   138
          READ(5.2)((COMP(J.I).I=1.14).J=1.5)                                  TNTSS   139
     2    FORMAT(8F10.0/6F10.0)                                                TNTSS   140
          IF(IAFT.NE.1)GOTO709                                                 TNTSS   141
          DO79I=1.14                                                           TNTSS   142
     708  YELLOW(I)=10.*COMP(3.I)/MW(I)                                        TNTSS   143
     709  CONTINUE                                                             TNTSS   144
          P1A=FIN(6.1)/MW(10)                                                  TNTSS   145
          P1B=FIN(6.2)/MW(10)                                                  TNTSS   146
          READ(5.6)NM                                                          TNTSS   147
     4    FORMAT(9I)                                                           TNTSS   148
          READ(5.1)TEMP                                                        TNTSS   149
          READ(5.1)VKM.VKMS                                                    TNTSS   150
          VOL(1)=VKM(1)                                                        TNTSS4   10
          VOL(2)=VKM(2)                                                        TNTSS4   11
          VOL(3)=VKMS                                                          TNTSS4   12
          VOL(4)=VKM(3)                                                        TNTSS4   13
          VOL(5)=VKMS                                                          TNTSS4   14
          VOL(6)=VKM(4)                                                        TNTSS4   15
          VOL(7)=VKM(5)                                                        TNTSS4   16
          VOL(8)=VKMS                                                          TNTSS4   17
          VOL(9)=VKM(6)                                                        TNTSS4   18
          VOL(10)=VKMS                                                         TNTSS4   19
          VOL(11)=VKM(7)                                                       TNTSS4   20
          VOL(12)=VKMS                                                         TNTSS4   21
          VOL(13)=VKM(8)                                                       TNTSS4   22
          VOL(14)=VKMS                                                         TNTSS4   23
     1428 FORMAT(8F10.0/6F10.0)                                                TNTSS   151
          READ(5.1411)EA0.E0A                                                  TNTSS   152
     1411 FORMAT(6F10.8)                                                       TNTSS   153
     1412 FORMAT(5F10.8)                                                       TNTSS   154
          DEL=.02                                                              TNTSS   155
```

```
                      NC=1*900C8                                                TNTS54    74
                      DO7C I=1,8                                                TNTSS     157
                      DO7I J=1,14                                               TNTSS     158
175                   ARRAY(J,I)=0.                                             TNTSS     159
                      DO72 K=1,5                                                TNTSS     160
                72    ARRAY(J,I)=ARRAY(J,I)+FIN(K,I)*COMP(K,J)*.01/RN(J)        TNTSS     161
                71    CONTINUE                                                  TNTSS     162
                      ARRAY(13,I)=ARRAY(13,I)+FIN(7,I)/RN(13)                   TNTSS     163
144             79    CONTINUE                                                  TNTSS     164
                      IF(IPRINT.EQ.1)                                           TNTSS     165
                     1WRITE(6,388) ((ARRAY(I,J),I=1,14),J=1,8)                  TNTSS     166
                388   FORMAT(1X14F8.3)                                          TNTSS     167
                      DO178I=1,6                                                TNTSS     168
185                   FAO(I)=EAO(I)/(1.-FAO(I))                                 TNTSS     169
                178   FOA(I)=FOA(I)/(1.-FOA(I))                                 TNTSS     170
                      DO171I=1,8                                                TNTSS     171
                      ZA=(1./TP-1./(TEMP(I)+273.3))/BB                          TNTSS     172
                      G1(I)=EXP(E2I*ZA)/AK12                                    TNTSS     173
194                   G3(I)=AK3W*EXP(E3W*ZA)                                    TNTSS     174
                      G4(I)=AK4W*EXP(E4W*ZA)                                    TNTSS     175
                      G35(I)=AK35*EXP(E35*ZA)                                   TNTSS     176
                      G45(I)=AK45*EXP(E45*ZA)                                   TNTSS     177
                      G5(I)=AK55*EXP(E55*ZA)                                    TNTSS     178
195                   G6(I)=AK65*EXP(ZA*E65)                                    TNTSS     179
                      G7(I)=AK7*EXP(E7*ZA)                                      TNTSS     180
                      G8(I)=AK8*EXP(E8*ZA)                                      TNTSS     181
                      G9(I)=AK9*EXP(E9*ZA)                                      TNTSS     182
                      G10(I)=AK10*EXP(E10*ZA)                                   TNTSS     183
200             171   CONTINUE                                                  TNTSS     184
                      DO 172 I=1,14                                             TNTSS     185
                      DO 173 J=1,14                                             TNTSS     186
                      AV(I,J)=AVI(I,J)                                          TNTSS     187
                 173  PV(I,J)=PVI(I,J)                                          TNTSS     188
205                   AV(I,15)=AVI(I,3)                                         TNTSS     189
                      PV(I,15)=PVI(I,3)                                         TNTSS     190
                 172  CONTINUE                                                  TNTSS     191
                      ITYPE=1                                                   TNTSS     192
                      IN=0                                                      TNTSS     193
210                   IV=0                                                      TNTSS     194
                      DO1491ISTGE=1,6                                           TNTSS     195
                      IN=IN+1                                                   TNTSS     196
                      IV=IV+2                                                   TNTSS     197
                      IF(ISTGE.EQ.1)GOTO1402                                    TNTSS     198
215                   IF(ISTGE.NE.3)GOTO1403                                    TNTSS     199
                1402  IN=IN+1                                                   TNTSS     200
                      IV=IV+1                                                   TNTSS     201
                1403  IV1=IV-1                                                  TNTSS     202
                      DO1404I=1,14                                              TNTSS     203
220                   A(I)=AV(I,IV1)                                            TNTSS     204
                1404  P(I)=PV(I,IV1)                                            TNTSS     205
                      CALL VESSEL                                               TNTSS     206
                1401  CONTINUE                                                  TNTSS     207
                      WRITE(6,383) ((FIN(I,J),J=1,8),I=1,7)                     TNTSS     208
225             383   FORMAT( 1H0INPUT MATRIX/6X  6HVESSEL,10X  2H14,8X  2H1P,9X  1H2,8 TNTSS     209
                     CX  2H3A,      8X  2H3B,9X  1H4,9X  1H5,9X  1H6/6X 10HWEAK WIT. ,8F TNTSS     210
                     C10.0/              6X  3HFR,,7X8F10.0/  5X 10HYELLOW WA,,8F10 TNTSS     211
                     C.0/ 5X 10HSTRONG WI,,       8F10.0/6X  5HOLEUM,5X,8F10.0/6X  7HTO TNTSS     212
```

```
                CLINGE,3XF10.0/6X  SHWATER,        5X8F10.0)                          TNTSS    213
230             WRITE(6,704) ((COMP(I,J),J=1,14),I=1,5)                             TNTSS    214
704   FORMAT(*0ACID STRENGTHS, WT. PCT,*/6X*COM,*,7X*AMNT*,2X*AMNT*,                TNTSS    215
     C  2X*AMNT*,2X*MCNT*,2X*ATNT*,2X*MTNT*,2X*TMRA*,2X*TMB*,                       TNTSS    216
     C 3X*HA,/30,2X*TOL*,2X*H2SO4 HNO3S04 H2O*,3X*SO3*/                             TNTSS    217
     C  4X*OLEUM WT. *,14F6.2/6X*FR,*,7X14F6.2/6X*YELLOW HA,*,14F6.2/               TNTSS    219
245  C  6X*STRONG NI,*,14F6.2/6X*OLEUM*,5X14F6.2)                                   TNTSS    219
                J=1                                                                 TNTSS    220
                WRITE(6,190)                                                        TNTSS    221
190   FORMAT(  1H1)                                                                 TNTSS    222
                DO1A7I=1,6                                                          TNTSS    223
260             WRITE(6,191)I                                                       TNTSS    224
191   FORMAT(  6HSTAGE,I2)                                                          TNTSS    225
                IF(I.NE.1.AND.I.NE.3)GOTO192                                        TNTSS    226
                WRITE(6,193)I,VKM(J),VKM(J+1),TEMP(J),TEMP(J+1)                     TNTSS    227
193   FORMAT(6X  6HNITRATOR,I2,  1H@,19X  6HNITRATOR,I2,  1H@/                      TNTSS    228
265  C          6X  6HVOL, =,F5.1,19X,  6HVOL, =,F5.1/6X  6HTEMP,=,F5.1,          TNTSS    229
     C             19X  6HTEMP,=,F5.1)                                            TNTSS    230
                J=J+1                                                               TNTSS    231
                GOTO196                                                             TNTSS    232
192   WRITE(6,195)I,VKM(J),TEMP(J)                                                  TNTSS    233
270   195  FORMAT(6X  8HNITRATOR,I2/6X  6HVOL, =,F5.1/6X  6HTEMP,=,F5.1)           TNTSS    234
194   J=J+1                                                                         TNTSS    235
                WRITE(6,196)I,VKMS,MC(I),EOA(I),EAO(I)                              TNTSS    236
196   FORMAT(  1H0,5X,  9HSEPARATOR,I2/6X  6HVOL, =F5.1/                            TNTSS    237
     C       6X 15HNOTCH SETTING =,I2/6X 11HENTRAINMENT/11X 15HORGANIC I           TNTSS    238
275  C  ACID,      FA,5/11X 15HACID IN ORGANIC ,FA,5)                               TNTSS    239
197   CONTINUE                                                                      TNTSS    240
780   CONTINUE                                                                      TNTSS    241
C     NITRATOR 1A                                                                   TNTSS    242
                IV=1                                                                TNTSS    243
280             ISTGE=1                                                             TNTSS    244
                IH=1                                                                TNTSS    245
                ITYPE=0                                                             TNTSS    246
                DO3213I=1,14                                                        TNTSS    247
                AI(I)=AM2(I)+A1A(I)                                                 TNTSS    248
3213  PI(I)=PM2(I)                                                                  TNTSS    249
                PI(15)=PI(15)+P1AI                                                  TNTSS    250
                CALL VESSEL                                                         TNTSS    251
C     NITRATOR 1B                                                                   TNTSS    252
                IV=2                                                                TNTSS    253
290             IB,=2                                                               TNTSS    254
                DO3214I=1,14                                                        TNTSS    255
                AII(I)= A1A(I)+A1BI(I)                                              TNTSS    256
3214  PII(I)= P1A(I)                                                                TNTSS    257
                PII(15)=PII(15)+P1AI                                                TNTSS    258
295             CALL NITSEP                                                         TNTSS    259
C     NITRATOR 2                                                                    TNTSS    260
                ISTGE=2                                                             TNTSS    261
                IV=6                                                                TNTSS    262
                IH=3                                                                TNTSS    263
300             DO3223I=1,14                                                        TNTSS    264
                AII(I)=AF1(I)+AM3(I)+A2I(I)                                         TNTSS    265
3223  PII(I)=PF1(I)+PM3(I)                                                          TNTSS    266
                CALL NITSEP                                                         TNTSS    267
C     NITRATOR 3A                                                                   TNTSS    268
305             ITYPE=0                                                             TNTSS    269
```

275

```
                ISTGE=3                                                  TNTSS  270
                IM=4                                                     TNTSS  271
                IV=4                                                     TNTSS  272
                DO 3233 I=1,14                                           TNTSS  273
  230           A(I)=AXM4(I)+AF2(I)+A3A(I)                               TNTSS  274
 3233           P(I)=PXM4(I)+PF2(I)                                      TNTSS  275
                CALL VFSSEL                                              TNTSS  276
                NITRATOR 3                                               TNTSS  277
                IM=5                                                     TNTSS  278
  295           IV=7                                                     TNTSS  279
                DO 3234 I=1,14                                           TNTSS  280
                A(I)= A3A(I)+A3B(I)                                      TNTSS  281
 3234           P(I)= P3A(I)                                             TNTSS  282
                CALL NITSEP                                              TNTSS  283
  300           NITRATOR 4                                               TNTSS  284
                IM=4                                                     TNTSS  285
                ISTGE=4                                                  TNTSS  286
                IV=9                                                     TNTSS  287
                DO 3263 I=1,14                                           TNTSS  288
  305           A(I)=AF3(I)+AXR5(I)+A4(I)                                TNTSS  289
 3263           P(I)=PF3(I)+PXR5(I)                                      TNTSS  290
                CALL NITSEP                                              TNTSS  291
                NITRATOR 5                                               TNTSS  292
                IV=11                                                    TNTSS  293
  310           IM=7                                                     TNTSS  294
                ISTGE=5                                                  TNTSS  295
                DO 3259 I=1,14                                           TNTSS  296
                A(I)=AF4(I)+AXR6(I)+A5(I)                                TNTSS  297
 3259           P(I)=PF4(I)+PXR6(I)                                      TNTSS  298
  315           CALL NITSEP                                              TNTSS  299
                NITRATOR 6                                               TNTSS  300
                ISTGE=6                                                  TNTSS  301
                IM=8                                                     TNTSS  302
                IV=13                                                    TNTSS  303
  320           DO 3263 I=1,14                                           TNTSS  304
                A(I)=AF5(I)+A6(I)                                        TNTSS  305
 3263           P(I)=PF5(I)                                              TNTSS  306
                WRITE(6,4207)                                            TNTSS  307
 4207           FORMAT(1H1)                                              TNTSS  308
  325           CALL NITSEP                                              TNTSS  309
                NC1=0                                                    TNTSS  310
                NC2=0                                                    TNTSS  311
                NC3=0                                                    TNTSS  312
                NC4=0                                                    TNTSS  313
  330           NC5=0                                                    TNTSS  314
                DO 2990 I=1,14                                           TNTSS  315
                AXR50(I)=AXR5(I)                                         TNTSS  316
                AXR40(I)=AXR4(I)                                         TNTSS  317
                AXR30(I)=AXR3(I)                                         TNTSS  318
  335           AXR20(I)=AXR2(I)                                         TNTSS  319
                PXR50(I)=PXR5(I)                                         TNTSS  320
                PXR40(I)=PXR4(I)                                         TNTSS  321
                PXR30(I)=PXR3(I)                                         TNTSS  322
                PXR20(I)=PXR2(I)                                         TNTSS  323
  340           2990 CONTINUE                                            TNTSS  324
                2404 NCS=NC5+1                                           TNTSS  325
                C    NITRATOR 5                                          TNTSS  326
```

```
                DO12431=1,14                                                    TNTSS  327
                AXP60(I)=AXP6(I)                                                TNTSS  328
345             PXP60(I)=PXP6(I)                                                TNTSS  329
                A11(I)=AF4(I)*AXP6(I)+A5I(I)                                    TNTSS  330
             1243 P11(I)=PF4(I)*PXP6(I)                                         TNTSS  331
                IN=7                                                            TNTSS  332
                IV=11                                                           TNTSS  333
                ISTAGE=5                                                        TNTSS  334
350             CALL NITSEP                                                     TNTSS  335
              C NITPATOR 6                                                      TNTSS  336
                ISTAGE=6                                                        TNTSS  337
                IN=8                                                            TNTSS  338
                IV=17                                                           TNTSS  339
355             DO12531=1,14                                                    TNTSS  340
                A11(I)=AF5(I)*A61(I)                                            TNTSS  341
             1253 P11(I)=PF5(I)                                                 TNTSS  342
                CALL NITSEP                                                     TNTSS  343
                IF(IPRNT.EQ.1)WRITE(6,3610)AXP6,PXP6                            TNTSS  344
360          3610 FORMAT(*0ITERATION FOR STAGE 6*/(1X14F8.3))                   TNTSS  345
                DO2402I=1,14                                                    TNTSS  346
                IF(ABS(AXP60(I)-AXP6(I)).GT.DEL)GOTO2403                        TNTSS  347
                IF(ABS(PXP60(I)-PXP6(I)).GT.DEL)GOTO2403                        TNTSS  348
365          2402 CONTINUE                                                      TNTSS  349
                NC5=0                                                           TNTSS  350
                IF(IPI.EQ.0)GOTO2410                                            TNTSS  351
                WRITE(6,3690)                                                   TNTSS  352
             3690 FORMAT(1X *ITERATION LOOP FOR STAGE 6 CONVERGED)              TNTSS  353
370             WRITE(6,3609)AXP6,PXP6,AXP5,PXP5                                TNTSS  354
              C,AXP60,PXP60                                                     TNTSS  355
             3609 FORMAT(1X14F8.3)                                              TNTSS  356
                GOTO2410                                                        TNTSS  357
             2403 DO 3407 I=1,14                                                TNTSS  358
375             AXP6(I)=AXP60(I)+FACT6*(AXP6(I)-AXP60(I))                       TNTSS  359
             3407 PXP6(I)=PXP60(I)+FACT6*(PXP6(I)-PXP60(I))                     TNTSS  360
                IF(NC5.LT.NC)GOTO2404                                           TNTSS  361
                WRITE(6,2405)                                                   TNTSS  362
             2405 FORMAT( 49H0ITERATION LOOP FOR NITPATOR 5 FAILED TO CONVERGE) TNTSS  363
380             STOP                                                            TNTSS  364
             2410 DO2411I=1,14                                                  TNTSS  365
                IF(ABS(AXP50(I)-AXP5(I)).GT.DEL)GOTO2413                        TNTSS  366
                IF(ABS(PXP50(I)-PXP5(I)).GT.DEL)GOTO2413                        TNTSS  367
             2411 CONTINUE                                                      TNTSS  368
385             NC4=0                                                           TNTSS  369
                IF(IPI.EQ.0)GOTO2420                                            TNTSS  370
                WRITE(6,3508)                                                   TNTSS  371
             3508 FORMAT(1X *ITERATION LOOP FOR STAGE 5 CONVERGED)              TNTSS  372
                WRITE(6,3609)AXP5,PXP5,AXP4,PXP4                                TNTSS  373
390           C,AXP50,PXP50                                                     TNTSS  374
                GOTO2420                                                        TNTSS  375
             2413 DO 3413 I=1,14                                                TNTSS  376
                AXP5(I)=AXP50(I)+FACT5*(AXP5(I)-AXP50(I))                       TNTSS  377
             3413 PXP5(I)=PXP50(I)+FACT5*(PXP5(I)-PXP50(I))                     TNTSS  378
395              IF(NC4.LT.NC)GOTO2412                                          TNTSS  379
                WRITE(6,2414)                                                   TNTSS  380
             2414 FORMAT( 49H0ITERATION LOOP FOR NITPATOR 4 FAILED TO CONVERGE) TNTSS  381
                STOP                                                            TNTSS  382
             2417 NC4=NC4+1                                                     TNTSS  383
```

```
                C     NITRATOR 4                                          TNTSS   384
                      IM=6                                                TNTSS   385
                      ISTAGE=4                                            TNTSS   386
                      IV=8                                                TNTSS   387
                      DO 1733 I=1,14                                      TNTSS   388
      405             AIR40(I)=AIR5(I)                                    TNTSS   389
                      PIR40(I)=PIR5(I)                                    TNTSS   390
                      AI(I)=AF3(I)+AIR5(I)+AA1(I)                         TNTSS   391
                1733  PI(I)=PF3(I)+PIR5(I)                                TNTSS   392
                      CALL NITSEP                                         TNTSS   393
      410             GOTO2624                                            TNTSS   394
                2629  DO 2621 I=1,14                                      TNTSS   395
                      IF(ABS(AIR40(I)-AIR4(I)).GT.DEL)GOTO2623            TNTSS   396
                      IF(ABS(PIR40(I)-PIR4(I)).GT.DEL)GOTO2623            TNTSS   397
                2621  CONTINUE                                            TNTSS   398
      415             NC3=9                                               TNTSS   399
                      IF(IPI.EQ.0)GOTO2630                                TNTSS   400
                      WRITE(6,3517)                                       TNTSS   401
                3402  FORMAT(/,' 3RD ITERATION LOOP FOR STAGE 4 CONVERGED') TNTSS   402
                      WRITE(6,3620,AIR4,PIR4,AIR3,PIR3                    TNTSS   403
      420           C,AIR40,PIR40                                         TNTSS   404
                      GOTO2624                                            TNTSS   405
                2623  DO 3621 I=1,14                                      TNTSS   406
                      AIR4(I)=AIR40(I)+FACT4*(AIR4(I)-AIR40(I))           TNTSS   407
                3621  PIR4(I)=PIR40(I)+FACT4*(PIR4(I)-PIR40(I))           TNTSS   408
      425             IF(NC3.LT.NC)GOTO2622                               TNTSS   409
                      WRITE(6,2624)                                       TNTSS   410
                2624  FORMAT(' 4TH ITERATION LOOP FOR NITRATOR 3 FAILED TO CONVERGE') TNTSS   411
                      STOP                                                TNTSS   412
                2622  NC3=NC3+1                                           TNTSS   413
      430       C     NITRATOR 3A                                         TNTSS   414
                      ISTAGE=3                                            TNTSS   415
                      IM=6                                                TNTSS   416
                      IV=6                                                TNTSS   417
                      ITYPE=0                                             TNTSS   418
      435             DO 1222 I=1,14                                      TNTSS   419
                      AIR4A(I)=AIR4(I)                                    TNTSS   420
                      PIR4A(I)=PIR4(I)                                    TNTSS   421
                      AI(I)=AIR4(I)+AF2(I)+AA1(I)                         TNTSS   422
                1222  PI(I)=PIR4(I)+PF2(I)                                TNTSS   423
      440             CALL VESSEL                                         TNTSS   424
                C     NITRATOR 3B                                         TNTSS   425
                      IS=5                                                TNTSS   426
                      IV=7                                                TNTSS   427
                      DO 1223 I=1,14                                      TNTSS   428
      445             AI(I)= A3A(I)+A3BI(I)                               TNTSS   429
                1223  PI(I)= P3A(I)                                       TNTSS   430
                      CALL NITSEP                                         TNTSS   431
                      GOTO2612                                            TNTSS   432
                2630  DO 2631 I=1,14                                      TNTSS   433
      450             IF(ABS(AIR30(I)-AIR3(I)).GT.DEL)GOTO2633            TNTSS   434
                      IF(ABS(PIR30(I)-PIR3(I)).GT.DEL)GOTO2633            TNTSS   435
                2631  CONTINUE                                            TNTSS   436
                      NC2=0                                               TNTSS   437
                      IF(IPI.EQ.0)GOTO2640                                TNTSS   438
      455             WRITE(6,3603)                                       TNTSS   439
                3603  FORMAT(' 7TH ITERATION LOOP FOR STAGE 3 CONVERGED') TNTSS   440
```

```
                WRITE(6,3600)AIR3,PIR3,AIR2,PIR2                        TNTSS   441
               F,AIR20,PIR20                                            TNTSS   442
                GOTO2644                                                TNTSS   443
      440     2637 DO 3637 I=1,14                                       TNTSS   444
                AIR3(I)=AIR30(I)+FACT3*(AIR3(I)-AIR30(I))               TNTSS   445
               3637 PIR3(I)=PIR30(I)+FACT3*(PIR3(I)-PIR30(I))           TNTSS   446
                IF(NC2.LT.NC)GOTO2632                                   TNTSS   447
                WRITE(6,2634)                                           TNTSS   448
      445       2634 FORMAT( 50H0ITERATION LOOP FOR NITRATOR 2 FAILED TO  CONVERGE)  TNTSS   449
                STOP                                                    TNTSS   450
               2632 NC2=NC2+1                                           TNTSS   451
               C    NITRATOR 2                                         TNTSS   452
                ISTGE=2                                                 TNTSS   453
      470       IN=3                                                    TNTSS   454
                IV=4                                                    TNTSS   455
                DO1213I=1,14                                            TNTSS   456
                AIR20(I)=AIR3(I)                                        TNTSS   457
                PIR20(I)=PIR3(I)                                        TNTSS   458
      475       AI(I)=AF1(I)*AIR3(I)+A2I(I)                             TNTSS   459
               1213 PII(I)=PF1(I)*PIR3(I)                               TNTSS   460
                CALL NITSEP                                             TNTSS   461
                GOTO2642                                                TNTSS   462
               2644 DO2641I=1,14                                        TNTSS   463
      480       IF(ABS(AIR20(I)-AIR2(I)).GT.DEL)GOTO2643                TNTSS   464
                IF(ABS(PIR20(I)-PIR2(I)).GT.DEL)GOTO2643                TNTSS   465
               2641 CONTINUE                                            TNTSS   466
                NC1=0                                                   TNTSS   467
                GOTO2648                                                TNTSS   468
      485       2643 DO 3643 I=1,14                                     TNTSS   469
                AIR2(I)=AIR20(I)+FACT2*(AIR2(I)-AIR20(I))               TNTSS   470
               3643 PIR2(I)=PIR20(I)+FACT2*(PIR2(I)-PIR20(I))           TNTSS   471
                IF(NC1.LT.NC)GOTO2642                                   TNTSS   472
                WRITE(6,2646)                                           TNTSS   473
      490       2646 FORMAT( 50H0ITERATION LOOP FOR NITRATOR 1 FAILED TO CONVERGE)  TNTSS   474
                STOP                                                    TNTSS   475
               2642 NC1=NC1+1                                           TNTSS   476
               C    NITRATOR 1A                                        TNTSS   477
                ISTGE=1                                                 TNTSS   478
      495       IN=1                                                    TNTSS   479
                IV=1                                                    TNTSS   480
                ITYPE=0                                                 TNTSS   481
                DO1202I=1,14                                            TNTSS   482
                AIR20(I)=AIR2(I)                                        TNTSS   483
      500       PIR20(I)=PIR2(I)                                        TNTSS   484
                AI(I)=AIR2(I)*AIA(I)                                    TNTSS   485
               1202 PII(I)=PIR2(I)                                      TNTSS   486
                PII(10)=PII(10)*PIA                                     TNTSS   487
                CALL NITSEP                                             TNTSS   488
      505       C    NITRATOR 1B                                        TNTSS   489
                IV=2                                                    TNTSS   490
                IN=2                                                    TNTSS   491
                DO1203I=1,14                                            TNTSS   492
                AII(I)= AIA(I)*AIBI(I)                                  TNTSS   493
      510       1203 PII(I)= PIA(I)                                     TNTSS   494
                PII(10)=PII(10)*PIBI                                    TNTSS   495
                CALL NITSEP                                             TNTSS   496
                GOTO2632                                                TNTSS   497
```

```
                2458 IF(IPI.NE.3)WRITE(6,2461)                                    TNTSS   498
      515       2461 FORMAT( 16H2NO HAVE ADDIVEN)                                 TNTSS   499
                2900 CONTINUE                                                     TNTSS   500
                     IF(ILIST.EQ.0)GOTO6000                                       TNTSS   501
                     IV=1                                                         TNTSS   502
                     WRITE(6,4960)                                                TNTSS   503
      520       4000 FORMAT( 2HN1,5X,9HPHASE COMPOSITIONS)                        TNTSS   504
                     DO7000ISTGF=1,6                                              TNTSS   505
                     IF(ISTGF.EQ.1)GOTO3901                                       TNTSS   506
                     IF(ISTGF.NE.3)GOTO3902                                       TNTSS   507
                3901 WRITE(6,4981)ISTGF                                           TNTSS   508
      525       4001 FORMAT(  9H0NITPATOR,I2,  14A)                               TNTSS   509
                     IV=IV+1                                                      TNTSS   510
                     WRITE(6,4002) (AV(I,IV),I=1,14),(PV(I,IV),I=1,10)            TNTSS   511
                     IF(IPRCH.NE.1) GO TO 1710                                    TNTSS6    4
                     WRITE(7,1429) (AV(I,IV),I=1,14), (PV(I,IV),I=1,14)           TNTSS   513
      530       1710 CONTINUE                                                     TNTSS   514
                4002 FORMAT(11X,                                                  TNTSS   515
                    C 11H   AMNT     MWT     ADWT     MDWT     ATWT     MTWT      TNB     TN TNTSS   516
                    CPA     MWT      TOL     H2SO4  MWH2SO4     H2O      SO3/     TNTSS   517
                    C    11H ACID PHASE,14F8.3/ 11H ORG. PHASE,10F8.3)            TNTSS   518
                     WRITE(6,4003)ISTGE                                           TNTSS   519
      535       4003 FORMAT(  9H0NITPATOR,I2,  14B)                               TNTSS   520
                     IV=IV+1                                                      TNTSS   521
                     WRITE(6,4002) (AV(I,IV),I=1,14),(PV(I,IV),I=1,10)            TNTSS   522
                     IF(IPRCH.NE.1) GO TO 1720                                    TNTSS6    5
                     WRITE(7,1429) (AV(I,IV),I=1,14), (PV(I,IV),I=1,14)           TNTSS   524
      540   1720 CONTINUE                                                         TNTSS   525
                     GOTO3902                                                     TNTSS   526
                3902 WRITE(6,4004)ISTGE                                           TNTSS   527
                4004 FORMAT(  9H0NITPATOR,I2)                                     TNTSS   528
      545            IV=IV+1                                                      TNTSS   529
                     WRITE(6,4002) (AV(I,IV),I=1,14),(PV(I,IV),I=1,10)            TNTSS   530
                     IF(IPRCH.NE.1) GO TO 1730                                    TNTSS6    6
                     WRITE(7,1429) (AV(I,IV),I=1,14), (PV(I,IV),I=1,14)           TNTSS   532
                1730 CONTINUE                                                     TNTSS   533
      550       3903 WRITE(6,4005)ISTGF,TSED(ISTGE)                               TNTSS   534
                4005 FORMAT( 10HPSEPARATOR,I2,10X, 13HTEMPERATURE =,F6.1)         TNTSS   535
                     IV=IV+1                                                      TNTSS   536
                     WRITE(6,4002) (AV(I,IV),I=1,14),(PV(I,IV),I=1,10)            TNTSS   537
                     IF(IPRCH.NE.1) GO TO 1740                                    TNTSS6    7
      555            WRITE(7,1429) (AV(I,IV),I=1,14), (PV(I,IV),I=1,14)           TNTSS   539
                1740 CONTINUE                                                     TNTSS   540
                1429 FORMAT(5F14.7/5E16.7/6F16.7)                                 TNTSS   541
                4900 FORMAT(11X,                                                  TNTSS   542
                    C 11H   AMNT     MWT     ADWT     MDWT     ATWT     MTWT      TNB     TN TNTSS   543
      560           CPA     MWT      TOL     H2SO4  MWH2SO4     H2O      SO3/     TNTSS   544
                    C    11H ACID PHASE,14F8.3/ 11H ORG. PHASE,10F8.3)            TNTSS   545
                3909 CONTINUE                                                     TNTSS   546
                     WRITE(6,4100)                                                TNTSS   547
                4100 FORMAT(1H1,65X,5HDATA)                                       TNTSS   548
      565            WRITE(6,4101) (I,G15(I),G16(I),G18(I),G19(I),G8(I),I=1,14)   TNTSS   549
                4101 FORMAT(7I,4HESSFL,4X,4HCOI,7I,4HBX,7I,4HTNP,7I,4HCO2,8X,4HQ)/TNTSS   550
                    C (1X,I10,4F10.4,3I,F10.7))                                   TNTSS4   25
                     S15=0.                                                       TNTSS   552
                     S14=0.                                                       TNTSS   553
      570            S1R=0.                                                       TNTSS   554
```

```
                    S10=0.                                                  TNTSS    555
                    DO 61 I=1,14                                            TNTSS    556
                    S15=S15+G15(I)                                          TNTSS    557
                    S16=S16+G16(I)                                          TNTSS    558
    570             S18=S18+G18(I)                                          TNTSS    559
                    S19=S19+G19(I)                                          TNTSS    560
                4107 CONTINUE                                               TNTSS    561
                    TCO2=S15                                                TNTSS    562
                    TH2O=S16                                                TNTSS    563
    580             TTMP=S19                                                TNTSS    564
                    TCO2=S18                                                TNTSS    565
                    WRITE(6,4107) S15,S16,S19,S19                           TNTSS    566
                4107 FORMAT(1X,6TOTAL=,4F10.4)                              TNTSS    567
                    WRITE(6,4007)                                           TNTSS    568
    585         4007 FORMAT(1////11X,'VESSEL TYPE CONSTANTS AND VOLUMETRIC FLOWS')  TNTSS4    26
                    WRITE(6,88)                                             TNTSS    570
                 88 FORMAT(1X,'VESSEL',5X,'A',10X,'P',10X,'T',12X,'TAU',12X,'F')  TNTSS4    27
                    K=0                                                     TNTSS    572
                    DO 88 IV=1,14                                           TNTSS    573
    590             VA=0.                                                   TNTSS    574
                    VP=0.                                                   TNTSS    575
                    DO 86 I=1,14                                            TNTSS    576
                    VA=VA+AV(I,IV)/MWO(I)                                   TNTSS    577
                 86 VP=VP+PV(I,IV)/MWO(I)                                   TNTSS    578
    595             VT=VA+VP                                                TNTSS    579
                    FV=VP/VT                                                TNTSS4    28
                    FA=VA/VT                                                TNTSS4    29
                    PT=0.                                                   TNTSS4    30
                    AT=0.                                                   TNTSS4    31
    600             DO 150 I=1,10                                           TNTSS4    32
                150 PT    =PT    +PV(I,IV)                                  TNTSS4    33
                    DO 160 I=1,14                                           TNTSS4    34
                160 AT=AT+AV(I,IV)                                          TNTSS4    35
                    PMIX    =PT    /VP                                      TNTSS4    36
    605             PMIXA=AT/VA                                             TNTSS4    37
                    IF(  I.EQ.IT(IV).EQ.9) FA=.755                          TNTSS4    38
                    IF(  I.EQ.IT(IV).EQ.8) FO=.245                          TNTSS4    39
                    WRITE(6,2A=FA*WMOL(IV)                                  TNTSS4    40
                    WMOLDO    =FO    *WMOL(IV)                              TNTSS4    41
    610             WMOLDO=WMOLDO+O*OP                                      TNTSS4    42
                    WMOLDA=WMOLDA*G*VA                                      TNTSS4    43
                    DO 151 I=1,14                                           TNTSS4    44
                    APA(I,IV)=AV(I,IV)/AT                                   TNTSS4    45
                151 APV(I,IV)=PV(I,IV)/PT                                   TNTSS4    46
    615             TPOUND=0.                                               TNTSS4    47
                    DO 153 I=1,10                                           TNTSS4    48
                    POUNDS(I,IV)=PMOLDO    *APV(I,IV)*MW(I)                 TNTSS4    49
                153 TPOUND=TPOUND+POUNDS(I,IV)                              TNTSS4    50
                    TTLPS(IV)=TPOUND                                        TNTSS4    51
    620             TPOPND=0.                                               TNTSS4    52
                    DO 167 I=1,15                                           TNTSS4    53
                    PACID(I,IV)=PMOLDA*APA(I,IV)*MW(I)                      TNTSS4    54
                    IF(I.EQ.9) PACID(I,IV)=0.                               TNTSS4    55
                167 TPOUND=TPOUND+PACID(I,IV)                               TNTSS4    56
    625             TTLPSA(IV)=TPOUND                                       TNTSS4    57
                    IF(I.NE.IT(IV).EQ.8)GOTO87                              TNTSS    580
                    K=K+1                                                   TNTSS    581
```

```
                TAU=WM(K)/QT                                                    TNTSS   582
                FORMAT                                                          TNTSS   583
      630     87  TAU=WMS/QT                                                    TNTSS   584
                85 WRITE(6,89) V,QA,QP,QT,TAU,F0                                TNTSS4   58
                88 FORMAT(1X,15,3F12.2,2F14.4)                                  TNTSS4   59
                   TTWTP=0.                                                     TNTSS4   60
                   TTNTP=0.                                                     TNTSS4   61
      635          TDNTA=0.                                                     TNTSS4   62
                   TTNTA=0.                                                     TNTSS4   63
                   TTTLBA=0.                                                    TNTSS4   64
                   TTTLMC=0.                                                    TNTSS4   65
                   DO 1530 I=1,14                                               TNTSS4   66
      640          TDNTP=TDNTP+PDUNDS(3,I)*PDUNDS(4,I)                          TNTSS4   67
                1530 TTNTP=TTNTP+PDUNDS(5,I)*PDUNDS(6,I)                        TNTSS4   68
                   DO 1630 I=1,14                                               TNTSS4   69
                   TDNTA=TDNTA+PACID(3,I)*PACID(4,I)                            TNTSS4   70
                1630 TTNTA=TTNTA+PACID(5,I)*PACID(6,I)                          TNTSS4   71
      645          TTNDT=TDNTP+TTNTA                                            TNTSS4   72
                   TTTNT=TTNTP+TTNTA                                            TNTSS4   73
                   DO 155 I=4,14                                                TNTSS4   74
                   TTTLBA=TTTLBA+TTLBAS(I)                                      TNTSS4   75
                155 TTTLMC=TTTLMC+TTLMS(I)                                      TNTSS4   76
      650          TTTTLB=TTTLMC+TTTLBA                                         TNTSS4   77
                   WRITE(6,4004) (I,SOL(I),I=1,14)                              TNTSS4   78
                4004 FORMAT(//1X,*SOLUBILITY OF NITRAMINE IN THE ACID PHASE*,//10X,  TNTSS4   79
                  F *WFSSFL*,10X,*MEGA*,//12X,I2,8X,F10.6))                     TNTSS4   80
                   WRITE(6,156) (I,I=1,14),((PDUNDS(K,L),L=1,14),K=1,10),       TNTSS4   81
      655          C (TTLBS(M),M=1,14),TTLMS,TDNTP,TTNTP                        TNTSS4   82
                 156 FORMAT(1HP,T69,4(4H****,A4))ISPERSED ORGANIC HOLDUPS********//T69,  TNTSS4   83
                   F *WFSSFL*,//1X,*COMPONENT*,6X,I1,1319,/10(I5,F14.2,13F9.2//12X,  TNTSS4   84
                   F *TOTAL*,F12.2,13F9.2,//2X,*TOTAL HOLDUP OF DISPERSED CLASS 7 MATE  TNTSS4   85
                   TOTAL IN NITRATION SECTION =*,F9.2,//2X,*TOTAL HOLDUP OF DISPERSED   TNTSS4   86
      660          &ONT IN  NITRATION SECTION =*,F9.2,//2X,*TOTAL HOLDUP OF DISPERSED   TNTSS4   87
                   STNT IN NITRATION SECTION =*,F9.2)                           TNTSS4   88
                   WRITE(6,164) (I,I=1,14),((PACID(K,L),L=1,14),K=1,10),        TNTSS4   89
                   C (TTLBSA(M),M=1,14),TTTBA,TDNTA,TTNTA,TTDNT,TTTNT,TTTTLB    TNTSS4   90
                 164 FORMAT(/////T69,4(4H****,A4))DISSOLVED ORGANIC HOLDUPS********.//168  TNTSS4   91
      665          F,*WFSSFL*,//1X,*COMPONENT*,6X,I1,1319,/10(I5,F14.2,13F9.2/12X,  TNTSS4   92
                   F *TOTAL *,F12.2,13F9.2,//2X,*TOTAL HOLDUP OF DISSOLVED CLASS 7 MATE  TNTSS4   93
                   IPIAL IN NITRATION SECTION =*,F9.2,//2X,*TOTAL HOLDUP DISSOLVED DNT  TNTSS4   94
                   2IN NITRATION SECTION =*,F9.2,//2X,*TOTAL HOLDUP OF DISSOLVED TNT I  TNTSS4   95
                   TN NITRATION SECTION =*,F9.2,////2X,*TOTAL HOLDUP OF ALL DNT IN NIT  TNTSS4   96
      670          &RATION SECTION =*,F9.2,//2X,*TOTAL HOLDUP OF ALL TNT IN NITRATION   TNTSS4   97
                   SSECTION =*,F9.2,//2X,*TOTAL HOLDUP OF ALL CLASS 7 MATERIAL IN NITR  TNTSS4   98
                   TRATION SECTION =*,F9.2)                                     TNTSS4   99
                   WRITE(6,4010)                                                TNTSS   587
                4010 FORMAT( 25H1********STREAM COMPOSITIONS)                   TNTSS   588
      675          DO 1104 ISTGE=1,6                                            TNTSS   589
                   DO 1104 I=1,14                                               TNTSS6    8
                   AIRLAS(I,ISTGE)=AIR(I,ISTGE)*WW(I)                           TNTSS6    9
                   PIRLAS(I,ISTGE)=PIR(I,ISTGE)*WW(I)                           TNTSS4   10
                   AXRLAS(I,ISTGE)=AXR(I,ISTGE)*WW(I)                           TNTSS6   11
      680          PXRLAS(I,ISTGE)=PXR(I,ISTGE)*WW(I)                           TNTSS6   12
                   AFLAS(I,ISTGE)=AF(I,ISTGE)*WW(I)                             TNTSS6   13
                   PFLAS(I,ISTGE)=PF(I,ISTGE)*WW(I)                             TNTSS6   14
                1104 CONTINUE                                                   TNTSS6   15
                   WRITE(6,4011)ISTGE,EOA(ISTGE),FAO(ISTGE)                     TNTSS   590
```

```
                4011 FORMAT(1H0,8STAGE,I2,5X,*EOA =*,F8.5,5X,*EAO =*,F8.5                TNTSS   591
                     C                        / 2HH INTERNAL ACID RECYCLE STREAM)         TNTSS   592
                      WRITE(6,4002) (AIR(I),I=1,14),(PIR(I,ISTGE),I=1,10)                TNTSS   593
                      WRITE(6,4004) (AIRLPS(I,ISTGE),I=1,14),(PIRLPS(I,ISTGE),I=1,10)    TNTSS4   16
                      WRITE(6,4012)                                                      TNTSS   594
  600           4012 FORMAT( 2HH EXTERNAL ACID RECYCLE STREAM)                           TNTSS   595
                      WRITE(6,4002) (AIR(I),I=1,14),(PIR(I,ISTGE),I=1,10)                TNTSS   596
                      WRITE(6,4004) (AIRLPS(I,ISTGE),I=1,14),(PIRLPS(I,ISTGE),I=1,10)    TNTSS6   17
                      WRITE(6,4013)                                                      TNTSS   597
                4013 FORMAT( 15H ORGANIC STREAM)                                         TNTSS   598
  605                 WRITE(6,4002) (AF (I,ISTGE),I=1,14),(PF (I,ISTGE),I=1,10)        TNTSS   599
                      WRITE(6,4004) (AFLPS(I,ISTGE),I=1,14),(PFLPS(I,ISTGE),I=1,10)    TNTSS4   18
                4004 FORMAT( 11H ACID PHASE,14F8.1/11H ORG. PHASE,10F8.1)               TNTSS6   19
                3005 CONTINUE                                                            TNTSS   600
                     C                                                                   TNTSS   601
  700                C                                                                   TNTSS   602
                     C     THIS SECTION OF THE PROGRAM CALCULATES VESSEL, STAGE, AND TRAIN TNTSS   603
                     C        MATERIAL BALANCES                                        TNTSS   604
                     C                                                                   TNTSS   605
                     C                                                                   TNTSS   606
  705                4000 IF(IMAL.EQ.0)GOTO6009                                        TNTSS   607
                      WRITE(6,4068)                                                      TNTSS   608
                4068 FORMAT(7HH0****ELEMENTAL MATERIAL BALANCES )                        TNTSS   609
                      WRITE(6,4006)                                                      TNTSS   610
                4006 FORMAT(*0OVERALL MATERIAL BALANCE*)                                 TNTSS   611
  710                 WRITE(6,4005)                                                      TNTSS   612
                      DO4007NATM=1,5                                                     TNTSS   613
                      TATM1=0.                                                           TNTSS   614
                      TATM0=0.                                                           TNTSS   615
                      DO4091I=1,14                                                       TNTSS   616
  715                 SUM1=PIR1(I)                                                       TNTSS   617
                      IF(I.EQ.10)SUM1=PIA1*PIM1                                          TNTSS   618
                      DO4092J=1,9                                                        TNTSS   619
                4092 SUM1=SUM1+ARRAY(I,J)                                                TNTSS   620
                      TATM1=TATM1+SUM1*ATOM(NATM,I)                                      TNTSS   621
  720           4091 TATM0=TATM0+(AF(I,6)*PF(I,6)+AIR(I,1)*PIR(I,1))*ATOM(NATM,I)      TNTSS   622
                      TATM0=TATM0+TCOX*GA(NATM,1)+TNOX*GA(NATM,2)+TTM**GA(NATM,3)+     TNTSS   623
                     C  TCO2*GA(NATM,4)                                                  TNTSS   624
                      IF(NATM.EQ.3)TATM1=TATM1+8.0**TNOX                                 TNTSS   625
                      DIF=TATM1-TATM0                                                    TNTSS   626
  725           4090 WRITE(6,4001)(HDR(I,NATM),I=1,2),TATP1,TATM0,DIF                   TNTSS   627
                      K=0                                                                TNTSS   628
                      J=-1                                                               TNTSS   629
                      DO4078ISTGE=1,6                                                    TNTSS   630
                      J=J+2                                                              TNTSS   631
  730                 K=K+1                                                              TNTSS   632
                      IF(ISTGE.EQ.2.OR.ISTGE.EQ.4)K=K+1                                  TNTSS   633
                      IF(ISTGE.EQ.2.OR.ISTGE.EQ.4)J=J+1                                  TNTSS   634
                      WRITE(6,4049) ISTGE                                                TNTSS   635
                4049 FORMAT(*0STAGE*,I2)                                                 TNTSS   636
  735                 WRITE(6,4005)                                                      TNTSS   637
                4005 FORMAT(* ELEMENT*,9X*MOLES IN*,7X*MOLES OUT*,6X*DIFFERENCE*)        TNTSS   638
                4001 FORMAT(1X,2A4,3F16.4)                                               TNTSS   639
                      DO4077NATM=1,5                                                     TNTSS   640
                      TATM1=0.                                                           TNTSS   641
  740                 TATM0=0.                                                           TNTSS   642
                      DO4077I=1,14                                                       TNTSS   643
```

```
                SUM1=ARRAY(I,5)                                          TNTSS   644
                TATM=TATM0*(AF(I,ISTGE)*PF(I,ISTGE)*AXR(I,ISTGE)*PXR(I,ISTGE))*  TNTSS   645
               C ATOM(MATM,I)                                            TNTSS   646
  745           IF(ISTGE.EQ.3)SUM1=SUM1*ARRAY(I,5)                       TNTSS   647
                IF(ISTGE.NE.1)GOTO4073                                   TNTSS   648
                SUM1=SUM1*ARRAY(I,2)*PXR(I)                              TNTSS   649
                IF(I.EQ.10) SUM1=SUM1*PIA*PIA                            TNTSS   650
                GOTO4075                                                 TNTSS   651
  750       4073 SUM1=SUM1*AF(I,ISTGE-1)*PF(I,ISTGE-1)                   TNTSS   652
            4075 IF(ISTGE.NE.4) SUM1=SUM1*AXR(I,ISTGE+1)*PXR(I,ISTGE+1)  TNTSS   653
            4072 TATM1=TATM1+SUM1*ATOM(MATM,I)                           TNTSS   654
                DO4574L=1,4                                              TNTSS   655
                SUM=GGS(J,L)*GGS(J+1,L)                                  TNTSS   656
  755           IF(ISTGE.EQ.1 .OR.ISTGE.EQ.3)SUM=SUM*GGS(J+2,L)          TNTSS   657
                IF(MATM.EQ.7.AND.L.EQ.2)TATM1=TATM1*RPP*SUM              TNTSS   658
            4574 TATM0=TATM0+SUM*GA(MATM,L)                              TNTSS   659
                DIF=TATM1-TATM0                                          TNTSS   660
            4071 WRITE(6,4001)(HDR(I,MATM),I=1,2),TATM1,TATM0,DIF        TNTSS   661
  760       4070 CONTINUE                                                TNTSS   662
                IV=0                                                     TNTSS   663
                IN=0                                                     TNTSS   664
                DO4998ISTGE=1,6                                          TNTSS   665
                IV=IV+1                                                  TNTSS   666
  765           IN=IN+1                                                  TNTSS   667
                WRITE(6,5999)IV                                          TNTSS   668
            5000 FORMAT(*0WFSSEL=*,I2)                                   TNTSS   669
                WRITE(6,4005)                                            TNTSS   670
                DO4996MATM=1,5                                           TNTSS   671
  770           TATM1=0.                                                 TNTSS   672
                TATM0=0.                                                 TNTSS   673
                DO4997L=1,4                                              TNTSS   674
            4997 TATM0=TATM0+GA(MATM,L)*GGS(IV,L)                        TNTSS   675
                IF(MATM.EQ.3)TATM1=TATM1*RPP*GGS(IV,2)                   TNTSS   676
  775           DO4971I=1,14                                             TNTSS   677
                TATM1=TATM1+ARRAY(I,IN)*ATOM(MATM,I)                     TNTSS   678
                IF(ISTGE.NE.1)TATM1=TATM1*(AF(I,ISTGE-1)*PF(I,ISTGE-1))*ATOM(MATM,  TNTSS   679
               C I)                                                      TNTSS   680
                IF(ISTGE.NE.4)TATM1=TATM1*(AXR(I,ISTGE+1)*PXR(I,ISTGE+1))*  TNTSS   681
  780          C ATOM(MATM,I)                                           TNTSS   682
                IF(ISTGE.EQ.1.OR.ISTGE.EQ.3)GOTO4004                     TNTSS   683
                TATM1=TATM1*(AIP(I,ISTGE)*PIP(I,ISTGE))*ATOM(MATM,I)     TNTSS   684
                GOTO4005                                                 TNTSS   685
            4004 IF(ISTGE.EQ.1.AND.I.EQ.10)TATM1=TATM1*PIA*ATOM(MATM,I)  TNTSS   686
  785       4005 TATM0=TATM0*(AV(I,IV)*PV(I,IV))*ATOM(MATM,I)            TNTSS   687
            4007 CONTINUE                                                TNTSS   688
                DIF=TATM1-TATM0                                          TNTSS   689
            4004 WRITE(6,4001)(HDR(I,MATM),I=1,2),TATM1,TATM0,DIF        TNTSS   690
                IF(ISTGE.NE.1.AND.ISTGE.NE.3)GOTO5010                    TNTSS   691
  790           IV=IV+1                                                  TNTSS   692
                IN=IN+1                                                  TNTSS   693
                WRITE(6,5000)IV                                          TNTSS   694
                WRITE(6,4005)                                            TNTSS   695
                DO4998MATM=1,5                                           TNTSS   696
  795           TATM1=0.                                                 TNTSS   697
                TATM0=0.                                                 TNTSS   698
                DO5021I=1,14                                             TNTSS   699
                TATM0=TATM0+(AV(I,IV)*PV(I,IV))*ATOM(MATM,I)             TNTSS   700
```

```
                TATMI=TATMI+(ARRAY(I,IM)*AIR(I,ISTGE)*PIR(I,ISTGE)+                TNTSS   701
A00           C AV(I,IV-1)*PV(I,IV-1))*ATOM(NATM,I)                               TNTSS   702
              IF(ISTGE.EQ.1)TATMI=TATMI+PXR1(I)*ATOM(NATM,I)                      TNTSS   703
           5002 IF(ISTGE.EQ.1.AND.I.EQ.10)TATMI=TATMI+P1R1*ATOM(NATM,I)           TNTSS   704
              DO5003L=1,4                                                         TNTSS   705
           5003 TATMO=TATMO+GA(NATM,L)*GGS(IV,L)                                  TNTSS   706
A05           IF(NATM.EQ.3)TATMI=TATMI+RPP*GGS(IV,2)                              TNTSS   707
              DIF=TATMI-TATMO                                                     TNTSS   708
           5001 WRITE(6,4001)(HDR(I,NATM),I=1,2),TATMI,TATMO,DIF                  TNTSS   709
           5010 IV=IV+1                                                           TNTSS   710
              WRITE(6,5000)IV                                                     TNTSS   711
A10           WRITE(6,4005)                                                       TNTSS   712
              DO5011NATM=1,5                                                      TNTSS   713
              TATMI=0.                                                            TNTSS   714
              TATMO=0.                                                            TNTSS   715
              DO5013L=1,4                                                         TNTSS   716
A15        5013 TATMO=TATMO+GA(NATM,L)*GGS(IV,L)                                  TNTSS   717
              IF(NATM.EQ.3)TATMI=TATMI+RPP*GGS(IV,2)                              TNTSS   718
              DO5012I=1,14                                                        TNTSS   719
              TATMI=TATMI+(AV(I,IV-1)*PV(I,IV-1))*ATOM(NATM,I)                    TNTSS   720
           5012 TATMO=TATMO+(AV(I,IV)*PV(I,IV))*ATOM(NATM,I)                      TNTSS   721
A20           DIF=TATMI-TATMO                                                     TNTSS   722
           5011 WRITE(6,4001)(HDR(I,NATM),I=1,2),TATMI,TATMO,DIF                  TNTSS   723
           4000 CONTINUE                                                          TNTSS   724
           6009 CONTINUE                                                          TNTSS   725
              C                                                                   TNTSS   726
              C                                                                   TNTSS   727
A25           C     THIS SECTION OF THE PROGRAM CALCULATES PERFORMANCE FUNCTIONS  TNTSS   728
              C                                                                   TNTSS   729
              C                                                                   TNTSS   730
              TNTI=0.                                                             TNTSS   731
A30           DO6017I=1,8                                                         TNTSS   732
           6017 TNTI=TNTI+PRAY(5,I)                                               TNTSS   733
              YIELD=100.*(PF6(5)+AF6(5)-TNTI)/(P1AI+P1BI)                         TNTSS   734
              TONT=PF6(3)+PF6(4)+AF6(3)+AF6(4)                                    TNTSS   735
              TONT=TONT*MW(3)                                                     TNTSS   736
A35           SUM=0.                                                              TNTSS   737
              DO 6025 I=1,6                                                       TNTSS   738
           6025 SUM=SUM+(AF6(I)+PF6(I))*MW(I)                                     TNTSS   739
              CONT=100.*TONT/SUM                                                  TNTSS   740
              CRUDE=0.                                                            TNTSS   741
A40           DO6018I=1,8                                                         TNTSS   742
           6018 CRUDE=CRUDE+(PF6(I)+PF6(I))*MW(I)                                 TNTSS   743
              DO 6027 I=9,14                                                      TNTSS   744
           6027 CRUDE=CRUDE+AF6(I)*MW(I)                                          TNTSS   745
              SPA=0.                                                              TNTSS   746
A45           SPP=0.                                                              TNTSS   747
              DO6019I=1,14                                                        TNTSS   748
              SPA=SPA+AXR1(I)*MW(I)                                               TNTSS   749
           6019 SPP=SPP+PXR1(I)*MW(I)                                             TNTSS   750
              TANR=AXR1(10)*MW(10)                                                TNTSS   751
              TPNR=PXR1(10)*MW(10)                                                TNTSS   752
A50           DO6020I=1,8                                                         TNTSS   753
              TANR=TANR+ AXR1(I)          *MW(I)                                  TNTSS   754
           6020 TPNR=TPNR+PXR1(I)*MW(I)                                           TNTSS   755
           6147 TOL=0.                                                            TNTSS   756
A55           SULP=0.                                                             TNTSS   757
```

```
                      WKN=0.                                                    TNTSS   758
                      STN=0.                                                    TNTSS   759
                      SUM=0.                                                    TNTSS   760
                      SPACID=SPA+SPP                                            TNTSS   761
      940             PCTNR=(TANR+TPNR)/SPACID*100.                             TNTSS   762
                      PCTNAD=TANR/SPA*100.                                      TNTSS   763
                      PCTD=(AXR(3)+AXR(4))*MW(3)*100./TANR                      TNTSS   764
                      DO6029J=1,8                                               TNTSS   765
                      TOL=TOL+FIN(6,J)                                          TNTSS   766
      965             SULP=SULP+FIN(5,J)                                        TNTSS   767
                      WKN=WKN+FIN(1,J)+FIN(2,J)                                 TNTSS   768
                 6029 STN=STN+FIN(4,J)                                          TNTSS   769
                      CTF=(CTL*TOL+CSL*SULP+CWN*WKN+CSN*STN)/(TOL*YIELD*MW(5)*.0001)  TNTSS   770
                      DO6030I=1,6                                               TNTSS   771
      970             KEY=0                                                     TNTSS   772
                 6028 II=1+KEY                                                  TNTSS   773
                      IJ=5+KEY                                                  TNTSS   774
                      PECN=0.                                                   TNTSS   775
                      IF(I.EQ.6)GOTO6032                                        TNTSS   776
      975             IX=I+1                                                    TNTSS   777
                      DO6031J=II,IJ,2                                           TNTSS   778
                      K=(J+1)/2                                                 TNTSS   779
                 6031 PECN=PECN+K*(AXR(J,IX)+PXR(J,IX))                         TNTSS   780
                 6032 IF(I.NE.1)GOTO6033                                        TNTSS   781
      990             FDN=1.+TNTI                                               TNTSS   782
                      IF(KEY.EQ.1)FDN=0.                                        TNTSS   783
                      GOTO6034                                                  TNTSS   784
                 6033 FDN=0.                                                    TNTSS   785
                      IY=I-1                                                    TNTSS   786
      995             DO6035J=II,IJ,2                                           TNTSS   787
                      K=(J+1)/2                                                 TNTSS   788
                 6035 FDN=FDN+K*(PF(J,IY)+AF(J,IY))                             TNTSS   789
                 6034 OUTN=0.                                                   TNTSS   790
                      DO6036J=II,IJ,2                                           TNTSS   791
     1000             K=(J+1)/2                                                 TNTSS   792
                 6036 OUTN=OUTN+K*(PF(J,I)+AF(J,I)+AXR(J,I)+PXR(J,I))           TNTSS   793
                      AR=OUTN-PECN-FDN                                          TNTSS   794
                      IF(KEY.EQ.1)GOTO6038                                      TNTSS   795
                      KEY=1                                                     TNTSS   796
     1005             SNA(I)=AR                                                 TNTSS   797
                      GOTO6028                                                  TNTSS   798
                 6038 SNN(I)=AR                                                 TNTSS   799
                 6030 CONTINUE                                                  TNTSS   800
                    C COMPUTATION OF ACTUAL ACIDITY                             TNTSS   801
     1020             DO6040I=1,6                                               TNTSS   802
                      TMOLES=AXR(9,I)                                           TNTS56   20
                      TLBS=TMOLES*MW(9)                                         TNTS56   21
                      DO6041J=11,14                                             TNTSS   804
                      TMOLES=TMOLES+AXR(J,I)                                    TNTS56   22
     1045             TLBS=TLBS+AXR(J,I)*MW(J)                                  TNTSS   805
                      AN(I)=100.*AXR(9,I)*MW(9)/TLBS                            TNTSS   806
                      AS(I)=100.*(AXR(11,I)+AXR(14,I))*MW(11)/TLBS              TNTSS   807
                      NTOS(I)=AXR(9,I)/(AXR(11,I)+AXR(14,I))                    TNTSS   808
                      ANS(I)=AXR(12,I)/TMOLES                                   TNTS56   23
     1060             PNS=100.*AXR(12,I)/TLBS*MW(12)                            TNTSS   809
                      TN(I)=AN(I)+0.4959*PNS                                    TNTSS   810
                      TS(I)=AS(I)+0.7718*PNS                                    TNTSS   811
```

```
      6040 TAS(I)=AS(I)+TN(I)*0.7782                                    TNTSS   812
           NTOSIA=AV(9,1)/(AV(1,1)+AV(14,1))                            TNTSS   813
           NTOS2A=AV(9,6)/(AV(1,6)+AV(14,6))                            TNTSS   814
           ANSIA=AV(12,1)/(AV(9,1)+AV(1,1)+AV(12,1)+AV(13,1)+AV(14,1))  TNTSS4   24
           ANS2A=AV(12,6)/(AV(9,6)+AV(1,6)+AV(12,6)+AV(13,6)+AV(14,6))  TNTSS6   25
     C     COMPUTATION OF MB DENSITY                                    TNTSS   815
           DO6845I=1,6                                                  TNTSS   816
           TLRS=MW(10)*AXR(10,I)                                        TNTSS   817
           TVOL=AF(10,I)/RHO(10)                                        TNTSS   818
           DO6846J=1,8                                                  TNTSS   819
           TLRS=TLRS+AXR(J,I)*MW(J)                                     TNTSS   820
      6846 TVOL=TVOL+AXR(J,I)/RHO(J)                                    TNTSS   821
      925  6845 RHONBS(I)=TLRS/TVOL                                     TNTSS   822
           WRITE(6,6850)YIELD,CRUDE,CONT,CTF,SPA,SPP,SPACID,PCTNB,PCTNRO,  TNTSS   823
          C PCTO,                                                       TNTSS   824
          1 (I,SNA(I),SNN(I),AN(I),AS(I),TN(I),TS(I),TAS(I),RHONBS(I),I=1,6)  TNTSS   825
      6850 FORMAT(*1$*****SUMMARY*/*0YIELD =*,F7.3,* MOLE PCT TOL CONVERSION T  TNTSS   826
      930 CO TNT*/                                                      TNTSS   827
          1 * LBS/HR CRUDE TNT =*,F7.2/* WT PCT DNT IN CRUDE TNT =*,F8.4/  TNTSS   828
          2 * RAW MATERIALS COST, $/LB OF  A-TNT =*,F10.6/              TNTSS   829
          3 *0SPENT ACID FLOW, LBS/HOUR*/6X,*ACID PH.*,F14.4/           TNTSS   830
          4 6X,*ORG. PH.*,F14.4/6X*TOTAL*,F17.4/* WT PCT TOTAL NB =*,F12.4/  TNTSS   831
      935 5 * WT PCT DISSOLVED NB =*,F8.4/                              TNTSS   832
          6 * WT PCT DNT IN DISSOLVED NB =*,F8.4//*0STAGE DATA*/        TNTSS   833
          6 *0STAGE   A-NITRATION   B-NITRATION   ACT NITRIC   ACT SULPHURIC  TNTSS   834
          7  TOT NITRIC   TOT SULPHURIC   TOTAL ACIDITY   NB DENSITY*/   TNTSS   835
          8 (1X,I3,F15.3,F14.3,F13.3,F15.3,F14.3,F15.3,F16.3,F14.3))    TNTSS   836
      940  IF(IAFT.EQ.0)GOTO80                                          TNTSS   837
           SUMO=0.                                                      TNTSS   838
           SUMA=MW(9)*AAS(9)                                            TNTSS   839
           DO81I=1,8                                                    TNTSS   840
      81   SUMO=SUMO+MW(I)*AAS(I)                                       TNTSS   841
      945  DO82I=11,14                                                  TNTSS   842
      82   SUMA=SUMA+MW(I)*AAS(I)                                       TNTSS   843
           PCTAS=100.*SUMO/(SUMO+SUMA)                                  TNTSS   844
           WRITE(6,83)PCTAS                                             TNTSS   845
      83   FORMAT(*0WT PCT NB FROM AFTER SEPARATOR =*,F10.5/* COMPOSITION*)  TNTSS   846
      950  WRITE(6,6860)AAS,(PAS(I),I=1,16)                            TNTSS   847
      80   CONTINUE                                                     TNTSS   848
           DO59I=1,8                                                    TNTSS   849
           Q=0.                                                         TNTSS   850
           DO41J=1,10                                                   TNTSS   851
      955  41   Q=Q+RATES(I,J)*DH(J)                                    TNTSS   852
           RTIO(I)=Q/.252                                               TNTSS   853
           Q=Q+(ETN(I,1)*FWN+FIN(2,I)*EFR+FIN(3,I)*EYE+FIN(5,I)*EOL)*.252  TNTSS   854
           GOTO(51,52,53,54,55,56,57,58),I                              TNTSS   855
      960  51   Q=Q+ENTH(AIP2,PIP2,TSEP2)-ENTH(A1A,P1A,T1A)             TNTSS   856
           GOTO59                                                       TNTSS   857
      52   Q=Q+ENTH(A1A,P1A,T1A)+ENTH(AIP1,PIP1,TSEP1)-ENTH(A1B,P1B,T1B)  TNTSS   858
           DLT=TSEP1-70.                                                TNTSS   859
           DO59J=1,10                                                   TNTSS   860
      59   Q=Q+CP(J)*PIP1(J)*DLT                                        TNTSS   861
      965  GOTO58                                                       TNTSS   862
      53   Q=Q+ENTH(AF1,PF1,TSEP1)+ENTH(AIP3,PIP3,TSEP3)+ENTH(AIR2,PIR2,TSEP2  TNTSS   863
          C)-ENTH(A2,P2,T2)                                             TNTSS   864
           GOTO58                                                       TNTSS   865
      54   Q=Q+ENTH(AF2,PF2,TSEP2)+ENTH(AIR4,PIP4,TSEP4)-ENTH(A3A,P3A,T3A)  TNTSS   866
```

```
                      GOTO55                                                    TNTSS   867
                55    Q=Q+ENTH(A3A,P3A,T3A)+ENTH(AIR3,PIR3,TSEP3)-ENTH(A3R,P3R,T3R)   TNTSS   868
                      GOTO57                                                    TNTSS   869
                56    Q=Q+ENTH(AF3,PF3,TSEP3)+ENTH(AXR5,PXR5,TSEP5)+           TNTSS   870
               C ENTH(AIR4,PIR4,TSEP4)-ENTH(A4,P4,T4)                           TNTSS   871
                      GOTO58                                                    TNTSS   872
                57    Q=Q+ENTH(AF4,PF4,TSEP4)+ENTH(AXR6,PXR6,TSEP6)+           TNTSS   873
               C ENTH(AIR5,PIR5,TSEP5)-ENTH(A5,P5,T5)                           TNTSS   874
                      GOTO58                                                    TNTSS   875
                58    Q=Q+ENTH(AF5,PF5,TSEP5)+ENTH(AIR6,PIR6,TSEP6)-ENTH(A6,P6,T6)   TNTSS   876
                59    RTU(I)=Q/.252                                           TNTSS   877
                      WRITE(6,61) (I,RTU(I),I=1,8)                            TNTSS   878
                61    FORMAT(/'0',ITRATOR HEAT DUTIES'/6X,'ITRATOR',5X,'BTU'/ TNTSS   879
               1 (1X,I9,F14.0))                                                 TNTSS   880
                      GO TO 4001                                              TNTSS   881
                      END                                                     TNTSS   882
```

SYMBOLIC REFERENCE MAP (R=1)

ENTRY POINTS
6153 TNTSIM

VARIABLES	SN	TYPE	RELOCATION						
304	AAS	REAL	ARRAY	AC	14701	AB	REAL		
0	AF	REAL	ARRAY	SOLV	15471	AFLBS	REAL	ARRAY	
0	AF1	REAL	ARRAY	SOLV	16	AF2	REAL	ARRAY	SOLV
34	AF3	REAL	ARRAY	SOLV	52	AF4	REAL	ARRAY	SOLV
70	AF5	REAL	ARRAY	SOLV	106	AF6	REAL	ARRAY	SOLV
0	AI	REAL	ARRAY	INPUT	0	AII	REAL	ARRAY	NTSP
124	AIP	REAL	ARRAY	SOLV	14751	AIPLBS	REAL	ARRAY	
124	AIP1	REAL	ARRAY	SOLV	142	AIP2	REAL	ARRAY	SOLV
160	AIP3	REAL	ARRAY	SOLV	176	AIP4	REAL	ARRAY	SOLV
214	AIP5	REAL	ARRAY	SOLV	232	AIP6	REAL	ARRAY	SOLV
112	AKA	REAL		Z	14543	AKR	REAL		
14544	AKC	REAL			113	AKEQ	REAL		Z
14545	AKEQOV	REAL			73	AKMA	REAL		Z
74	AKMATL	REAL		Z	61	AK10	REAL		Z
46	AK12	REAL		Z	53	AK3S	REAL		Z
47	AK3W	REAL		Z	54	AK4S	REAL		Z
50	AK4W	REAL		Z	51	AK5S	REAL		Z
52	AK6S	REAL		Z	57	AK7	REAL		Z
44	AKR	REAL		Z	101	AK9	REAL		Z
17344	AN	REAL	ARRAY		15741	ANS	REAL	ARRAY	
14705	ANS1A	REAL			14706	ANS3A	REAL		
0	ARRAY	REAL	ARRAY	X	17354	AS	REAL	ARRAY	
14616	AT	REAL			16052	ATOM	REAL	ARRAY	
0	AV	REAL	ARRAY	AC	16160	AVI	REAL	ARRAY	
250	AXP	REAL	ARRAY	SOLV	15271	AXPLBS	REAL	ARRAY	
250	AXP1	REAL	ARRAY	SOLV	266	AXP2	REAL	ARRAY	SOLV
17036	AXP20	REAL	ARRAY		304	AXP3	REAL	ARRAY	SOLV
17052	AXP30	REAL	ARRAY		322	AXP4	REAL	ARRAY	SOLV
17070	AXP40	REAL	ARRAY		340	AXP5	REAL	ARRAY	SOLV
17106	AXP50	REAL	ARRAY		356	AXP6	REAL	ARRAY	SOLV
17124	AXP60	REAL	ARRAY		0	A1A	REAL	ARRAY	AC
0	A1AI	REAL	ARRAY	X	16	A1B	REAL	ARRAY	AC
16	A1BI	REAL	ARRAY	X	34	A1S	REAL	ARRAY	AC
52	A2	REAL	ARRAY	AC	34	A2I	REAL	ARRAY	X
70	A2S	REAL	ARRAY	AC	106	A3A	REAL	ARRAY	AC
52	A3AI	REAL	ARRAY	X	124	A3P	REAL	ARRAY	AC
70	A3BI	REAL	ARRAY	X	142	A3S	REAL	ARRAY	AC
160	A4	REAL	ARRAY	AC	196	A4I	REAL	ARRAY	X
174	A4S	REAL	ARRAY	AC	214	A5	REAL	ARRAY	AC
124	A5I	REAL	ARRAY	X	232	A5S	REAL	ARRAY	AC
250	A6	REAL	ARRAY	AC	142	A6I	REAL	ARRAY	X
266	A6S	REAL	ARRAY	AC	14741	BTU	REAL	ARRAY	
17024	BTUO	REAL	ARRAY		14652	CONT	REAL	-	
17420	COMP	REAL	ARRAY		16	CP	REAL	ARRAY	Z
14653	CPRIDE	REAL			12175	CSL	REAL		
12177	CSN	REAL			14670	CTF	REAL		
12174	CTL	REAL			12176	CWN	REAL		
6	DEL	REAL		VECTOR	34	DM	REAL	ARRAY	Z
14645	DIF	REAL			14714	DLT	REAL		
1126	EAO	REAL	ARRAY	SOLV	1004	EAOP	REAL	ARRAY	SOLV
12201	EEP	REAL			1134	EOA	REAL	ARRAY	SOLV

VARIABLES	SN	TYPE	RELOCATION						
1012	FOAP	REAL	ARRAY	SOLV	12203	EOL	REAL		
12200	FWN	REAL			12202	FYW	REAL		
71	F10	REAL		Z	62	E23	REAL		Z
55	F1S	REAL		Z	63	E3N	REAL		Z
56	F4S	REAL		Z	64	E4W	REAL		Z
65	F5S	REAL		Z	66	E6S	REAL		Z
67	F7	REAL		Z	70	E8	REAL		Z
102	F9	REAL		Z	14614	FA	REAL		
1262	FACD	REAL	ARRAY	SOLV	14546	FACT2	REAL		
14555	FACT3	REAL			14554	FACT4	REAL		
14553	FACT5	REAL			14552	FACT6	REAL		
72	FD	REAL		Z	14676	FDN	REAL		
17250	FIN	REAL	ARRAY		110	FMAX	REAL		Z
14613	FO	REAL			14546	FOV	REAL		
14026	GA	REAL	ARRAY		1020	G65	REAL	ARRAY	SOLV
0	G1	REAL	ARRAY	PAR	110	G10	REAL	ARRAY	PAR
1020	G15	REAL	ARRAY	SOLV	1036	G16	REAL	ARRAY	SOLV
1054	G1A	REAL	ARRAY	SOLV	1072	G19	REAL	ARRAY	SOLV
10	G3	REAL	ARRAY	PAR	30	G3S	REAL	ARRAY	PAR
20	G4	REAL	ARRAY	PAR	40	G4S	REAL	ARRAY	PAR
50	G5	REAL	ARRAY	PAR	60	G6	REAL	ARRAY	PAR
70	G7	REAL	ARRAY	PAR	100	G8	REAL	ARRAY	PAR
120	G9	REAL	ARRAY	PAR	16014	HDR	INTEGER	ARRAY	
14550	I	INTEGER			10	IAFT	INTEGER		VECTOR
11	ICHECK	INTEGER		VECTOR	7	IE	INTEGER		VECTOR
0	IFLG	INTEGER	ARRAY	FLAG	14672	II	INTEGER		
12	III	INTEGER		DUM	14673	IJ	INTEGER		
14562	ILIST	INTEGER			14563	IMPAL	INTEGER		
4	IN	INTEGER		VECTOR	14723	INIT	INTEGER	ARRAY	
14564	IPI	INTEGER			14565	IPNCH	INTEGER		
1	IPONT	INTEGER		VECTOR	3	ISTGE	INTEGER		VECTOR
14560	ISTOP	INTEGER			0	ITYPE	INTEGER		VECTOR
5	IV	INTEGER		VECTOR	14572	IVI	INTEGER		
14675	IX	INTEGER			14677	IY	INTEGER		
14551	J	INTEGER			14570	K	INTEGER		
14671	KEY	INTEGER			14637	L	INTEGER		
14640	M	INTEGER			14623	MHOLDA	INTEGER		
14542	MHOLDO	REAL			15747	MW	REAL	ARRAY	
14641	MATN	INTEGER			2	NC	INTEGER		VECTOR
14573	NC1	INTEGER			14574	NC2	INTEGER		
14575	NC3	INTEGER			14576	NC4	INTEGER		
14577	NC5	INTEGER			14547	NDS	INTEGER		
774	ND	INTEGER	ARRAY	SOLV	14561	NSET	INTEGER		
14715	NTOS	REAL	ARRAY		14540	NTOSIA	REAL		
14541	NTOS3A	REAL			14700	OUTN	REAL		
20426	PACID	REAL	ARRAY		304	PAS	REAL	ARRAY	PC
14717	PCTAS	REAL			14667	PCTD	REAL		
14665	PCTNB	REAL			14666	PCTNBD	REAL		
374	PF	REAL	ARRAY	SOLV	15615	PFLAS	REAL	ARRAY	
374	PF1	REAL	ARRAY	SOLV	412	PF2	REAL	ARRAY	SOLV
430	PF3	REAL	ARRAY	SOLV	446	PF4	REAL	ARRAY	SOLV
464	PF5	REAL	ARRAY	SOLV	502	PF6	REAL	ARRAY	SOLV
21	PI	REAL	ARRAY	INPUT	16	PII	REAL	ARRAY	NTSP
520	PIA	REAL	ARRAY	SOLV	15075	PIPLBS	REAL	ARRAY	
520	PIB1	REAL	ARRAY	SOLV	536	PIB2	REAL	ARRAY	SOLV
554	PIB3	REAL	ARRAY	SOLV	572	PIB4	REAL	ARRAY	SOLV
610	PIB5	REAL	ARRAY	SOLV	626	PIB6	REAL	ARRAY	SOLV

VARIABLES	SN	TYPE	RELOCATION						
14706	PNS	REAL			17760	POUNDS	REAL	ARRAY	
14615	PT	REAL			0	PV	REAL	ARRAY	PC
14562	PVI	REAL	ARRAY		644	PXR	REAL	ARRAY	SOLV
15345	PXPLBS	REAL	ARRAY		644	PXR1	REAL	ARRAY	SOLV
662	PXR2	REAL	ARRAY	SOLV	17142	PXR20	REAL	ARRAY	
700	PXR3	REAL	ARRAY	SOLV	17160	PXR30	REAL	ARRAY	
716	PXR4	REAL	ARRAY	SOLV	17176	PXR40	REAL	ARRAY	
734	PXR5	REAL	ARRAY	SOLV	17214	PXR50	REAL	ARRAY	
752	PXR6	REAL	ARRAY	SOLV	17232	PXR60	REAL	ARRAY	
0	P1A	REAL	ARRAY	PC	14546	P1AI	REAL		
14	P1B	REAL	ARRAY	PC	14567	P1BI	REAL		
34	P1S	REAL	ARRAY	PC	52	P2	REAL	ARRAY	PC
70	P2S	REAL	ARRAY	PC	106	P3A	REAL	ARRAY	PC
124	P3B	REAL	ARRAY	PC	142	P3S	REAL	ARRAY	PC
160	P4	REAL	ARRAY	PC	176	P4S	REAL	ARRAY	PC
214	P5	REAL	ARRAY	PC	232	P5S	REAL	ARRAY	PC
250	P6	REAL	ARRAY	PC	266	P6S	REAL	ARRAY	PC
14713	P	REAL			14610	QA	REAL		
14611	QP	REAL			0	QQ	REAL	ARRAY-	000
14612	QT	REAL			0	R	REAL	ARRAY	DUM
1142	RATES	REAL	ARRAY	SOLV	14674	RECN	REAL		
0	RHO	REAL	ARRAY	Z	14620	RHOA	REAL		
17612	RHONRS	REAL	ARRAY		14617	RHOP	REAL		
0	RHO1	REAL		Z	11	RHO10	REAL		Z
12	RHO11	REAL		Z	13	RHO12	REAL		Z
14	RHO13	REAL		Z	15	RHO14	REAL		Z
1	RHO2	REAL		Z	2	RHO3	REAL		Z
3	RHO4	REAL		Z	4	RHO5	REAL		Z
5	RHO6	REAL		Z	6	RHO7	REAL		Z
7	RHO8	REAL		Z	10	RHO9	REAL		Z
111	RR	REAL		Z	14547	RRP	REAL		
100	RR	REAL		Z	75	SA	REAL		Z
76	SB	REAL		Z	77	SC	REAL		Z
100	SD	REAL		Z	101	SF	REAL		Z
102	SG	REAL		Z	103	SH	REAL		Z
104	SI	REAL		Z	105	SJ	REAL		Z
17340	SNA	REAL	ARRAY		17404	SNM	REAL	ARRAY	
1110	SOL	REAL	ARRAY	SOLV	14654	SPA	REAL		
14656	SPACID	REAL			14655	SPP	REAL		
14663	STN	REAL			14661	SULP	REAL		
14646	SUM	REAL			14711	SUMA	REAL		
14644	SUMI	REAL			14710	SUMO	REAL		
14400	S15	REAL			14401	S16	REAL		
14402	S18	REAL			14403	S19	REAL		
14456	TANR	REAL			17342	TAS	REAL	ARRAY	
14502	TATMI	REAL			14463	TATMO	REAL		
14625	TAU	REAL			14404	TCOI	REAL		
14407	TCO2	REAL			14451	TDNT	REAL		
14470	TDNTA	REAL			14426	TDNTP	REAL		
0	TEMP	REAL	ARRAY	PARA	15770	TITLE	INTEGER	ARRAY	
14703	TLPS	REAL			14702	TMOLES	REAL		
17370	TN	REAL	ARRAY		14405	TNOX	REAL		
14647	TNTI	REAL			14660	TOL	REAL		
14657	TPNR	REAL			14624	TPOUND	REAL		
107	TR	REAL		Z	17376	TS	REAL	ARRAY	
770	TSEP	REAL	ARRAY	SOLV	770	TSEP1	REAL		SOLV
771	TSEP2	REAL		SOLV	772	TSEP3	REAL		SOLV

```
VARIABLES      SN  TYPE          RELOCATION
   773  TSFP4      REAL              SOLV          774  TSFPS      REAL              SOLV
   775  TSFP6      REAL              SOLV        14634  TTDNT      REAL
 20174  TTLRS      REAL      ARRAY               20442  TTLRSA     REAL      ARRAY
 14604  TTNN       REAL                          14631  TTNTA      REAL
 14627  TTNTP      REAL                          14632  TTTLBA     REAL
 14633  TTTLRS     REAL                          14635  TTTNT      REAL
 14636  TTTTLR     REAL                          14707  TVOL       REAL
     1  T1A        REAL              PARA            1  T1B        REAL              PARA
     2  T2         REAL              PARA            3  T3A        REAL              PARA
     4  T3B        REAL              PARA            5  T4         REAL              PARA
     6  T5         REAL              PARA            7  T6         REAL              PARA
     0  V          REAL      ARRAY   E0          14671  VHOLDA     REAL
 14622  WWRLDO     REAL                           10  WKN        REAL      ARRAY   PARA
    20  WKRS       REAL              PARA        17526  WOL        REAL      ARRAY
 14662  WRN        REAL                          17564  XP         REAL      ARRAY
 20212  XPA        REAL      ARRAY               1270  YELLOW     REAL      ARRAY   SOLV
 14650  YIELD      REAL                          14571  ZA         REAL

FILE NAMES          MODE
     0  INPUT                 2041  OUTPUT              4102  PUNCH               0  TAPES     FMT
  2041  TAPE6      FMT        4102  TAPE7      FMT

EXTERNALS           TYPE    ARGS
        FNTN        REAL       3                    EXP        REAL      1 LIBRARY
        MTTSEP                 0                    VESSEL               0

INLINE FUNCTIONS    TYPE    ARGS
        ABS         REAL       1  INTRIN

STATEMENT LABELS
12230  1       FMT          12453  2       FMT          12663  4       FMT
12621  7       FMT          12570  39      FMT              0  41
12006  50                   11647  51                  11656  52
11701  53                   11716  54                  11730  55
11742  56                   11757  57                  11774  58
     0  59                  14503  61      FMT          6276  65
12562  66      FMT              0  70                      0  71
     0  72                  11607  80                      0  81
     0  82                  14457  83      FMT         10140  85
     0  86                  10136  87                  13620  88      FMT
13640  89      FMT              0  150                     0  151
     0  153                 13783  154     FMT             0  155
     0  160                      0  163                 13770  164     FMT
     0  170                      0  171                     0  172
     0  173                      0  187                 13026  190     FMT
13834  191     FMT           6780  192                 13050  193     FMT
 6706  194                  13072  195     FMT         13110  196     FMT
12417  300     FMT          12507  301     FMT         12527  302     FMT
12731  303     FMT          12766  304     FMT         12366  305     FMT
12721  700     FMT              0  780         INACTIVE 12630  701     FMT
     0  708                  6362  709                     0  1104
     0  1202                     0  1203                    0  1213
     0  1222                     0  1223                    0  1233
     0  1241                     0  1253                    0  1401
  6575  1402                 6600  1403                    0  1404
12711  1411    FMT          12713  1412    FMT         12700  1420    FMT  NO REFS
13511  1429    FMT              6  1530                    0  1630
```

STATEMENT LABELS

7424	1710		7453	1720		7701	1730		
7730	1740		0	2300		0	2402		
7200	2403		7116	2404		13174	2405	FMT	
7217	2410		0	2411		7262	2412		
7203	2417		13230	2414	FMT	7304	2420		
0	2421		7347	2422		7330	2423		
13264	2424	FMT	7404	2430		0	2431		
7447	2432		7430	2433		13320	2434	FMT	
7471	2440		0	2441		7527	3442		
7510	2447		13332	2444	FMT	7565	2450		
13344	2451	FMT	0	3213		0	3214		
0	3221		0	3233		0	3234		
0	3243		0	3253		0	3263		
0	3401		0	3413		0	3423		
0	3431		0	3443		13150	3600	FMT	
13206	3601	FMT	13242	3602	FMT	13276	3603	FMT	
13167	3609	FMT	13140	3610	FMT	0	3900		
7401	3901		7654	3902		7701	3903		
0	3905		13353	4003	FMT	13363	4001	FMT	
13400	4002	FMT	13426	4043	FMT	13447	4004	FMT	
13471	4005	FMT	14161	4009	FMT	14002	4010	FMT	
14074	4011	FMT	14122	4012	FMT	14144	4013	FMT	
14172	4049	FMT	0	4070		0	4071		
0	4072		10571	4073		0	4074		
10574	4075		14225	4040	FMT	14242	4091	FMT	
14233	4085	FMT	14202	4086	FMT	0	4090		
0	4091		0	4092		0	4093		
10743	4094		10752	4095		0	4096		
0	4097		0	4098		13542	4100	FMT	
13560	4101	FMT	0	4102		13600	4103	FMT	
13131	4207	FMT	14260	5000	FMT	0	5001		
0	5002		0	5003		11077	5010		
0	5011		0	5012		0	5013		
13515	4000	FMT	6274	6001		13606	6003	FMT	
13552	4004	FMT	10420	6008		11154	6009		
0	4017		0	6018		0	6019		
0	4020		0	6025		0	6027		
11112	4028		0	6029		0	6030		
0	4031		11337	6032		11346	6033		
11165	4034		0	6035		0	6036		
11414	4038		0	6040		0	6041		
0	4045		0	6046		14361	6050	FMT	
0	4147	INACTIVE	0	0000	INACTIVE				

COMMON BLOCKS LENGTH

FLAG	4
DATA	17
INPUT	34
MTSP	20
ADD	14
EQ	22
X	112
PC	214
AC	214
SOLV	710
NUM	11
VECTOR	10

COMMON BLOCKS	LENGTH
7	7A
PAR	AR

STATISTICS

PROGRAM LENGTH	125150	5453
BUFFER LENGTH	61470	3171
COMMON LENGTH	30140	1568

```
      SUBROUTINE NITSEP                                                 TNTSS    883
      DIMENSION AIRO(14),PIRO(14)                                       TNTSS    884
      DIMENSION AIR(14),AXR(14),AF(14),PIR(14),PXR(14),PF(14)           TNTSS    885
      COMMON/FLAG/IFLG(6)                                               TNTSS    886
    5 COMMON/VECTOR/ITYPE,IPONT,NC,ISTGE,IN,IV,DEL,IE,IAFT,ICHECK       TNTSS    887
      COMMON/SOLV/AF(14,6),AIO(14,6),AXR(14,6),PF(14,6),PIR(14,6),      TNTSS    888
     C PXR(14,6),TSEP(6),        NO(6),EAOP(6),EOAP(6)                  TNTSS    889
     C ,G15(14),G16(14),G18(14),G19(14),SOL(14)                         TNTSS4   101
     C ,FAO(6),EOA(6),RATES(8,10),FACD(6),YELLOW(14)                    TNTSS    891
   10 COMMON/PF/PV(14,15)                                               TNTSS    892
      COMMON/AC/AV(14,15)                                               TNTSS    893
      COMMON/NTSP/AI(14),PI(14)                                         TNTSS    894
      COMMON/INPUT/A(17),P(17)                                          TNTSS    895
      EQUIVALENCE (AF(1),AF(1,1)),(AIR(1),AIR(1,1)),(AXR(1),            TNTSS    896
   15 C AXR(1,1)),(PF(1),PF(1,1)),(PIR(1),PIR(1,1)),(PXR(1),            TNTSS    897
     C PXR(1,1))                                                        TNTSS    898
      ICOUNT=0                                                          TNTSS    899
      IVO=IV                                                            TNTSS    900
   40 IV=IV+1                                                           TNTSS    901
   20 DO17I=1,14                                                        TNTSS    902
      AI(I)=AV(I,IVO)                                                   TNTSS    903
   17 PI(I)=PV(I,IVO)                                                   TNTSS    904
      ITYPE=1                                                           TNTSS    905
      CALL VESSEL                                                       TNTSS    906
   25 IF(ICOUNT)19,19,21                                                TNTSS    907
   21 IF(ICOUNT-NC)25,25,26                                             TNTSS    908
   25 CONTINUE                                                          TNTSS    909
      IF(IPONT.EQ.1)WRITE(6,500)ISTGE,(AIR(I,ISTGE),I=1,14),(PIR(I,     TNTSS    910
     C ISTGE),I=1,10)                                                   TNTSS    911
   30 500 FORMAT(*0INTERNAL RECYCLE FOR STAGE*,I2/* AIR*,14F8.3/* PIR*,  TNTSS    912
     C 1*F8.3)                                                          TNTSS    913
      DO31I=1,14                                                        TNTSS    914
      IF(ABS(AIR(I,ISTGE)-AIO(I))-DEL)30,30,29                          TNTSS    915
   30 IF(ABS(PIR(I,ISTGE)-PIO(I))-DEL)31,31,29                          TNTSS    916
   35 31 CONTINUE                                                       TNTSS    917
      RETURN                                                            TNTSS    918
   26 WRITE(6,27)ISTGE,NC                                               TNTSS    919
   27 FORMAT( 32H0INTERNAL RECYCLE LOOP FOR STAGE,I2, 23H FAILED TO CONV TNTSS    920
     CERGE  IN,I3, 11H ITERATIONS)                                      TNTSS    921
   40 IFLG(ISTGE)=1                                                     TNTSS    922
      RETURN                                                            TNTSS    923
   29 CONTINUE                                                          TNTSS    924
   19 CONTINUE                                                          TNTSS    925
   20 ICOUNT=ICOUNT+1                                                   TNTSS    926
   45 IF(ISTGE.NE.1) GO TO 55                                           TNTSS    927
      IF(IAFT.EQ.0)GOTO59                                               TNTSS    928
      IVA=IV                                                            TNTSS    929
      IV=15                                                             TNTSS    930
      DO41I=1,14                                                        TNTSS    931
   50 AI(I)=AXR(I)*YELLOW(I)                                            TNTSS    932
   41 PI(I)=PXR(I)                                                      TNTSS    933
      CALL VESSEL                                                       TNTSS    934
      IV=IVA                                                            TNTSS    935
   59 IV=IV-1                                                           TNTSS    936
   55 DO75I=1,14                                                        TNTSS    937
      AIRO(I)=AIR(I,ISTGE)                                              TNTSS    938
   75 PIRO(I)=PIR(I,ISTGE)                                              TNTSS    939
```

```
                IF(ISTGF.NE.1)GOTO36                                    TNTSS   940
                IF(IAFT.EQ.0)GOTO37                                     TNTSS   941
60              DO46I=1,14                                              TNTSS   942
                AI(I)=AII(I)*AIRO(I)                                    TNTSS   943
           44   PI(I)=PII(I)*PIRO(I)+Pv(I,15)                           TNTSS   944
                GOTO45                                                  TNTSS   945
           37   DO64I=1,14                                              TNTSS   946
65              AI(I)=AII(I)*AIRO(I)                                    TNTSS   947
           64   PI(I)=PII(I)*PIRO(I)+PsM1(I)                            TNTSS   948
                GOTO45                                                  TNTSS   949
           36   DO47I=1,14                                              TNTSS   950
                AI(I)=AII(I)*AIRO(I)                                    TNTSS   951
70         47   PI(I)=PII(I)*PIRO(I)                                    TNTSS   952
           45   ITYPE=0                                                 TNTSS   953
                CALL VFSSEL                                             TNTSS   954
                GOTO40                                                  TNTSS   955
                END                                                     TNTSS   956
```

SYMBOLIC REFERENCE MAP (R=1)

ENTRY POINTS
1 HITSFP

VARIABLES	SN	TYPE		RELOCATION					
0	AF	REAL	ARRAY	SOLV	0	AF1	REAL	ARRAY	SOLV
0	AI	REAL	ARRAY	INPUT	0	AII	REAL	ARRAY	NTSP
124	AIR	REAL	ARRAY	SOLV	221	AIRO	REAL	ARRAY	
124	AIR1	REAL	ARRAY	SOLV	0	AV	REAL	ARRAY	AC
250	AXR	REAL	ARRAY	SOLV	250	AXR1	REAL	ARRAY	SOLV
6	DEL	REAL		VECTOR	1126	EAO	REAL	ARRAY	SOLV
1004	FAOP	REAL	ARRAY	SOLV	1134	EOA	REAL	ARRAY	SOLV
1012	FOAP	REAL	ARRAY	SOLV	1262	FACD	REAL	ARRAY	SOLV
1020	G15	REAL	ARRAY	SOLV	1036	G16	REAL	ARRAY	SOLV
1054	G1R	REAL	ARRAY	SOLV	1072	G19	REAL	ARRAY	SOLV
217	I	INTEGER			10	IAFT	INTEGER		VECTOR
11	ICHECK	INTEGER		VECTOR	215	ICOUNT	INTEGER		
7	IF	INTEGER		VECTOR	0	IFLG	INTEGER	ARRAY	FLAG
4	IN	INTEGER		VECTOR	1	IPMNT	INTEGER		VECTOR
3	ISTGE	INTEGER		VECTOR	0	ITYPE	INTEGER		VECTOR
5	IV	INTEGER		VECTOR	220	IVA	INTEGER		
216	IVO	INTEGER			2	NC	INTEGER		VECTOR
776	PO	INTEGER	ARRAY	SOLV	374	PF	REAL	ARRAY	SOLV
374	PF1	REAL	ARRAY	SOLV	21	PI	REAL	ARRAY	INPUT
14	PII	REAL	ARRAY	NTSP	520	PIR	REAL	ARRAY	SOLV
237	PIRO	REAL	ARRAY		520	PIR1	REAL	ARRAY	SOLV
0	PV	REAL	ARRAY	PC	644	PXR	REAL	ARRAY	SOLV
644	PXR1	REAL	ARRAY	SOLV	1142	RATES	REAL	ARRAY	SOLV
1110	SOL	REAL	ARRAY	SOLV	770	TSEP	REAL	ARRAY	SOLV
1270	YELLOW	REAL	ARRAY	SOLV					

FILE NAMES	MODE
TAPE6	FMT

EXTERNALS	TYPE	ARGS
VESSEL		0

INLINE FUNCTIONS	TYPE	ARGS	
ABS	REAL	1	INTRIN

STATEMENT LABELS

0	17			62	19		0	20	INACTIVE
0	21	INACTIVE		0	25	INACTIVE	56	26	
203	27	FMT		62	29		0	30	INACTIVE
0	31			0	35		144	36	
131	37			4	40		0	41	
0	44			155	45		0	46	
0	47			103	50		166	500	FMT

COMMON BLOCKS	LENGTH
FLAG	6
VECTOR	10
SOLV	710
PC	210
AC	210
NTSP	20

SYMBOLIC REFERENCE MAP (R=1)

ENTRY POINTS
1 NITSEP

VARIABLES	SN	TYPE	RELOCATION							
0	AF	REAL	ARRAY	SOLV	0	AFI	REAL	ARRAY	SOLV
0	AI	REAL	ARRAY	INPUT	0	AII	REAL	ARRAY	NTSP
124	AIP	REAL	ARRAY	SOLV	221	AIPO	REAL	ARRAY	
124	AIPI	REAL	ARRAY	SOLV	0	AV	REAL	ARRAY	AC
250	AXP	REAL	ARRAY	SOLV	250	AXPI	REAL	ARRAY	SOLV
6	DEL	REAL		VECTOR	1126	EAO	REAL	ARRAY	SOLV
1004	FAOP	REAL	ARRAY	SOLV	1134	EOA	REAL	ARRAY	SOLV
1012	FOAP	REAL	ARRAY	SOLV	1242	FACO	REAL	ARRAY	SOLV
1020	G15	REAL	ARRAY	SOLV	1036	G16	REAL	ARRAY	SOLV
1054	G18	REAL	ARRAY	SOLV	1072	G19	REAL	ARRAY	SOLV
217	I	INTEGER			10	IAFT	INTEGER		VECTOR
11	ICHECK	INTEGER		VECTOR	215	ICOUNT	INTEGER	-	
7	IF	INTEGER		VECTOR	0	IFLG	INTEGER	ARRAY	FLAG
4	IN	INTEGER		VECTOR	1	IPRNT	INTEGER		VECTOR
3	ISTGE	INTEGER		VECTOR	0	ITYPE	INTEGER		VECTOR
5	IV	INTEGER		VECTOR	220	IVA	INTEGER		
216	IVO	INTEGER			2	NC	INTEGER		VECTOR
776	PO	INTEGER	ARRAY	SOLV	374	PF	REAL	ARRAY	SOLV
374	PFI	REAL	ARRAY	SOLV	21	PI	REAL	ARRAY	INPUT
14	PII	REAL	ARRAY	NTSP	520	PIP	REAL	ARRAY	SOLV
237	PIPO	REAL	ARRAY		520	PIPI	REAL	ARRAY	SOLV
0	PV	REAL	ARRAY	PC	644	PXP	REAL	ARRAY	SOLV
644	PXPI	REAL	ARRAY	SOLV	1142	RATES	REAL	ARRAY	SOLV
1110	SOL	REAL	ARRAY	SOLV	770	TSEP	REAL	ARRAY	SOLV
1270	YELLOW	REAL	ARRAY	SOLV					

FILE NAMES MODE
TAPE6 FMT

EXTERNALS	TYPE	ARGS
VESSEL		0

INLINE FUNCTIONS	TYPE	ARGS	
ABS	REAL	1	INTRIN

STATEMENT LABELS

0	17			62	19		0	20	INACTIVE
0	21	INACTIVE		0	25	INACTIVE	56	26	
203	27	FMT		62	29		0	30	INACTIVE
0	31			0	35		144	36	
131	37			4	40		0	41	
0	44			155	45		0	46	
0	47			103	50		166	500	FMT

COMMON BLOCKS	LENGTH
FLAG	6
VECTOR	10
SOLV	710
PC	210
AC	210
NTSP	20

COMMON %LOCKS LENGTH
INPUT 36

STATISTICS
PROGRAM LENGTH 255B 173
COMMON LENGTH 2270B 1208

```
                      SUBROUTINE VESSEL                                                 TNTSS     957
                      REAL MWAVGA,MWAVGP                                                TNTSS     958
                      REAL MW(17)                                                       TNTSS     959
                      DIMENSION FF(10)                                                  TNTSS     960
     5                DIMENSION V(22),PI(17),AI(17),P(14),A(14),VD(22),R(10)            TNTSS     961
                      DIMENSION DD(8),AR(8),PX(8)                                       TNTSS     962
                      COMMON/DDD/DD(14)                                                 TNTSS     963
                      COMMON/PAR/F1(8),F3(8),F4(8),F35(8),F45(8),F5(8),F6(8),F7(8),     TNTSS     964
                     C F8(8),F10(8),F9(8)                                               TNTSS     965
    10                COMMON/EQ/A1,A2,A3,A4,A5,A6,A7,A8,A9,AS04,A12,AL,P1,P2,P3,P4,P5,P6 TNTSS     966
                     C,P7,P8,P9,P10                                                     TNTSS     967
                      COMMON/PC/PV(14,15)                                               TNTSS     968
                      COMMON/AC/AV(14,15)                                               TNTSS     969
                      COMMON/FAPA/TEMP(8),VKW(8),VKMS                                   TNTSS     970
    15                COMMON/SOLV/AF(14,6),AIP(14,6),AXR(14,6),PF(14,6),PIR(14,6),      TNTSS     971
                     C PXP(14,6),ISEP(6),       MD(6),EAOP(6),EOAP(6),                 TNTSS     972
                     C  G15(14),G16(14),G18(14),G19(14),SOL(14)                         TNTSS4    102
                     C ,EAO(6),EOA(6),RATES(9,18),FACD(6),YELLOW(14)                    TNTSS     974
                      COMMON/VECTOR/ITYPE,IPRNT,NC,ISTGE,IN,IV,DEL,IE,IAFT,ICHECK       TNTSS     975
    20                COMMON/INPUT/AI1,AI2,AI3,AI4,AI5,AI6,AI7,AI8,AI9,AI10,AI11,       TNTSS     976
                     C  AI12,AI13,AI14,AI15,AI16,AI17, PI1,PI2,PI3,PI4,PI5,PI6,PI7,PI8, TNTSS     977
                     C  PI9,PI10,PI11,PI12,PI13,PI14,PI15,PI16,PI17                     TNTSS     978
                      COMMON/Z/ RHO1,RHO2,RHO3,RHO4,RHO5,RHO6,RHO7,RHO8,RHO9,RHO10,     TNTSS     979
                     C RHO11,RHO12,RHO13,RHO14,CP(14),DM(10),AK12,AK3W,AK4W,AK5S,AK6S,  TNTSS     980
    25               C AK3S,AK4S,E3S,E4S,                                               TNTSS     981
                     C AK7,AK8,AK10,E2I,E3W,E4W,E5S,E6S,E7,E8,E10,FD,AKNA,AKNATL,SA,SB, TNTSS     982
                     C SC,SD,SE,SG,SM,SI,SJ,RW,TR,FMAX,RP,AKA,AKEQ                      TNTSS4    103
                      COMMON/DD14/P1,P2,P3,P4,P5,P6,P7,P8,P9,P10,III                    TNTSS     984
                      EQUIVALENCE (V(1),A1) ,(AI1,AI(1)),(PI1,PI(1)),(R1,R(1))          TNTSS     986
    30                EQUIVALENCE (ISEP,IST6F)                                          TNTSS     987
                      EQUIVALENCE (AKMAP,SB)                                            TNTSS     988
                      EQUIVALENCE (AKEQ3,SJ),(AKEQ4,SC)                                 TNTS,5      1
                      DATA XA,XB,XC,XD,XE,XF/3.62,.01823,3.80A,7.716,8.452,6.292/       TNTSS     989
                      DATA AKECON/1.495/                                                TNTSS4    104
    35                DATA FF    /0.,.06547,.16547,.29179,.42961,.57059,.70821,.83453,  TNTSS     992
                     C .93976,1./                                                       TNTSS     993
                      DATAMW/2*17.,2*182,,2*27,,213,,258,,63,,92,,98,,127,,18,,80,,     TNTSS     994
                     C 3*1./                                                            TNTSS     995
                      DATA DLA/.05/                                                     TNTSS     996
    40                IF(IPRNT.EQ.1)WRITE(6,6600)(AI(I),I=1,14),(PI(I),I=1,10),ISTGE    TNTSS     997
                 6600 FORMAT(*0AI*,14F9.4/* PI*,10F9.4,5X,*STAGE*,I2)                   TNTSS     998
                      AKEQ1=SM                                                          TNTSS3      5
                      AKEQ2=AKEQ                                                        TNTSS3      6
                      FACT=1.                                                           TNTSS    1000
    45                NC=50                                                             TNTSS4    105
                      ITR=0                                                             TNTSS    1001
                      IF(IV.EQ.4) ITR=1                                                 TNTSS4    106
                      IF(IV.EQ.4) FACT=.5                                               TNTSS4    107
                   10 DO157I=1,14                                                       TNTSS    1002
    50                A(I)=AV(I,IV)                                                     TNTSS    1003
                  157 P(I)=PV(I,IV)                                                     TNTSS    1004
                      DO160I=1,8                                                        TNTSS    1005
                      V(I)=A(I)                                                         TNTSS    1006
                  160 V(I+12)=P(I)                                                      TNTSS    1007
    55                AS04=A(11)+A(14)                                                  TNTSS    1008
                      A9=A(9)                                                           TNTSS    1009
                      A12=A(12)                                                         TNTSS    1010
```

```
                      AL=A(13)-A(14)                                                    TNTSS  1011
                      P9=P(9)                                                           TNTSS  1012
                      P10=P(10)                                                         TNTSS  1013
                      ICOUNT=0                                                          TNTSS  1014
                      G1=F1(IN)                                                         TNTSS  1015
                      G3=F3(IN)                                                         TNTSS  1016
                      GA=FA(IN)                                                         TNTSS  1017
                      G3S=F3S(IN)                                                       TNTSS  1018
                      GAS=FAS(IN)                                                       TNTSS  1019
                      G5=F5(IN)                                                         TNTSS  1020
                      G6=F6(IN)                                                         TNTSS  1021
                      G7=F7(IN)                                                         TNTSS  1022
                      G8=F8(IN)                                                         TNTSS  1023
                        G9=F9(IN)                                                       TNTSS  1024
                      G10=F10(IN)                                                       TNTSS  1025
                      TKEL=TEMP(IN)+273.3                                               TNTSS  1026
                      IF(ITYPE)140,140,141                                              TNTSS  1027
                  141 FVK=VKMS                                                          TNTSS  1028
                      GOTO167                                                           TNTSS  1029
                  140 FVK=VKM(IN)                                                       TNTSS  1030
                  142 ICOUNT=ICOUNT+1                                                   TNTSS  1031
                      IF(ICOUNT-NC) 163,163,164                                         TNTSS  1032
                  163 CONTINUE                                                          TNTSS  1033
                      IF(A9.LT.1.) A9=1.                                                TNTSS  1034
                      DO161I=1,22                                                       TNTSS  1035
                  161 V0(I)=V(I)                                                        TNTSS  1036
                  172 IF(AL)30,31,31                                                    TNTSS  1037
                   30 A13=0.                                                            TNTSS  1038
                      A14=-AL                                                           TNTSS  1039
                      GOTO32                                                            TNTSS  1040
                   31 A13=AL                                                            TNTSS  1041
                      A14=0.                                                            TNTSS  1042
                   32 CONTINUE                                                          TNTSS  1043
                      A11=A5A4-A14                                                      TNTSS  1044
                      IF(A11.LT.1.) A11=1.                                              TNTSS  1045
                C     COMPUTE TOTAL FLOWS                                               TNTSS  1046
                      ANR=0.                                                            TNTSS  1047
                      PNR=0.                                                            TNTSS  1048
                      DO1001I=1,P                                                       TNTSS  1049
                      ANR =ANR+ABS(V(I))                                                TNTSS  1050
                 1000  PNR=PNR+ABS(V(I+12))                                            TNTSS  1051
                      PNR=PNR+ABS(P10)                                                  TNTSS  1052
                      IF(ANR.LT..01) ANR=.01                                            TNTSS  1053
                      IF(PNR.LT.1.) PNR=1.                                              TNTSS  1054
                      PT=PNR+ABS(P9)                                                    TNTSS  1055
                      AT=ANR +ABS(A9)+ABS(A13)+ABS(A12)+A13+A14                         TNTSS  1056
                      IF(AT.LT.1.)AT=1.                                                 TNTSS  1057
                C     COMPUTE DENSITIES                                                 TNTSS  1058
                      QA=A1/RHO1+A2/RHO2+A3/RHO3+A4/RHO4+A5/RHO5+A6/RHO6+A9/RHO9+       TNTSS  1059
                     C A11/RHO11+A12/RHO12+A13/RHO13+A14/RHO14+A7/RHO7+A8/RHO8          TNTSS  1060
                      QP=P1/RHO1+P2/RHO2+P3/RHO3+P4/RHO4+P5/RHO5+P6/RHO6+P9/RHO9       TNTSS  1061
                     C +P10/RHO10+P7/RHO7+P8/RHO8                                       TNTSS  1062
                      IF(QA.LT.1.) QA=1.                                                TNTSS  1063
                      IF(QP.LT.1.) QP=1.                                                TNTSS  1064
                      IF(ITYPE)11,11,12                                                 TNTSS  1065
                   11 FA=QA/(QA+QP)                                                     TNTSS  1066
                      GOTO13                                                            TNTSS  1067
```

```
                      12  FA=.755                                                  TNTSS   1068
                     13   FP=1.-FA                                                 TNTSS   1069
                    C     COMPUTE MOLE FRACTIONS                                   TNTSS   1070
                          ATI=1./AT                                                TNTSS   1071
                          X13=A13*ATI                                              TNTSS   1072
                          X1=A1*ATI                                                TNTSS   1073
                          X2=A2*ATI                                                TNTSS   1074
                          X5=A5*ATI                                                TNTSS   1075
                          X6=A6*ATI                                                TNTSS   1076
                          X9=A9*ATI                                                TNTSS   1077
                          X14=A14*ATI                                              TNTSS   1078
                    C     COMPUTE XEQA                                             TNTSS   1079
                          PP= -7.42+.01023*TKEL-3.000*X13+7.716*(X1+X2)-8.452*(X5+X6)-  TNTSS4   108
                         C 5.592*X9                                                TNTSS4   109
                          IF(PP.GT.300.) PP=300.                                   TNTSS   1081
                          IF(PP.LT.-250.) PP=-250.                                 TNTSS   1082
                          XEQA=10.**PP                                             TNTSS   1083
                    C     COMPUTE ETA                                              TNTSS   1084
                          IF(ITYPE.15.15.16                                        TNTSS   1085
                     15   ETAA=FVK*FP*AKMA                                         TNTSS   1086
                          ETAP=FVK*FP*AKMAP                                        TNTSS   1087
                          ETA=1./(1./ETAP+1./(ETAA*XEQA))                          TNTSS   1088
                          ETATL=FVK*FP*AKMATL                                      TNTSS   1089
                    C     COMPUTE D                                                TNTSS   1090
                          ZA=ETA/PMB                                               TNTSS   1091
                          ZB=ETA/AMB                                               TNTSS   1092
                          D1=ZA*P1-ZB*A1                                           TNTSS   1093
                          D2=ZA*P2-ZB*A2                                           TNTSS   1094
                          D3=ZA*P3-ZB*A3                                           TNTSS   1095
                          D4=ZA*P4-ZB*A4                                           TNTSS   1096
                          D5=ZA*P5-ZB*A5                                           TNTSS   1097
                          D6=ZA*P6-ZB*A6                                           TNTSS   1098
                          D7=ZA*P7-ZB*A7                                           TNTSS   1099
                          D8=ZA*P8-ZB*A8                                           TNTSS   1100
                          D10=ETATL*P10/PMB                                        TNTSS   1101
                          GOTO17                                                   TNTSS   1102
                     16   D1=0.                                                    TNTSS   1103
                          D2=0.                                                    TNTSS   1104
                          D3=0.                                                    TNTSS   1105
                          D4=0.                                                    TNTSS   1106
                          D5=0.                                                    TNTSS   1107
                          D6=0.                                                    TNTSS   1108
                          D7=0.                                                    TNTSS   1109
                          D8=0.                                                    TNTSS   1110
                          D10=0.                                                   TNTSS   1111
                     17   CONTINUE                                                 TNTSS   1112
                    C     COMPUTE M                                                TNTSS   1113
                          AINV=A1+A2+A3+A4+A5+A6+A7+A8                             TNTSS   1114
                          AMNR=AT*XEQA-AINV-D1-D2-D3-D4-D5-D6-D7-D8                TNTSS   1115
                          IF(IPRNT.EQ.1)                                           TNTSS   1116
                         CWRITE(6,304)AT,PT,AMB,PMB,AINB,AMNR,XEQA,D1,D2,D3,D4,D5,D6,D7,D8  TNTSS   1117
                         C,D10                                                     TNTSS   1118
                      304 FORMAT(' AT,PT,AMB,PMB,AINB,AMNB,XEQA',7F12.5/           TNTSS   1119
                         C ' D1-8,D10',9F12.5)                                     TNTSS   1120
                    C     COMPUTE GAMMA                                            TNTSS4   110
                          F=A9/QA                                                  TNTSS4   111
                          V=A13/QA                                                 TNTSS   1130
```

```
                      S=A11/SA                                                  TNTSS3      7
                      IF(A14.GT.0.) GO TO 1361                                  TNTSS    1131
                C                                                               TNTSS    1132
      175       C                                                               TNTSS    1133
                C     SULPHURIC + WATER SYSTEM                                  TNTSS    1134
                C                                                               TNTSS    1135
                      YL=0.                                                     TNTSS4    112
                      YU=S                                                      TNTSS4    113
      180             DO 1300 I=1,40                                            TNTSS4    114
                      Y=(YL+YU)/2.                                              TNTSS4    115
                      X=(Y*Y-AKE02*(S-Y)*(W-Y))/(2.*AKE02*(S-Y)+Y)              TNTSS4    116
                      IF(X.LE.0..OR.X.LE.(Y-W)/2.) GO TO 1305                   TNTSS4    117
                      GO TO 1306                                                TNTSS4    118
      185       1305  X=Y                                                       TNTSS4    119
                      GO TO 1308                                                TNTSS4    120
                1306  IF(X.GE.F.OR.X.GE.Y) GO TO 1307                           TNTSS4    121
                      GO TO 1309                                                TNTSS4    122
                1307  YU=Y                                                      TNTSS4    123
      190             GO TO 1300                                                TNTSS4    124
                1308  AK1=X*Y*(W-2.*X-Y)/((F-X)*(S-Y))                          TNTSS4    125
                      IF(ABS(AK1-AKE01).LT..01) GO TO 1312                      TNTSS4    126
                      IF(AK1.LT.AKE01) GO TO 1310                               TNTSS4    127
                      YU=Y                                                      TNTSS4    128
      195             GO TO 1300                                                TNTSS4    129
                1310  YL=Y                                                      TNTSS4    130
                1300  CONTINUE                                                  TNTSS4    131
                1312  CH2=X                                                     TNTSS4    132
                      CHSO4=Y                                                   TNTSS4    133
      200             CH2O=W-X                                                  TNTSS4    134
                      CH2SO4=S-Y                                                TNTSS4    135
                      CHSO3=F-X                                                 TNTSS4    136
                      CH2O2=W-X-(Y-X)                                           TNTSS4    137
                      A17=CH02*QA                                               TNTSS4    138
      205             Q=X/F                                                     TNTSS4    139
                      GO TO 2341                                                TNTSS    1155
                1361  F=A9/QA                                                   TNTSS    1156
                      P=(A11-A14)/QA                                            TNTSS    1157
                      C=A14/QA                                                  TNTSS    1158
      210       C                                                               TNTSS5      2
                C     SULFURIC + OLEUM SYSTEM (REGION 1)                        TNTSS5      3
                C                                                               TNTSS5      4
                      IF(A9.GT..5*A14) GO TO 2337                               TNTSS5      5
                      CH02=F                                                    TNTSS5      6
      215             CHSO3=0.                                                  TNTSS5      7
                      CH2SO4=B+F                                                TNTSS5      8
                      CH2O2=F                                                   TNTSS5      9
                      CHSO4=0.                                                  TNTSS5     10
                      CH2O=0.                                                   TNTSS5     11
      220             A17=CH02*QA                                               TNTSS5     12
                      Q=1.                                                      TNTSS5     13
                      GO TO 2341                                                TNTSS5     14
                C                                                               TNTSS5     15
                C     SULFURIC + OLEUM SYSTEM (REGION 3)                        TNTSS5     16
      225       C                                                               TNTSS5     17
                2337  IF(A9.LE.A14) GO TO 3300                                  TNTSS5     18
                      X=F                                                       TNTSS5     19
                      XL=.5*C                                                   TNTSS5     20
```

```
                      AC=A+3.*C                                                 TNTSSS     21
  230                 CR=.5*R+1.5*C                                             TNTSSS     22
                      DO 2330 I=1,40                                            TNTSSS     23
                      X=(XU+XL)/2.                                              TNTSSS     24
                      Y=AKE04*X*(2.*X-C)**2/(F-X)                               TNTSSS     25
                      IF(Y.LE.(C-X)) GO TO 2339                                 TNTSSS     26
  235                 GO TO 2340                                                TNTSSS     27
                 2339 XL=X                                                      TNTSSS     28
                      GO TO 2330                                                TNTSSS     29
                 2340 IF(Y.GE.(CR-X)) GO TO 2343                                TNTSSS     30
                      GO TO 2344                                                TNTSSS     31
  240            2343 XU=X                                                      TNTSSS     32
                      GO TO 2330                                                TNTSSS     33
                 2344 AK3=X*(Y+X-C)*(2.*X-C)**2/((F-X)*(BC-2.*X-2.*Y)**2)       TNTSSS     34
                      IF(ABS(AK3-AKE03).LT.1.) GO TO 2348                       TNTSSS     35
                      IF(AK3.LT.AKE03) GO TO 2345                               TNTSSS     36
  245                 XU=X                                                      TNTSSS     37
                      GO TO 2330                                                TNTSSS     38
                 2345 XL=X                                                      TNTSSS     39
                 2330 CONTINUE                                                  TNTSSS     40
                 2348 CW07=X                                                    TNTSSS     41
  250                 CWS207=Y                                                  TNTSSS     42
                      CW1107=F-X                                                TNTSSS     43
                      CW1?=?*X-C                                                TNTSSS     44
                      CW2S06=AC-2.*X-2.*Y                                       TNTSSS     45
                      CWS04=2.*X-C                                              TNTSSS     46
  255                 A107=CW02*DA                                              TNTSSS     47
                      Q=CW02/F                                                  TNTSSS     48
                      GO TO 2341                                                TNTSSS     49
                C                                                               TNTSSS     50
                C     SULFURIC + OLEUM SYSTEM (REGION 2)                        TNTSSS     51
  260           C                                                               TNTSSS     52
                 3300 XL=.5*F                                                   TNTSSS     53
                      IF((F-.5*C).LT.XU) XU=F-.5*C                              TNTSSS     54
                      XL=0.                                                     TNTSSS     55
                      FC=2.*F-C                                                 TNTSSS     56
  265                 CF=F-F                                                    TNTSSS     57
                      DO 2350 I=1,20                                            TNTSSS     58
                      X=(XL+XU)/2.                                              TNTSSS     59
                      AK4=X*(CF+X)/((F-X)*(FC-2.*X)**2)                         TNTSSS     60
                      IF(AK4.LT.AKE04) GO TO 2351                               TNTSSS     61
  270 .               XU=X                                                      TNTSSS     62
                      GO TO 2350                                                TNTSSS     63
                 2351 XL=X                                                      TNTSSS     64
                 2350 CONTINUE                                                  TNTSSS     65
                      CW02=F-X                                                  TNTSSS     66
  275                 CW1107=X                                                  TNTSSS     67
                      CWS207=2*F+X                                              TNTSSS     68
                      CWS06=FC-2.*X                                             TNTSSS     69
                      CW1?=0.                                                   TNTSSS     70
                      CW2S06=0.+C                                               TNTSSS     71
  280                 A107=CW02*DA                                              TNTSSS     72
                      Q=CW02/F                                                  TNTSSS     73
                 2341 GAMMA=FVRHOFA*Q*Q**AKA/(QA*QA)                            TNTSS3     37
                      G3D=G3S*GAMMA                                             TNTSS4    140
                      G4D=G4S*GAMMA                                             TNTSS4    141
  285                 G5G=G5*GAMMA                                              TNTSS     1238
```

```
                      G66=GA+GAMMA                                                TNTSS   1239
                      G7G=G7+FVKM+FA+(    A17)/(QA+QA)                            TNTSS4   142
                      G8P=G8+FVKM+FA+(    A17)/(QA+QA)                            TNTSS4   143
                      G10P=G10+FVKM+FA+(    A17)/(QA+QA)                          TNTSS4   144
          200         G9G=G9+GAMMA                                                TNTSS   1243
                      AM9 =AT+XEQA                                                TNTSS   1244
                      IF(AMMA)130,131,131                                         TNTSS   1245
          130         CA=AMMA/AMB                                                 TNTSS   1246
                      CR=0.                                                       TNTSS   1247
          205         GOTO132                                                     TNTSS   1248
          131         CA=0.                                                       TNTSS   1249
                      CR=AMMA/PMA                                                 TNTSS   1250
          132         CONTINUE                                                    TNTSS   1251
                      IF(ITYPE)133,133,134                                        TNTSS   1252
          300         134 C1=0.                                                   TNTSS   1253
                      C1P=0.                                                      TNTSS   1254
                      C10=0.                                                      TNTSS   1255
                      C1A=0.                                                      TNTSS   1256
                      GOTO135                                                     TNTSS   1257
          305         133 C1=FTA                                                  TNTSS   1258
                      C1P=FTATL/PMA                                               TNTSS   1259
                      C10=C1/PMB                                                  TNTSS   1260
                      C1A=C1/AMB                                                  TNTSS   1261
          135         P10=P110/(1.+C1P)                                           TNTSS   1262
          310         Q10=C1P*P10                                                 TNTSS   1263
                      P2=G1*Q10                                                   TNTSS   1264
                      R1=Q10-P2                                                   TNTSS   1265
                      AX1=1.+C1A-CA                                               TNTSS   1266
                      C11=AX1+G3D                                                 TNTSS   1267
          315         C12=-C10-CR                                                 TNTSS   1268
                      R1=A11                                                      TNTSS   1269
                      R2=P11*R1                                                   TNTSS   1270
                      C22=1.+C10    +CR                                           TNTSS   1271
                      C21=CA-C1A                                                  TNTSS   1272
          320         P1=(C21*R1-C11*R2)/(C21*C12-C11*C22)                        TNTSS   1273
                      A1=(R1-C12*P1)/C11                                          TNTSS   1274
                      III=III+1                                                   TNTSS   1275
                      P3=G3D*A1                                                   TNTSS   1276
                      IF(P3.LT.0.)P3=0.                                           TNTSS   1277
          325         AM1=CA*A1+CR*P1                                             TNTSS   1278
                      D1=C10*P1-C1A*A1                                            TNTSS   1279
                      IF(IPPNT.EQ.1)                                              TNTSS   1280
                     1WRITE(6,382) AM1,D1,R3,A1,P1,R1                             TNTSS   1281
          382         FORMAT(1H  A=1,D1,R3,A1,P1,R1,3F12.5,E16.5,2F12.5)          TNTSS   1282
          330         R1=A12                                                      TNTSS   1283
                      R2=R12*R2                                                   TNTSS   1284
                      C11=AX1+G4D                                                 TNTSS   1285
                      P2=(C21*R1-C11*R2)/(C21*C12-C11*C22)                        TNTSS   1286
                      A2=(R1-C12*P2)/C11                                          TNTSS   1287
          335         R4=G4D*A2                                                   TNTSS   1288
                      IF(R4.LT.0.)R4=0.                                           TNTSS   1289
                      R1=A13*R3                                                   TNTSS   1290
                      R2=P13                                                      TNTSS   1291
                      C11=AX1+G5G+G7G+G8P+G9G                                     TNTSS   1292
          340         P3=(C21*R1-C11*R2)/(C21*C12-C11*C22)                        TNTSS   1293
                      A3=(R1-C12*P3)/C11                                          TNTSS   1294
                      RBA=GRD*A3                                                  TNTSS   1295
```

```
                R7A=G7G*A3                                                      TNTSS  1296
                R5 =G5G*A3                                                      TNTSS  1297
      345       IF(R7A.LT.0.) R7A=0.                                            TNTSS  1298
                IF(RRA.LT.0.) RRA=0.                                            TNTSS  1299
                IF(R5.LT.0.)R5=0.                                               TNTSS  1300
                R6GA=G6G*A3                                                     TNTSS  1301
                B1=A14*R4                                                       TNTSS  1302
      350       R2=R14                                                          TNTSS  1303
                C11=A11*G6G+G7G+G8P+G9G                                         TNTSS  1304
                P4=(C21*B1-C11*B2)/(C21*C12-C11*C22)                            TNTSS  1305
                A4=(B1-C12*P4)/C11                                              TNTSS  1306
                R4M=G8P*A4                                                      TNTSS  1307
      355       R7M=G7G*A4                                                      TNTSS  1308
                R6 =G6G*A4                                                      TNTSS  1309
                R9GM=G9G*A4                                                     TNTSS  1310
                R9G=R9GM+R9GA                                                   TNTSS  1311
                IF(R7M.LT.0.) R7M=0.                                            TNTSS  1312
      360       IF(R4M.LT.0.) R4M=0.                                            TNTSS  1313
                IF(R6.LT.0.)R6=0.                                               TNTSS  1314
                RR=RRA+RRM                                                      TNTSS  1315
                R7=R7*+R7M                                                      TNTSS  1316
                B1=A15*R5                                                       TNTSS  1317
      365       R2=R15                                                          TNTSS  1318
                C11=A11*4.*G1(P                                                 TNTSS  1319
                P5=(C21*B1-C11*B2)/(C21*C12-C11*C22)                            TNTSS  1320
                A5=(B1-C12*P5)/C11                                              TNTSS  1321
                R10A=G10P*A5                                                    TNTSS  1322
      370       IF(R10A.LT.0.) R10A=0.                                          TNTSS  1323
                B1=A14*R6                                                       TNTSS  1324
                B2=R16                                                          TNTSS  1325
                P6=(C21*B1-C11*B2)/(C21*C12-C11*C22)                            TNTSS  1326
                A6=(B1-C12*P6)/C11                                              TNTSS  1327
      375       R10M=G10P*A6                                                    TNTSS  1328
                IF(R10M.LT.0.) R10M=0.                                          TNTSS  1329
                R10=R10A+R10M                                                   TNTSS  1330
                C11=A11                                                         TNTSS  1331
                B1=A17*R10                                                      TNTSS  1332
      380       R2=R17                                                          TNTSS  1333
                P7=(C21*B1-C11*B2)/(C21*C12-C11*C22)                            TNTSS  1334
                A7=(B1-C12*P7)/C11                                              TNTSS  1335
                B1=A19*R10*2.                                                   TNTSS  1336
                B2=R18                                                          TNTSS  1337
      385       P8=(C21*B1-C11*B2)/(C21*C12-C11*C22)                            TNTSS  1338
                A8=(B1-C12*P8)/C11                                              TNTSS  1339
                C5=11.*R7*14.5 *R8*9.*R10                                       TNTSS  1340
                C5=C5*14.5*R9G                                                  TNTSS  1341
                R9=R1*C5                                                        TNTSS  1342
      390       C5P=C5-R9                                                       TNTSS  1343
                C4=B14*P1*P4.P5*R4                                              TNTSS  1344
                AL=A113-A114*C4*15.*R7*16.5 *R8-(.67*.33*RP)*R9*12.*R10         TNTSS  1345
                AL=AL*16.5*R9G                                                  TNTSS  1346
                A12=A112*C5P                                                    TNTSS  1347
      395       A5D4=A111*A114-C5P                                              TNTSS  1348
                C6=1.5*A13*DT/(AT*A11)                                          TNTSS  1349
                A9=(A19*P19-C4-13.*R7-17.5 *R8-9. *R10*(.33*.67*RP)*R9)/(11.*C6) TNTSS  1350
                A9=A9-12.5*R9G/(11.*C6)                                         TNTSS  1351
                R9=C6*A9                                                        TNTSS  1352
```

```
      DO1AA1=1,22                                                       TNTSS  1353
      IF(ABS(V(I)-V0(I))-DLA)100,100,173                                TNTSS  1354
  172 CONTINUE                                                          TNTSS  1355
      IF(IPRNT.EQ.1) WRITE(6,9910)IV,FACT,Q,R                           TNTSS  1356
 9910 FORMAT(' VESSEL',I3,' CONVERGED, FACT =',F10.5,5X,'Q =',F8.5/     TNTSS  1357
     C 1X10F10.4)                                                       TNTSS  1358
  169 DO185I=1,14                                                       TNTSS  1359
      A(I)=0.                                                           TNTSS  1360
  185 P(I)=0.                                                           TNTSS  1361
      DO186I=1,8                                                        TNTSS  1362
      A(I)=V(I)                                                         TNTSS  1363
  186 P(I)=V(I+12)                                                      TNTSS  1364
      IF(AL)190,191,191                                                 TNTSS  1365
  190 A(13)=0.                                                          TNTSS  1366
      A(14)=-AL                                                         TNTSS  1367
      GOTO192                                                           TNTSS  1368
  191 A(13)=AL                                                          TNTSS  1369
      A(14)=0.                                                          TNTSS  1370
  192 CONTINUE                                                          TNTSS  1371
      A(9)=A9                                                           TNTSS  1372
      A(11)=AS04-A(14)                                                  TNTSS  1373
      A(12)=A12                                                         TNTSS  1374
      P(9)=P9                                                           TNTSS  1375
      P(10)=P10                                                         TNTSS  1376
      IF(IV.EQ.15)GOTO150                                               TNTSS  1377
      QQ(IV)=Q                                                          TNTSS  1378
      G15P=6.*R7+7.*R8                                                  TNTSS  1379
      G15P=G15P+7.*R96                                                  TNTSS  1380
      G15(IV)=G15P                                                      TNTSS  1381
      G16(IV)=R9*.67*(1.-RP)                                            TNTSS  1382
      G18(IV)=R7                                                        TNTSS  1383
      G19(IV)=R10                                                       TNTSS  1384
      SOL(IV)=XEQA                                                      TNTSSA  145
      IF(ITYPE)80,80,81                                                 TNTSS  1385
   81 ZA=9.                                                             TNTSS  1386
      ZB=0.                                                             TNTSS  1387
      DO82I=1,8                                                         TNTSS  1388
   82 ZA=ZA+P(I)*CP(I)                                                  TNTSS  1389
      DO83I=1,14                                                        TNTSS  1390
   83 ZB=ZB+A(I)*CP(I)                                                  TNTSS  1391
      DO84I=1,10                                                        TNTSS  1392
   84 ZP=ZP+HW(I)*B(I)                                                  TNTSS  1393
      TSEP(ISEP)=TEMP(IN)+ZB/ZA                                         TNTSS  1394
      IF(IE)109,109,110                                                 TNTSS  1395
  109 CONTINUE                                                          TNTSS  1396
      PTI=1./PT                                                         TNTSS  1397
      X3=A3*ATI                                                         TNTSS  1398
      X4=A4*ATI                                                         TNTSS  1399
      X7=A7*ATI                                                         TNTSS  1400
      X11=A11*ATI                                                       TNTSS  1401
      X8=A8*ATI                                                         TNTSS  1402
      X12=A12*ATI                                                       TNTSS  1403
      X13=A13*ATI                                                       TNTSS  1404
      Y1=P1*PTI                                                         TNTSS  1405
      Y2=P2*PTI                                                         TNTSS  1406
      Y3=P3*PTI                                                         TNTSS  1407
      Y4=P4*PTI                                                         TNTSS  1408
```

```
                      YS=P5*PTI                                                  TNTSS   1409
                      YS=P6*PTI                                                  TNTSS   1410
                      Y7=P7*PTI                                                  TNTSS   1411
      440             YA=PA*PTI                                                  TNTSS   1412
                      Y9=P9*PTI                                                  TNTSS   1413
                      Y10=P10*PTI                                                TNTSS   1414
                      RMAVGA=X1*RM(1)+X2*RM(2)+X3*RM(3)+X4*RM(4)+X5*RM(5)+X6*RM(6)+  TNTSS   1415
                     + X7*RM(7)+XA*RM(8)+X9*RM(9)+X11*RM(11)+X12*RM(12)+X13*RM(13)+  TNTSS   1416
      465            2 X14*RM(14)                                               TNTSS   1417
                      RMAVGP=Y1*RM(1)+Y2*RM(2)+Y3*RM(3)+Y4*RM(4)+YS*RM(5)+Y6*RM(6)+  TNTSS   1418
                     1 Y7*RM(7)+YA*RM(8)+Y9*RM(9)+Y10*RM(10)                     TNTSS   1419
                      NBTCH=NB(ISEP)+1                                           TNTSS   1420
                      RVOL=FMAX*FF(NBTCH)                                        TNTSS   1421
      470             RTO=RT/AT                                                  TNTSS   1422
                      RTL=RTO*RMAVGP/RMAVGA                                      TNTSS   1423
                      TLI=RT*RMAVGP+AT*RMAVGA                                    TNTSS   1424
                      RHOO=RT/OP                                                 TNTSS   1425
                      RHLO=RHOO*RMAVGP                                           TNTSS   1426
      475             DPR=AT/AA-RT/OP                                            TNTSS   1427
                      CXX=1.3753*0.23063*RTL-0.01512*RHLO-0.25607*DPR            TNTSS   1428
                      EAO4      =-0.17805+1.8497*RTO-0.75339*RTL+4.869E-6*TLI+   TNTSS   1429
                     1 0.22976*RHOO                                              TNTSS   1430
                      IF(EAO4.LT.0.)EAO4=0.                                      TNTSS   1431
      480             EXX=EAO4/(1.-EAO4)                                         TNTSS   1432
                      FLW=0.                                                     TNTSS   1433
                      FMG=1.                                                     TNTSS   1434
                       DO1I=1,20                                                 TNTSS   1435
                      FIR=(FLW+FMG)*.5                                           TNTSS   1436
      485             FOG=CXX+0.42907*FIR                                        TNTSS   1437
                      FOGC=FOG                                                   TNTSS   1438
                      IF(FOG.GT.1.)FOG=1.                                        TNTSS   1439
                      IF(FOG.LT.0.)FOG=0.                                        TNTSS   1440
                      TPR=FOG*PT                                                 TNTSS   1441
      490             TPF=PT-TPR                                                 TNTSS   1442
                      TAF=EXX*TPF                                                TNTSS   1443
                      TAR=AT-TAF                                                 TNTSS   1444
                      CX2=FIR/(1.-FIR)                                           TNTSS   1445
                      TPIR=TPR/(1.+CX2)                                          TNTSS   1446
      495             TPIR=TPR-TPIR                                              TNTSS   1447
                      TAIR=TAR/(1.+CX2)                                          TNTSS   1448
                      TAIR=TAR-TAIR                                              TNTSS   1449
                      CVOL=TAIR*QA/AT*TPIR*QR/PT                                 TNTSS   1450
                      IF(CVOL.GT.RVOL)GOTO2                                      TNTSS   1451
      500             FLW=FIR                                                    TNTSS   1452
                      GOTO1                                                      TNTSS   1453
                  2   FMG=FIR                                                    TNTSS   1454
                  1   CONTINUE                                                   TNTSS   1455
                      EOA(ISEP)=IPIR/(TPIR+TAIR)                                 TNTSS   1456
      505             EAO(ISEP)=EAO4                                             TNTSS   1457
                      WRITE(4,5) ISEP,EOA(ISEP),EAO(ISEP)                        TNTSS   1458
                  5   FORMAT(* ISEP,EOA,EAO*,I5,2F14.6)                          TNTSS   1459
                      EOAP(ISEP)=EOA(ISEP)/(1.-EOA(ISEP))                        TNTSS   1460
                      EAOP(ISEP)=EAO(ISEP)/(1.-EAO(ISEP))                        TNTSS   1461
      510         110 CONTINUE                                                   TNTSS   1462
                      FAR=(1.-EAOP(ISEP)*PT/AT)/(1.-EOAP(ISEP)*EAOP(ISEP))       TNTSS   1463
                      IF(FAR)142,143,143                                         TNTSS   1464
                  142 FAR=0.                                                     TNTSS   1465
```

```
                  143  IF(FAR.GT.1.)FAR=1.                                    TNTSS   1466
515                    FAR1=1.-FAR                                            TNTSS   1467
                       FP0=1.-FAR*EQAP(ISEP) *AT/PT                           TNTSS   1468
                       IF(FP0)144,145,145                                     TNTSS   1469
                  144  FP0=0.                                                 TNTSS   1470
                  145  IF(FP0.GT.1.)FP0=1.                                    TNTSS   1471
520                    FP01=1.-FP0                                            TNTSS   1472
                       QT=QA*FAR*(1.-FP0)*QP                                  TNTSS   1473
                       NOTCH=NO(ISEP)+1                                       TNTSS   1474
                       FRAC=FMAX*FF(NOTCH)/QT                                 TNTSS   1475
                       IF(FRAC.GT.1.)FRAC=1.                                  TNTSS   1476
525                    FR=1.-FRAC                                             TNTSS   1477
                       IF(IPRNT.EQ.1)                                         TNTSS   1478
                      CWRITE(6,170) EQAP(ISEP),EAQP(ISEP),PT,AT,QT,FF(NOTCH),QA,QP,  TNTSS   1479
                      C FMAX,                                                 TNTSS   1480
                      C FRAC,FR,FAR,FAR1,FP0,FP01                             TNTSS   1481
530               170  FORMAT(* EQAP,EAQP,PT,AT,QT,FF,QA,QP,FMAX*,9F10.4/    TNTSS   1482
                      C * FRAC,FR,FAR,FAR1,FP0,FP01*,6F10.5)                  TNTSS   1483
                       DO146I=1,14                                            TNTSS   1484
                       AIR(I,ISEP)=A(I)*FAR*FRAC                              TNTSS   1485
                       PIR(I,ISEP)=P(I)*FP01*FRAC                             TNTSS   1486
535                    AXR(I,ISEP)=A(I)*FAR*FR                                TNTSS   1487
                       PXR(I,ISEP)=P(I)*FP01*FR                               TNTSS   1488
                       AF(I,ISEP)=A(I)*FAR1                                   TNTSS   1489
                       PF(I,ISEP)=P(I)*FP0                                    TNTSS   1490
                  146  CONTINUE                                               TNTSS   1491
540                    GOTO85                                                 TNTSS   1492
                   88  DO14J=1,10                                            TNTSS   1493
                   14  RATES(IN,J)=R(J)                                      TNTSS   1494
                   85  CONTINUE                                              TNTSS   1495
                       IF(IPRNT)150,150,151                                   TNTSS   1496
545                151  IF(ITYPE)152,152,153                                  TNTSS   1497
                    152  IF(IN.EQ.7) GO TO 1520                             TNTSS   1498
                       IF(IN.NE.7) GO TO 150                                  TNTSS   1499
                  1520 WRITE(6,154)IN,      ICOUNT                            TNTSS   1500
                   154  FORMAT( 17H0NITRATION VESSEL,I2,                      TNTSS   1501
550                    C   5X 12HITERATIONS =,I3)                             TNTSS   1502
                       GOTO155                                                TNTSS   1503
                    153  IF(ISEP.EQ.5) GO TO 1530                           TNTSS   1504
                       IF(ISEP.NE.5) GO TO 154                                TNTSS   1505
                  1530 WRITE(6,156)ISEP,TSEP(ISEP),ICOUNT                     TNTSS   1506
555                156  FORMAT( 10H0SEPARATOR,I2,10X 13HTEMPERATURE =,F7.2,5X 12HITERATION TNTSS   1507
                      CS =,   I3)                                             TNTSS   1508
                   155  WRITE(6,187)V,GISP,R9,R7,R10                          TNTSS   1509
                   187  FORMAT(5X  2HA1,7X  2HA2,7X  2HA3,7X  2HA4,7X  2HA5,7X  2HA6,7X  2 TNTSS   1510
                      CHA7,7X  2HA8,     7X  2HA9,6X  4HA$04,6X  3HA12,6X  2HAL,7X  2HP1/1 TNTSS   1511
560                   CX13F9.3/5X  2HP2,7X  2HP3,      7X  2HP4,7X  2HP5,7X  2HP6,7X  2HP7 TNTSS   1512
                      C,7X  2HPR,7X  2HP9,7X  3HP10,4X  6HCO1.33,      4X  5HR01.5,5X  3HT TNTSS   1513
                      CNW,4X  3HCO2/1X13F9.3)                                 TNTSS   1514
                   150  DO159I=1,14                                           TNTSS   1515
                       AV(I,IV)=A(I)                                          TNTSS   1516
565                 159  PV(I,IV)=P(I)                                        TNTSS   1517
                  C     THE FOLLOWING CALCULATIONS ARE TO CHECK THE AGREEMENT  TNTSS   1518
                  C     WITH THE ORIGINAL EQUATIONS                            TNTSS   1519
                       IF(ICHECK.NE.1) GO TO 1234                             TNTSS   1520
                       SPWR=P(10)                                             TNTSS   1521
570                    SAWR=0.                                                TNTSS   1522
```

```
                      DO208I=1,8                                                        TNTSS   1523
                      SPNR=SPNP*P(I)                                                    TNTSS   1524
                  208 SANR=SANR*A(I)                                                    TNTSS   1525
                      AT=SANR                                                           TNTSS   1526
                      DO701I=9,14                                                       TNTSS   1527
                  701 AT=AT*A(I)                                                        TNTSS   1528
                      PP=-7.679*.01023*TKEL-7.80R*A(13)/AT+7.716*(A(1)+A(2))/AT         TNTSS   1529
                     C -R.452*(A(5)+A(6))/AT-6.202*A(9)/AT                              TNTSS   1530
                      XEQA=10.**PP                                                      TNTSS   1531
                      SANPC=AT*XEQA                                                     TNTSS   1532
                      PT=SPNP*P(9)                                                      TNTSS   1533
                      WRITE(6,700) IV,TKEL,AT,SANR,SANPC,PNR,PT,A,P,(A(I),I=1,14),      TNTSS   1534
                     C (P(I),I=1,14)                                                    TNTSS   1535
                  700 FORMAT(*0VESSEL*,13,5X,*TKEL*,F6.1,5X,*AT*,F14.4,5X,*SANR*,       TNTSS   1536
                     C F14.4,5X,*SANPC*,F14.4/* PNR*,F14.4,5X,*PT*,F14.4/* A *,14F9.2/ TNTSS   1537
                     C * P *,14F9.2/* A*,14F9.2/* P*,14F9.2)                           TNTSS   1538
                      PNR=SPNR                                                          TNTSS   1539
                      ANR=SANR                                                          TNTSS   1540
                      SUM=0.                                                            TNTSS   1541
                      WRITE(6,756) R1,R2,R3,R4,R5,R6,R7,R8,R9,R10,R9G,RP,CS,CSP,AS04,   TNTSS   1542
                     C C6,C4                                                            TNTSS   1543
                  756 FORMAT(* R1-10,R9G*,11F10.4/* RP,CS,CSP,AS04,C6,C4*,6F10.4)       TNTSS   1544
                      IF(ITYPE.EQ.0)GOTO350                                             TNTSS   1545
                      DO751I=1,8                                                        TNTSS   1546
                  751 DD(I)=0.                                                          TNTSS   1547
                      DI0=0.                                                            TNTSS   1548
                      GOTO352                                                           TNTSS   1549
                  350 ETA=1./(1./ETAP+1./(ETAA*XEQA))                                   TNTSS   1550
                      ZA=ETA/PNR                                                        TNTSS   1551
                      ZB=ETA/ANR                                                        TNTSS   1552
                      DO709I=1,8                                                        TNTSS   1553
                      DD(I)=ZA*P(I)-ZB*A(I)                                             TNTSS   1554
                  208 SUM=SUM+DD(I)                                                     TNTSS   1555
                      DI0=ETATL*P(10)/PNR                                               TNTSS   1556
                  352 AMNR=SANPC-AINR-SUM                                               TNTSS   1557
                      IF(AMNR)337,333,333                                               TNTSS   1558
                  338 CA=AMNR/ANR                                                       TNTSS   1559
                      CP=0.                                                             TNTSS   1560
                      GO TO 332                                                         TNTSS   1561
                  331 CA=0.                                                             TNTSS   1562
                      CP=AMNR/PNR                                                       TNTSS   1563
                  332 CONTINUE                                                          TNTSS   1564
                      DO 337 I=1,8                                                      TNTSS   1565
                  337 AM(I)=CA*A(I)+CP*P(I)                                             TNTSS   1566
                      P2=G1*010                                                         TNTSS   1567
                      AX1=A[(1)        -G3G*A(1)+DD(1)+AM(1)                            TNTSS   1568
                      PR1=010-22                                                        TNTSS   1569
                      PR1=G3G*A(1)                                                      TNTSS   1570
                      WRITE(6,382) AM(1),DD(1),RR3,A(1),P(1),PR1                        TNTSS   1571
                      AX2=A[(2)    -G4D*A(2)+DD(2)+AM(2)                                TNTSS   1572
                      AX3=A[(3)+G3D*A(1)-G5G*A(3)-G7G*A(3)-G8P*A(3)+DD(3)+AM(3)         TNTSS   1573
                      AX4=A[(4)+G4D*A(2)-G6G*A(4)-G7G*A(4)-G8P*A(4)+DD(4)+AM(4)         TNTSS   1574
                      AX5=A[(5)+G5G*A(3)-4.*G10P*A(5)+DD(5)+AM(5)                       TNTSS   1575
                      AX6=A[(6)+G6G*A(4)-4.*G10P*A(6)+DD(4)+AM(6)                       TNTSS   1576
                      AX7=A[(7)+G19P*(A(5)+A(4))+DD(7)+AM(7)                            TNTSS   1577
                      AX8=A[(8)+7.*G10P*(A(5)+A(6))+DD(8)+AM(8)                         TNTSS   1578
                      PR7=G7G*(A(3)+A(4))                                               TNTSS   1579
```

```
                PRA=G4P*(A(3)+A(4))                                              TNTSS   1580
                PR10=G10P*(A(5)+A(6))                                            TNTSS   1581
  630           PR9=(11.*RR7+14.5*RR8+9.*RR10)*F0                                TNTSS   1582
                RR9G=G9G*(A(3)+A(4))                                             TNTSS   1583
                DO220I=1,8                                                       TNTSS   1584
  220           PX(I)=PI(I)-DD(I)-AM(I)                                          TNTSS   1585
                PX(1)=PX(1)+D10-R2                                               TNTSS   1586
  635           PX(2)=PX(2)+R2                                                   TNTSS   1587
                PX9=1.5I*A(13)*A(9)*PT/(AT*A(11))                                TNTSS   1588
                AX9=AI(9)+PI(9)-P(9)-D10-G3D*A(1)-G4D*A(2)-G5G*A(3)-G6G*A(4)-    TNTSS   1589
               C 13.*RR7-12.5*RRA-9.*RR10-12.5*RR9G+(.33+.67*RP)*RR9             TNTSS   1590
                PX10=PI(10)-D10                                                  TNTSS   1591
  640           AX12=AI(12)+(1.-F0)*(13.*RR7+14.5*RR8+9.*RR10)                   TNTSS   1592
                AXL=AI(13)-AI(14)+D10+G3D*A(1)+G4D*A(2)+G5G*A(3)+G6G*A(4)+       TNTSS   1593
               C 15.*RR7+14.5*RRA-(.67+.33*RP)*RR9+12.*PR10                      TNTSS   1594
                WRITE(6,355)D0,D10,XEQA,AM,AMNR,AINB,AX1,AX2,AX3,AX4,AX5,AX6,    TNTSS   1595
               C AX7,AX8,AX9,AX12,AXL,PX,PX9,PX10                                TNTSS   1596
  645       355 FORMAT(* D0=D10*,9F10.4,3X,*XEQA*,F10.5/* AM*,8F10.4,3X,*AMNR*,   TNTSS   1597
               C F10.4,3X,*AINB*,F10.4/* AX1-9*,9F10.4,*   AX12,AXL*,2F10.4/     TNTSS   1598
               C* PX1-10*,10F10.4)                                               TNTSS   1599
                WRITE(6,361) G1,G3,G4,G5,G6,G7,G8,G9,G10,G3D,G4D,G5G,G6G,        TNTSS   1600
               C G7G,G8P,G9G,G10P                                                TNTSS   1601
  650       361 FORMAT(* G1,G3,G4,G5,G6,G7,G8,G9,G10*/1X9F12.2/                  TNTSS   1602
               C * G3D,G4D,G5G,G6G,G7G,G8P,G9G,G10P*/1X8F12.4)                    TNTSS   1603
            1234 RETURN                                                          TNTSS   1604
             173 IF(ITR)162,162,174                                              TNTSS   1605
             174 DO175I=1,22                                                     TNTSS   1606
  655        175 V(I)=V0(I)+FACT*(V(I)-V0(I)  )                                  TNTSS   1607
                GOTO162                                                          TNTSS   1608
             164 ITR=ITR+1                                                       TNTSS   1609
                FACT=.5*FACT                                                     TNTSS   1610
                IF(ITR-5)18,18,1690                                              TNTSS   1611
  660           WRITE(6,167)IV                                                   TNTSS   1612
            167 FORMAT(  7H0VESSEL,I3, 19H FAILED TO CONVERGE)                   TNTSS   1613
                GOTO169                                                          TNTSS   1614
                END                                                              TNTSS   1615
```

SYMBOLIC REFERENCE MAP (R=1)

ENTRY POINTS
1 VESSEL

VARIABLES	SN	TYPE	RELOCATION						
3516	A	REAL	ARRAY		0	AF	REAL	ARRAY	SOLV
0	AI	REAL	ARRAY	INPUT	3231	AINB	REAL		
124	AIP	REAL	ARRAY	SOLV	0	AI1	REAL		INPUT
11	AI10	REAL		INPUT	12	AI11	REAL		INPUT
13	AI12	REAL		INPUT	14	AI13	REAL		INPUT
15	AI14	REAL		INPUT	16	AI15	REAL		INPUT
17	AI16	REAL		INPUT	20	AI17	REAL		INPUT
1	AI2	REAL		INPUT	2	AI3	REAL		INPUT
3	AI4	REAL		INPUT	4	AI5	REAL		INPUT
5	AI6	REAL		INPUT	6	AI7	REAL		INPUT
7	AI8	REAL		INPUT	10	AI9	REAL		INPUT
112	AKA	REAL		Z	113	AKEQ	REAL		Z
2402	AKFOOV	REAL			3143	AKEQ1	REAL		
3144	AKEQ2	REAL			105	AKEQ3	REAL		Z
77	AKEQ4	REAL		Z	73	AKMA	REAL		Z
76	AKMAP	REAL		Z	74	AKMATL	REAL		Z
3242	AK1	REAL			61	AK10	REAL		Z
46	AK12	REAL		Z	3262	AK3	REAL		
53	AK3S	REAL		Z	47	AK3W	REAL		Z
3265	AK4	REAL			54	AK4S	REAL		Z
50	AK4W	REAL		Z	51	AK5S	REAL		Z
52	AK6S	REAL		Z	57	AK7	REAL		Z
60	AK8	REAL		Z	13	AL	REAL		EQ
3572	AM	REAL	ARRAY		3232	AMNB	REAL		
3314	AMI	REAL			3170	ANB	REAL		
11	ASQ4	REAL		EQ	3173	AT	REAL		
3200	ATI	REAL			0	AV	REAL	ARRAY	AC
3444	AXL	REAL			250	AXR	REAL	ARRAY	SOLV
3305	AX1	REAL			3443	AX12	REAL		
3424	AX2	REAL			3425	AX3	REAL		
3426	AX4	REAL			3427	AX5	REAL		
3430	AX6	REAL			3431	AX7	REAL		
3432	AXR	REAL			3441	AX9	REAL		
0	A1	REAL		EQ	3167	A11	REAL		
12	A12	REAL		EQ	3165	A13	REAL		
3166	A14	REAL			3251	A17	REAL		
1	A2	REAL		EQ	2	A3	REAL		EQ
3	A4	REAL		EQ	4	A5	REAL		EQ
5	A6	REAL		EQ	6	A7	REAL		EQ
7	A8	REAL		EQ	10	A9	REAL		EQ
3253	B	REAL			3260	BC	REAL		
3310	BI	REAL			3311	B2	REAL		
3254	C	REAL			3277	CA	REAL		
3261	CB	REAL			3264	CF	REAL		
3247	CHN03	REAL			3244	CHS04	REAL		
3255	CHS207	REAL			3250	CN20	REAL		
3246	CH2S04	REAL			3245	CH30	REAL		
3243	CN02	REAL			16	CP	REAL	ARRAY	Z
3300	CP	REAL			3405	CVOL	REAL		
3304	CXX	REAL			3460	CX2	REAL		
3301	C2	REAL			3304	C1A	REAL		

VARIABLES	SN	TYPE	RELOCATION						
3303	C10	REAL			3342	C1P	REAL		
3306	C11	REAL			3307	C12	REAL		
3313	C21	REAL			3312	C22	REAL		
3330	C4	REAL			3326	C5	REAL		
3327	C5P	REAL			3331	C6	REAL		
3562	CD	REAL	ARRAY		6	DEL	REAL		VECTOR
34	DH	REAL	ARRAY	Z	2403	DLA	REAL		
3363	DMM	REAL			3220	D1	REAL		
3230	D10	REAL			3221	D2	REAL		
3222	D3	REAL			3223	D4	REAL		
3224	D5	REAL			3225	D6	REAL		
3226	D7	REAL			3227	D8	REAL		
1126	FA0	REAL	ARRAY	SOLV	1004	EAOP	REAL	ARRAY	SOLV
3365	FA04	REAL			1134	EOA	REAL	ARRAY	SOLV
1012	EOAP	REAL	ARRAY	SOLV	3214	ETA	REAL		
3212	ETAA	REAL			3213	ETAP	REAL		
3215	ETATL	REAL			3366	EXX	REAL		
71	F10	REAL		Z	62	E21	REAL		Z
55	F3S	REAL		Z	63	F3W	REAL		Z
56	F4S	REAL		Z	64	E4W	REAL		Z
65	F5S	REAL		Z	66	E6S	REAL		Z
67	F7	REAL		Z	70	E8	REAL		Z
3233	F	REAL			3176	FA	REAL		
1262	FACD	REAL	ARRAY	SOLV	3145	FACT	REAL		
3406	FAR	REAL			3407	FAR1	REAL		
3263	FC	REAL			72	FD	REAL		Z
3466	FF	REAL	ARRAY		3370	FMG	REAL		
3371	FIR	REAL			3367	FLW	REAL		
110	FMAX	REAL		Z	3372	FOG	REAL		
3373	FOGC	REAL			3177	FP	REAL		
3410	FPO	REAL			3411	FPO1	REAL		
3414	FR	REAL			3413	FRAC	REAL		
3164	FWKM	REAL			0	F1	REAL	ARRAY	PAR
110	F10	REAL	ARRAY	PAR	10	F3	REAL	ARRAY	PAR
30	F3S	REAL	ARRAY	PAR	20	F4	REAL	ARRAY	PAR
40	F4S	REAL	ARRAY	PAR	50	F5	REAL	ARRAY	PAR
60	F6	REAL	ARRAY	PAR	70	F7	REAL	ARRAY	PAR
100	F8	REAL	ARRAY	PAR	120	F9	REAL	ARRAY	PAR
3266	GAMMA	REAL			3150	G1	REAL		
3162	G10	REAL			3275	G10P	REAL		
1020	G15	REAL	ARRAY	SOLV	3332	G15P	REAL		
1036	G16	REAL	ARRAY	SOLV	1054	G18	REAL	ARRAY	SOLV
1072	G19	REAL	ARRAY	SOLV	3151	G3	REAL		
3267	G30	REAL			3153	G3S	REAL		
3152	G4	REAL			3270	G4D	REAL		
3154	G4S	REAL			3155	G5	REAL		
3271	G5G	REAL			3156	G6	REAL		
3272	G6G	REAL			3157	G7	REAL		
3273	G7G	REAL			3160	G8	REAL		
3274	GAP	REAL			3161	G9	REAL		
3276	G9G	REAL			3142	I	INTEGER		
10	IAFT	INTEGER		VECTOR	11	ICHECK	INTEGER		VECTOR
3147	ICOUNT	INTEGER			7	IE	INTEGER		VECTOR
12	III	INTEGER		DUM	4	IN	INTEGER		VECTOR
1	IPOINT	INTEGER		VECTOR	3	ISEP	INTEGER		VECTOR
3	ISTGE	INTEGER		VECTOR	3146	ITR	INTEGER		
0	ITYPE	INTEGER		VECTOR	5	IV	INTEGER		VECTOR

VARIABLES	SN	TYPE	RELOCATION
3415	.I	INTEGER	
3140	*MAVGA	REAL	
2	*C	INTEGER	VECTOR
3354	*NOTCH	INTEGER	
374	PF	REAL ARRAY	SOLV
520	PIP	REAL ARRAY	SOLV
32	PI10	REAL	INPUT
34	PI12	REAL	INPUT
36	PI14	REAL	INPUT
40	PI16	REAL	INPUT
22	PI2	REAL	INPUT
24	PI4	REAL	INPUT
26	PI6	REAL	INPUT
30	PI8	REAL	INPUT
3171	PMB	REAL	
3172	PT	REAL	
0	PV	REAL ARRAY	PC
644	PXP	REAL ARRAY	SOLV
3440	P.9	REAL	
25	P10	REAL	EQ
16	P3	REAL	EQ
20	P5	REAL	EQ
22	P7	REAL	EQ
24	P9	REAL	EQ
3174	QA	REAL	
0	QQ	REAL ARRAY	QQQ
0	R	REAL ARRAY	DUM
3362	RHL0	REAL	
0	RHO1	REAL	Z
12	RHO11	REAL	Z
14	RHO13	REAL	Z
1	RHO2	REAL	Z
3	RHO4	REAL	Z
5	RHO6	REAL	Z
7	RHO8	REAL	Z
111	RP	REAL	Z
3422	RR1	REAL	
3423	RR3	REAL	
3434	RR8	REAL	
3437	RR9G	REAL	
3356	RT0	REAL	
0	R1	REAL	DUM
3324	R10A	REAL	
1	R2	REAL	DUM
3	R4	REAL	DUM
5	R6	REAL	DUM
3316	R7A	REAL	
7	RR	REAL	DUM
3320	RRM	REAL	
3323	RRG	REAL	
3322	RRGM	REAL	
75	SA	REAL	Z
3420	SANBC	REAL	
77	SC	REAL	Z
101	SE	REAL	Z
103	SH	REAL	Z
105	SJ	REAL	Z
3445	RV	REAL ARRAY	
3141	RWAVGP	REAL	
776	NO	INTEGER ARRAY	SOLV
3500	P'	REAL ARRAY	
21	PI	REAL ARRAY	INPUT
21	PI1	REAL	INPUT
33	PI11	REAL	INPUT
35	PI13	REAL	INPUT
37	PI15	REAL	INPUT
41	PI17	REAL	INPUT
23	PI3	REAL	INPUT
25	PI5	REAL	INPUT
27	PI7	REAL	INPUT
31	PI9	REAL	INPUT
3210	PP	REAL	
3333	PTI	REAL	
3402	PX	REAL ARRAY	
3442	PX10	REAL	
14	P1	REAL	EQ
15	P2	REAL	EQ
17	P4	REAL	EQ
21	P6	REAL	EQ
23	PP	REAL	EQ
3252	Q	REAL	
3175	QP	REAL	
3412	QT	REAL	
1142	RATES	REAL ARRAY	SOLV
3361	RHO0	REAL	
11	RHO10	REAL	Z
13	RHO12	REAL	Z
15	RHO14	REAL	Z
2	RHO3	REAL	Z
4	RHO5	REAL	Z
6	RHO7	REAL	Z
10	RHO9	REAL	Z
186	RR	REAL	Z
3435	RR10	REAL	
3433	RR7	REAL	
3436	RR9	REAL	
3357	RTL	REAL	
3355	RWOL	REAL	
11	R10	REAL	DUM
3325	R10M	REAL	
2	R3	REAL	DUM
4	R5	REAL	DUM
6	R7	REAL	DUM
3321	R7M	REAL	
3315	RRA	REAL	
10	RR	REAL	DUM
3317	RRGA	REAL	
3235	S	REAL	
3417	SANB	REAL	
76	SB	REAL	Z
100	SD	REAL	Z
102	SG	REAL	Z
104	SI	REAL	Z
1110	SOL	REAL ARRAY	SOLV

VARIABLES	SN	TYPE	RELOCATION						
3416	CPNB	REAL				3421	CWH	REAL	
3376	TAF	REAL				3404	TAIR	REAL	
3377	TAP	REAL				3403	TAIR	REAL	
0	TEMP	REAL	ARRAY	PARA		3163	TKEL	REAL	
3360	TLI	REAL				3375	TPF	REAL	
3402	TPIR	REAL				3374	TPR	REAL	
3401	TPIR	REAL				107	TR	REAL	Z
770	TSEP	REAL	ARRAY	SOLV		0	V	REAL	ARRAY E0
10	VKM	REAL	ARRAY	PARA		20	VKMS	REAL	PARA
3534	W0	REAL	ARRAY			3234	W	REAL	
3241	X	REAL				2374	XA	REAL	
2375	XA	REAL				2376	XC	REAL	
2377	XD	REAL				2400	XE	REAL	
3211	XEQA	REAL				2401	XF	REAL	
3257	XL	REAL				3256	XU	REAL	
3202	X1	REAL				3317	X11	REAL	
3341	X12	REAL				3201	X13	REAL	
3207	X14	REAL				3203	X2	REAL	
3334	X3	REAL				3315	X4	REAL	
3204	X5	REAL				3205	X6	REAL	
3336	X7	REAL				3340	X8	REAL	
3206	X9	REAL				3240	Y	REAL	
1270	YELLOW	REAL	ARRAY	SOLV		3236	YL	REAL	
3237	YU	REAL				3342	Y1	REAL	
3353	Y10	REAL				3343	Y2	REAL	
3344	Y3	REAL				3345	Y4	REAL	
3346	Y5	REAL				3347	Y6	REAL	
3350	Y7	REAL				3351	Y8	REAL	
3352	Y9	REAL				3216	ZA	REAL	
3217	ZB	REAL							

FILE NAMES	MODE
TAPE6	FMT

INLINE FUNCTIONS	TYPE	ARGS	
ABS	REAL	1	INTRIN

STATEMENT LABELS

1640	1		1637	2		2517	5	FMT	
0	11	INACTIVE	247	12		251	13		
0	14		0	15	INACTIVE	362	16		
367	17		23	18		0	30		INACTIVE
121	31		123	32		1755	80		
0	81	INACTIVE	0	82		0	83		
0	84		1762	85		0	109		INACTIVE
1668	110		0	130	INACTIVE	721	131		
724	132		730	133		0	134		INACTIVE
735	135		101	140		0	141		INACTIVE
0	142	INACTIVE	1670	143		0	144		INACTIVE
1703	145		0	146		2004	150		
0	151	INACTIVE	0	152	INACTIVE	1773	153		
2564	154	FMT	2002	155		2000	156	FMT	
0	157		0	159		0	160		
0	161		103	162		0	163		INACTIVE
2365	164		3060	167	FMT	1323	169		
0	172	INACTIVE	2355	173		0	174		INACTIVE
0	175		0	185		0	186		

STATEMENT LABELS

2620	187	FMT	0	188		0	190	INACTIVE
1340	191		1342	192		0	200	
0	201		0	204		0	220	
2662	900	FMT	0	330	INACTIVE	2126	331	
2131	332		0	333		2075	350	
0	351		2117	352		2777	355	FMT
2730	356	FMT	3042	361	FMT	2545	370	FMT
2464	382	FMT	2443	384	FMT	2354	1234	
472	1300		446	1305		450	1306	
456	1307		456	1308		471	1310	
475	1312		511	1341		1778	1520	
1776	1530		0	1690	INACTIVE	0	1900	
527	2317		601	2338		555	2339	
557	2340		667	2341		562	2343	
564	2344		600	2345		604	2348	
651	2350		650	2351		621	3300	
2412	4600	FMT	2501	9910	FMT			

COMMON BLOCKS LENGTH

000	14
PAR	88
FO	22
PC	210
AC	210
PARA	17
SOLV	710
VECTOR	10
INPUT	34
7	76
NUM	11

STATISTICS

PROGRAM LENGTH	76120	1090
COMMON LENGTH	25720	1402

```
      FUNCTION ENTH(A,P,TP)                                              TMTSS   1616
      DIMENSION A(14),P(14),X(14),Y(14)                                  TMTSS   1617
      REAL LAS,LASE                                                      TNTSS   1618
      COMMON/Z/ RM01,RM02,RM03,RM04,RM05,RM06,RM07,RM08,RM09,RM010,      TNTSS   1619
     C RM11,RM012,RM013,RM014,CP(14),DM(10),AK12,AK3W,AK4W,AK5S,AK6S,    TNTSS   1620
     C AK7S,AK8S,E3S,E4S,                                                TNTSS   1621
     C AK7,AK8,AK10,EZ1,E3W,E4W,E5S,E6S,E7,E8,E10,FB,AKHA,AKHATL,SA,SB,  TNTSS   1622
     C SC,SD,SE,SG,SH,SI,SJ,RR,TR,FMAX,BP,AKA,AKE0                      TNTSS4   146
      EQUIVALENCE (CP(11),CP11),(CP(9),CP9),(CP(14),CP14),               TNTSS   1624
     C (CP(13),CP13),(CP(12),CP12)                                       TNTSS   1625
      DATA X/-129.,-133.,-134.,-137.,-134.,-128.,-115.,-98.,-75.,-45.,   TNTSS   1626
     C 0.,60.,160.,260./                                                 TNTSS   1627
      DATA Y/-127.,-127.,-129.,-130.,-124.,-120.,-108.,-91.,-72.,-47.,   TNTSS   1628
     C -25.,-5.,20.,40./                                                 TNTSS   1629
      DLT=TP-20.                                                         TNTSS   1630
      LAS=90.*A(1)+63.*A(9)+18.*A(13)+80.*A(14)                          TNTSS   1631
      ENTH=0.                                                            TNTSS   1632
      IF(LAS.LT.1.)GOTO3                                                 TNTSS   1633
      LASE=90.*(A(1)+A(14))+63.*A(9)                                     TNTSS   1634
      WTA=LASE/LAS                                                       TNTSS   1635
      F=(WTA-.45)/.05                                                    TNTSS   1636
      J=F                                                                TNTSS   1637
      F=F-FLOAT(J)                                                       TNTSS   1638
      ENTH0=X(J)+(X(J+1)-X(J))*F                                         TNTSS   1639
      ENTH2=Y(J)+(Y(J+1)-Y(J))*F                                         TNTSS   1640
      WTH=63.*A(9)/LASE                                                  TNTSS   1641
      ENTH=LAS*(ENTH0+(ENTH2-ENTH0)*WTH/.2)*.252                         TNTSS   1642
     C +DLT*(A(11)*CP11+A(9)*CP9+A(13)*CP13+A(14)*CP14)                  TNTSS   1643
    3 DO1I=1,10                                                          TNTSS   1644
      IF(I.EQ.9)GOTO2                                                    TNTSS   1645
      T=A(I)*P(I)                                                        TNTSS   1646
      GOTO1                                                              TNTSS   1647
    2 T=P(I)                                                             TNTSS   1648
    1 ENTH=ENTH+T*DLT*CP(I)                                              TNTSS   1649
      ENTH=ENTH+DLT*CP12*A(12)                                           TNTSS   1650
      RETURN                                                             TNTSS   1651
      END                                                                TNTSS   1652
```

SYMBOLIC REFERENCE MAP (R=1)

ENTRY POINTS
4 ENTH

VARIABLES	SN	TYPE	RELOCATION						
0	A	REAL	ARRAY	F.P.	112	AKA	REAL		Z
113	AKEQ	REAL		Z	73	AKMA	REAL		Z
74	AKMATL	REAL		Z	61	AK1S	REAL		Z
46	AK12	REAL		Z	53	AK3S	REAL		Z
47	AK3N	REAL		Z	54	AK4S	REAL		Z
50	AK4N	REAL		Z	51	AK5S	REAL		Z
52	AK6S	REAL		Z	57	AP7	REAL		Z
60	AK8	REAL		Z	16	CP	REAL	ARRAY	Z
30	CP11	REAL		Z	31	CP12	REAL		Z
32	CP13	REAL		Z	33	CP14	REAL		Z
26	CP9	REAL		Z	34	DN	REAL	ARRAY	Z
126	ELT	REAL			123	ENTH	REAL		
132	ENTH0	REAL			133	ENTH2	REAL		
71	F10	REAL		Z	62	EZI	REAL		Z
55	F3S	REAL		Z	63	E3N	REAL		Z
56	F4S	REAL		Z	64	E4N	REAL		Z
65	F5S	REAL		Z	66	E6S	REAL		Z
67	F7	REAL		Z	70	E8	REAL		Z
130	F	REAL			72	FD	REAL		Z
110	FMAX	REAL		Z	135	I	INTEGER		
131	J	INTEGER			124	LBS	REAL		
125	LOSE	REAL			0	P	REAL	ARRAY	F.P.
0	RH01	REAL		Z	11	RH010	REAL		Z
12	RH011	REAL		Z	13	RH012	REAL		Z
14	RH013	REAL		Z	15	RH014	REAL		Z
1	RH02	REAL		Z	2	RH03	REAL		Z
3	RH04	REAL		Z	4	RH05	REAL		Z
5	RH06	REAL		Z	6	RH07	REAL		Z
7	RH08	REAL		Z	10	RH09	REAL		Z
111	RP	REAL		Z	100	RP	REAL		Z
75	SA	REAL		Z	76	SB	REAL		Z
77	SC	REAL		Z	100	SD	REAL		Z
101	SE	REAL		Z	102	SG	REAL		Z
103	SH	REAL		Z	104	SI	REAL		Z
105	SJ	REAL		Z	136	T	REAL		
0	TP	REAL		F.P.	107	TR	REAL		Z
127	VTA	REAL			134	VTH	REAL		
137	X	REAL	ARRAY		155	Y	REAL	ARRAY	

INLINE FUNCTIONS	TYPE	ARGS
FLOAT	REAL	1 INTPIN

STATEMENT LABELS
101 1 100 2 66 3

COMMON BLOCKS	LENGTH
7	76

STATISTICS
PROGRAM LENGTH 1738 123
COMMON LENGTH 1148 76

LISTING OF DATA DECK

```
24.8        3553330.    372403.     124.5       504.76      .09         2.1         .0001
1P000000.   10000000.   22000.      19000.
85.9        24800.      17462.      9700.       6500.       5040.       7000.       1.
.68         15500.      0.          1.547       0.          7000.       .08         1.51
60000.      .9          743.3       27500.      5000.       418.        .65         .6
.2          .1          .1          50.         1.495       1.
    .21522646E+00   .8294911E-02    .41790835E-01   .1969340E-02    .2326701E-01
    .12425728E-02   .1197501E-05    .4192564E-05    .1693838E-02    0.
    .90833564E-02   .72344644E+01   .2158946E-03    0.
    .20084617E-02   .8484839E+00    .7953856E+01    .1853772E+00    .2237119E+01
    .11021463E+00   .1361186E-03    .4023557E-03    .5584231E+01    .3788531E-02
    0.              0.              0.              0.
    .16331846E+00   .6329752E-02    .2782711E-01    .1324854E-02    .1578576E-01
    .93642629E-03   .8437177E-05    .2831157E-05    .1723383E-02    0.
    .11571346E-03   .8412154E+01    .2538323E-03    0.
    .23609721E-02   .9997714E+00    .4002695E+01    .1981967E+00    .2259384E+01
    .12867898E+00   .1357684E-03    .4072912E-03    .5227897E+01    .1125365E-02
    0.              0.              0.              0.
    .16323472E+00   .5502921E-02    .2792942E-01    .2141892E-02    .1578542E-01
    .93885558E-03   .8438769E-06    .2831431E-05    .1723232E+02    0.
    .11571346E-03   .8412154E+01    .2538323E-03    0.
    .23609721E-02   .9997714E+00    .4002695E+01    .1981964E+00    .2259384E+01
    .12867898E+00   .1357684E-03    .4072913E-03    .5227882E+01    .1125365E-02
    0.              0.              0.              0.
    .42421146E-01   .9579418E-03    .7831818E-03    .2790504E-01    .4491863E+00
    .24813467E-01   .2714285E-04    .9142179E-04    .2855232E+02    0.
    .16819099E-03   .1892634E-02    .1544613E-03    0.
    .23022555E-01   .6427913E-01    .3234119E+02    .1151152E+01    .1873512E+02
    .10821103E+01   .1131866E-02    .3395418E-02    .9520513E+01    .6621969E-06
    0.              0.              0.              0.
    .16099777E-03   .2136797E-05    .8184181E-04    .2789308E-01    .4530698E+00
    .24852146E-01   .2714285E-04    .8284797E-04    .2851045E+02    0.
    .16819711E-03   .1892915E-02    .1544971E-03    0.
    .23022555E-01   .6427913E-01    .3234298E+02    .1151213E+01    .1873612E+02
    .10821103E+01   .1131866E-02    .3395598E-02    .9518314E+01    .6621969E-06
    0.              0.              0.              0.
    .39677776E-05   .3727274E-06    .1054428E+01    .7295593E-01    .3988827E+01
    .22153644E+00   .2479297E-01    .7418877E-03    .2748837E+02    0.
    .94645508E+02   .5336712E+01    0.              .1493373E+02
    .33540542E-02   .9194927E-04    .2136369E+02    .5184438E+00    .2744830E+02
    .15466468E+01   .1725844E-02    .5175132E-02    0.              .2249254E-09
    0.              0.              0.              0.
    .80450208E-04   .1871781E-04    .5056667E+01    .7996201E-01    .1843620E+02
    .57887778E-04   .4231019E-03    .1869306E-02    .3645713E+02    0.
    .17697644E+03   .1284449E+02    0.              .8842643E+01
    .43911772E-05   .1757346E-06    .1858464E+02    .2942631E+00    .3033323E+02
    .28948752E+01   .2288875E-02    .6866584E-02    0.              .1377263E-12
    0.              0.              0.              0.
    .51394273E-13   .2787457E-13    .3361967E+01    .3118727E-01    .1164259E+02
    .60240136E+00   .7179384E-03    .2153814E-02    .3244768E+02    0.
    .17687751E+03   .1367858E+02    0.              .6331878E+01
    .63013777E-05   .1757346E-06    .1867322E+02    .2950451E+00    .3042558E+02
    .21124638E+01   .2304831E-02    .6928494E-02    0.              .1377263E-12
    0.              0.              0.              0.
    .53795708E-13   .2888721E-13    .1491833E+01    .1341059E-01    .1440889E+02
    .46474429E+00   .1991719E-03    .3245156E-02    .5033451E+02    0.
    .17713343E+03   .6321457E+01    0.              .7198746E+02
    .88114198E-04   .2670382E-09    .4146365E+01    .3745823E-01    .3983829E+02
    .18284768E+01   .2991875E-02    .8975624E-02    0.              .4962952E-16
    0.              0.              0.              0.
    .28487798E-18   .2882488E-17    .5781444E+01    .2845365E-02    .1566905E+02
```

```
 .642[illegible]E+00   .1727[illegible]E-02   .3467163E-02   .5819492E+02   0.
 .1727[illegible]E-01   .6545214E+01   0.   .7078775E+02
 .8831418E-00   .2670[illegible]E-00   .4153[illegible]E+01   .374877RE-01   .4083573E+02
 .1837964E+01   .3807891E-02   .9823672E-02   0.   .6962952E-16
 0.   0.   0.   0.
 .1521369E-15   .1736[illegible]E-15   .1915978E-02   .1040993E-02   .1000014E+02
 .[illegible]256876E+00   .9642557E-03   .2832747E-02   .3908715E-02   0.
 .9679615E-02   .1824678E+01   0.   .6233184E-02
 .1888451E-10   .[illegible]517[illegible]E-12   .[illegible]2655[illegible]E-02   .4589232E-02   .4293243E+02
 .1[illegible]7[illegible]E+01   .4[illegible]E-02   .1215915E-01   0.   .1572996E-19
 0.   0.   0.   0.
 .9681[illegible]E-21   .9914431E-21   .3288158E-01   .1813678E-03   .1011337E+02
 .[illegible]3187[illegible]E-02   .1111[illegible]E-02   .[illegible]3417214E-02   .3971318E-02   0.
 .9607[illegible]E-02   .1857[illegible]E+01   0.   .6211741E-02
 .1[illegible]8451E-10   .[illegible]517[illegible]E-12   .[illegible]2668[illegible]E-02   .4589609E-02   .4296996E+02
 .1[illegible]1E+01   .4[illegible]E-02   .1217154E-01   0.   .1572996E-19
 0.   0.   0.   0.
 .5774427E-10   .1[illegible]E-10   .2297[illegible]E-01   .7763093E-04   .7990087E+01
 .3613427E+00   .[illegible]E-[illegible]   .2574211E-02   .3435483E-02   0.
 .7220[illegible]E+02   .1647568E+00   0.   .5364277E-02
 .1874845E-13   .[illegible]1777[illegible]E-15   .[illegible]5[illegible]E-01   .2918972E-03   .2962424E+02
 .1244557E+01   .[illegible]E-02   .9557365E-02   0.   .3093139E-23
 0.   0.   0.   0.
 .1[illegible]E-26   .1210245E-26   .7267474E-02   .4583500E-05   .8004017E+01
 .3449911E+00   .1941650E-02   .[illegible]1269[illegible]E-02   .3433815E-02   0.
 .7231484E+02   .1516[illegible]E+00   0.   .5361439E-02
 .1874845E-13   .[illegible]1777[illegible]E-15   .[illegible]5[illegible]E-01   .2919002E-03   .2962948E+02
 .1244[illegible]E+01   .[illegible]E-02   .9559409E-02   0.   .3093139E-23
 0.   0.   0.   0.
1.        1.        1.2       1.2       1.5
 1
OPTIMUM CONDITIONS----DEVELOPED ON 7-21-72
 111
1500.                1900.
498.
          1000.
                                1000.     320.      400.      220.      900.
                                                                       10000.
1763.     587.
500.
0.
64.                                       44.
0.
64.                                       46.
                                          .5
5.5                  10.                  84.
0.
64.                                       2.
0.
5.23                 57.1                           37.67
115 21
51.       31.       64.       83.       85.       90.       95.       110.
52.1      57.1      48.1      51.5      52.1      53.5      60.2      60.2
78.1
0.        .15615    .13918    .02421    .01950    .00477
.00871    .02787    .09552    .03047    .04133    .04715
```

******INPUT DATA******

RATE CONSTANTS

PROGRAM OUTPUT

K12	K3W	K4W	K5S	K4S	K5S	K6S	K7	K8	K10
26.30	3553730.66	372863.00	10000.00	10000000.00	124.50	506.76	.00	2.10	.00

K9	KA	KC	KFO	KFOW
.300000	.100000	.100000	50.000000	1.495000

ACTIVATION ENERGIES

E2I	E3W	E4W	E5S	E4S	E5S	E6S	E7	E8	E10
00.	26000.	17462.	22000.	10000.	9300.	6500.	5040.	7000.	1.

CONSTANTS

A	B	C	D	E	G	H	I	J
.481550.00	0.00	1.00	0.00	7400.00	.00	1.5160000.00		

GAS LAW CONSTANT = .08
REFERENCE TEMPERATURE = 461.27 DEG R
MASS TR. COEFF. = 27500.0
MASS TR. COEFF. (TAR) = 5900.0
EFFECT OF REACTION FOR HMOSAA DECOMPOSITION = .6500
DRAG COEFFICIENT = .600

PHYSICAL PROPERTIES

COMPONENT	MOL. WT.	DENSITY	MT. CAP.	REACTION	MT. OF REACTION
1	137.0	.50	21.60	1	13930.
2	137.0	.50	21.60	2	13120.
3	182.0	.64	29.90	3	13750.
4	182.0	.66	29.90	4	9900.
5	227.0	.69	33.00	5	11760.
6	227.0	.65	33.00	6	14520.
7	273.0	.69	33.00	7	237600.
8	250.0	.68	33.00	8	321000.
9	83.0	1.40	1.01	9	13200.
10	92.0	.55	15.90	10	0.
11	00.0	1.15	15.55		
12	127.0	1.15	15.55		
13	18.0	1.00	0.16		
14	00.0	1.15	16.30		

[redacted] [redacted] OPTIMUM CONDITIONS----DEVELOPED ON 3-21-72

[redacted]

[redacted]	1A	1B	2	3A	3B	4	5	6
[redacted]	[redacted]	-0.	1000.	-0.	-0.	-0.	-0.	-0.
FD.	[redacted]	-0.	-0.	-0.	-0.	-0.	-0.	-0.
YELLOW MG.	-0.	[redacted]	-0.	-0.	-0.	-0.	-0.	-0.
STOPPING MI.	-0.	-0.	-0.	1000.	320.	400.	220.	900.
OLEUM	-0.	-0.	-0.	-0.	-0.	-0.	-0.	10000.
[redacted]	[redacted]	[redacted]	-0.	-0.	-0.	-0.	-0.	-0.
WATER	[redacted]	-0.	-0.	-0.	-0.	-0.	-0.	-0.

ACID STRENGTHS, WT. PCT.

COMP.	AMMT	DMMT	ADMT	MDMT	ATMT	MTMT	TMMA	TMM	MMB3	TML	M2SO4	MMDSO4	M2O	SO3
[redacted]	[redacted]	-0.00	[redacted]	-0.00	-0.00	[redacted]	-0.00	-0.00	56.00	-0.00	[redacted]	-0.00	44.00	-0.00
FD.	[redacted]	-0.00	-0.00	-0.00	-0.00	[redacted]	-0.00	-0.00	56.00	-0.00	-0.00	-0.00	46.00	-0.00
YELLOW MG.	[redacted]	-0.00	[redacted]	[redacted]	.50	[redacted]	-0.00	-0.00	5.50	-0.00	10.0[redacted]	-0.00	84.00	-0.00
STOPPING MI.	[redacted]	-0.00	[redacted]	-0.00	-0.00	[redacted]	-0.00	-0.00	96.00	-0.00	-0.00	-0.00	2.00	-0.00
OLEUM	[redacted]	-0.00	[redacted]	-0.00	-0.00	[redacted]	-0.00	-0.00	5.23	-0.00	57.10	-0.00	-0.00	37.67

STAGE 1

MIXATOR 1A	MIXATOR 1B
VOL. = 52.1	VOL. = 52.1
TEMP.= 51.8	TEMP.= 33.8

SEPARATOR 1
VOL. = 29.1
MATCH SETTING = 1
ENTRAINMENT
ORGANIC IN ACID .00071
ACID IN ORGANIC 5.09898

STAGE 2

MIXATOR 2
VOL. = 69.1
TEMP.= 44.8

SEPARATOR 2
VOL. = 29.1
MATCH SETTING = 1
ENTRAINMENT
ORGANIC IN ACID .02787
ACID IN ORGANIC .15615

STAGE 3

MIXATOR 3A	MIXATOR 3B
VOL. = 53.5	VOL. = 52.1
TEMP.= 81.4	TEMP.= 85.8

SEPARATOR 3
VOL. = 28.1
MATCH SETTING = 5
ENTRAINMENT
ORGANIC IN ACID .00632
ACID IN ORGANIC .13918

STAGE 4

MIXATOR 4
VOL. = 53.5
TEMP.= 88.4

SEPARATOR 4
VOL. = 28.1
MATCH SETTING = 5
ENTRAINMENT
ORGANIC IN ACID .03967
ACID IN ORGANIC .12621

STAGE 5

MIXATOR 5
VOL. = 68.2
TEMP.= 85.9

SEPARATOR 5
VOL. = 29.1
MATCH SETTING = 2
ENTRAINMENT
ORGANIC IN ACID .04133
ACID IN ORGANIC .11958

STAGE 6

NITRATOR A
WR$_o$ = 69.2
TEMP$_o$=110.9

SEPARATOR A
WR$_o$ = 29.1
BATCH SETTING = 1
ENTRAINMENT
ORGANIC IN ACID .4715
ACID IN ORGANIC .03477

*****PHASE COMPOSITIONS

NITRATOR 1A

	ANNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.343	.215	.816	.388	.256	.003	.000	.003	9.686	0.000	97.966	7.311	162.704	0.000
ORG. PHASE	14.561	.584	5.402	.372	2.467	.143	.000	.000	2.453	.007				

NITRATOR 1B

	ANNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.227	.087	.354	.604	.427	.001	.000	.000	5.781	0.000	115.864	8.558	252.527	0.000
ORG. PHASE	23.826	.759	5.516	.384	2.734	.146	.000	.000	1.702	.003				

SEPARATOR 1 TEMPERATURE = 77.0

	ANNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.226	.086	.355	.605	.427	.001	.000	.000	5.779	0.000	115.864	8.558	252.529	0.000
ORG. PHASE	23.826	.759	5.516	.384	2.734	.146	.000	.000	1.702	.003				

NITRATOR 2

	ANNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.082	.103	1.542	.057	1.117	.052	.000	.000	17.927	0.000	122.767	9.098	77.432	0.000
ORG. PHASE	.223	.087	30.992	1.109	19.952	1.010	.000	.000	4.264	.000				

SEPARATOR 2 TEMPERATURE = 65.5

	ANNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.082	.103	1.458	.041	1.120	.066	.000	.000	17.756	0.000	122.789	9.157	77.660	0.000
ORG. PHASE	.223	.087	30.994	1.109	19.961	1.011	.000	.000	4.239	.000				

NITRATOR 3A

	ANNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.088	.088	2.212	.051	4.125	.211	.000	.000	32.036	0.000	91.268	5.151	0.000	18.764
ORG. PHASE	.088	.088	17.815	.418	32.347	1.697	.000	.001	0.000	.000				

NITRATOR 3B

	ANNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.088	.088	3.761	.054	13.757	.687	.000	.000	62.429	0.000	239.445	18.016	0.000	15.494
ORG. PHASE	.088	.088	14.792	.211	54.124	2.697	.000	.001	0.000	.000				

SEPARATOR 3 TEMPERATURE = 93.2

	ANNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.088	.088	2.742	.017	15.512	.707	.000	.000	60.245	0.000	241.349	18.526	0.000	13.048
ORG. PHASE	.088	.088	14.835	.211	54.342	2.712	.000	.001	0.000	.000				

NITRATOR 4

	ANNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.088	.088	1.328	.011	17.280	.811	.000	.000	65.213	0.000	192.120	5.448	0.000	98.163
ORG. PHASE	.088	.088	3.254	.026	43.072	1.978	.000	.001	0.000	.000				

SEPARATOR 4 TEMPERATURE = 93.3

	ANNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.088	.088	.532	.003	18.485	.812	.000	.000	64.337	0.000	192.906	5.639	0.000	97.186
ORG. PHASE	.088	.088	3.260	.026	44.020	1.985	.000	.001	0.000	.000				

NITRATOR 5

	ANNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.088	.088	.288	.001	18.732	.465	.000	.000	34.150	0.000	93.203	.781	0.000	64.442
ORG. PHASE	.088	.088	.891	.004	45.083	1.990	.000	.001	0.000	.000				

SEPARATOR 5 TEMPERATURE = 96.1

	ANNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.088	.088	.453	.000	18.462	.465	.000	.000	33.959	0.000	93.376	.820	0.000	64.230
ORG. PHASE	.088	.088	.892	.004	45.039	1.992	.000	.001	0.000	.000				

NITRATOR 6

	ANNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.000	.000	.025	.000	10.781	.461	.000	.000	25.358	0.000	71.522	.151	0.000	53.957
ORG. PHASE	.000	.000	.072	.000	30.477	1.303	.000	.001	0.000	.000				

SEPARATOR 6 TEMPERATURE = 110.2

	ANNT	MNNT	ADNT	MDNT	ATNT	MTNT	TNB	TNBA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.000	.000	.072	.000	10.788	.460	.000	.000	25.330	0.000	71.547	.155	0.000	53.927
ORG. PHASE	.000	.000	.072	.000	30.488	1.303	.000	.001	0.000	.000				

GAS DATA

VESSEL	COX	NOX	TNM	CO2	Q
1	.0000	.0039	.0003	.0000	.0047134
2	.0000	.0008	.0008	.0000	.0017689
3	.0000	.0006	.0000	.0000	.0016771
4	.1594	.0577	.0010	.0000	.4890113
5	.0011	.0291	.0005	.0000	.4777425
6	3.7199	1.3364	.0175	.0000	.9999992
7	2.9849	1.0717	.0136	.0000	.9999986
8	.7654	.2538	.0032	.0000	.9999987
9	1.6781	.5291	.0062	.0000	.9999998
10	.2439	.0958	.0011	.0000	.9999998
11	.5080	.1832	.0020	.0000	.9999999
12	.0534	.0193	.0002	.0000	.9999999
13	.1792	.0616	.0025	.0000	1.0000000
14	.0041	.0022	.0000	.0000	1.0000000
TOTAL	10.1139	3.6385	.0460	.0002	

VESSEL TIME CONSTANTS AND VOLUMETRIC FLOWS

VESSEL	QA	QP	QT	TAU	FO
1	147.34	55.39	202.73	.2570	.2732
2	147.34	68.77	256.11	.2934	.2685
3	187.34	68.77	256.11	.0785	.2450
4	156.13	125.32	281.45	.1789	.4453
5	156.46	125.35	281.80	.0714	.2450
6	137.76	124.71	262.47	.2039	.4751
7	324.81	174.62	499.23	.1044	.3494
8	322.68	175.35	498.02	.0484	.2450
9	352.12	121.76	473.78	.1129	.2570
10	351.15	122.16	473.31	.8425	.2450
11	189.76	121.68	311.45	.1933	.3907
12	189.57	121.78	311.35	.8646	.2450
13	154.89	79.60	234.49	.2567	.3395
14	154.96	79.64	234.60	.8857	.2450

SOLUBILITY OF NITROGEN IN THE ACID PHASE

VESSEL	XEQA
1	.691023
2	.688837
3	.688837
4	.711820
5	.711726
6	.662278
7	.651424
8	.650635
9	.652823
10	.652651
11	.655915
12	.655707
13	.669436
14	.669357

••••••••••DISPERSED ORGANIC HOLDUPS••••••••••

	VESSEL													
	1	2	3	4	5	6	7	8	9	10	11	12	13	14
	[illegible]	441.72	235.83	5.71	1.20	.01	.00	.00	.00	.00	.00	.00	.00	.00
	[illegible]	21.16	7.45	.17	.04	.00	.00	.00	.00	.00	.00	.00	.00	.00
3	[illegible]	204.23	71.89	963.66	221.68	669.51	280.95	75.83	66.88	23.91	31.36	6.56	3.37	.81
4	17.41	14.28	5.89	34.58	7.97	15.28	4.01	1.08	.54	.19	.15	.03	.01	.00
5	155.83	126.25	44.44	778.13	177.11	1486.69	1279.82	346.44	1124.57	402.82	2014.08	421.69	1775.84	427.95
6	8.32	6.72	2.37	36.28	8.52	78.53	63.89	17.29	58.78	18.16	87.33	18.28	75.91	18.29
7	.87	.68	.28	.88	.88	.91	.91	.09	.91	.08	.02	.08	.02	.00
8	.87	.68	.27	.01	.88	.03	.02	.01	.03	.01	.06	.01	.06	.02
9	39.72	21.81	7.68	45.91	18.48	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	.11	.06	.03	.30	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
TOTAL	1076.12	1136.15	364.71	1858.79	427.19	2250.97	1629.71	448.64	1242.74	445.11	2133.00	446.59	1855.21	447.08

TOTAL HOLDUP OF DISPERSED CLASS 7 MATERIAL IN NITRATION SECTION = 13176.23

TOTAL HOLDUP OF DISPERSED DNT IN NITRATION SECTION = 2964.52

TOTAL HOLDUP OF DISPERSED TNT IN NITRATION SECTION = 11056.88

••••••••••DISSOLVED ORGANIC HOLDUPS••••••••••

	VESSEL													
COMPONENT	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	12.31	6.24	2.51	.85	.19	.00	.00	.00	.00	.00	.00	.00	.00	.00
2	.36	.21	.07	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
3	5.31	1.00	.01	46.14	25.39	81.18	69.46	16.94	27.28	4.84	7.23	.76	1.17	.04
4	.37	.14	.27	1.76	.72	1.87	.99	.14	.22	.02	.03	.00	.00	.00
5	3.24	1.23	.58	39.14	24.31	184.27	317.90	155.35	468.55	176.68	465.78	193.28	618.42	224.45
6	.17	.07	.03	1.99	1.64	9.67	15.87	7.32	28.76	7.76	28.19	8.28	26.43	9.66
7	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.01	.00
8	.00	.00	.00	.00	.00	.00	.01	.00	.01	.00	.01	.01	.02	.01
9	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TOTAL	21.44	9.07	3.00	92.09	51.86	276.99	404.42	179.75	508.82	189.30	493.26	202.33	646.05	236.16

TOTAL HOLDUP OF DISSOLVED CLASS 7 MATERIAL IN NITRATION SECTION = 3201.04

TOTAL HOLDUP DISSOLVED DNTIN NITRATION SECTION = 294.87

TOTAL HOLDUP OF DISSOLVED TNT IN NITRATION SECTION = 2906.72

TOTAL HOLDUP OF ALL DNT IN NITRATION SECTION = 3262.59

TOTAL HOLDUP OF ALL TNT IN NITRATION SECTION = 14053.60

TOTAL HOLDUP OF ALL CLASS 7 MATERIAL IN NITRATION SECTION = 16457.27

*****STREAM COMPOSITIONS

STAGE 1 EOA = .03871 FAO = 0.20000

INTERNAL ACID RECYCLE STREAM

	AMMT	WMMT	ADMT	WDMT	ATMT	WTMT	TMP	TMPA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.133	.041	.040	.001	.046	.000	.000	.000	.042	0.000	16.876	1.247	36.782	0.000
ORG. PHASE	.027	.001	.004	.000	.031	.000	.000	.000	.007	.000				
ACID PHASE	4.5	.1	1.5	.1	.9	.0	.0	.9	53.0	0.0	1653.0	158.3	662.1	0.0
ORG. PHASE	3.6	.1	1.2	.1	.7	.0	.0	.1	.1	.0				

EXTERNAL ACID RECYCLE STREAM

	AMMT	WMMT	ADMT	WDMT	ATMT	WTMT	TMP	TMPA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.193	.065	.047	.004	.253	.001	.000	.000	4.930	0.000	98.988	7.312	215.746	0.000
ORG. PHASE	.156	.005	.037	.001	.219	.001	.000	.000	.012	.000				
ACID PHASE	24.5	.7	8.5	.0	33.2	.3	.0	.0	311.1	0.0	9700.8	920.6	3883.4	0.0
ORG. PHASE	21.6	.7	5.8	.5	4.2	.2	.0	.0	.7	.0				

ORGANIC STREAM

	AMMT	WMMT	ADMT	WDMT	ATMT	WTMT	TMP	TMPA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	4.[illegible]	[illegible]	[illegible]	4.[illegible]	8.[illegible]	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ORG. PHASE	22.[illegible]	.763	5.472	.381	2.712	.144	.000	.000	1.688	.003				
ACID PHASE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ORG. PHASE	3129.5	183.2	996.3	69.3	615.7	32.8	.0	.0	186.4	.3				

STAGE 2 EOA = .12797 FAO = .15615

INTERNAL ACID RECYCLE STREAM

	AMMT	WMMT	ADMT	WDMT	ATMT	WTMT	TMP	TMPA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.288	.088	.234	.087	.188	.011	.000	.000	2.051	0.000	19.784	1.478	12.478	0.000
ORG. PHASE	.206	.062	.171	.028	.365	.019	.000	.000	.078	.000				
ACID PHASE	.0	.0	62.4	1.2	63.8	2.4	.0	.0	179.6	0.0	1931.0	186.7	224.5	0.0
ORG. PHASE	.6	.0	156.2	3.7	83.1	5.2	.0	.0	4.9	.0				

EXTERNAL ACID RECYCLE STREAM

	AMMT	WMMT	ADMT	WDMT	ATMT	WTMT	TMP	TMPA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.288	.088	1.164	.433	1.598	.053	.000	.000	14.174	0.000	97.957	7.318	61.995	0.000
ORG. PHASE	.229	.091	2.843	.112	1.829	.093	.000	.000	.388	.000				
ACID PHASE	.0	.0	211.9	4.0	282.9	12.0	.0	.0	893.0	0.0	9599.8	929.4	1115.9	0.0
ORG. PHASE	2.8	.1	515.8	18.5	413.1	21.8	.0	.0	24.5	.0				

ORGANIC STREAM

	AMMT	WMMT	ADMT	WDMT	ATMT	WTMT	TMP	TMPA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.288	.088	.849	.382	.646	.003	.000	.000	.738	0.000	5.848	.377	3.195	0.000
ORG. PHASE	.198	.184	27.586	.987	17.675	.900	.000	.000	3.772	.000				
ACID PHASE	.0	.0	15.9	.3	11.5	.6	.0	.0	46.0	0.0	494.7	47.8	57.5	0.0
ORG. PHASE	27.1	.0	5823.2	179.7	4812.3	204.2	.0	.1	237.6	.0				

STAGE 3 EOA = .09532 FAO = .13918

INTERNAL ACID RECYCLE STREAM

	AMMT	WMMT	ADMT	WDMT	ATMT	WTMT	TMP	TMPA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.288	.093	1.193	.418	8.478	.400	.000	.000	14.824	0.000	139.534	10.709	0.000	7.534
ORG. PHASE	.868	.288	6.308	.343	14.199	.584	.000	.000	0.000	.000				
ACID PHASE	.0	.0	214.8	1.7	1943.9	92.8	.0	.0	2193.9	0.0	13674.4	1360.0	0.0	603.0
ORG. PHASE	.0	.0	888.6	11.4	3656.6	182.5	.0	.1	0.0	.0				

EXTERNAL ACID RECYCLE STREAM

	AMMT	WMMT	ADMT	WDMT	ATMT	WTMT	TMP	TMPA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.288	.093	.828	.607	4.[illegible]	.287	.000	.000	24.429	0.000	97.883	7.512	0.000	5.288
ORG. PHASE	.868	.288	3.[illegible]	.544	11.[illegible]	.544	.000	.000	0.000	.000				
ACID PHASE	.0	.0	150.7	1.7	1381.9	65.1	.0	.0	1539.0	0.0	9582.5	954.1	0.0	423.0
ORG. PHASE	.3	.0	541.4	8.8	2566.1	128.0	.0	.0	0.0	.0				

ORGANIC STREAM

	AMMT	WMMT	ADMT	WDMT	ATMT	WTMT	TMP	TMPA	HNO3	TOL	H2SO4	HNOSO4	H2O	SO3
ACID PHASE	.288	.088	.836	.000	.247	.012	.000	.000	.991	0.000	3.972	.305	0.000	.215
ORG. PHASE	.288	.088	7.353	.195	26.934	1.344	.000	.000	0.000	.000				
ACID PHASE	.0	.0	6.1	.0	54.1	2.6	.0	.0	62.4	0.0	389.2	30.7	0.0	17.2
ORG. PHASE	.4	.0	1338.2	19.1	6113.9	305.1	.0	.1	0.0	.0				

STAGE 4 EOA = .09867 FAO = .92421

INTERNAL ACID RECYCLE STREAM

ACID PHASE	.000	.000	.706	.602	11.579	.508	.000	.000	.000	40.302	0.000	120.939	3.532	0.000	40.879
ORG. PHASE	.000	.001	.495	.004	6.681	.301	.000	.000	.000	0.000	.000				
ACID PHASE	.0	.0	72.1	.1	2620.5	115.4	.0	.1	2539.8	0.0	11842.3	660.6	0.0	4878.3	
ORG. PHASE	.0	.0	98.0	.7	1516.6	68.4	.0	.0	0.0	.0					

EXTERNAL ACID RECYCLE STREAM

ACID PHASE	.003	.000	.235	.001	6.441	.301	.000	.000	23.678	0.000	71.596	2.093	0.000	36.870	
ORG. PHASE	.002	.302	.233	.002	1.058	.178	.000	.000	0.000	.000					
ACID PHASE	.0	.0	42.7	.2	1557.3	68.4	.0	.0	1504.3	0.0	7016.4	265.0	0.0	2885.6	
ORG. PHASE	.0	.0	57.3	.4	893.6	40.5	.0	.0	0.0	.0					

ORGANIC STREAM

ACID PHASE	.000	.000	.012	.000	.045	.002	.000	.000	.157	0.000	.471	.014	0.000	.237	
ORG. PHASE	.000	.000	2.672	.028	33.381	1.595	.000	.001	0.000	.000					
ACID PHASE	.0	.0	.7	.0	1.7	.4	.0	.0	9.9	0.0	46.1	1.7	0.0	19.0	
ORG. PHASE	.0	.0	369.9	3.7	7527.6	361.6	.1	.2	0.0	.0					

STAGE 5 EOA = .26137 EAO = .01958

INTERNAL ACID RECYCLE STREAM

ACID PHASE	.000	.000	.017	.000	3.546	.152	.000	.000	11.187	0.000	38.541	.260	0.000	21.004	
ORG. PHASE	.000	.000	.052	.000	2.733	.117	.000	.000	0.000	.000					
ACID PHASE	.0	.0	3.2	.0	895.0	34.5	.0	.0	699.7	0.0	2993.0	34.0	0.0	1680.6	
ORG. PHASE	.0	.0	9.5	.0	617.6	26.6	.0	.0	0.0	.0					

EXTERNAL ACID RECYCLE STREAM

ACID PHASE	.000	.000	.016	.000	7.254	.311	.000	.000	22.719	0.000	62.478	.540	0.000	42.971	
ORG. PHASE	.000	.000	.107	.001	5.529	.240	.000	.000	0.000	.000					
ACID PHASE	.0	.0	6.5	.0	1644.6	70.6	.0	.1	1431.3	0.0	6122.1	69.6	0.0	3437.7	
ORG. PHASE	.0	.0	19.5	.1	1254.1	54.4	.0	.0	0.0	.0					

ORGANIC STREAM

ACID PHASE	.000	.000	.024	.000	.142	.002	.000	.000	.133	0.000	.365	.003	0.000	.251	
ORG. PHASE	.000	.000	.732	.004	37.737	1.635	.000	.001	0.000	.000					
ACID PHASE	.0	.0	.0	.0	9.6	.4	.0	.0	8.4	0.0	35.8	.4	0.0	20.1	
ORG. PHASE	.0	.0	133.2	.6	8552.4	371.1	.1	.3	0.0	.0					

STAGE 6 EOA = .26715 EAO = .02477

INTERNAL ACID RECYCLE STREAM

ACID PHASE	.000	.000	.003	.000	1.438	.072	.000	.000	3.962	0.000	11.192	.024	0.000	8.436	
ORG. PHASE	.000	.000	.003	.000	1.082	.051	.000	.000	0.000	.000					
ACID PHASE	.1	.0	.1	.0	381.1	14.3	.0	.0	249.6	0.0	1096.8	3.1	0.0	674.9	
ORG. PHASE	.0	.0	.5	.0	272.9	11.7	.0	.0	0.0	.0					

EXTERNAL ACID RECYCLE STREAM

ACID PHASE	.000	.000	.002	.000	9.193	.388	.000	.000	21.350	0.000	60.305	.131	0.000	45.453	
ORG. PHASE	.000	.000	.015	.000	6.478	.277	.000	.000	0.000	.000					
ACID PHASE	.0	.0	.4	.0	2064.0	88.1	.0	.1	1345.1	0.0	5909.9	16.6	0.0	3636.3	
ORG. PHASE	.0	.0	2.8	.0	1671.5	62.9	.0	.1	0.0	.0					

ORGANIC STREAM

ACID PHASE	.000	.000	.000	.000	.008	.000	.000	.000	.018	0.000	.050	.000	0.000	.038	
ORG. PHASE	.000	.000	.004	.000	22.888	.975	.000	.001	0.000	.000					
ACID PHASE	.0	.0	.0	.0	1.7	.1	.0	.0	1.1	0.0	4.9	.0	0.0	3.0	
ORG. PHASE	.0	.0	9.8	.0	5177.3	221.3	.1	.2	0.0	.0					

******ELEMENTAL MATERIAL BALANCES

OVERALL MATERIAL BALANCE

ELEMENT	MOLES IN	MOLES OUT	DIFFERENCE
CARBON	1[illegible].5952	1[illegible].5431	-.0370
HYDROGEN	764.6177	764.6177	-.0005
OXYGEN	826.8590	826.9636	-.1127
NITROGEN	58.1036	58.2573	-.0617
SULPHUR	196.3732	196.3879	-.0147

STAGE 1

ELEMENT	MOLES IN	MOLES OUT	DIFFERENCE
CARBON	220.6350	220.6250	.0100
HYDROGEN	441.2660	441.2994	-.0334
OXYGEN	757.1520	757.2586	-.1067
NITROGEN	58.4760	58.6960	-.0200
SULPHUR	196.2974	196.2995	-.0119

STAGE 2

ELEMENT	MOLES IN	MOLES OUT	DIFFERENCE
CARBON	391.5760	391.6006	-.0237
HYDROGEN	668.7660	668.7818	-.0161
OXYGEN	833.6655	833.7327	-.0672
NITROGEN	157.[illegible]369	157.[illegible]618	-.0278
SULPHUR	119.[illegible]939	119.[illegible]915	-.0095

STAGE 3

ELEMENT	MOLES IN	MOLES OUT	DIFFERENCE
CARBON	415.[illegible]394	415.8692	-.0102
HYDROGEN	590.4926	590.5536	.0608
OXYGEN	879.8729	879.7951	.0959
NITROGEN	199.2661	199.2739	-.0078
SULPHUR	115.1933	115.1761	.0091

STAGE 4

ELEMENT	MOLES IN	MOLES OUT	DIFFERENCE
CARBON	346.5414	346.5419	-.0005
HYDROGEN	419.5952	419.5841	.0111
OXYGEN	772.4268	772.4076	.0173
NITROGEN	171.5419	171.5425	-.0008
SULPHUR	118.4813	118.4806	.0007

STAGE 5

ELEMENT	MOLES IN	MOLES OUT	DIFFERENCE
CARBON	375.7464	375.7458	.0013
HYDROGEN	417.0558	417.0521	.0038
OXYGEN	771.2692	771.2375	.0868
NITROGEN	183.5966	183.5966	-.0007
SULPHUR	196.4187	196.4599	.0008

STAGE 6

ELEMENT	MOLES IN	MOLES OUT	DIFFERENCE
CARBON	2[illegible].[illegible]582	239.0712	-.0130
HYDROGEN	362.7507	362.7746	-.0169
OXYGEN	691.4191	691.4399	-.0298
NITROGEN	141.7863	141.7589	-.0064
SULPHUR	195.9725	195.9774	-.0058

VESSEL 1

ELEMENT	MOLES IN	MOLES OUT	DIFFERENCE
CARBON	183.2719	183.2619	.0099
HYDROGEN	712.3869	712.4449	-.0581
OXYGEN	701.0184	701.1198	-.1004

NITROGEN	57.2761	57.2753	-.0152
OXYGEN	145.2472	145.[illegible]	-.0097

VESSEL 3

ELEMENT	MOLES IN	MOLES OUT	DIFFERENCE
CARBON	238.2186	238.2186	.0000
HYDROGEN	971.2478	971.2478	.0000
OXYGEN	479.5460	479.5413	-.0046
NITROGEN	68.7999	68.7999	-.0068
SULPHUR	126.6782	126.6726	-.0072

VESSEL 1

ELEMENT	MOLES IN	MOLES OUT	DIFFERENCE
CARBON	238.2154	238.2154	.0000
HYDROGEN	971.2479	971.2479	.0000
OXYGEN	979.5613	979.5613	.0000
NITROGEN	68.7999	68.7999	0.0000
SULPHUR	126.6726	126.6726	0.0000

VESSEL 4

ELEMENT	MOLES IN	MOLES OUT	DIFFERENCE
CARBON	391.6583	391.6837	-.0237
HYDROGEN	765.[illegible]	765.[illegible]	-.0145
OXYGEN	967.7936	967.8615	-.0079
NITROGEN	164.0791	164.0554	-.0278
SULPHUR	131.8572	131.8657	-.0095

VESSEL 5

ELEMENT	MOLES IN	MOLES OUT	DIFFERENCE
CARBON	391.3226	391.3226	.0000
HYDROGEN	765.[illegible]	765.6481	.0084
OXYGEN	967.6423	967.6615	.0098
NITROGEN	164.7964	164.7964	.0000
SULPHUR	131.8657	131.8657	.0000

VESSEL 6

ELEMENT	MOLES IN	MOLES OUT	DIFFERENCE
CARBON	615.[illegible]93	615.[illegible]05	-.0616
HYDROGEN	578.[illegible]151	578.[illegible]046	.0205
OXYGEN	861.[illegible]339	861.[illegible]469	.0360
NITROGEN	164.[illegible]000	164.[illegible]984	-.0097
SULPHUR	115.1233	115.[illegible]82[illegible]	.0999

VESSEL 7

ELEMENT	MOLES IN	MOLES OUT	DIFFERENCE
CARBON	632.8421	632.8737	-.0046
[illegible]	1928.[illegible]85[illegible]	1928.[illegible]6[illegible]5	.0265
[illegible]	1760.5327	1760.[illegible]43[illegible]	.0036
[illegible]	332.[illegible]951	332.[illegible]722	-.0071
[illegible]	272.9535	272.[illegible]651	.0042

VESSEL 8

ELEMENT	MOLES IN	MOLES OUT	DIFFERENCE
CARBON	429.4721	429.[illegible]721	.0000
[illegible]	1874.[illegible]568	1874.[illegible]642	.0039
[illegible]	1[illegible]3.[illegible]481	1[illegible].[illegible]795	.0064
[illegible]	331.[illegible]748	331.[illegible]748	0.0000
[illegible]	272.[illegible]663	272.[illegible]663	-.0000

VESSEL 9

ELEMENT	MOLES IN	MOLES OUT	DIFFERENCE
CARBON	484.[illegible]283	484.[illegible]313	-.0595
HYDROGEN	[illegible].[illegible]367	[illegible].[illegible]2[illegible]	.0004
OXYGEN	1856.9832	1856.[illegible]4[illegible]	.0148
NITROGEN	272.[illegible]896	272.[illegible]112	-.0030
SULPHUR	235.7722	[illegible].[illegible]2[illegible]	.0097

VESSEL10

ELEMENT	MOLES IN	MOLES OUT	DIFFERENCE
CARBON	684.8738	684.8738	.0000
HYDROGEN	845.8281	845.8277	.0014
OXYGEN	1692.3980	1692.3955	.0025
NITROGEN	271.8276	271.8276	0.0000
SULPHUR	295.7315	295.7315	.0000

VESSEL11

ELEMENT	MOLES IN	MOLES OUT	DIFFERENCE
CARBON	621.0060	621.0081	-.0013
HYDROGEN	523.6263	523.6230	.0033
OXYGEN	1032.6366	1032.6306	.0043
NITROGEN	216.6271	216.6279	-.0007
SULPHUR	158.6271	158.6263	.0008

VESSEL12

ELEMENT	MOLES IN	MOLES OUT	DIFFERENCE
CARBON	621.1772	621.1772	.0000
HYDROGEN	523.6230	523.6227	.0003
OXYGEN	1031.5119	1031.5109	.0005
NITROGEN	216.6168	216.6168	.0000
SULPHUR	158.6263	158.6263	.0000

VESSEL13

ELEMENT	MOLES IN	MOLES OUT	DIFFERENCE
CARBON	321.8738	321.8840	-.0136
HYDROGEN	396.7163	396.7311	-.0168
OXYGEN	783.5921	783.6128	-.0298
NITROGEN	156.8176	156.8260	-.0066
SULPHUR	125.6266	125.6295	-.0042

VESSEL14

ELEMENT	MOLES IN	MOLES OUT	DIFFERENCE
CARBON	321.8161	321.8161	.0000
HYDROGEN	396.7311	396.7311	.0000
OXYGEN	783.2959	783.2959	.0001
NITROGEN	156.7685	156.7685	.0000
SULPHUR	125.6295	125.6295	.0000

YIELD = 80.233 MOLE PCT FOR CONVERSION TO TNT
LBS/HR FEED TNT =5619.46
WT PCT TNT IN CRUDE TNT = .1823
RAW MATERIALS COST, $/LB OF A-TNT = .850660

SPENT ACID FLOW, LBS/HOUR
ACID BY, 13445.0063
DOC, BY, 36.5586
TOTAL 14081.6649
WT PCT TOTAL NO3 = .5997
WT PCT DISSOLVED AB = .2826
WT PCT TNT IN DISSOLVED NO = 77.1986

STAGE DATA

STAGE	A-NITRATION	B-NITRATION	ACT NITRIC	ACT SULPHURIC	TOT NITRIC	TOT SULPHURIC	TOTAL ACTIVITY	NO DENSITY
1	26.737	1.772	2.098	65.448	5.205	70.275	69.691	73.869
2	22.995	.797	7.123	76.571	10.795	82.287	84.982	87.092
3	14.162	.703	12.784	80.830	16.096	86.717	93.368	90.076
4	3.787	.276	12.980	90.397	14.818	92.155	101.385	90.603
5	1.375	.095	12.948	93.423	13.253	93.909	103.736	90.771
6	.502	.083	12.731	95.817	12.487	95.135	104.672	90.799

NITRATOR HEAT ENTITIES
NITRATOR BTU
1 1681161.
2 798836.
3 2004861.
4 1611211.
5 1266367.
6 876633.
7 413611.
8 -179278.

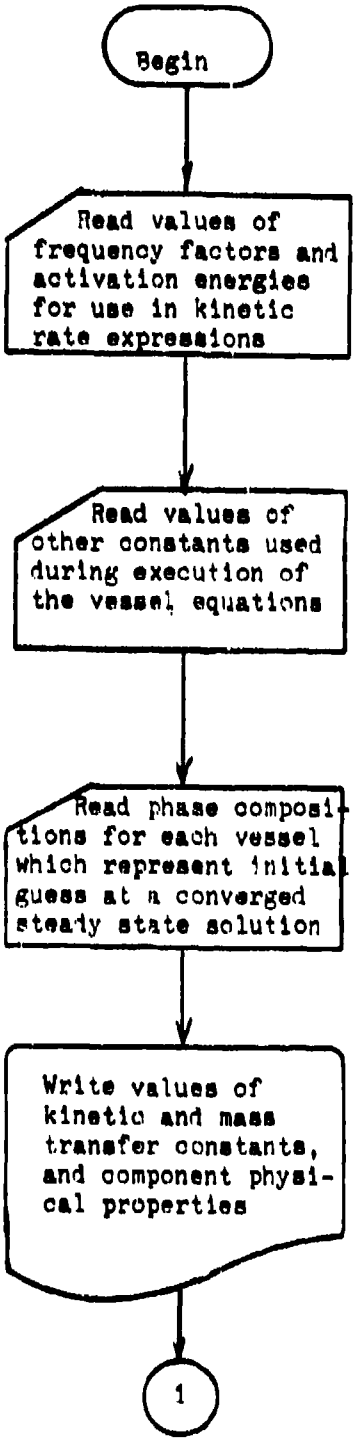
NUMBER OF VESSEL EQUATION ITERATIONS FOR THIS DATA SET 6230

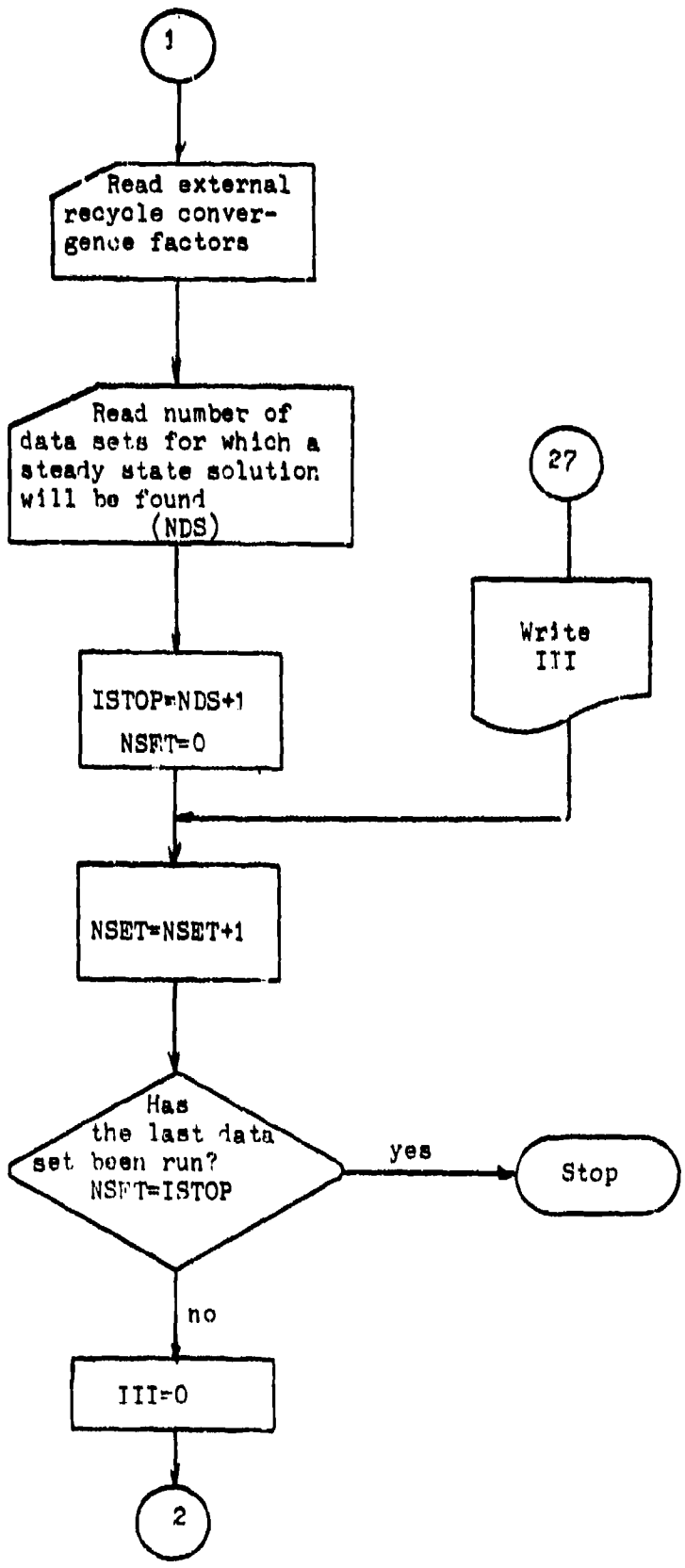
APPENDIX G

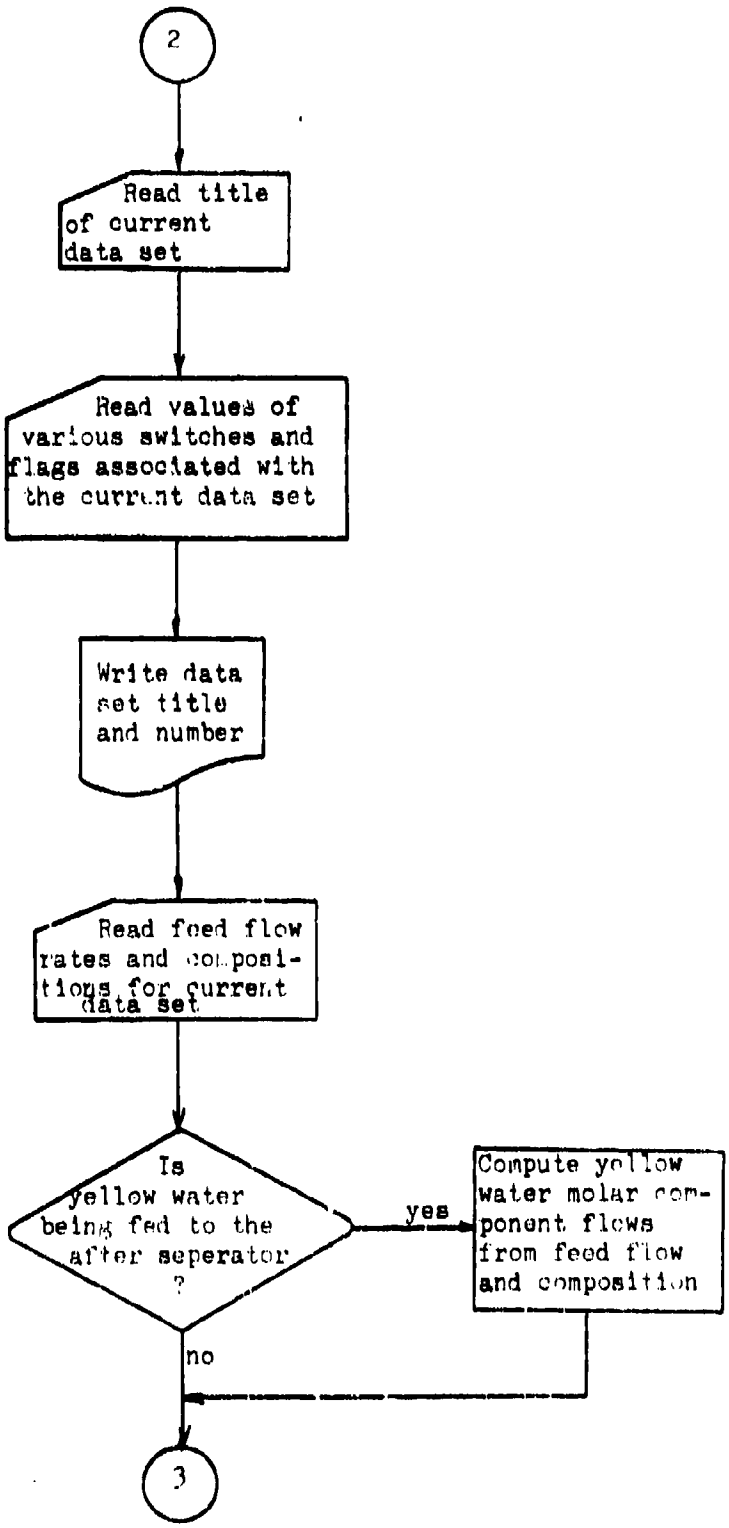
Steady State Simulation--Program Flowchart

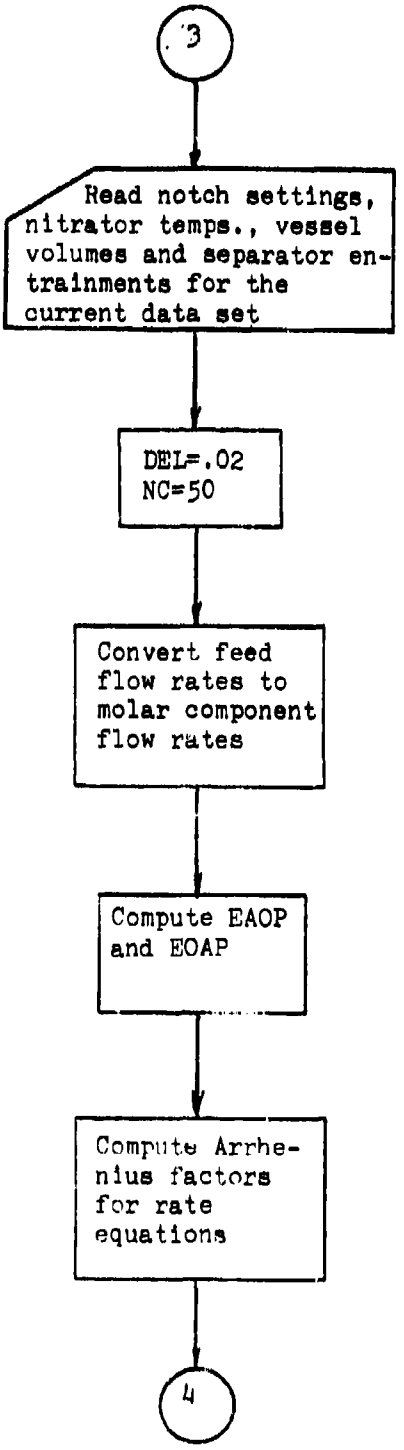
Preceding page blank

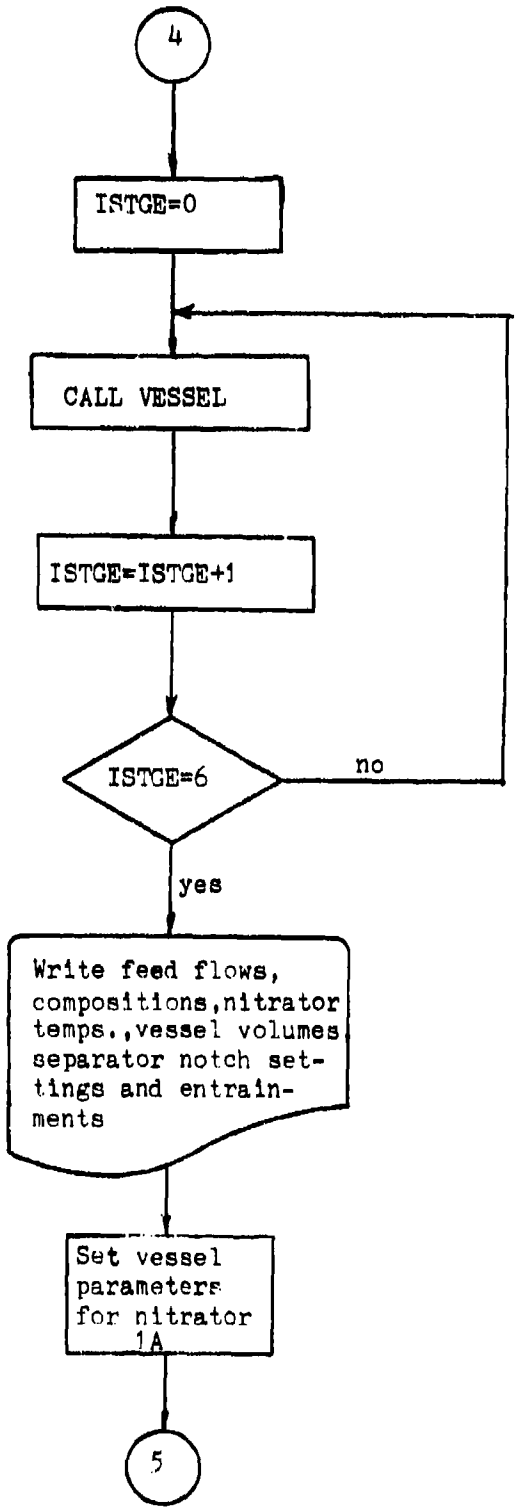
Main Program

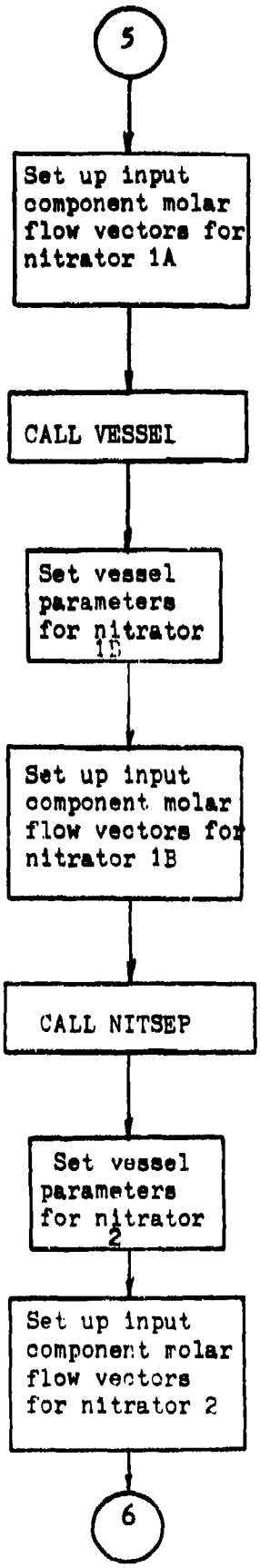


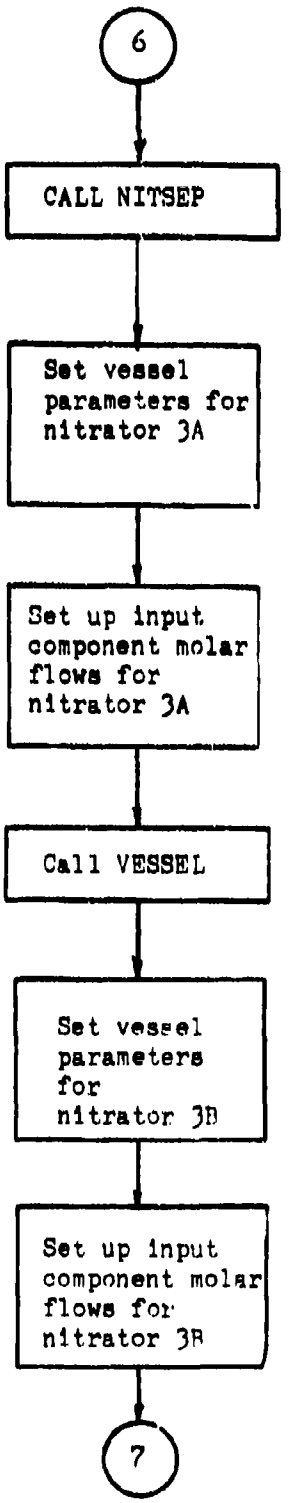

1
Read external recycle convergence factors
Read number of data sets for which a steady state solution will be found (NDS)
27
Write III
ISTOP=NDS+1
NSET=0
NSET=NSET+1
Has the last data set been run? NSET=ISTOP
yes
Stop
no
III=0
2

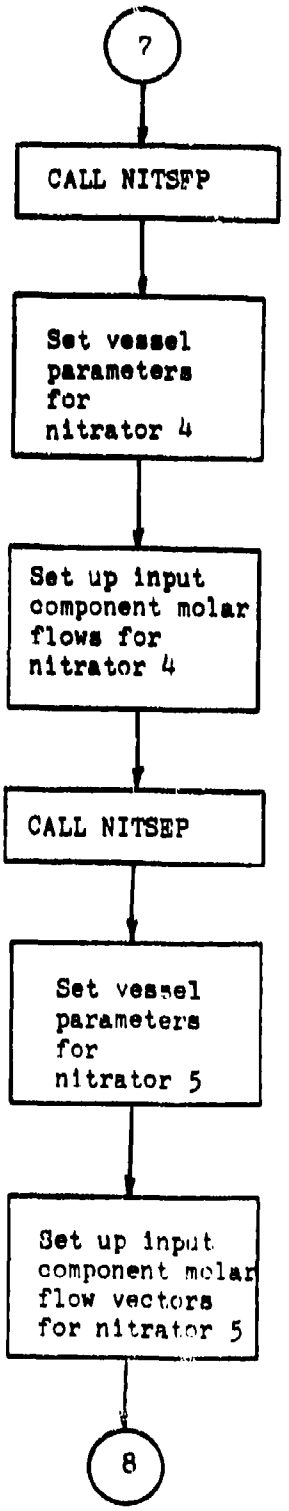

2
Read title of current data set
Read values of various switches and flags associated with the current data set
Write data set title and number
Read feed flow rates and compositions for current data set
Is yellow water being fed to the after seperator ?
yes
Compute yellow water molar component flows from feed flow and composition
no
3

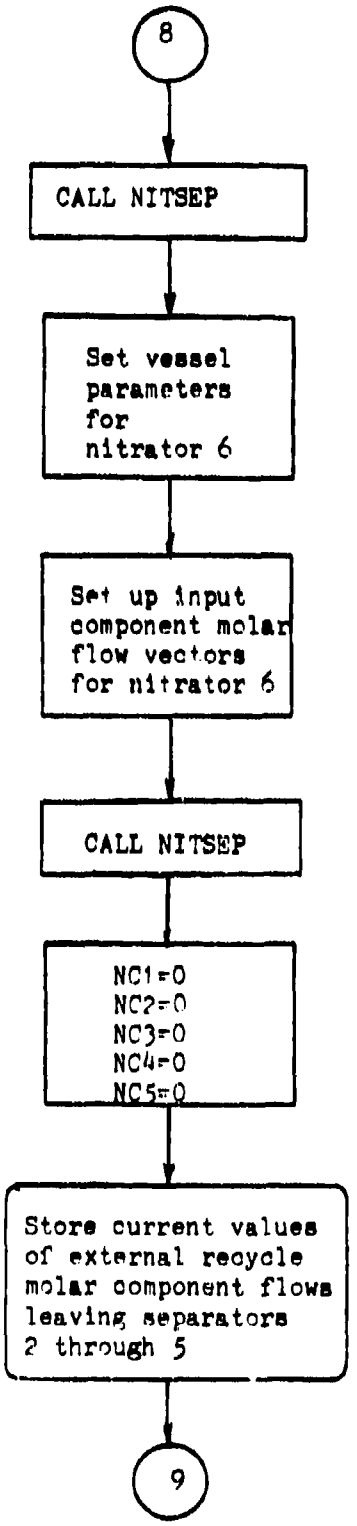

3
Read notch settings, nitrator temps., vessel volumes and separator entrainments for the current data set
DEL=.02
NC=50
Convert feed flow rates to molar component flow rates
Compute EAOP and EOAP
Compute Arrhenius factors for rate equations
4

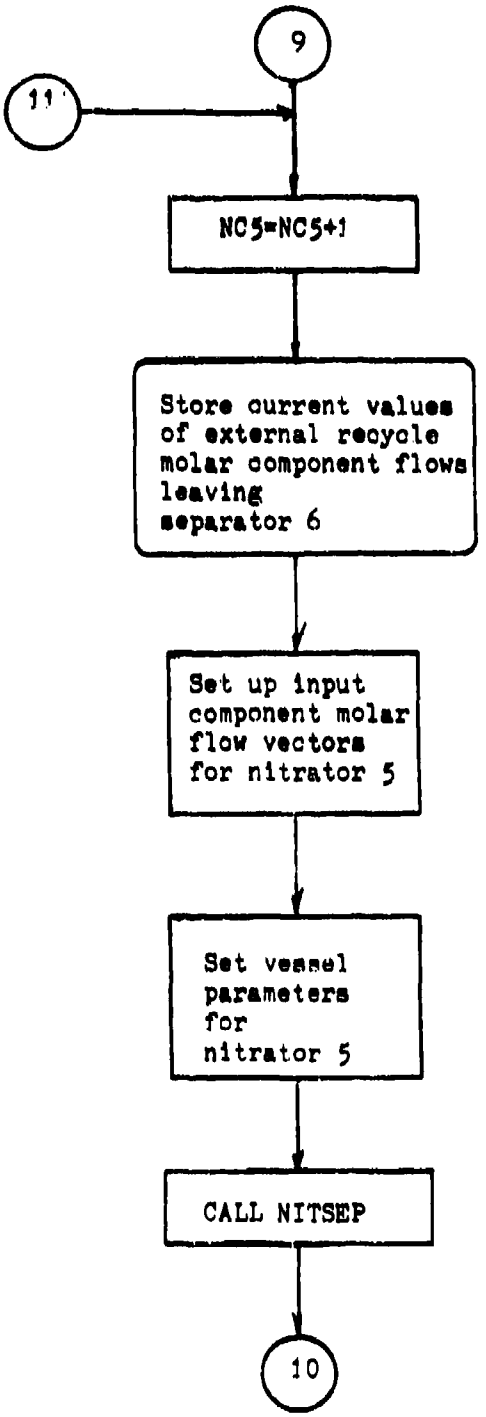

4
ISTGE=0
CALL VESSEL
ISTGE=ISTGE+1
ISTGE=6
no
yes
Write feed flows, compositions, nitrator temps., vessel volumes separator notch settings and entrainments
Set vessel parameters for nitrator 1A
5

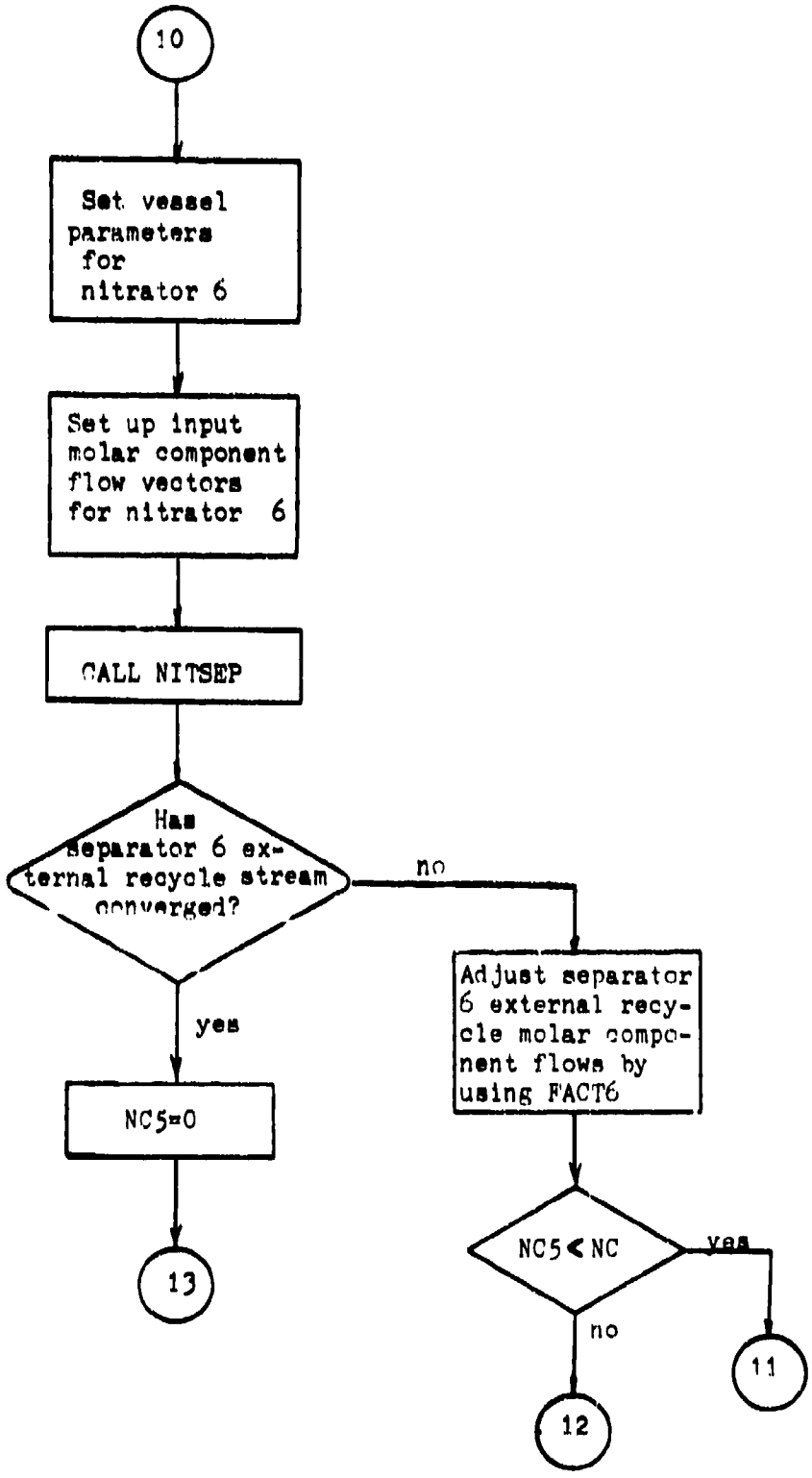

5
Set up input component molar flow vectors for nitrator 1A
CALL VESSEL
Set vessel parameters for nitrator 1
Set up input component molar flow vectors for nitrator 1B
CALL NITSEP
Set vessel parameters for nitrator 2
Set up input component molar flow vectors for nitrator 2
6

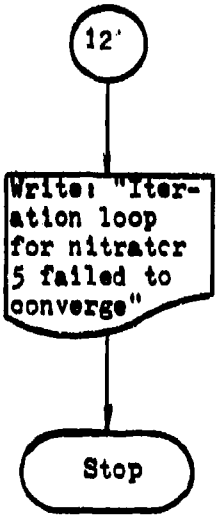

6
CALL NITSEP
Set vessel parameters for nitrator 3A
Set up input component molar flows for nitrator 3A
Call VESSEL
Set vessel parameters for nitrator 3B
Set up input component molar flows for nitrator 3B
7

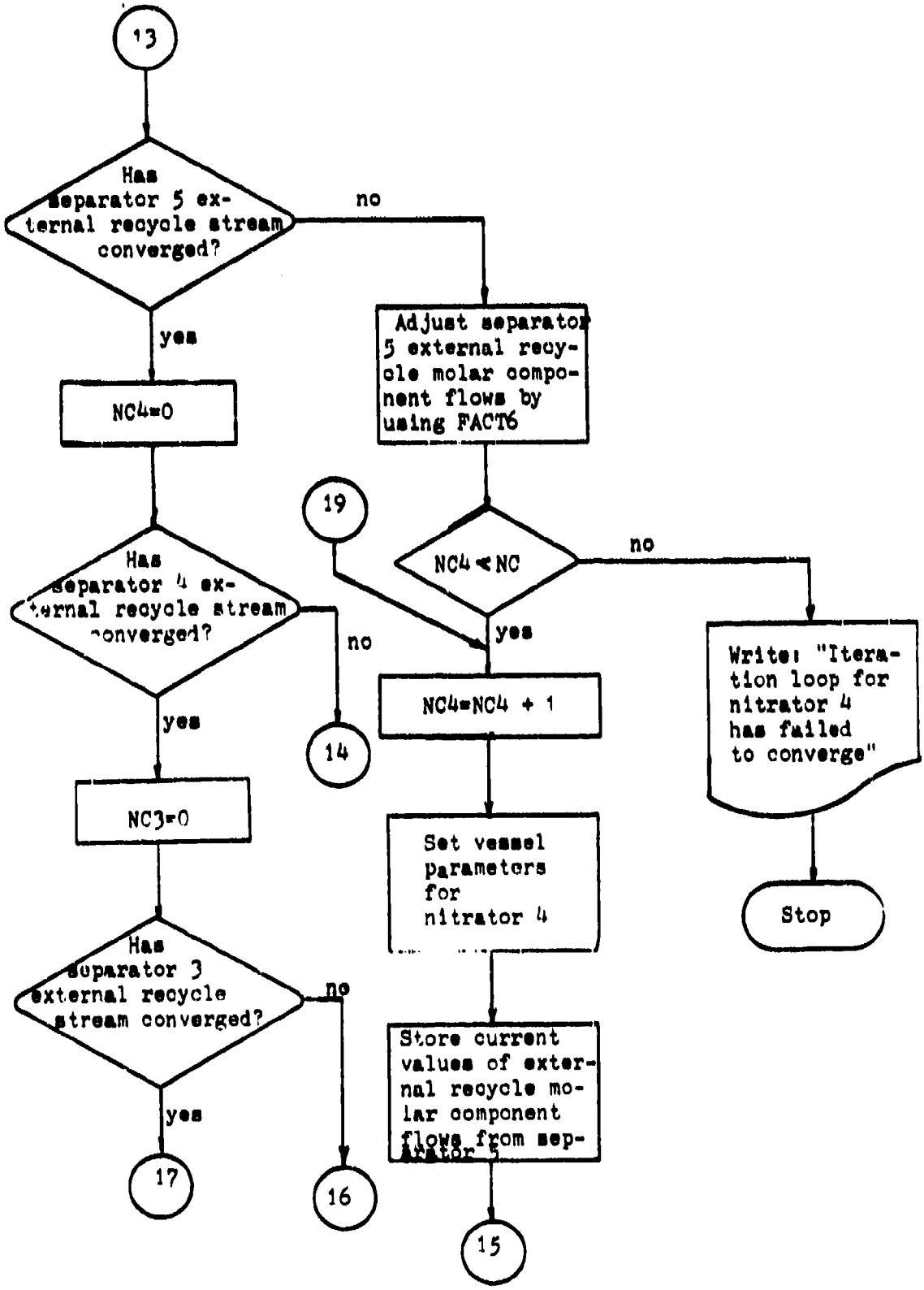

7
CALL NITSFP
Set vessel parameters for nitrator 4
Set up input component molar flows for nitrator 4
CALL NITSEP
Set vessel parameters for nitrator 5
Set up input component molar flow vectors for nitrator 5
8

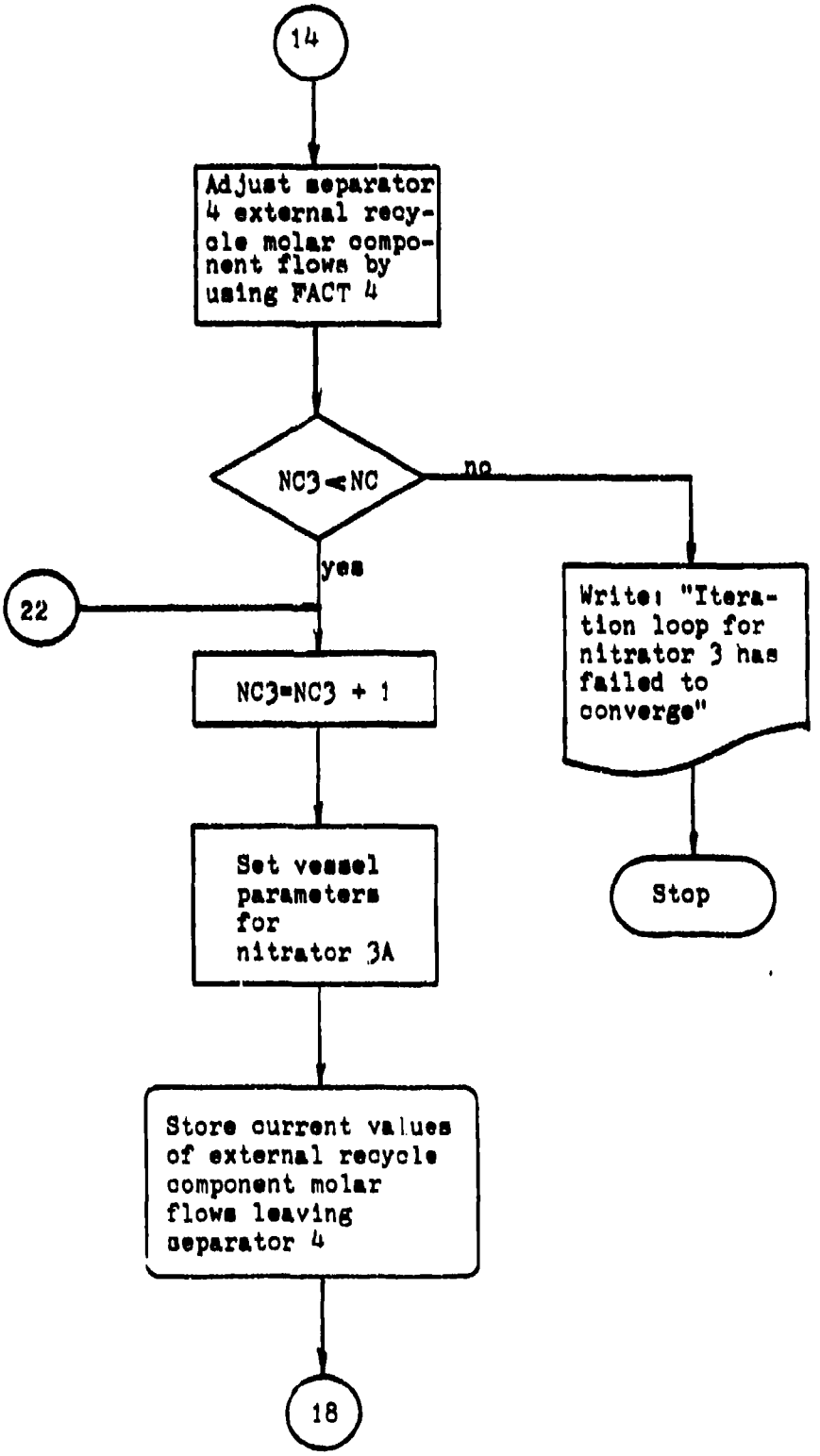

8
CALL NITSEP
Set vessel parameters for nitrator 6
Set up input component molar flow vectors for nitrator 6
CALL NITSEP
NC1=0
NC2=0
NC3=0
NC4=0
NC5=0
Store current values of external recycle molar component flows leaving separators 2 through 5
9

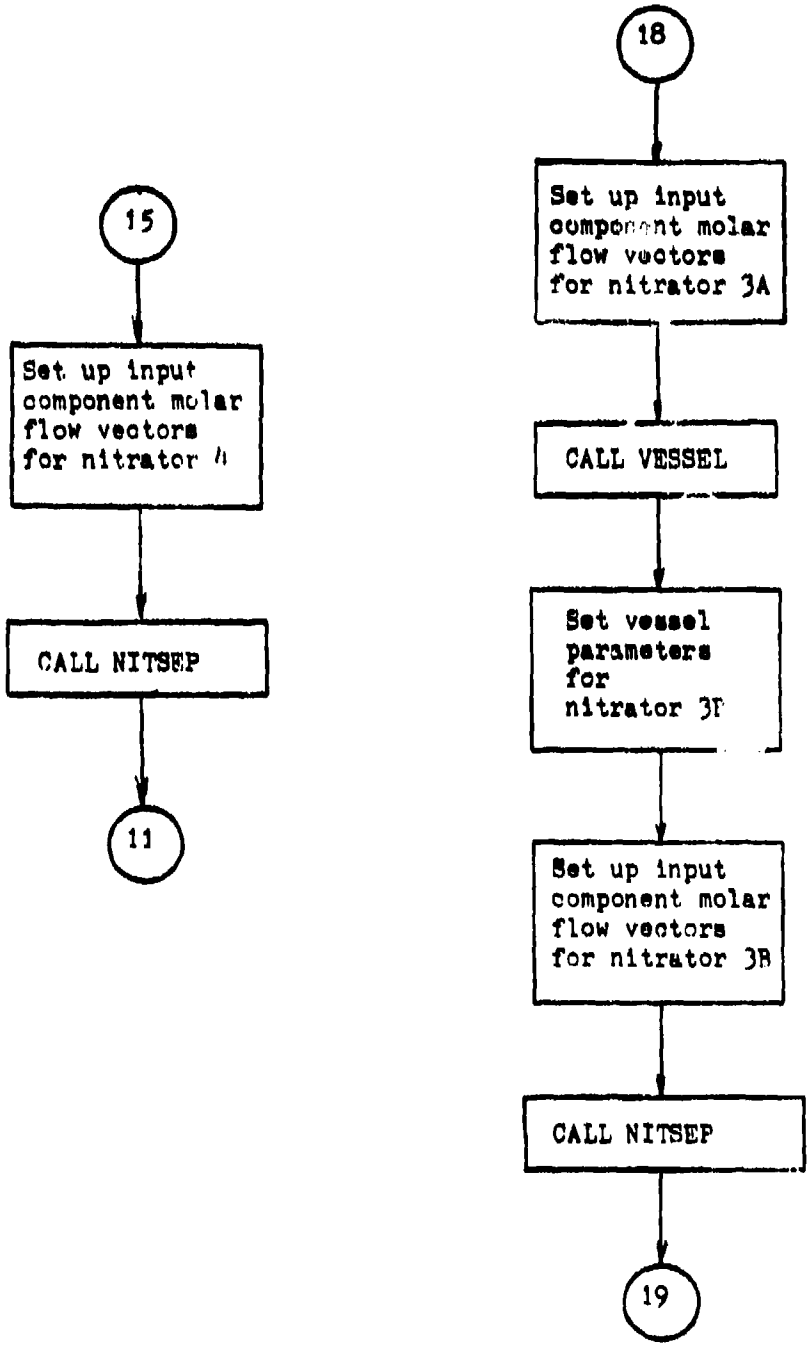

9
11
NC5=NC5+1
Store current values of external recycle molar component flows leaving separator 6
Set up input component molar flow vectors for nitrator 5
Set vessel parameters for nitrator 5
CALL NITSEP
10

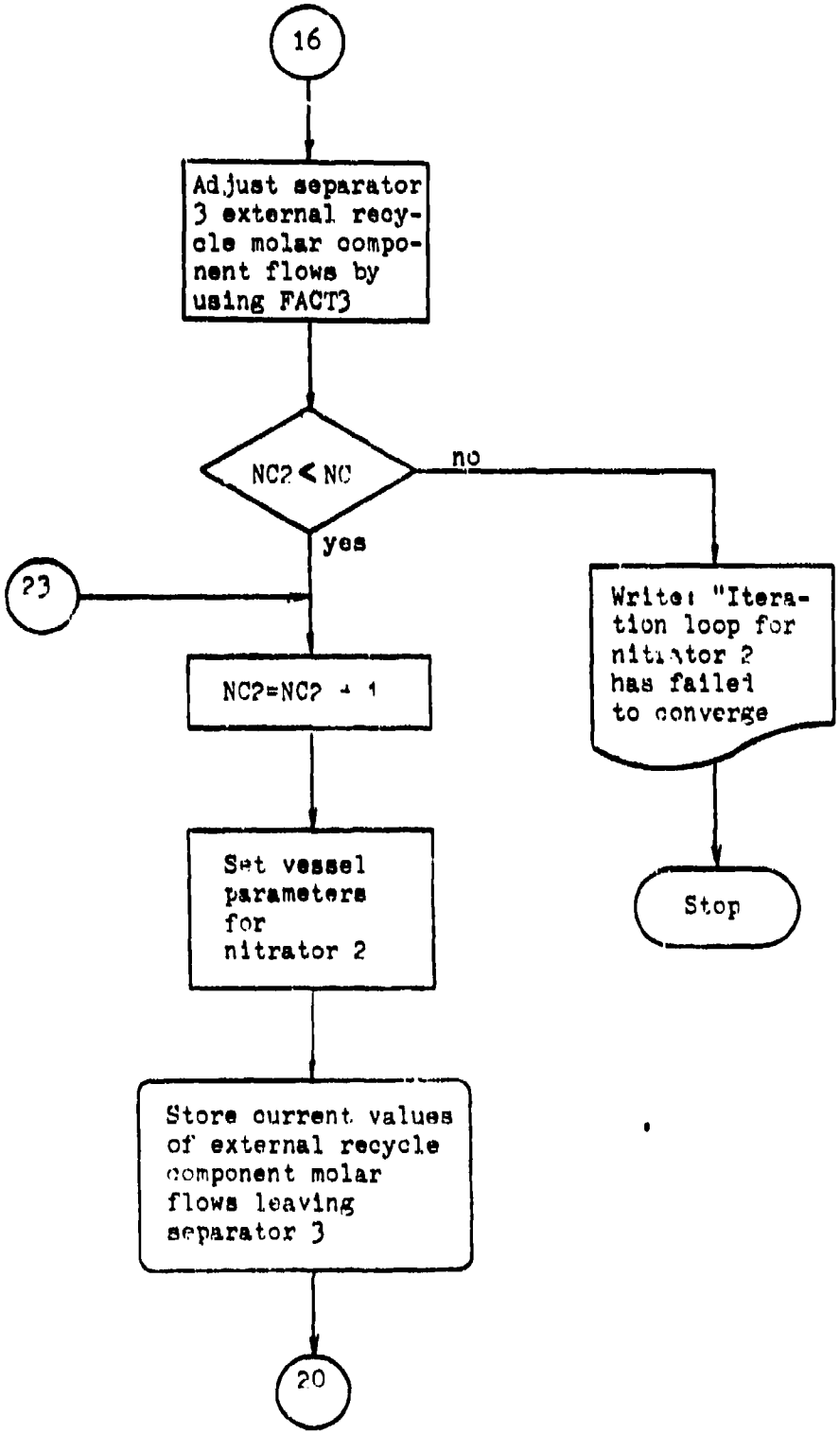

10
Set vessel parameters for nitrator 6
Set up input molar component flow vectors for nitrator 6
CALL NITSEP
Has separator 6 external recycle stream converged?
no
yes
Adjust separator 6 external recycle molar component flows by using FACT6
NC5=0
13
NC5 < NC
yes
no
11
12

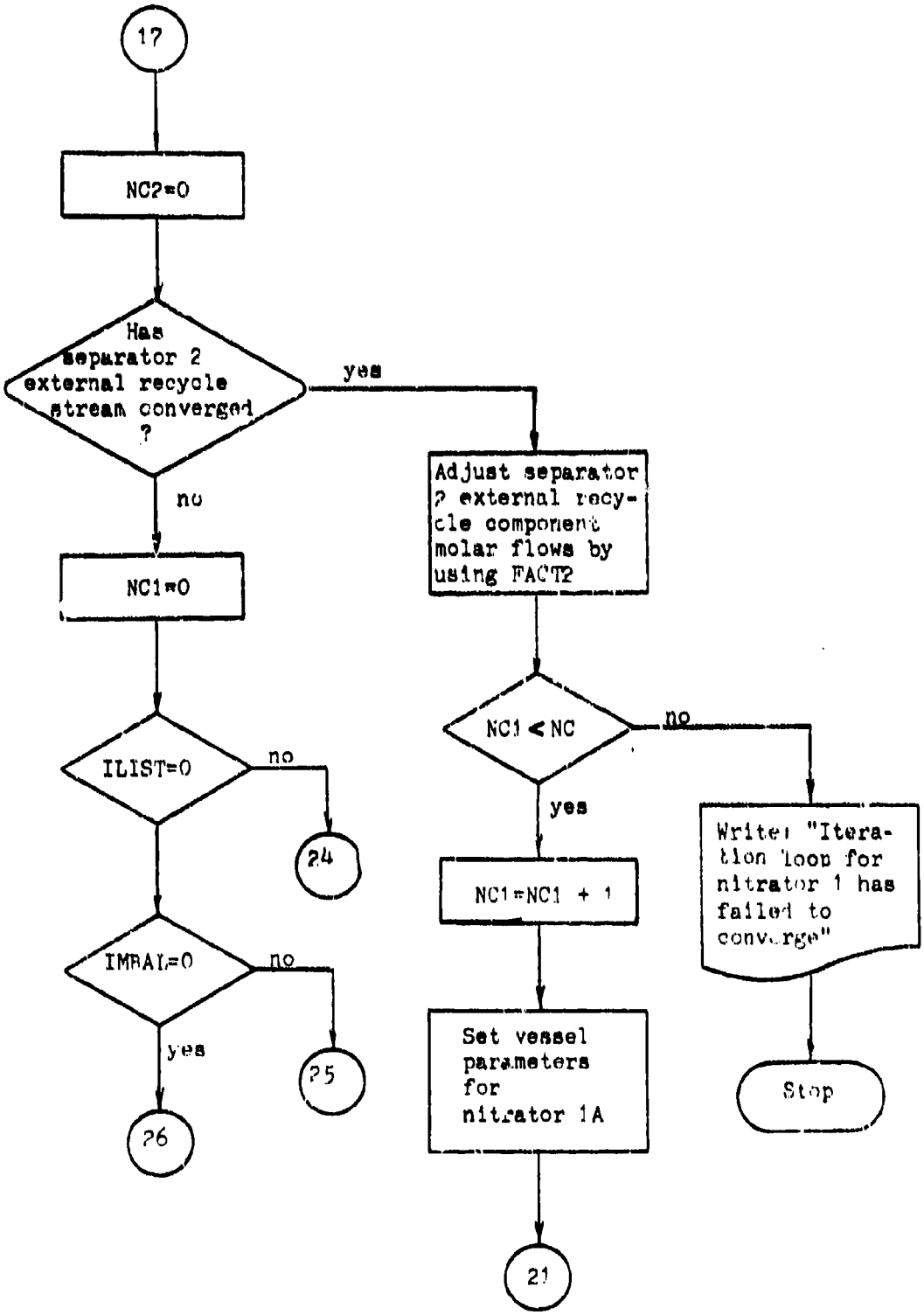

12'
Write: "Iter-
ation loop
for nitrater
5 failed to
converge"
Stop

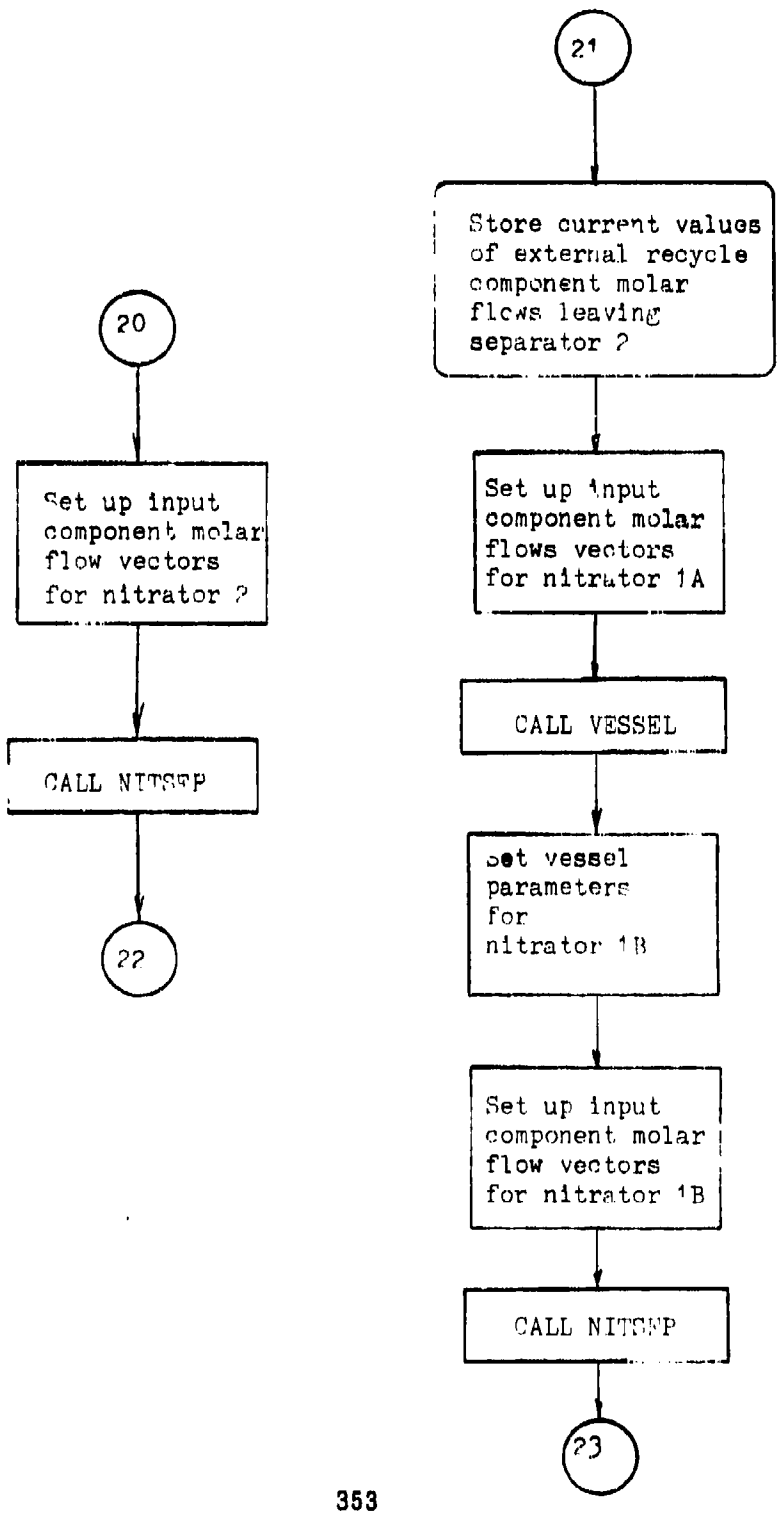

13
Has separator 5 external recycle stream converged?
no
yes
Adjust separator 5 external recycle molar component flows by using FACT6
NC4=0
19
NC4 < NC
no
yes
Has separator 4 external recycle stream converged?
no
yes
NC4=NC4 + 1
Write: "Iteration loop for nitrator 4 has failed to converge"
14
NC3=0
Set vessel parameters for nitrator 4
Stop
Has separator 3 external recycle stream converged?
no
yes
Store current values of external recycle molar component flows from separator 5
17
16
15

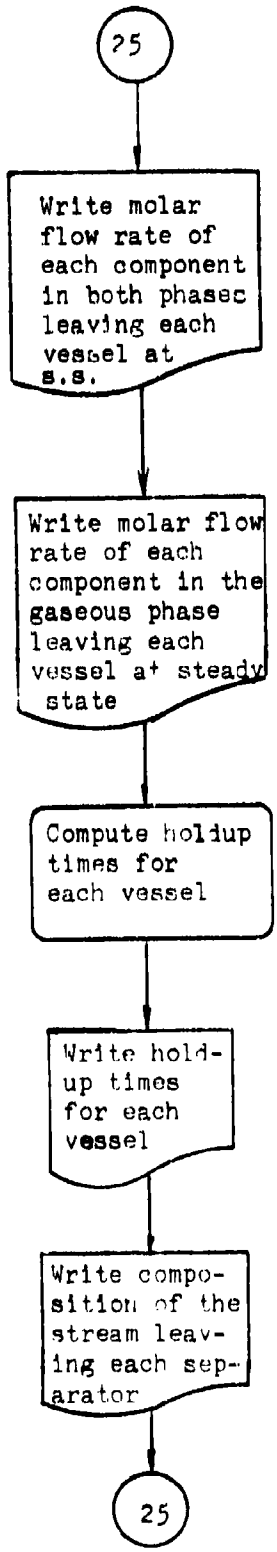

14
Adjust separator 4 external recycle molar component flows by using FACT 4
NC3<NC
no
yes
22
Write: "Iteration loop for nitrator 3 has failed to converge"
NC3=NC3 + 1
Stop
Set vessel parameters for nitrator 3A
Store current values of external recycle component molar flows leaving separator 4
18

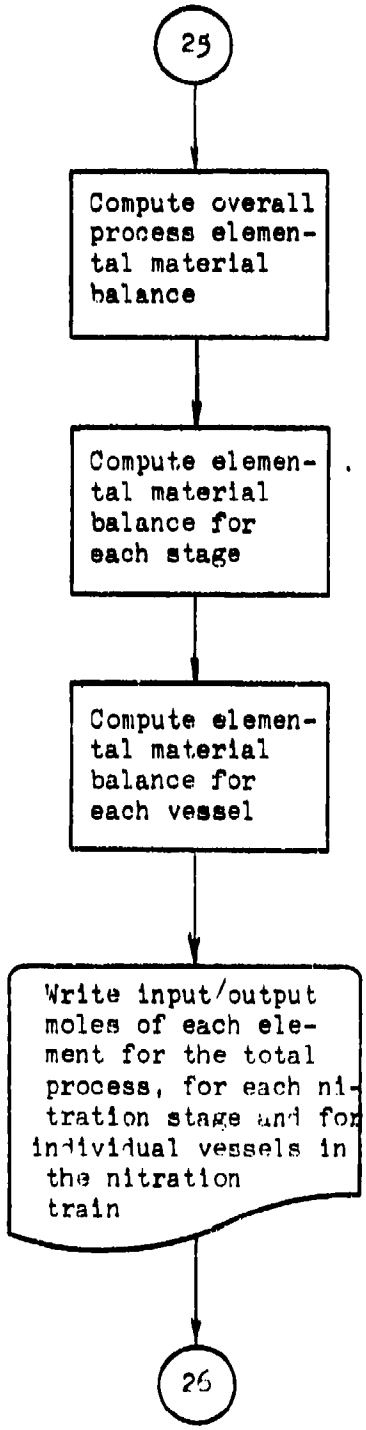

15
Set up input component molar flow vectors for nitrator A
CALL NITSEP
11
18
Set up input component molar flow vectors for nitrator 3A
CALL VESSEL
Set vessel parameters for nitrator 3B
Set up input component molar flow vectors for nitrator 3B
CALL NITSEP
19

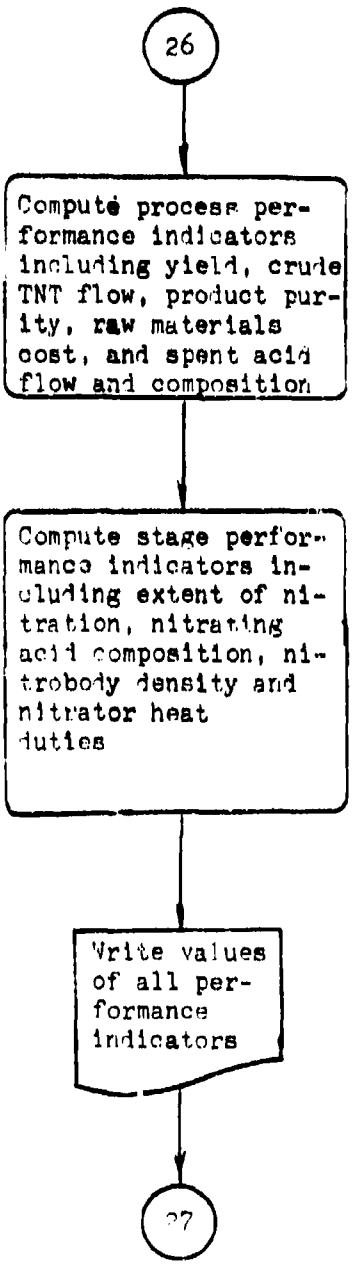

16
Adjust separator 3 external recycle molar component flows by using FACT3
NC2 ≤ NC
no
yes
23
Write: "Iteration loop for nitrator 2 has failed to converge
NC2=NC2 + 1
Stop
Set vessel parameters for nitrator 2
Store current values of external recycle component molar flows leaving separator 3
20


17
NC2=0
Has separator 2 external recycle stream converged ?
yes
no
Adjust separator 2 external recycle component molar flows by using FACT2
NC1=0
NC1 < NC
no
yes
ILIST=0
no
24
IMBAL=0
no
yes
25
26
NC1=NC1 + 1
Write "Iteration loop for nitrator 1 has failed to converge"
Set vessel parameters for nitrator 1A
Stop
21

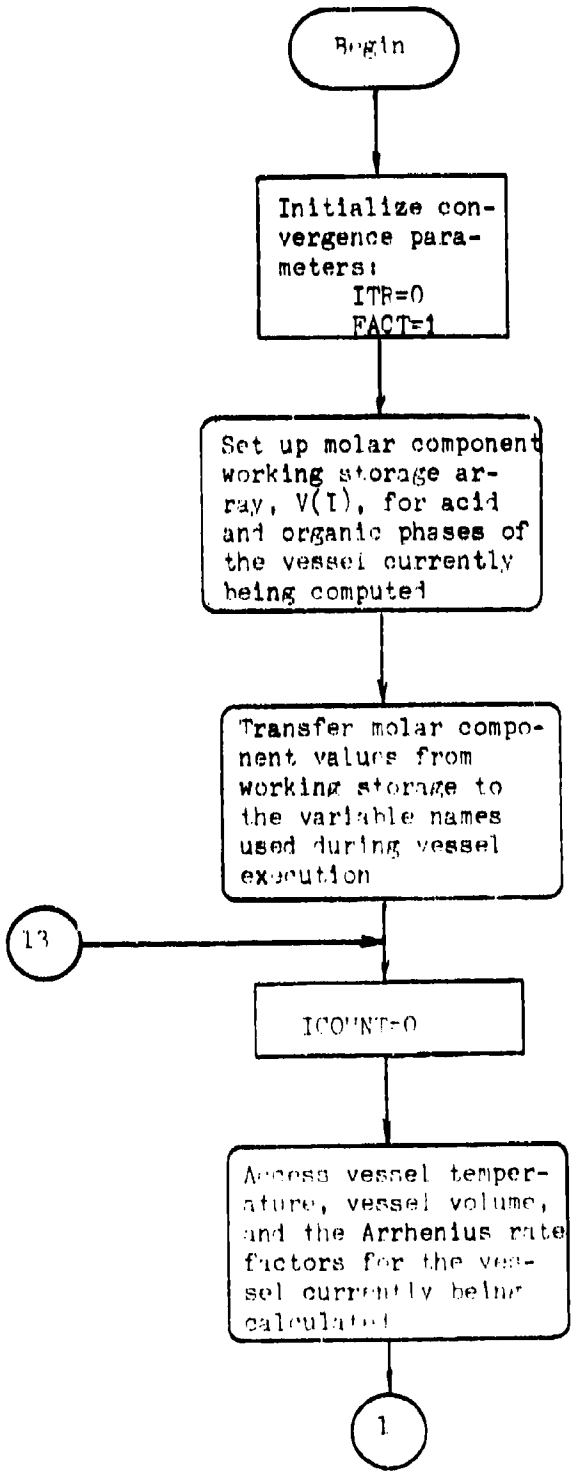

20
Set up input component molar flow vectors for nitrator 2
CALL NITSEP
22
21
Store current values of external recycle component molar flows leaving separator 2
Set up input component molar flows vectors for nitrator 1A
CALL VESSEL
Set vessel parameters for nitrator 1B
Set up input component molar flow vectors for nitrator 1B
CALL NITSEP
23

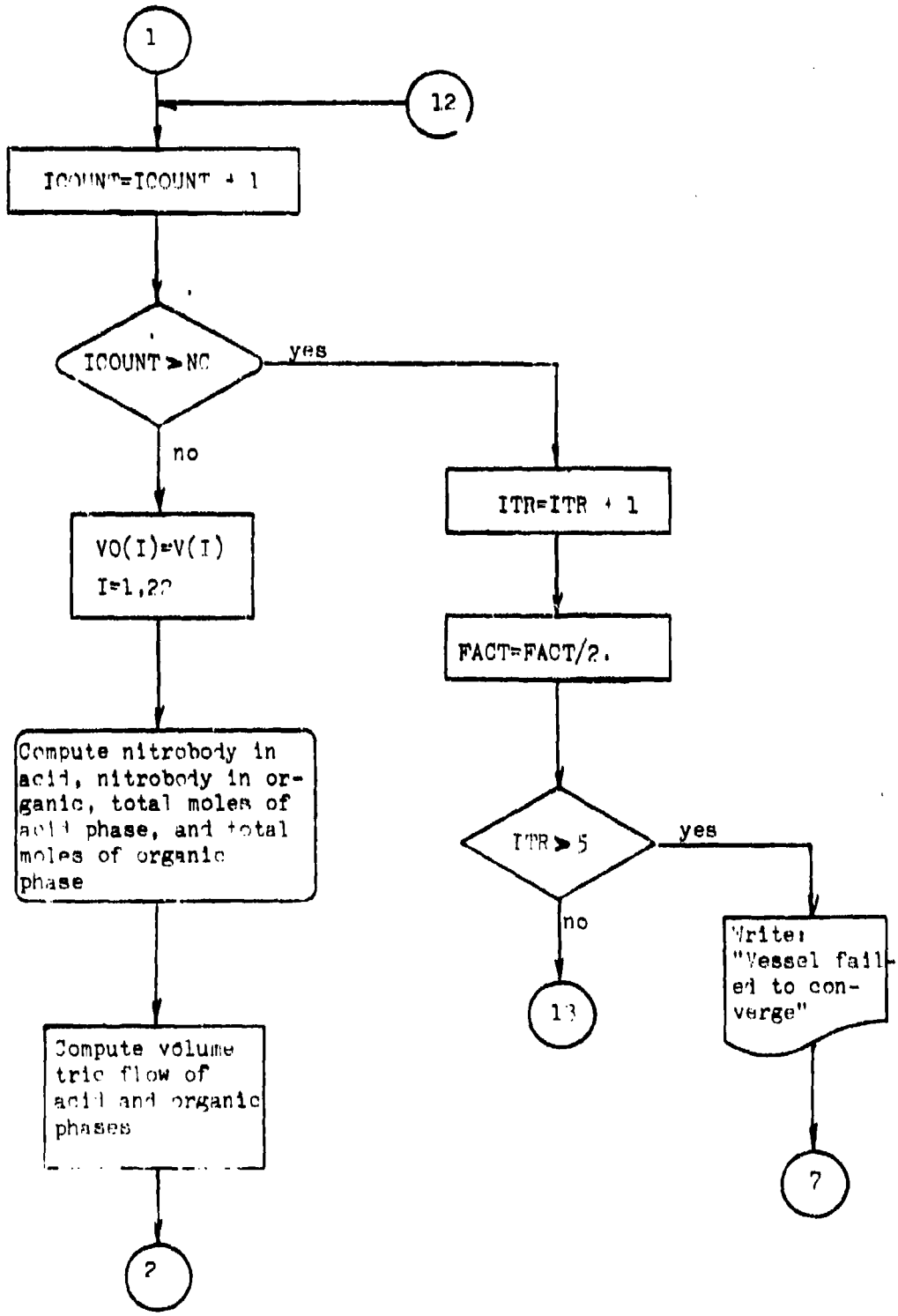

25
Write molar flow rate of each component in both phasec leaving each vessel at s.s.
Write molar flow rate of each component in the gaseous phase leaving each vessel at steady state
Compute holiup times for each vessel
Write hold-up times for each vessel
Write compo-sition of the stream leav-ing each sep-arator
25

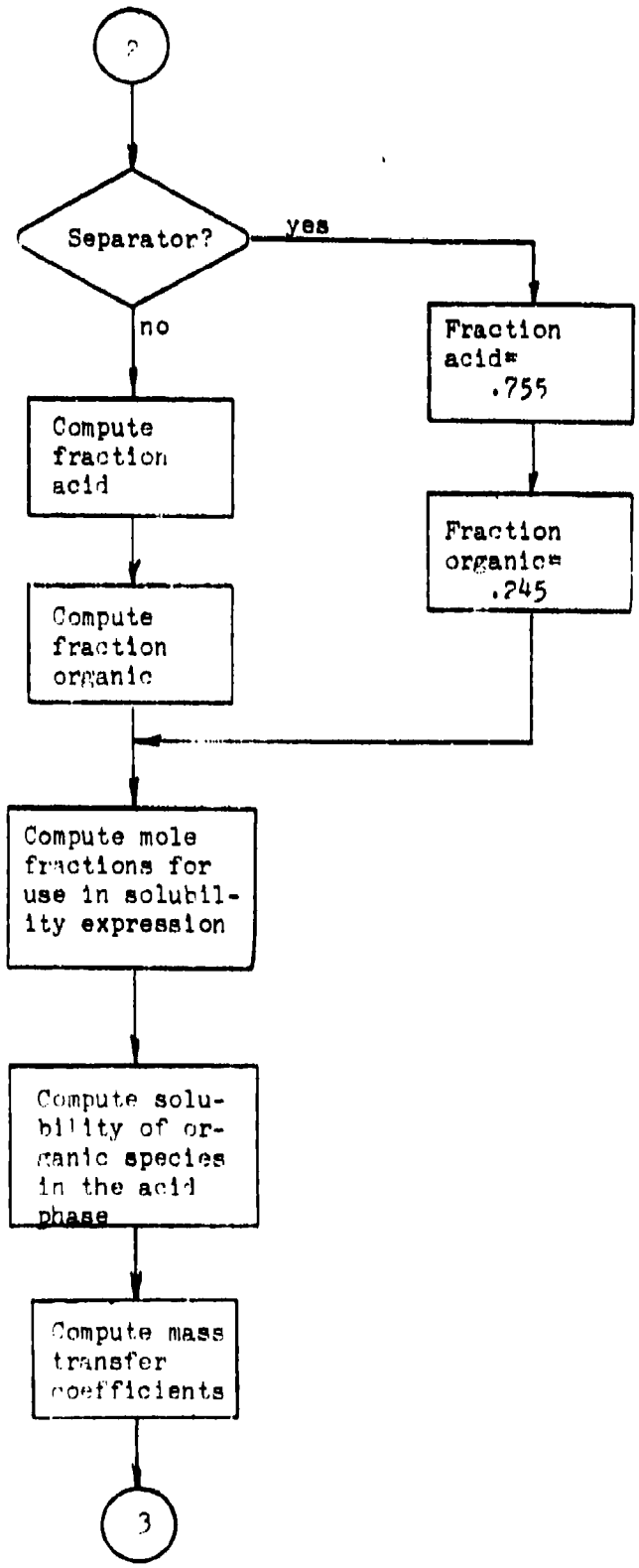

25
Compute overall process elemental material balance
Compute elemental material balance for each stage
Compute elemental material balance for each vessel
Write input/output moles of each element for the total process, for each nitration stage and for individual vessels in the nitration train
26

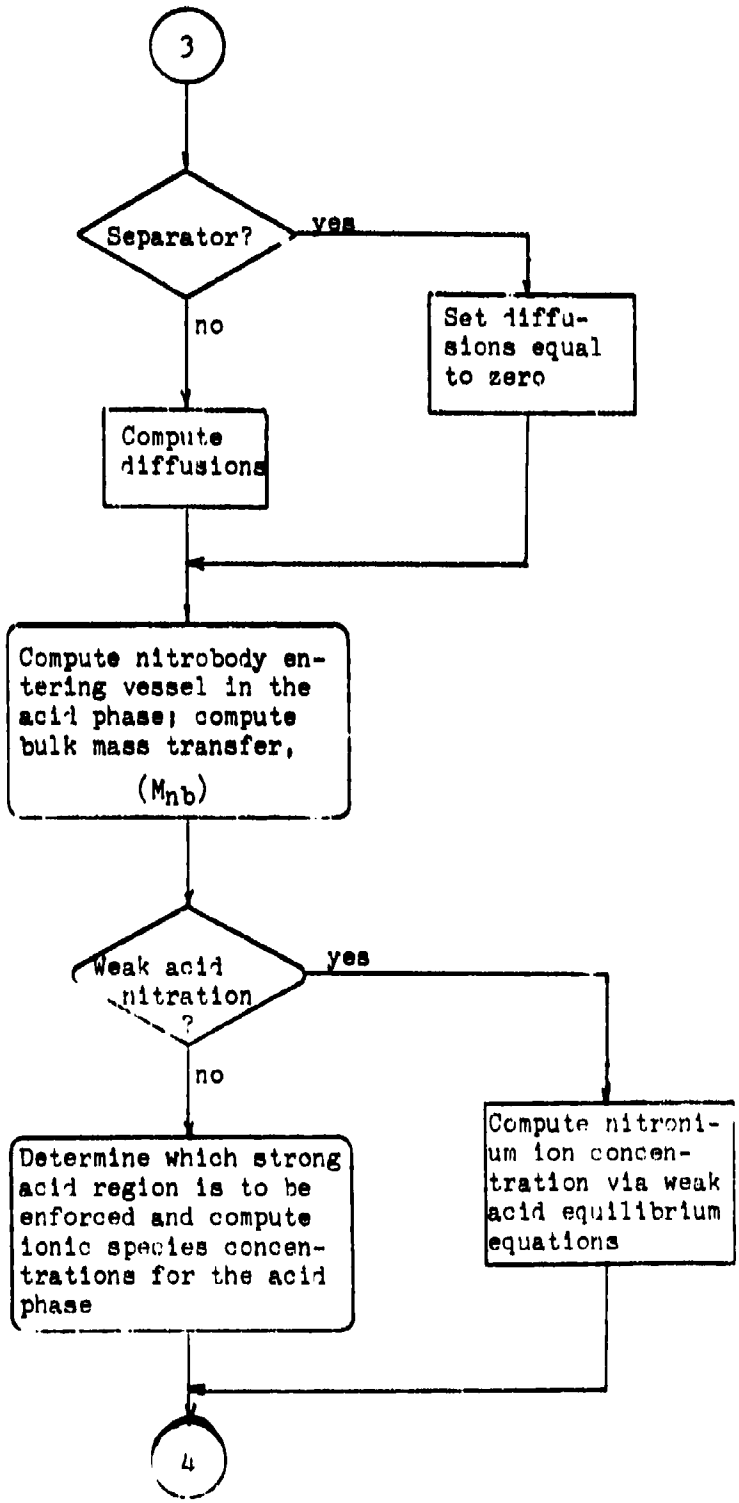

26
Compute process performance indicators including yield, crude TNT flow, product purity, raw materials cost, and spent acid flow and composition
Compute stage performance indicators including extent of nitration, nitrating acid composition, nitrobody density and nitrator heat duties
Write values of all performance indicators
27

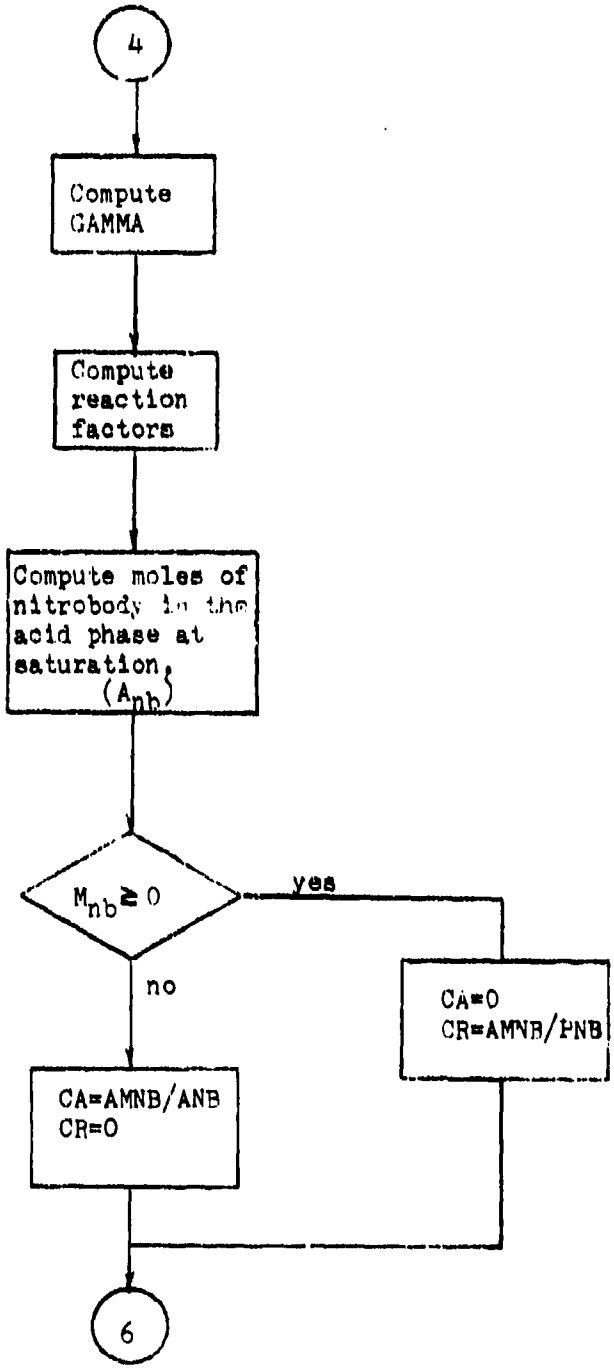
Subroutine VESSEL

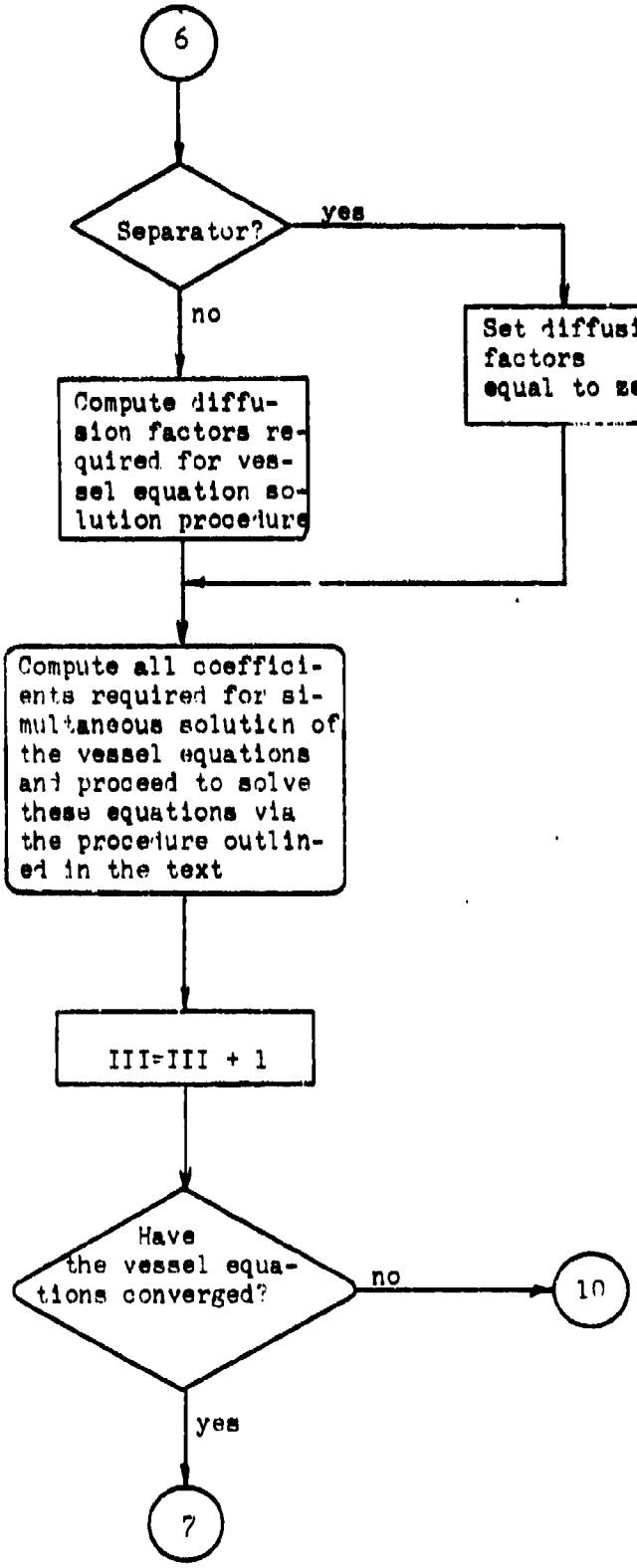


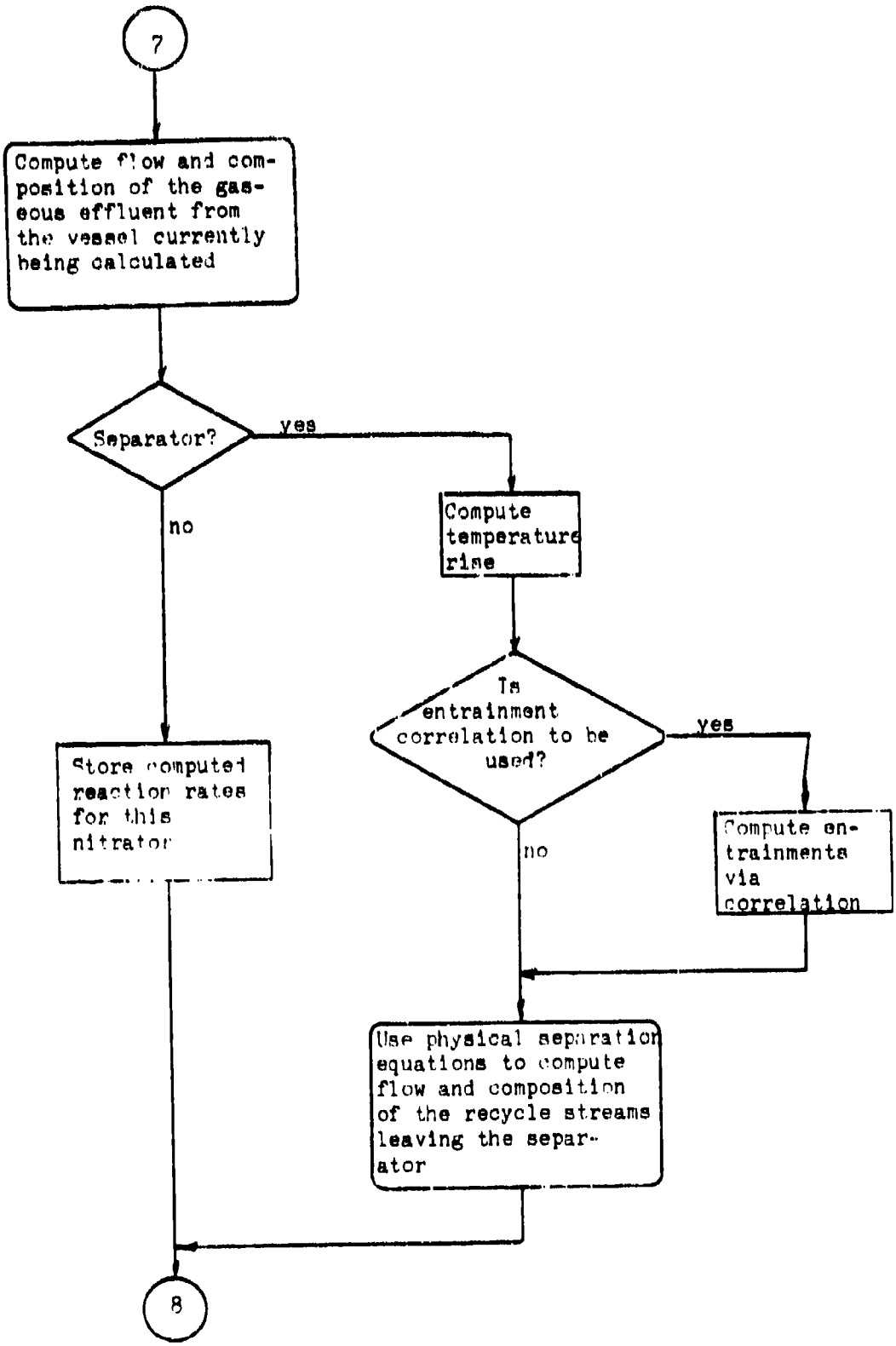

1
12
ICOUNT=ICOUNT + 1
ICOUNT ≥ NC
yes
no
VO(I)=V(I)
I=1,20
Compute nitrobody in acid, nitrobody in organic, total moles of acid phase, and total moles of organic phase
Compute volume tric flow of acid and organic phases
2
ITR=ITR + 1
FACT=FACT/2.
ITR ≥ 5
yes
no
13
Write "Vessel failed to converge"
7

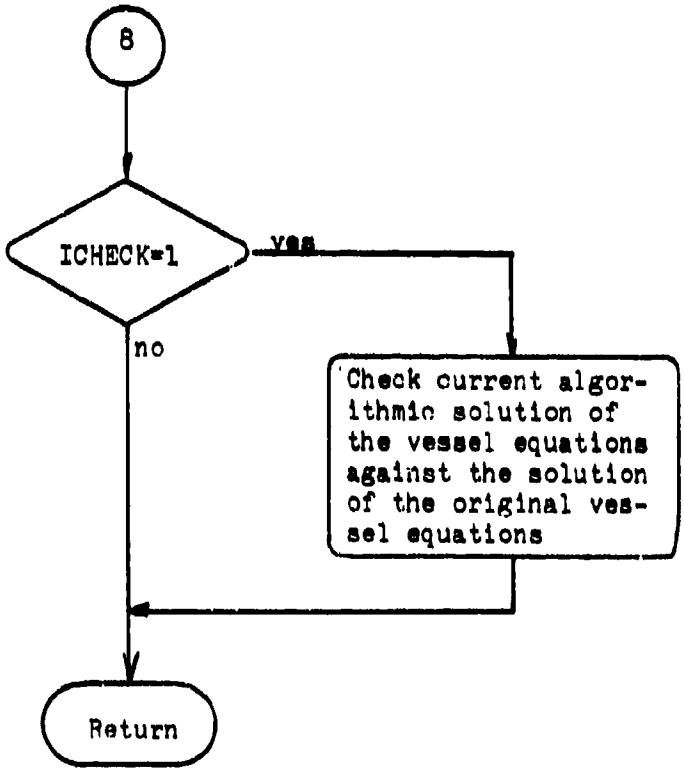

2
Separator?
yes
no
Fraction acid= .755
Compute fraction acid
Fraction organic= .245
Compute fraction organic
Compute mole fractions for use in solubility expression
Compute solubility of organic species in the acid phase
Compute mass transfer coefficients
3

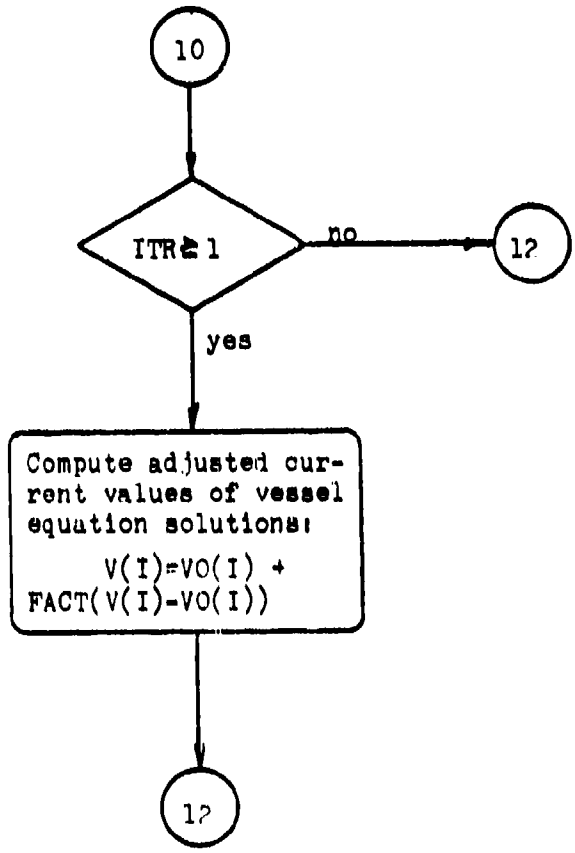

3
Separator?
yes
no
Set diffusions equal to zero
Compute diffusions
Compute nitrobody entering vessel in the acid phase; compute bulk mass transfer, (M_{nb})
Weak acid nitration ?
yes
no
Compute nitronium ion concentration via weak acid equilibrium equations
Determine which strong acid region is to be enforced and compute ionic species concentrations for the acid phase
4


4
Compute GAMMA
Compute reaction factors
Compute moles of nitrobody in the acid phase at saturation, (A_{nb})
$M_{nb} \geq 0$
yes
no
CA=0
CR=AMNB/PNB
CA=AMNB/ANB
CR=0
6

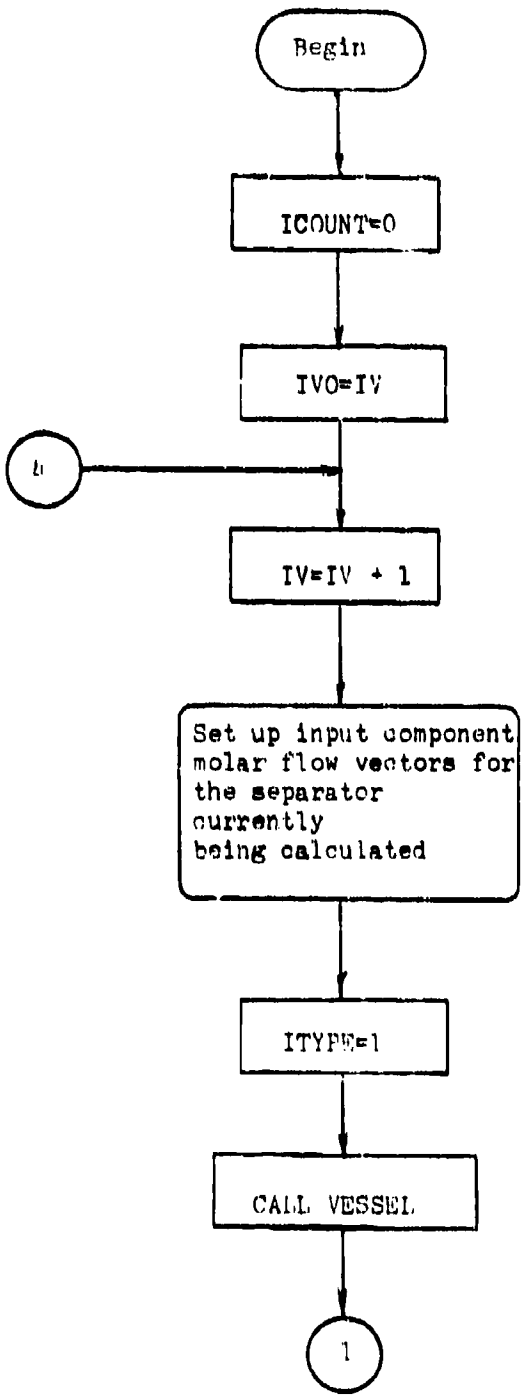

6
Separator?
yes
no
Set diffusion factors equal to zero
Compute diffusion factors required for vessel equation solution procedure
Compute all coefficients required for simultaneous solution of the vessel equations and proceed to solve these equations via the procedure outlined in the text
III=III + 1
Have the vessel equations converged?
no
10
yes
7

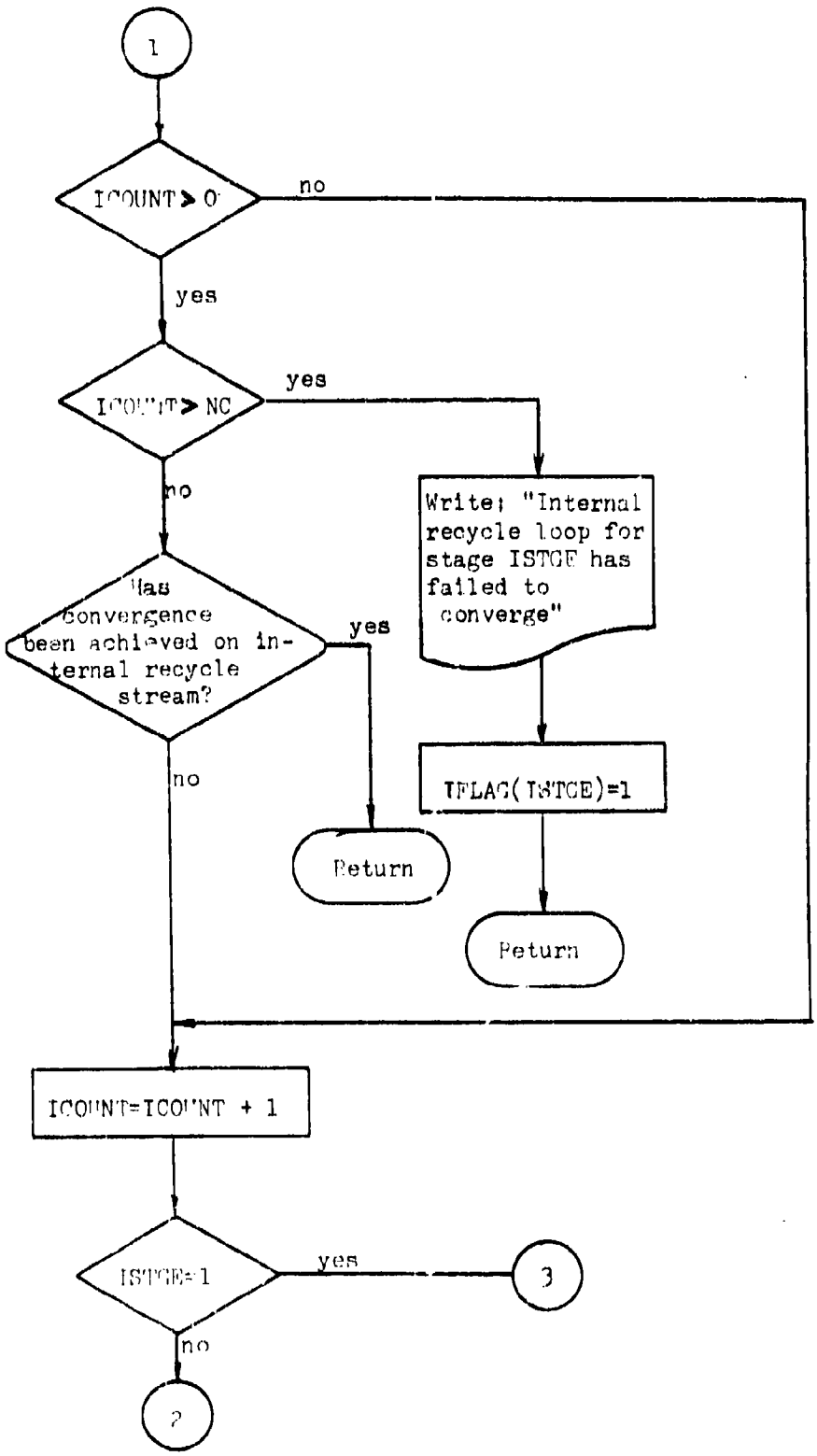

7
Compute flow and composition of the gaseous effluent from the vessel currently being calculated
Separator?
yes
no
Compute temperature rise
Is entrainment correlation to be used?
yes
no
Store computed reaction rates for this nitrator
Compute entrainments via correlation
Use physical separation equations to compute flow and composition of the recycle streams leaving the separator
8

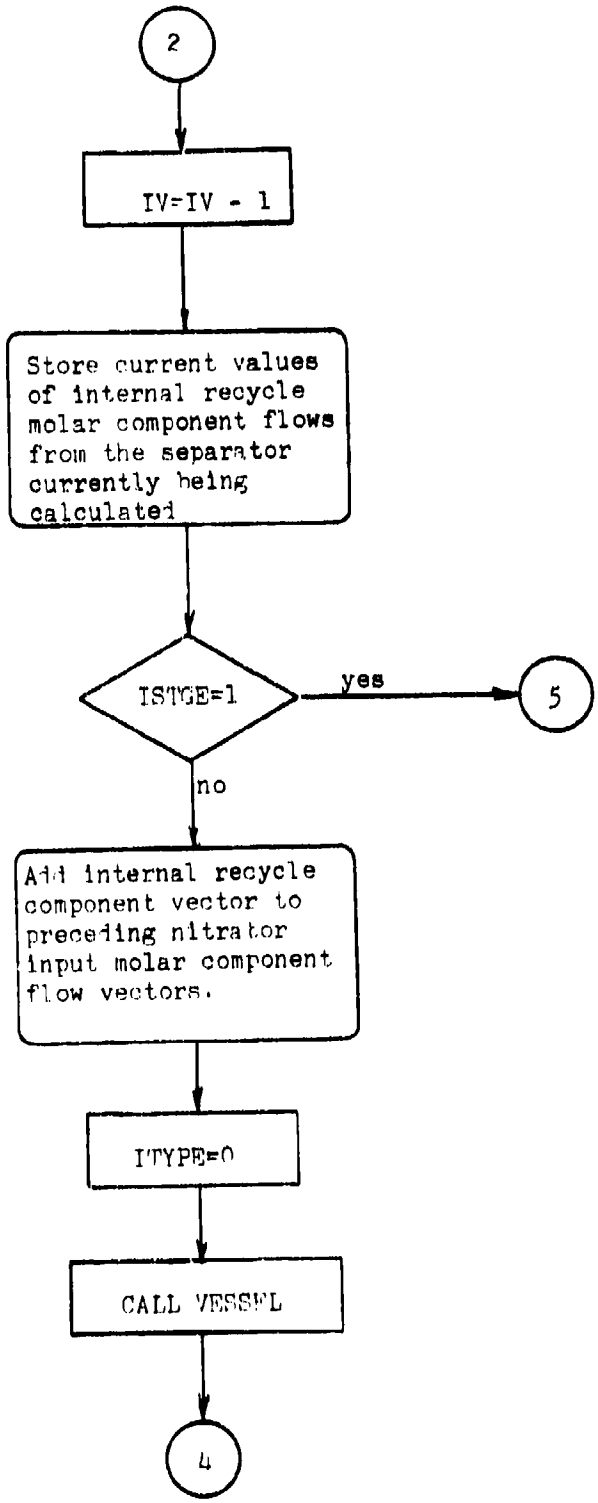

8
ICHECK=1
yes
no
Check current algorithmic solution of the vessel equations against the solution of the original vessel equations
Return

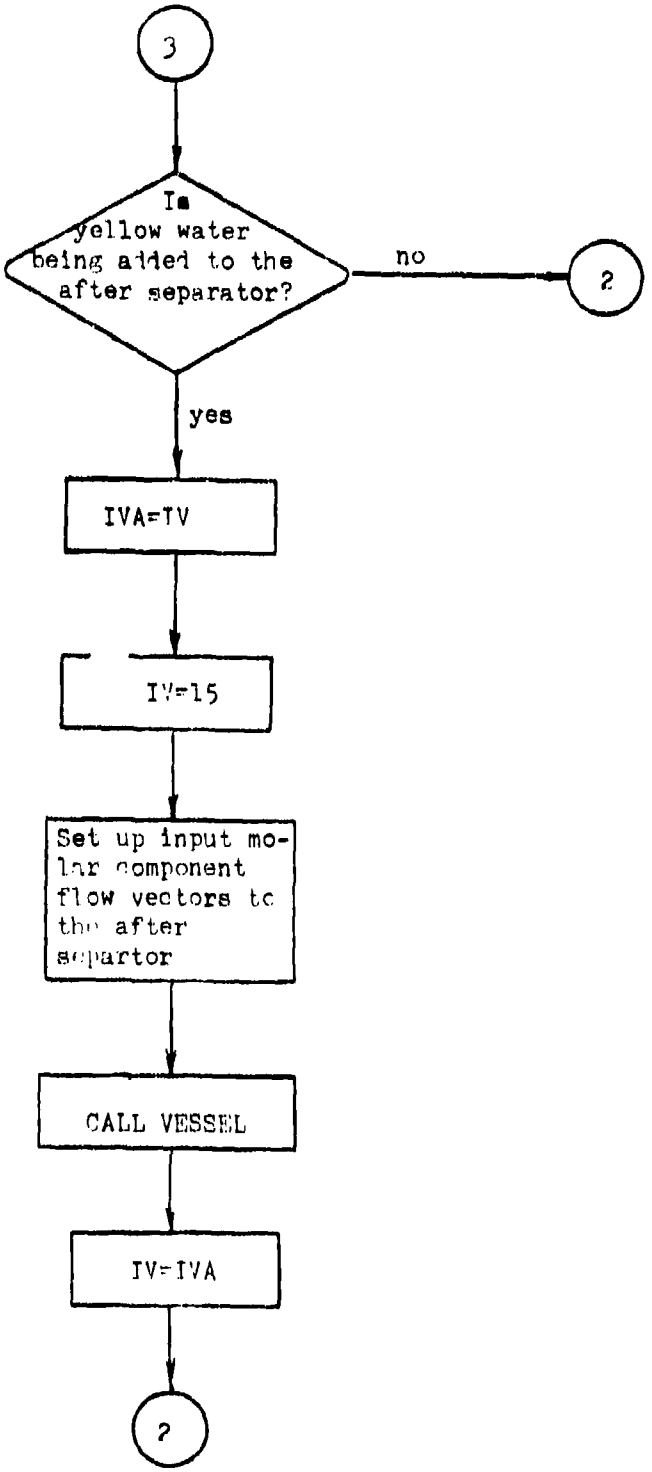

10
ITR≥1
no
12
yes
Compute adjusted current values of vessel equation solutions:
V(I)=VO(I) + FACT(V(I)-VO(I))
12

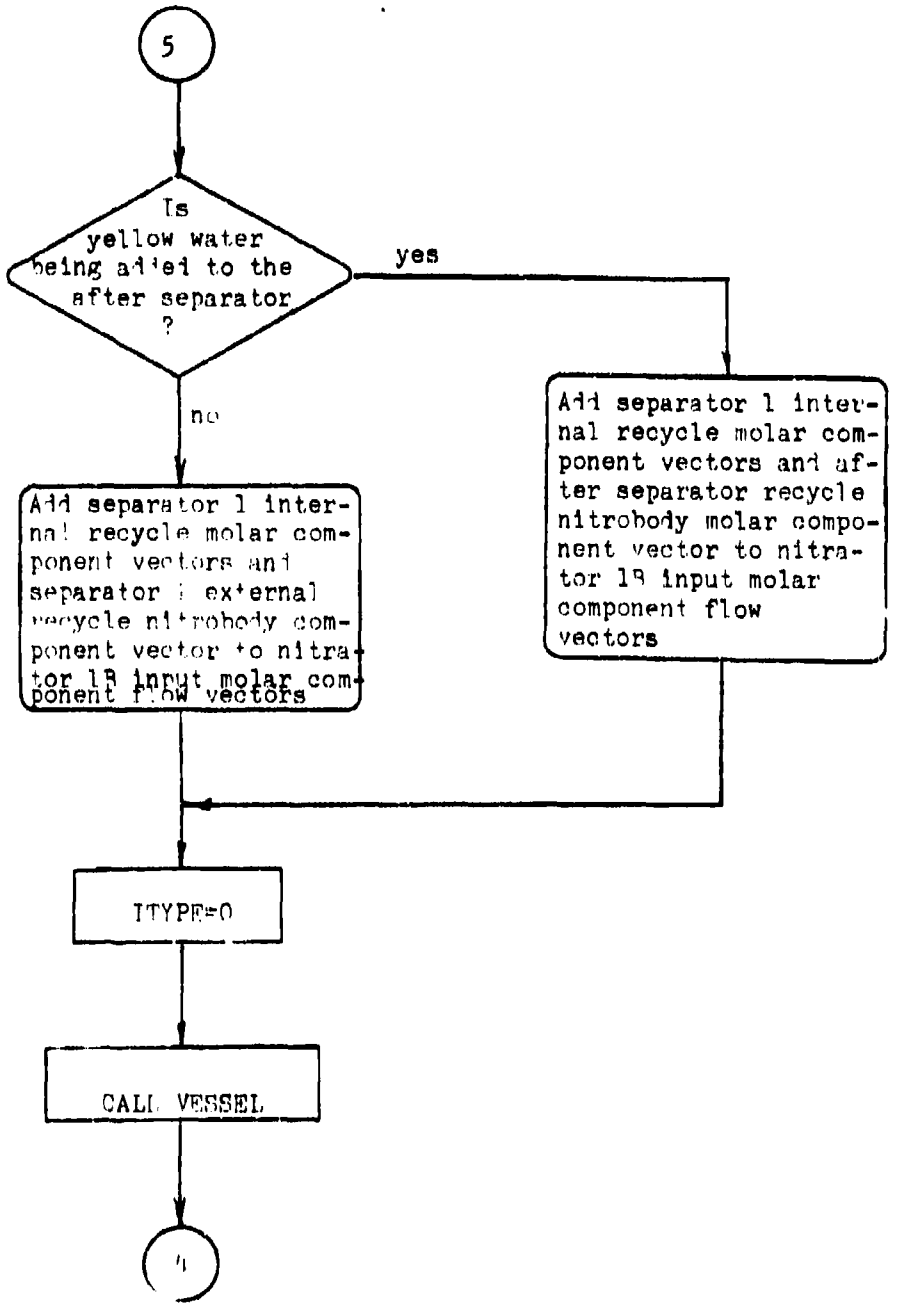
Subroutine NITSEP



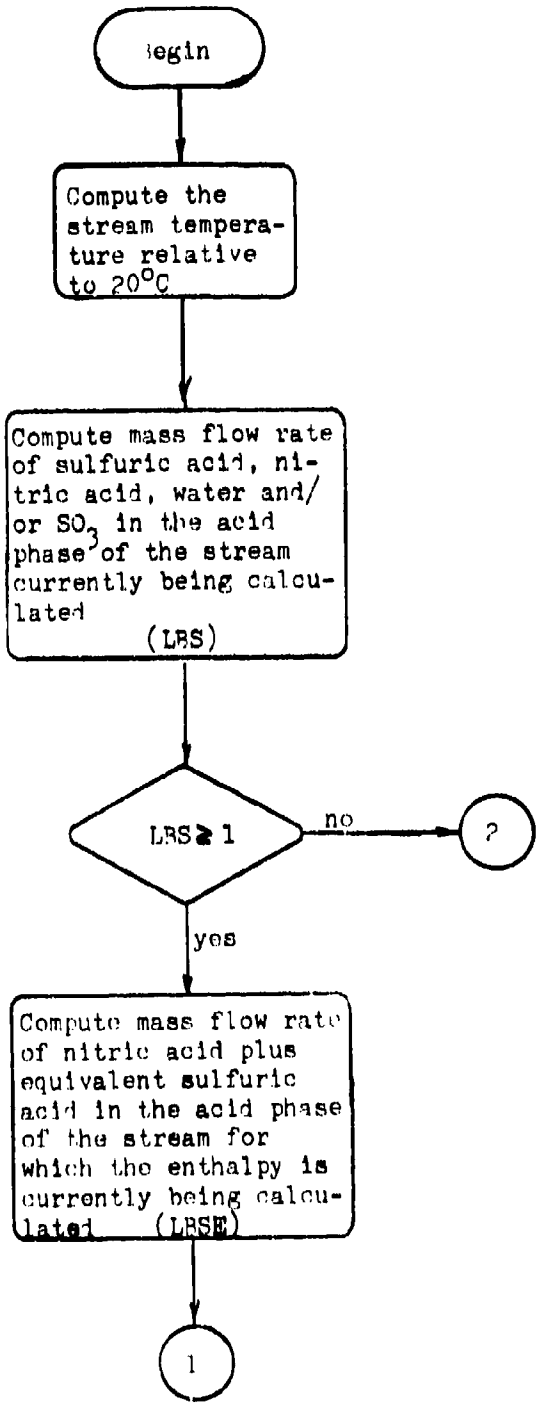

1
ICOUNT > 0
no
yes
ICOUNT > NC
yes
no
Has convergence been achieved on internal recycle stream?
yes
no
Write: "Internal recycle loop for stage ISTGE has failed to converge"
IFLAG(ISTGE)=1
Return
Return
ICOUNT=ICOUNT + 1
ISTGE=1
yes
3
no
2

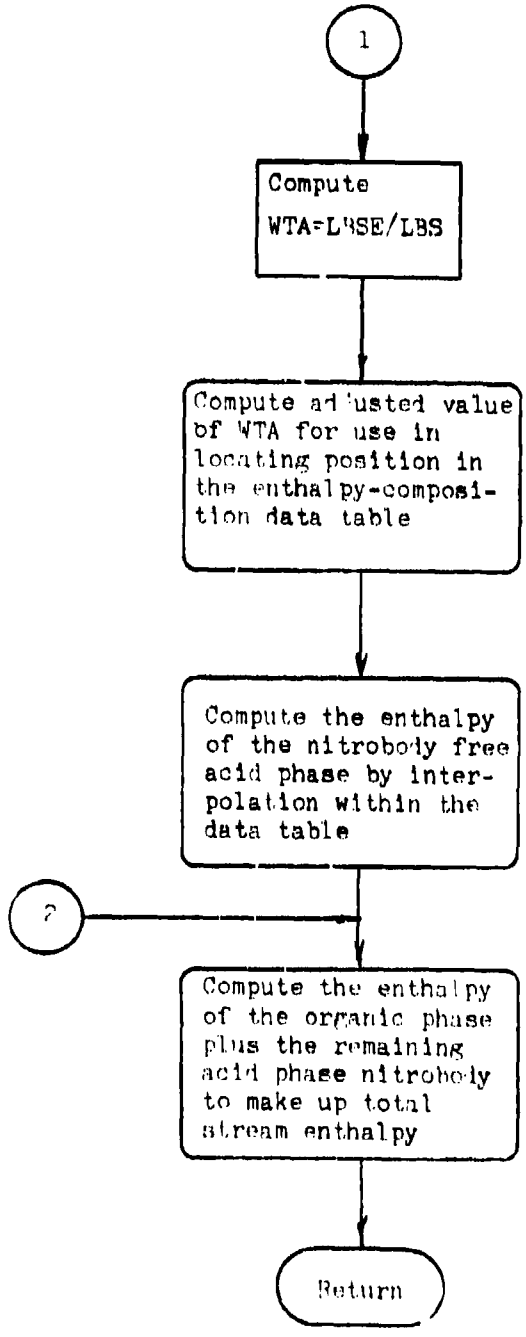

2
IV=IV - 1
Store current values of internal recycle molar component flows from the separator currently being calculated
ISTGE=1
yes
5
no
Add internal recycle component vector to preceding nitrator input molar component flow vectors.
ITYPE=0
CALL VESSEL
4


3
Is yellow water being added to the after separator?
no
2
yes
IVA=IV
IV=15
Set up input molar component flow vectors to the after separtor
CALL VESSEL
IV=IVA
2


5
Is yellow water being added to the after separator ?
yes
no
Add separator 1 internal recycle molar component vectors and after separator recycle nitrobody molar component vector to nitrator 1B input molar component flow vectors
Add separator 1 internal recycle molar component vectors and separator 1 external recycle nitrobody component vector to nitrator 1B input molar component flow vectors
ITYPE=0
CALL VESSEL
4

Function ENTH




1
Compute
WTA=L*SE/LBS
Compute adjusted value of WTA for use in locating position in the enthalpy-composition data table
Compute the enthalpy of the nitrobody free acid phase by interpolation within the data table
2
Compute the enthalpy of the organic phase plus the remaining acid phase nitrobody to make up total stream enthalpy
Return

APPENDIX H

Steady State Simulation--Program Nomenclature

Main Program

AAS (I)	moles/hr of component i in the acid phase flowing from the after separator
AB	extent of nitration (either α or m) across the stage currently being calculated (moles/hr NO_2^+ added to the ring)
AF (I,J)	moles/hr of component i in the entrained acid phase of the organic stream flowing from separator j
AFLBS (I,J)	same as AF but in units of lbs/hr
AF1 (I)	moles/hr of component i in the entrained acid phase of the organic stream flowing from separator 1
AF2 (I)	same as AF1 but for separator 2
AF3 (I)	same as AF1 but for separator 3
AF4 (I)	same as AF1 but for separator 4
AF5 (I)	same as AF1 but for separator 5
AF6 (I)	same as AF1 but for separator 6
AI (I)	total acid phase moles/hr of component i flowing into a nitrator which is followed by another nitrator
AII (I)	total acid phase moles/hr (less acid phase of internal recycle) of component i flowing into a nitrator which is followed by a separator
AIR (I,J)	moles/hr of component i in the acid phase of the internal recycle stream flowing from separator j

AIR LBS (I,J)	same as AIR but in units of lbs/hr
AIR1 (I)	moles/hr of component i in the acid phase of the internal recycle stream flowing from separator 1
AIR2 (I)	same as AIR1 but for separator 2
AIR3 (I)	same as AIR1 but for separator 3
AIR4 (I)	same as AIR1 but for separator 4
AIR5 (I)	same as AIR1 but for separator 5
AIR6 (I)	same as AIR1 but for separator 6
AKA	general rate factor for all nitration reactions. Also, if Bennett's strong acid rate expression is used, the coefficient of the bisulfate ion concentration
AKB	coefficient of the sulfuric acid concentration in Bennett's rate expression
AKC	coefficient of the pyrosulfuric ion concentration in Bennett's rate expression
AKEQ	equilibrium constant for the sulfuric acid-water dissociation reaction
AKEQOV	equilibrium constant for the dissociation of a mixture of sulfuric and pyrosulfuric acids to ionic species. NOT USED
AKMA	acid phase mass transfer coefficient
AKMATL	mass transfer coefficient for toluene
AK10	rate constant for reaction 10
AK12	ratio of rate constants for reactions 1 & 2

AK3S	rate constant for reaction 3 in strong acid
AK3W	rate constant for reaction 3 in weak acid NOT USED
AK4S	rate constant for reaction 4 in strong acid
AK4W	rate constant for reaction 4 in weak acid NOT USED
AK5S	rate constant for reaction 5
AK6S	rate constant for reaction 6
AK7	rate constant for reaction 7
AK8	rate constant for reaction 8
AK9	NOT USED
AN(I)	percent actual nitric acid in the acid phase of the external recycle stream flowing from the ith separator
ANS(I)	mole fraction nitrosylsulfuric acid in the acid phase of the external recycle stream flowing from the ith separator
ANS1A	mole fraction nitrosylsulfuric acid in the acid phase flowing from nitrator 1A
ANS3A	mole fraction nitrosylsulfuric acid in the acid phase flowing from nitrator 3A
ARRAY(I,J)	moles/hr of component i in the raw material feedstocks flowing to nitrator j
AS(I)	percent sulfuric acid and SO_3 (as equivalent sulfuric) in the acid phase of the external recycle stream flowing from the ith separator

AT	total moles/hr of acid phase flowing from the vessel for which the holdup is being computed
ATØM(I,J)	number of i-type atoms in component j
AV(I,J)	moles/hr of component i in the total acid phase flowing from vessel j
AVI(I,J)	first guess at converged value of moles/hr of component i in the acid phase flowing from vessel j
AXR(I,J)	moles/hr of component i in the acid phase of the external recycle stream flowing from separator j
AXRLBS(I,J)	same as AXR but in units of lbs/hr
AXR1(I)	moles/hr of component i in the acid phase of the external recycle stream flowing from separator 1
AXR2(I)	same as AXR1 but for separator 2
AXR2Ø(I)	previous value of AXR2(I) to which current value is compared during the external recycle convergence procedure
AXR3(I)	same as AXR1 but for separator 3
AXR3Ø(I)	same as AXR2Ø bit fpr AXR3
AXR4(I)	same as AXR1 but for separator 4
AXR4Ø(I)	same as AXR2Ø but for AXR4
AXR5(I)	same as AXR1 but for separator 5
AXR5Ø(I)	same as AXR2Ø but for AXR5
AXR6 (I)	same as AXR1 but for separator 6

AXR6Ø (I)	same as AXR2Ø but for AXR6
A1A (I)	moles/hr of component i in the total acid phase flowing from nitrator 1A
A1AI (I)	moles/hr of component i flowing into nitrator 1A from the raw material feedstocks
A1B (I)	same as A1A but for nitrator 1B
A1BI (I)	same as A1AI but for nitrator 1B
A1S (I)	moles/hr of component i in the total acid phase flowing from separator 1
A2 (I)	same as A1A but for nitrator 2
A2I (I)	same as A1AI but for nitrator 2
A2S (I)	same as A1S but for separator 2
A3A (I)	same as A1A but for nitrator 3A
A3AI (I)	same as A1AI but for nitrator 3A
A3B (I)	same as A1A but for nitrator 3B
A3BI (I)	same as A1AI but for nitrator 3B
A3S (I)	same as A1S but for separator 3
A4 (I)	same A1A but for nitrator 4
A4I (I)	same as A1AI but for nitrator 4
A4S (I)	same as A1S but for separator 4
A5 (I)	same as A1A but for nitrator 5
A5I (I)	same as A1AI bur for nitrator 5
A5S (I)	same as A1S but for separator 5

A6(I)	same as A1A but for nitrator 6
A6I(I)	same as A1AI but for nitrator 6
A6S(I)	same as A1S but for separator 6
BTU(I)	total heat load in nitrator i, BTU/hr
BTUQ(I)	heat evolved in nitrator i which is due to chemical reaction only, BTU/hr
CDNT	weight % DNT in the nitrobody stream flowing from separator 6 on and acid free basis
COMP(I,J)	weight % component i in raw material feedstock type j
CP(I)	heat capacity of component i, BTU/lb-mole/°K
CRUDE	total mass flow rate (lbs/hr) of the organic stream from separator 6
CSL	cost of oleum, $/lb
CSN	cost of strong nitric acid, $/lb
CTF	cost of raw materials per unit of TNT produced, $/lb α-TNT
CTL	cost of toluene, $/lb
CWN	cost of weak nitric acid, $/lb
DEL	convergence tolerance for components in acid recycle streams
DH(I)	heat of reaction for reaction i, BTU/lb-mole of reactant
DIF	storage variable for the difference between atoms of a given type in and atoms of that type out during material balance calculations

DLT	temperator of separator 1 referenced to 20°C
EAØ (I)	molar ratio of acid phase in the organic stream to total organic stream flowing from the ith separator
EAØP (I)	molar ratio of acid phase to organic phase in the organic stream flowing from the ith separator
EFR	enthalpy of mixing for fume recovery acid
EØA (I)	molar ratio of organic phase in the external recycle stream to the total external recycle stream flowing from the ith separator
EØAP (I)	molar ratio of organic phase to acid phase in the external recycle stream flowing from the ith separator
EØL	enthalpy of mixing for oleum
EWN	enthalpy of mixing for weak nitric acid
EYW'	enthalpy of mixing for yellow water
E10	activation energy for reaction 10
E21	ratio of activation energy for reaction 2 to that of reaction 1
E3S	activation energy for reaction 3
E3W	NOT USED
E4S	activation energy for reaction 4
E4W	NOT USED
E5S	activation energy for reaction 5
E6S	activation energy for reaction 6

E7	activation energy for reaction 7
E8	activation energy for reaction 8
E9	NOT USED
FA	volume fraction of acid phase in the vessel for which holdup is being calculated
FACD(I)	NOT USED
FACT2	relaxation factor used in convergence of the external recycle from separator 2
FACT3	same as FACT2 but for separator 3
FACT4	same as FACT2 but for separator 4
FACT5	same as FACT2 but for separator 5
FACT6	same as FACT2 but for separator 6
FD	extent of reaction for the decomposition of nitrosylsulfuric acid
FDN	moles/hr of ring associated NO_2 groups flowing into a nitration stage with the organic stream from the previous stage
FIN(I,J)	lbs/hr of feedstock i to nitration vessel j
FMAX	maximum possible volumetric flow rate of material through any internal recycle pipe
FØ	volume fraction of organic phase in the vessel for which holdup is being calculated
FØV	NOT USED
GA(I,J)	number of i-type atoms in gaseous product j

CGS (I,J)	moles/hr of gaseous product j evolved in vessel i
G1 (I)	ratio of the Arrhenius coefficients in the kinetic rate expressions for reactions 1 and 2 in the ith nitrator
G10 (I)	Arrhenius coefficient for reaction 10 in nitrator i
G15 (I)	moles/hr of $CO_{1,8}$ evolved from vessel i
G16 (I)	moles/hr of NO_x evolved from vessel i
G18 (I)	moles/hr of TNM evolved from vessel i
G19 (I)	moles/hr of CO_2 evolved from vessel i
G3 (I)	NOT USED
G3S (I)	Arrhenius coefficient for reaction 3 in nitrator i
G4 (I)	NOT USED
G4S (I)	same as G3S but for reaction 4
G5 (I)	same as G3S bur for reaction 5
G6 (I)	same as G3S but for reaction 6
G7 (I)	same as G3S but for reaction 7
G8 (I)	same as G3S but for reaction 8
G9 (I)	Zero
HDR (I,J)	array used to store alphanumeric headings for chemical elements in material balance printout
I	general index integer
IAFT	after separator switch. If equal to 1 then after separator is considered in the simulation as a dilution vessel to which 1000 lb/hr of yellow water is added

ICHECK	check calculation switch. If equal to 1 then check calculations are performed on the vessel equations in SUBROUTINE VESSEL
IE	entrainment correlation switch. If equal to 0 then entrainment correlation is used instead of assuming fixed values for entrainments
IFLG (I)	set equal to 1 whenever internal recycle loop for stage i does not converge
II	index used in calculation of extent of nitration in each stage
III	number of passes through SUBROUTINE VESSEL required to reach a converged solution
IJ	index used in calculation of extent of nitration in each stage
ILIST	printout switch. If equal to 1 printout of phase compositions, gas flows, vessel time constants, volumetric flows, acid phase solubility, vessel holdups and stream compositions is obtained
IMBAL	material balance switch. If equal to 1 chemical element balances are carried out on the entire nitration section, each individual nitration stage, and each individual vessel
IN	nitrator number
INIT (I)	vessel index. Has value of 1 if vessel is a nitrator and 0 if vessel is a separator
IPI	intermediate printout switch. If equal to 1 a printout of external recycle molar component flows after each iteration will be given

IPNCH	punch switch. If equal to zero no punched output. If equal to 1 final steady state (i.e. values of component molar flows for both phases in each vessel) is punched out for use as initial conditions in dynamic simulation or new first guess in steady state simulation
IPRNT	SUBROUTINE VESSEL printout switch. If equal to 1 gives a variety of debug printout which can be used to analyze problems associated with the vessel equations
ISTGE	stage number
ISTØP	equal to number of data sets plus 1. Program execution is terminated when NSET = ISTØP
ITYPE	equal to 0 for a nitrator and 1 for a separator
IV	vessel number
IV1	vessel number used during initial determination of recycle streams from first guess values of component molar phase flows
IX	index used in calculation of extent of nitration in each stage
IY	index used in calculation of extent of nitration in each stage
J	general index integer used for a variety of counting purposes
K	general index integer used for a variety of counting purposes
KEY	index which indicates whether extent of alpha or meta nitration is to be determined in a given stage
L	vessel index used in holdup calculation printout

M	vessel index used in holdup calculation printout
MHØLDA	total moles of acid phase holdup in the vessel currently being calculated
MHØLDØ	total moles of organic phase holdup in the vessel currently being calculated
MW(I)	molecular weight of component i
NATM	index of atomic species used in elemental material balance calculations
NC	maximum number of iterations allowed on any given recycle (internal or external) convergence loop
NC1	running sum of iterations on external recycle loop for separator 2
NC2	running sum of iterations on external recycle loop for separator 3
NC3	running sum of iterations on external recycle loop for separator 4
NC4	running sum of iterations on external recycle loop for separator 5
NC5	running sum of iterations on external recycle loop for separator 6
NDS	number of sets of operating conditions for which a steady state solution is desired in a given simulation run
NØ(I)	notch setting on the internal recycle gate valve for separator i
NSET	number of the data set for which the steady state solution is currently being determined

NTOS (I)	molar ratio of nitric acid to the sum of sulfuric acid and SO_3 in the external recycle stream flowing from the ith separator
NTØS1A	molar ratio of nitric acid to the sum of sulfuric acid and SO_3 in the acid phase flowing from nitrator 1A
NTØS3A	same as NTOS1A but for nitrator 3A
ØUTN	moles/hr of ring associated NO_2 groups flowing out of a given nitration stage
PACID (I,J)	pounds of component i held up in the acid phase of vessel j
PAS (I)	moles/hr of component i in the organic phase flowing from the after separator
PCTAS	weight % dissolved nitrobody in the acid phase flowing from the after separator under the condition of 1000 lb/hr of yellow water added to the after separator
PCTD	weight % DNT in the organic components dissolved in the acid phase flowing from separator 1
PCTNB	weight % total nitrobody contained in the acid stream flowing from separator 1 to the after separator
PCTNBD	weight % dissolved nitrobody contained in the acid stream flowing from separator 1 to the after separator
PF (I,J)	moles/hr of component i in the organic phase of the organic stream flowing from separator j
PFLBS (I,J)	same as PF but in units of lb/hr

PF1(I)	moles/hr of component i in the organic phase of the organic stream flowing from separator 1
PF2(I)	same as PF1 but for separator 2
PF3(I)	same as PF1 but for separator 3
PF4(I)	same as PF1 but for separator 4
PF5(I)	same as PF1 but for separator 5
PF6(I)	same as PF1 but for separator 6
PI(I)	total organic phase moles/hr of component i flowing into a nitrator which is followed by another nitrator
PII(I)	total organic phase moles/hr of component i (less organic phase of internal recycle) flowing into a nitrator which is followed by another separator
PIR(I,J)	moles/hr of component i in the organic phase of the internal recycle stream flowing from separator j
PIRLBS(I,J)	same as PIR but in units of lb/hr
PIR1(I)	moles/hr of component i in the organic phase of the internal recycle stream flowing from separator 1
PIR2(I)	same as PIR1 but for separator 2
PIR3(I)	same as PIR1 but for separator 3
PIR4(I)	same as PIR1 but for separator 4
PIR5(I)	same as PIR1 but for separator 5
PIR6(I)	same as PIR1 but for separator 6

PNS	weight % nitrosylsulfuric acid in the acid phase of the external recycle stream flowing from a given separator
PØUNDS (I,J)	pounds of component i held up in the organic phase of vessel j
PT	total moles/hr of organic phase flowing from the vessel for which the holdup is being computed
PV (I,J)	moles/hr of component i in the total organic phase flowing from vessel j
PVI (I,J)	first guess at converged value of moles/hr of component i in the organic phase flowing from vessel j
PXR (I,J)	moles/hr of component i in the organic phase of the external recycle stream flowing from separator j
PXRLBS (I,J)	same as PXR but in units of lb/hr
PXR1 (I)	moles/hr of component i in the organic phase of the external recycle stream flowing from separator 1
PXR2 (I)	same as PXR1 but for separator 2
PXR2Ø (I)	previous value of PXR2 (I) to which current value is compared during the external recycle convergence procedure
PXR3 (I)	same as PXR1 but for separator 3
PXR3Ø (I)	same as PXR2Ø but for separator 3
PXR4 (I)	same as PXR1 but for separator 4
PXR4Ø (I)	same as PXR2Ø but for separator 4
PXR5 (I)	same as PXR1 but for separator 5
PXR5Ø (I)	same as PXR2Ø but for separator 5

PXR6 (I)	same as PXR1 but for separator 6
PXR60 (I)	same as PXR20 but for separator 6
P1A (I)	moles/hr of component i in the total organic phase flowing from nitrator 1A
P1AI	moles/hr toluene to nitrator 1A
P1B (I)	same as P1A but for nitrator 1B
P1BI	moles/hr toluene to nitrator 1B
P1S (I)	moles/hr of component i in the total organic phase flowing from separator 2
P2 (I)	moles/hr of component i in the total organic phase flowing from nitrator 2
P2S (I)	same as P1S but for separator 2
P3A (I)	same as P2 but for nitrator 3A
P3B (I)	same as P2 but for nitrator 3B
P3S (I)	same as P1S but for separator 3
P4 (I)	same as P2 but for nitrator 4
P4S (I)	same as P1S but for separator 4
P5 (I)	same as P2 but for nitrator 5
P5S (I)	same as P1S but for separator 5
P6 (I)	same as P2 but for nitrator 6
P6S (I)	same as P1S but for nitrator 6
Q	accumulation term used in calculation of nitrator heat loads

QA	ft^3/hr of total acid phase flowing from the vessel for which holdup is being computed
QP	same as QA but for organic phase
QQ(I)	fraction nitric acid converted to nitronium ion in vessel i
QT	ft^3/hr of total material flowing from the vessel for which holdup is being computed
R(I)	rate of reaction for reaction i in the vessel currently being simulated by SUBRØUTINE VESSEL
RATES(I,J)	rate of reaction for reaction j in nitrator i
RECN	moles/hr of ring associated NO_2 groups flowing into a nitration stage with the external recycle from the next higher stage
RHØ(I)	molar density of component i
RHØA	molar density of the acid phase in the vessel for which holdup is being calculated
RHØNBS(I)	mass density of the nitrobody dissolved in the acid phase of the external recycle stream flowing from the ith separator
RHØP	molar density of the organic phase in the vessel for which holdup is being calculated
RHØ1	equivalent to RHØ(1)
RHØ10	equivalent to RHØ(10)
RHØ11	equivalent to RHØ(11)
RHØ12	equivalent to RHØ(12)
RHØ13	equivalent to RHØ(13)

RHØ14	equivalent to RHØ(14)
RHØ2	equivalent to RHØ(2)
RHØ3	equivalent to RHØ(3)
RHØ4	equivalent to RHØ(4)
RHØ5	equivalent to RHØ(5)
RHØ6	equivalent to RHØ(6)
RHØ7	equivalent to RHØ(7)
RHØ8	equivalent to RHØ(8)
RHØ9	equivalent to RHØ(9)
RP	coefficient of the molecular oxygen term in reaction 9
RPP	precomputed constant based on RP which is used in material balance calculations
RR	ideal gas law constant
SA	adjustable constant. NOT USED
SB	equivalent to KMAP
SC	equivalent to AKEQ4 in SUBRØUTINE VESSEL
SD	adjustable constant. NOT USED
SE	equivalent to AK9. NOT USED
SG	equivalent to E9. NOT USED
SH	equivalent to AKEQ1 in SUBRØUTINE VESSEL
SI	adjustable constant. NOT USED

SJ	equivalent to AKEQ3 in SUBRØUTINE VESSEL
SNA (I)	net moles/hr of ring associated alpha NO_2 groups flowing through the ith nitration stage. Extent of alpha-nitration in nitration stage i
SNM (I)	same as SNA but for meta-nitration
SOL (I)	saturation solubility of total organic components in the acid phase of vessel i
SPA	mass flow rate of the acid phase of the external recycle stream (spent acid) from separator 1
SPACID	mass flow rate of the total external recycle stream from separator 1
SPP	mass flow rate of the organic phase of the external recycle stream from separator 1
STN	total flow rate (lb/hr) of strong nitric acid into the process from all raw material feed streams
SULP	total flow rate (lb/hr) of oleum into the process from all raw material feed streams
SUM	total molar flow rate of gasses evolved in the nitration stage for which material balance calculations are being executed. Also the moles/hr of organics flowing from separator 6 with the organic stream
SUMA	mass flow rate acid components of the acid phase from the after separator when the after separator option is used
SUMI	accumulation term for input streams used during material balance calculations (moles/hr)
SUMØ	mass flow rate of organic components in the acid phase from the after separator when the after separator option is used

S15	total moles/hr of $CO_{1.6}$ evolved in nitration section
S16	total moles/hr of NO_x evolved in the nitration section
S18	total moles/hr of TNM evolved in the nitration section
S19	total moles/hr of CO_2 evolved in the nitration section
TANB	total moles/hr of dissolved organics in the acid phase of the external recycle flowing from separator 1
TAS(I)	total acidity of the acid phase of the external recycle stream flowing from separator i
TATMI	total moles/hr of a given atomic specie entering that section of the process over which an elemental material balance is being computed
TATMØ	total moles/hr of a given atomic specie exiting that section of the process over which an elemental material balance is being computed
TAU	holdup time in a given vessel
TCØX	equivalent to S15
TCO2	equivalent to S19
TDNT	total mass flow rate of DNT in the organic stream from separator 6
TDNTA	total pounds of DNT held up in the acid phase of all process vessels
TDNTP	total pounds of DNT held up in the organic phase of all process vessels

TEMP (I)	temperature of the ith nitrator
TITLE (I)	alphanumeric identifying information for a given data set
TLBS	total lb/hr of acid components in the acid phase of the external recycle stream flowing from the separator for which acid composition calculations are being executed
TMØLES	same as TLBS but in units of moles/hr
TN (I)	weight % total nitric acid in the acid phase of the external recycle stream flowing from the ith separator on an organic free basis
TNØX	equivalent to S16
TNTI	moles/hr of TNT entering the nitration section with feed material
TØL	lb/hr toluene fed to the nitration section
TPNB	total moles/hr of organic components in the organic phase of the external recycle stream flowing from separator 1
TPØUND	accumulation term for total pounds of organic material held up in either the acid or organic phase of the vessel for which holdup calculations are being executed
TR	reference temperature
TS (I)	weight % total sulfuric acid plus SO_3 (as equivalent sulfuric) in the acid phase of the external recycle stream flowing from the ith separator on an organic free basis
TSEP (I)	temperature of the ith separator
TSEP1	equivalent to TSEP (1)

TSEP2	equivalent to TSEP (2)
TSEP3	equivalent to TSEP (3)
TSEP4	equivalent to TSEP (4)
TSEP5	equivalent to TSEP (5)
TSEP6	equivalent to TSEP (6)
TTDNT	total pounds of DNT held up in all process vessels
TTLBS (I)	total pounds of organic phase held up in the ith vessel
TTLBSA (I)	total pounds of organic components held up in the acid phase of the ith vessel
TTNM	equivalent to S18
TTNTA	total pounds of TNT held up in the acid phase of all process vessels
TTNTP	total pounds of TNT held up in the organic phase of all process vessels
TTTLBA	total pounds of organic components held up in the acid phase of all process vessels between and including nitrator 2 and separator 6
TTTLBS	total pounds of organic phase held up in all process vessels between and including nitrator 2 and separator 6
TTTNT	total pounds of TNT held up in all process vessels
TTTTLB	total pounds of organic components (in both acid and organic phases) held up in all process vessels between and including nitrator 2 and separator 6
TVØL	volumetric flow of the organic compounds in the acid phase of the external recycle stream flowing from a separator for which nitrobody density is being computed

T1A	temperature of nitrator 1A
T1B	temperature of nitrator 1B
T2	temperature of nitrator 2
T3A	temperature of nitrator 3A
T3B	temperature of nitrator 3B
T4	temperature of nitrator 4
T5	temperature of nitrator 5
T6	temperature of nitrator 6
V(I)	storage vector for current values of the i component flow terms generated in SUBRØUTINE VESSEL
VHØLDA	volume of acid phase held up in a given vessel
VHØLDØ	volume of organic phase held up in a given vessel
VKM(I)	working volume of the ith nitrator
VKMS	working volume of any separator
VØL(I)	working volume of the ith vessel
WKN	total flow rate (lb/hr) of weak nitric acid into the process from all raw material feed stream
XP(I,J)	mole fraction of component i in the organic phase within vessel j
XPA(I,J)	mole fraction of component i in the acid phase within vessel j
YELLØW(I)	moles/hr of component i in the yellow water fed to the after separator whenever the after separator option is chosen.

YIELD	moles α -TNT in the organic stream flowing from separator 6 per mole of toluene fed to the process (expressed as %)
ZA	temperature coefficient in the exponent of the Arrhenius rate law

Subroutine NITSEP

The definitions of the following variables are identical to those in the main program: AF(I,J), AF1(I), AI(I), AII(I), AIR(I,J), AIR1(I), AV(I,J), AXR(I), AXR1(I), DEL, EAØ(I), EAØP(I), EØA(I), EØAP(I), FACD(I), G15(I), G16(I), G18(I), G19(I), I, IAFT, ICHECK, IE, IFLG(I), IN, IPRNT, ISTGE, ITYPE, IV, NØ(I), PF(I,J), PF1(I), PI(I), PII(I), PIR(I,J), PIR1(I), PV(I,J), PXR(I), PXR1(I), RATES(I,J), SØL(I), TSEP(I), YELLOW(I),

Remaining variables are defined as follows:

AIRØ(I)	previous value of AIR(I,J) to which current value is compared during the internal recycle convergence procedure for stage j
ICOUNT	counter for iterations of internal recycle convergence loop
IVA	vessel index for separator 1 used whenever after separator is included in the simulation
IVØ	vessel index for the nitrator which preceeds the separator for which internal recycle convergence is being executed
PIRØ(I)	previous value of PIR(I,J) to which current value is compared during the internal recycle convergence procedure for stage j

Subroutine VESSEL

The definitions of the following variables are identical to those in the main program: AF(I,J), AI(I), AIR(I,J), AKA, AKEQ, AKEQOV, AKMA, AKMAP, AKMATL, AK10, AK12, AK3S, AK3W, AK4S, AK4W, AK4S, AK6S, AK7, AK8, AV(I,J), AXR(I,J), CP(I), DEL, DH(I), EAØ(I), EAØP(I), EØA(I), EØAP(I), E10, E12, E3S, E3W, E4S, E4W, E5S, E6S, E7, E8, FACD(I,J), FP, FMAX, G15(I), G16(I), G18(I), G19(I), I, IAFT, ICHECK, IE, III, IN, IPRINT, ISTGE, ITYPE, IV, J, MN(I), NØ(I), PF(I,J), PI(I), PIR(I,J), PV(I,J), PXR(I,J), QQ(I), R(I), RATES(I,J), RHØ1, RHØ10, RHØ12, RHØ13, RHØ14, RHØ2, RHØ3, RHØ4, RHØ5, RHØ6, RHØ7, RHØ8, RHØ9, RP, RR, SA, SB, SC, SD, SE, SG, SH, SI, SJ, SØL(I), TEMP(I), TR, TSEP(I), V(I), VKM(I), VKMS, YELLØW(I)

The definitions of the following variables are identical to other variables defined in the main program:

Variable in VESSEL	Variable in main program
AI1 thru AI17	AI(1) thru AI(17)
F1(I) thru F10(I)	G1(I) thru G10(I)
ISEP	ISTGE
PI1 thru PI17	PI(1) thru PI(17)
R1 thru R10	R(1) thru R(10)

Remaining variables are defined as follows:

A(I)	moles/hr of component i in the acid phase flowing from the vessel currently being simulated
AINB	moles/hr of organic components in the combined acid phase flowing to the vessel currently being simulated
AKEQ1	equilibrium constant for the dissociation of nitric acid in aqueous sulfuric acid
AKEQ2	equilibrium constant for the dissociation of sullfuric acid in an aqueous system
AKEQ3	equilibirum constant for dissociation of nitric acid in anhydrous sulfuric acid

AKEQ4	equilibrium constant for the recombination of nitronium and bisulfate ions in anydrous acid mixtures
AK1	computed value of AKEQ1 obtained from interval halving procedure
AK3	computed value of AKEQ3 obtained from interval halving procedure
AK4	computed value of AKEQ4 obtained from interval halving procedure
AL	moles/hr water in the acid phase flowing from the vessel currently being simulated; negative values represent moles/hr SO_3
AM(I)	moles/hr of component i transferred from the organic phase into the acid phase by bulk mass transfer in the vessel currently being simulated. Used in check calculations only
AMNB	total moles/hr of organic components transferred from the organic to acid phase by bulk mass transfer in the vessel currently being simulated
AM1	moles/hr α -MNT transferred from the organic phase into the acid phase by bulk mass transfer in the vessel currently being simulated
ANB	moles/hr organic components in the acid phase flowing from the vessel currently being simulated
ASØ4	combined moles/hr of H_2SO_4 and SO_3 in the acid phase flowing from the vessel currently being simulated
AT	total moles/hr of acid phase flowing from the vessel currently being simulated
ATI	reciprocal of AT

AXL	same as AL but used only in check calculations
AX1	1. + C1A-CA
AX1 thru AX9	same as A1 thru A9 but used only in check calculations
AX12	same as A12 but used only in check calculations
A1	moles/hr α MNT in the acid phase flowing from the vessel currently being simulated
A2	same as A1 but for m MNT
A3	same as A1 but for α DNT
A4	same as A1 but for m MNT
A5	same as A1 but for α TNT
A6	same as A1 but for m TNT
A7	same as A1 but for TNBX
A8	same as A1 but for TNB
A9	moles/hr nitric acid in the acid phase flowing from the vessel currently being simulated
A11	same as A9 but for H_2SO_4
A12	same as A9 but for nitrosylsulfuric acid
A13	same as A9 but for water
A14	same as A9 but for SO_3
A17	moles/hr nitronium ion in the acid phase flowing from the vessel currently being simulated
B	free sulfuric acid concentration in oleum in the vessel currently being simulated

BC	B + (3 x C)
B1	term representing moles/hr of an organic component flowing into a vessel with the combined acid phase plus the amount of that component formed by reaction
B2	moles/hr of an organic component flowing into a vessel with the combined organic phase
C	concentration of pyrosulfuric acid in the vessel currently being simulated
CA	ratio of AMNB to ANB (constant used in determining bulk mass transfer during simulataneous solution of vessel equations)
CB	(.5 x B) + (1.5 x C)
CF	C - F
CHNØ3	equilibrium concentration of nitric acid in the acid phase of the vessel currently being simulated (moles/cf^3)
CHSØ4	same as CHNØ3 but for bisulfate ion
CHS2Ø7	same as CHNØ3 but for pyrosulfate ion
CH2Ø	same as CHNØ3 but for water
CH2SO4	same as CHNØ3 but for sulfuric acid
CH3Ø	same as CHNØ3 but for hydronium ion
CNØ2	same as CHNØ3 but for nitronium ion
CR	ratio of AMNB to PNB. Constant used in determination of bulk mass transfer during simultaneous solution of vessel equations
CVØL	computed volumetric flow of an internal recycle stream based on entrainment correlation

CXX	correlation used to determine fraction organic entrained in the internal recycle stream
CX2	ratio of fraction internal recycle to fraction external recycle used in entrainment correlation
C1	equal to overall mass transfer coefficient (ETA) during simultaneous solution of vessel equations
C1A	coefficient equal to C1/ANB used during simultaneous solution of vessel equations
C1Ø	coefficient equal to C1/PNB used during simultaneous solution of vessel equations
C1P	coefficient related to toluene diffusion which is used during simultaneous solution of vessel equations
C11	coefficient equal to acid phase mass transfer plus the sum of the reaction coefficients used during simultaneous solution of the vessel equations
C12	coefficient equal to (- C1Ø - CR) used during simultaneous solution of the vessel equations
C21	coefficient equal to (CA - C1A) used during simultaneous solution of the vessel equations
C22	coefficient equal to (1 + C1Ø + CR) used during simultaneous solution of the vessel equations
C4	equal to the sum of reaction rates R1 thru R6. Represents the moles/hr water produced by reactions 1 thru 6
C5	moles/hr nitrosylsulfuric acid produced by oxidation reactions
C5P	net moles/hr nitrosylsulfuric acid produced after decomposition takes place

C6	organic phase nitric acid solubility coefficient
DD(I)	rate of diffusion of organic component i. Used only in check calculations
DLA	convergence tolerance for components in both acid and organic phases flowing from the vessel currently being simulated
DRM	difference in molar densities between the acid and organic phases used in the entrainment correlation
D1	moles/hr of α MNT which diffuse from the organic into the acid phase in the vessel currently being simulated. Negative values means diffusion is from acid to organic phase
D10	moles/hr of toluene which diffuse from the bulk organic phase to the acid-organic interface
D2	same as D1 but for mMNT
D3	same as D1 but for α DNT
D4	same as D1 but for mDNT
D5	same as D1 but for α TNT
D6	same as D1 but for mTNT
D7	same as D1 but for TNBX
D8	same as D1 but for TNB
EAØ4	molar ratio of acid phase in the organic stream to total organic stream, based on the entrainment correlation
ETA	overall mass transfer coefficient in the vessel currently being simulated

ETAA	acid phase mass transfer coefficient in the vessel currently being simulated
ETAP	organic phase mass transfer coefficient in the vessel currently being simulated
ETATL	mass transfer coefficient for toluene in the organic phase
EXX	ratio acid phase to organic phase in the organic stream, based on the entrainment correlation
F	initial concentration of nitric acid prior to establishment of equilibrium conditions in the vessel currently being simulated
FA	volume fraction acid phase in the vessel currently being simulated
FACT	relaxation factor used in convergence procedure for composition of phases flowing from the vessel currently being simulated
FAR	fraction of the total acid phase flowing from a separator that is recycled for the separator currently being simulated
FAR1	fraction of the total acid phase flowing from a separator that is entrained in the organic stream which flows to the next nitrator for the separator currently being simulated
FC	constant equal to (2 x F) - C used in computation of nitronium ion equilibrium concentration in region 2 for the vessel currently being simulated
FF(I)	cross sectional area fraction corresponding to the ith notch setting on the gate valve in the internal recycle line of the separator currently being simulated

FHG	upper boundary value of internal recycle fraction computed using the entrainment coefficient
FIR	internal recycle fraction computed using the entrainment correlation for the separator currently being simulated
FLW	same as FHG except lower boundary value
FØG	molar ratio of organic phase in the acid recycle streams to total organic phase flowing from the separator currently being simulated (based on entrainment correlation)
FOGC	current value of FØG
FP	volume fraction of organic phase in the vessel currently being simulated
FPØ	molar fraction of the total organic phase flowing from a separator which appears in the organic stream for the separator currently being simulated
FPØ1	molar fraction of the total organic phase flowing from a separator which appears in the recycled acid streams for the separator currently being simulated
FR	volume fraction of the combined recycled acid streams which is external recycle for the separator currently being simulated
FRAC	volume fraction of the combined recycled acid streams which is internal recycle for the separator currently being simulated
FVKM	volume of the vessel currently being simulated
GAMMA	acid concentration factor for all nitration reactions in the vessel currently being simulated

G1	equivalent to F1(I) where I is the index of the nitrator currently being simulated or the index of the nitrator preceding the separator currently being simulated
G10	same as G1 but for F10(I)
G10P	rate of reaction 10 per mole of TNT in the acid phase flowing from the vessel currently being simulated
G15P	equivalent to G15(I) where I is the index of the vessel currently being simulated
G3	same as G1 but for F3(I)
G3D	rate of reaction 3 per mole of α MNT in the acid phase flowing from the vessel currently being simulated
G3S	same as G1 but for F3S(I)
G4	same as G1 but for F4(I)
G4D	rate of reaction 4 per mole of mMNT in the acid phase flowing from the vessel currently being simulated
G4S	same as G1 but for F4S(I)
G5	same as G1 but for F5(I)
G5G	rate of reaction 5 per mole of α DNT in the acid phase flowing from the vessel currently being simulated
G6	same as G1 but for F6(I)
G6G	rate of reaction 6 per mole of mDNT in the acid phase flowing from the vessel currently being simulated

G7	same as G1 but for F7(I)
G7G	rate of reaction 7 per mole of DNT in the acid phase flowing from the vessel currently being simulated
G8	same as G1 but for F8(I)
G8P	rate of reaction 8 per mole of DNT in the acid phase flowing from the vessel currently being simulated
G9	same as G1 but for F9(I)
G9G	zero
ICØUNT	number of passes made through suoroutine VESSEL during a particular convergence iteration for the vessel currently being simulated
ITR	number of convergence iterations executed for the vessel currently being simulated. Five iterations, each consisting of NC passes through VESSEL are allowed
MWAVGA	average molecular weight of the acid phase flowing from the separator which is being simulated and for which entrainment is being determined via the correlation
MWAVGP	same as MWAVGA but for the organic phase
NC	maximum number of passes through VESSEL allowed per iteration during vessel equation convergence procedure
NØTCH	value of NØ(I) where I is the index of the separator currently being simulated
P(I)	moles/hr of component i in the organic phase flowing from the vessel currently being simulated

PNB	moles/hr of combined organic components in the organic phase flowing from the vessel currently being simulated
PP	exponent of the nitrobody-in-acid solubility correlation
PT	moles/hr of combined organic components in both the acid and organic phases flowing from the vessel currently being simulated
PTI	the reciprocal of PT. Used for computation of entrainment via the correlation
PX(I)	same as P(I) for components 1 thru 8 but used only in check calculations
PX10	same as P(10) but used only in check calculations
PX9	same as P(9) but used only in check calculations
P1	moles/hr α MNT in the organic phase flowing from the vessel currently being simulated
P10	same as P1 but for toluene
P2	same as P1 but for mMNT
P3	same as P1 but for α DNT
P4	same as P1 but for mDNT
P5	same as P1 but for α TNT
P6	same as P1 but for mTNT
P7	same as P1 but for TNBX
P8	same as P1 but for TNB
P9	same as P1 but for nitric acid

Q	fraction of molecular nitric acid converted to nitronium ion in the vessel currently being simulated
QA	ft^3/hr of acid phase flowing from the vessel currently being simulated
QP	ft^3/hr of organic phase flowing from the vessel currently being simulated
QT	volumetric flow (ft^3/hr) of combined internal plus external recycle streams flowing from the separator currently being simulated
RHLØ	mass density (lb/ft^3) of the organic phase flowing from the separator currently being simulated and for which entrainment is being determined via the correlation
RHØØ	same as RHLØ but molar density ($moles/ft^3$)
RR1	same as R1 but used only for check calculation
RR10	same as R10 but used only for check calculation
RR3	same as RR1 but for R3
RR7	same as RR1 but for R7
RR8	same as RR1 but for R8
RR9	same as RR1 but for R9
RR9G	same as RR1 but for R9G
RTL	mass ratio of organic to acid phase in the separator currently being simulated and for which entrainment is being calculated via the correlation
RTØ	same as RTL but molar ratio

RVØL	maximum volumetric flow of internal recycle stream possible for a given notch setting in the separator currently being simulated and for which entrainment is being calculated via the correlation
R10A	rate of reaction 10 for α TNT in the vessel currently being simulated
R10M	rate of reaction 10 for mTNT in the vessel currently being simulated
R7A	rate of reaction 7 for mDNT in the vessel currently being simulated
R8A	rate of reaction 8 for α DNT in the vessel currently being simulated
R8M	rate of reation 8 for mDNT in the vessel currently being simulated
R9G	zero
R9GA	zero
R9GM	zero
S	initial concentration (moles/ft^3) of total sulfuric acid in the acid phase of the vessel currently being simulated
SANB	same as ANB but used only in check calculations
SANBC	same as SANB but based on computed solubility
SPNB	same as PNB but used only in check calculations
SUM	sum of the individual organic component diffusions used only in the check calculations
TAF	moles/hr of entrained acid phase (based on the correlation) contained in the organic stream flowing from the separator currently being simulated

TAIR	moles/hr of acid phase (based on the correlation) contained in the internal recycle stream flowing from the separator currently being simulated
TAR	moles/hr of acid phase (based on the correlation) contained in the combined internal and external recycle streams flowing from the separator currently being simulated
TAXR	moles/hr of acid phase (based on the correlation) contained in the external recycle stream flowing from the separator currently being simulated
TKEL	temperature (in Degrees Kelvin) of the vessel currently being simulated
TLI	total mass flow (lb/hr) through the separator currently being simulated and for which entrainment is being computed via the correlation
TPF	moles/hr of organic phase (based on the correlation) contained in the organic stream flowing from the separator currently being simulated
TPIR	moles/hr of entrained organic phase (based on the correlation) contained in the internal recycle stream flowing from the separator currently being simulated
TPR	moles/hr of entrained organic phase (based on the correlation) contained in the combined recycle streams flowing from the separator currently being simulated
TPXR	moles/hr of entrained organic phase (based on the correlation) contained in the external recycle stream flowing from the separator currently being simulated

VØ(I)	storage vector for the values of the i component molar flows generator on the previous pass through VESSEL for the vessel currently being simulated
W	concentration (moles/ft^3) of water in the vessel currently being simulated
X	computed equilibrium concentration of nitronium ion in the acid phase under aqueous conditions and under conditions of oleum region 3. Also equilibrium concentration at molecular nitric acid in oleum region 2
XA	NOT USED
XB	NOT USED
XC	NOT USED
AD	NOT USED
XE	NOT USED
XEQA	equilibrium solubility of organic material (nitrobody) in the acid phase of the vessel currently being simulated
XF	NOT USED
XL	Lower boundary value used in an interval halving convergence procedure
XU	upper boundary valued used in an interval halving convergence procedure
X1	mole fraction α MNT in the acid phase of the vessel currently being simulated
X11	same as X1 but for sulfuric acid
X12	same as X1 but for nitrosylsulfuric acid

X13	same as X1 but for water
X14	same as X1 but for SO_3
X2	same as X1 but for mMNT
X3	same as X1 but for α DNT
X4	same as X1 but for mDNT
X5	same as X1 but for α TNT
X6	same as X1 but for mTNT
X7	same as X1 but for TNBX
X8	same as X1 but for TNB
X9	same as X1 but for nitric acid
Y	equilibrium concentration of the pyrosulfate ion in the acid phase of the vessel being simulated under conditons of oleum region 3
YL	lower boundary value used in an interval halving convergence procedure
YU	upper boundary value used in an interval halving convergence procedure
Y1	mole fraction of α MNT in the organic phase of the vessel currently being simulated
Y10	same as Y1 but for toluene
Y2	same as Y1 but for mMNT
Y3	same as Y1 but for α DNT
Y4	same as Y1 but for mDNT
Y5	same as Y1 but for α TNT

Y6	same as Y1 but for MTNT
Y7	same as Y1 but for TNBX
Y8	same as Y1 but for TNB
Y9	same as Y1 but for nitric acid
ZA	diffusion coefficient for organic components in the organic phase
ZB	diffusion coefficient for organic components in the acid phase

Function ENTH

The definitions of the following variables are identical to those in the main program: AKA, AKEQ, AKMA, AKMATL, AK10, AK12, AK3S, AK3W, AK4S, AK4W, AK5S, AK6S, AK7, AK8, CP(I), DH(I), E10, E21, E3S, E3W, E4S, E4W, E5S, E6S, E7, E8, FD, FMAX, RHØ1, RHØ10, RHØ11, RHØ12, RHØ13, RHØ14, RHØ2, RHØ3, RHØ4, RHØ5, RHØ6, RHØ7, RHØ8, RHØ9, RP, RR, SA, SB, SC, SD, SE, SG, SH, SI, SJ, TR

Remaining variables are defined as follows:

A(I)	moles/hr of component I in the acid phase of the stream for which the enthalpy is currently being calculated
CP11	equivalent to CP(11)
CP12	equivalent to CP(12)
CP13	equivalent to CP(13)
CP14	equivalent to CP(14)
CP9	equivalent to CP(9)
DLT	temperature of the vessel (relative to 20°C) for which the enthalpy of a particular exiting stream is currently being calculated

ENTH	enthalpy of the stream currently being calculated (kcal/hr)
ENTHØ	enthalpy of mixing of the acid components in the acid phase of the stream currently being calculated based on the zero nitric curve of the McKinley and Brown data (kcal/lb)
ENTH2	same as ENTHØ but based on the 20% nitric curve
F	adjusted weight fraction (nitrobody free basis) of nitric plus equivalent sulfuric acid in the acid phase of the stream currently being calculated
I	general index integer
J	general index integer
LBS	lb/hr of nitric acid, sulfuric acid, water and SO_3 flowing with the acid phase of the stream for which the enthalpy is currently being calculated
LBSE	lb/hr of nitric acid plus equivalent sulfuric acid in the acid phase of the stream for which the enthalpy is currently being calculated
P(I)	moles/hr of component i in the organic phase of the stream for which the enthalpy is currently being calculated
T	moles/hr of a given organic component in the combined acid and organic phases (i.e., in the total stream) of the stream for which the enthalpy is currently being calculated
TP	temperature of the vessel for which the enthalpy of a particular exiting stream is being calculated
WTA	LBSE/LBS; nitrobody free weight fraction of nitric plus equivalent sulfuric acid in the acid phase of the stream for which the enthalpy is currently being calculated

WTN	weight fraction of nitric acid in the nitric plus equivalent sulfuric acid portion of the acid phase of the stream for which the enthalpy is currently being calculated
X(I)	the ith data point on the zero % nitric curve from the enthalpy-concentration data of McKinley and Brown
Y(I)	the ith data point on the 20% nitric curve form the enthalpy-concentration data of McKinley and Brown

APPENDIX I

Steady State Simulation--Input Data Format

CARD	DATA READ	FORMAT
1	AK12, AK3W, AK4W, AK5S, AK6S, AK7, AK8, AK10	8F10.0
2	AK3S, AK4S, E3S, E4S	8F10.0
3	E21, E3W, E4W, E5S, E6S, E7, E8, E10	8F10.0
4	SA, SB, SC, SE, SG, SH, SI	8F10.0
5	SJ, RR, TR, AKMA, AKMATL, FMAX FD, RP	8F10.0
6	AKA, AKS, AKC, AKEQ, AKEQOV, FOV	8F10.0
7, 8	AVI(I,1), I=1,14	8F10.0/8F10.0
9,10	PVI(I,1), I=1,14	8F10.0/8F10.0
11,12	AVI(I,2), I=1,14	8F10.0/8F10.0
13,14	PVI(I,2), I=1,14	8F10.0/8F10.0
15,16	AVI(I,3), I=1,14	8F10.0/8F10.0
17,18	PVI(I,3), I=1,14	8F10.0/8F10.0
19,20	AVI(I,4), I=1,14	8F10.0/8F10.0
21,22	PVI(I,4), I=1,14	8F10.0/8F10.0
23,24	AVI(I,5), I=1,14	8F10.0/8F10.0
25,26	PVI(I,5), I=1,14	8F10.0/8F10.0
27,28	AVI(I,6), I=1,14	8F10.0/8F10.0
29,30	PVI(I,6), I=1,14	8F10.0/8F10.0
31,32	AVI(I,7), I=1,14	8F10.0/8F10.0
33,34	PVI(I,7), I=1,14	8F10.0/8F10.0
35,36	AVI(I,8), I=1,14	8F10.0/8F10.0
37,38	PVI(I,8), I=1,14	8F10.0/8F10.0
39,40	AVI(I,9), I=1,14	8F10.0/8F10.0
41,42	PVI(I,9), I=1,14	8F10.0/8F10.0
43,44	AVI(I,10), I=1,14	8F10.0/8F10.0

CARD	DATA READ	FORMAT
45,46	PVI(I,10), I=1,14	8F10.0/6F10.0
47,48	AVI(I,11), I=1,14	8F10.0/6F10.0
49,50	PVI(I,11), I=1,14	8F10.0/6F10.0
51,52	AVI(I,12), I=1,14	8F10.0/6F10.0
53,54	PVI(I,12), I=1,14	8F10.0/6F10.0
55,56	AVI(I,13), I=1,14	8F10.0/6F10.0
57,58	PVI(I,13), I=1,14	8F10.0/6F10.0
59,60	AVI(I,14), I=1,14	8F10.0/6F10.0
61,62	PVI(I,14), I=1,14	8F10.0/6F10.0
63	FACT 6, FACT 5, FACT 4, FACT 3, FACT 2	5F10.0
64	NDA	I2
65	TITLE	20A4
66	IPRNT, EI, ILIST, IMBAL, IPI, IAFT, IPNCH, ICHECK	9I1
67	FIN(1,J), J=1,8	8F10.0
68	FIN(2,J), J=1,8	8F10.0
69	FIN(3,J), J=1,8	8F10.0
70	FIN(4,J), J=1,8	8F10.0
71	FIN(5,J), J-1,8	8F10.0
72	FIN(6,J), J=1,8	8F10.0
73	FIN(7,J), J=1,8	8F10.0
74-83	((COMP(J,I), I=1,14), J=1,5)	8F10.0/6F10.0
84	NO(I), I=1,6	6I
85	TEMP(I), I=1,8	8F10.0
86	VKM(I), I=1,8	8F10.0
87	VKMS	F10.0
88	EAO(I), I=1,6	6F10.0
89	EOA(I), I=1,6	6F10.0

APPENDIX J

Parameter Fitting

Preceding page blank

Table J1

Nitration snapshot

B-Line - 8/18/71 - 1:30 pm

	Nitrator Temperature	Separator Temperature	Recycle Setting	Weak Nitric Flows, lbs/hr	Strong Nitric Flows, lbs/hr
1A	51	51		500 from Fume Recovery 2445 from SAR	
1B	44	51	1		
2	76	66	1	3467 from SAR	
3A	80				7
3B	86	78	5		43
4	89	94	2		202
5	96	103	2		144
6	104	104	1		1118
Toluene	2418 lbs/hr		No fresh water added		
Oleum	12300 lbs/hr		Yellow water to 1A - 1200 lbs/hr		

Acid Analysis - Acid Phase

	Yellow Water	Spent	1B	2	3B	4	5	6
Total Acidity	11.97	74.68	72.78	88.49	98.26	100.86	103.28	103.17
Total Sulfuric	8.28	67.22	66.67	78.65	84.93	88.32	90.53	90.95
Actual Nitric	4.76	3.63	5.89	10.60	13.86	13.97	15.15	15.42
$HNOSO_4$		12.00	1.96	4.11	6.58	4.33	2.50	0.57
Water	86.98	26.41	26.54	9.81	-0.29	-3.28	-6.16	-6.50
Nitrobody		0.38	0.49	7.12	23.18	16.12	19.04	20.27
Acid Density			1.619	1.716		1.786	1.798	1.790

Table J1 (Cont'd)

Acid Analysis - Nitrobody Phase

	1B	2	3B	4	5	6
Total Acidity	4.88	9.37	4.88	1.06	0.71	0.16
Total Sulfuric	0.70	1.51	1.54	0.61	0.60	0.12
Actual Nitric	4.97	9.98	3.96	0.28	0.14	0.05
$HNOSO_4$	0.81	0.24	0.66	0.66	0.33	0
Water and Nitrobody	99.42	88.33	93.99	98.99	99.17	99.83
Separator Density	1.208	1.366	1.430			

Gas Analysis

	Gas Chromatography - Percentage by Volume					MSA Billionaire		Total Toluene
	CO_2	O_2	N_2	CO	N_2O	NO_x	TNM	Loss
Sample 1	6.89	17.62	63.38	5.07	0.46	3.0	610	7.5
Sample 2	6.24	17.84	63.31	4.21	0.37	3.2	490	6.5

Total Gas Flow - 687 cu ft/min

Acid Phase

Oxidation Products (Wt $)

Compound	Spent Acid	1B	2	3B	4	5	6
Trinitrobenzene	0.50	0.04	0.22	0.14	0.02	0.01	

Table J1 (Cont'd)

Nitrobody in Acid Phase

Compound	Spent Acid	1B	2	3B	4	5	6
2-MNT	25.67	43.93					
3-MNT	1.94	3.04					
4-MNT	19.04	28.36					
TOTAL MNT	46.65	75.33					
*PNM	2.06						
2,6-DNT	5.72	3.67	10.63	3.28	0.54	0.06	0.01
2,5-DNT	0.19	0.07	0.56	0.31	0.12	0.03	0.05
2,4-DNT	33.03	16.75	84.50	36.42	10.99	1.50	0.16
3,5-DNT				0.03	0.01		0.04
3,4-DNT			0.84	0.37	0.05	0.01	
TOTAL DNT	38.94	20.49	96.53	40.41	11.71	1.60	0.26
2,4,6-TNT	11.84	4.13	2.85	57.89	86.20	95.72	96.69
2,3,5-TNT				0.02	0.02	0.04	0.05
2,4,5-TNT			0.33	1.16	1.49	1.76	2.02
2,3,4-TNT			0.06	0.39	0.57	0.84	1.01
TOTAL TNT	11.84	4.13	3.24	59.46	88.28	98.36	99.72

*PNM – phenylnitromethane resulting from methyl group nitration of toluene

Table J1 (Cont'd)

Nitrobody Phase

Oxidation Products (Wt %)

Compound	1B	2	3B	4	5	6
Trinitrobenzene	0.02	0.30	0.37	0.25	0.19	0.08

Analysis of Nitrobody Phase

Compound	1B	2	3B	4	5	6
Toluene	0.28					
2-MNT	45.98					
3-MNT	2.87					
4-MNT	28.26					
TOTAL MNT	77.11					
2,6-DNT	2.31	10.99	4.13	0.89	0.10	0.01
2,5-DNT	0.12	0.47	0.13	0.13	0.04	0.01
2,4-DNT	15.65	58.12	25.35	9.12	1.47	0.16
3,5-DNT			0.02	0.01	0.001	0.04
3,4-DNT	0.12	1.28	0.55	0.12	0.01	
TOTAL DNT	18.20	70.86	30.36	10.27	1.62	0.22
2,4,6-TNT	4.23	28.50	66.92	86.39	94.64	96.00
2,3,5-TNT			0.02	0.03	0.05	0.06
2,4,5-TNT		0.25	1.64	2.85	2.29	2.32
2,3,4-TNT		0.10	0.69	1.02	1.22	1.33
TOTAL TNT	4.23	28.85	69.27	89.49	98.20	99.71
Separator - Density	1.208	1.366	1.430			

Table J2

Final values of parameters

Parameter	Coded Name	Value	Units
k_{12}	AK12	88.9	dimensionless
k_{3s}	AK3S	1.8×10^{7}	hr^{-1}
k_{4s}	AK4S	1.0×10^{7}	hr^{-1}
k_{55s}	AK5S	124.5	hr^{-1}
k_{6s}	AK6S	506.8	hr^{-1}
k_{7}	AK7	.09	hr^{-1}
k_{8}	AK8	2.1	hr^{-1}
k_{10}	AK10	.001	hr^{-1}
k_{a}	AKA	.2	$(ft^3)\ (lb\text{-}moles)^{-1}$
K_{eq1}	SH	.03	$(lb\text{-}moles)\ (ft^3)^{-1}$
K_{eq2}	AKEQ	50.	dimensionless
K_{eq3}	SJ	6.0×10^{4}	$(lb\text{-}moles)^3\ (ft^3)^{-2}$
K_{eq4}	SC	0.	$(ft^3)\ (lb\text{-}moles)^{-1}$
E_{21}	E21	88.9	$(Kcal)\ (lb\text{-}mole)^{-1}$
E_{3s}	E3S	2.2×10^{4}	$(Kcal)\ (lb\text{-}mole)^{-1}$
E_{4s}	E4S	1.0×10^{4}	$(Kcal)\ (lb\text{-}mole)^{-1}$
E_{5s}	E5S	9.3×10^{3}	$(Kcal)\ (lb\text{-}mole)^{-1}$
E_{6s}	E6S	6.5×10^{3}	$(Kcal)\ (lb\text{-}mole)^{-1}$
E_{7}	E7	$5.0 \times 4 \times 10^{3}$	$(Kcal)\ (lb\text{-}mole)^{-1}$

Parameter	Coded Name	Value	Units
E_8	E8	7.0×10^3	$(\text{Kcal})\,(\text{lb-mole})^{-1}$
E_{10}	E10	1.0	$(\text{Kcal})\,(\text{lb-mole})^{-1}$
$k_m a$	AKMA	2.75×10^4	$[(\text{lb-moles})\,(\text{hr})^{-1}(\text{ft}^3)^{-1}] \times [(\text{ft}^3)\,(\text{ft}^3)^{-1}]$
$(k_m a)_p$	AKMAP	1.55×10^4	$[(\text{lb-moles})\,(\text{hr})^{-1}(\text{ft}^3)^{-1}] \times [(\text{ft}^3)\,(\text{ft}^3)^{-1}]$
$(k_m a)_{Tol}$	AKMATL	5.0×10^3	$[(\text{lb-mole})\,(\text{hr})^{-1}(\text{ft}^3)^{-1}] \times [(\text{ft}^3)\,(\text{ft}^3)^{-1}]$
i	SI	1.51	dimensionless
F_D	FD	.65	dimensionless
RP	RP	.6	dimensionless

APPENDIX K

Steady State Optimization

Preceding page blank

Table K1

Independent variables

Variable	Rank
Weak Nitric Acid to 1A	6
Weak Nitric Acid to 1B	20
Weak Nitric Acid to 2	5
Fume Recovery Nitric Acid to 1A	18
Fume Recovery Nitric Acid to 1B	19
Yellow Water to 1A	22
Yellow Water to 1B	28
Yellow Water to 2	17
Fresh Water to 1A	26
Fresh Water to 2	27
Strong Nitric Acid to 3A	4
Strong Nitric Acid to 3B	12
Strong Nitric Acid to 4	3
Strong Nitric Acid to 5	11
Strong Nitric Acid to 6	2
Oleum to 6	1
Concentration of Weak Nitric Acid	13
Concentration of Fume Recovery Nitric Acid	10
Concentration of Strong Nitric Acid	9
Sulfuric Content of Oleum	8
Temperature of Nitrator 1A	7
Temperature of Nitrator 1B	25
Temperature of Nitrator 2	21
Temperature of Nitrator 3A	14
Temperature of Nitrator 3B	15

Table K1 (Cont'd)

Variable	Rank
Temperature of Nitrator 4	23
Temperature of Nitrator 5	24
Temperature of Nitrator 6	16
Recycle Valve Notch Setting in Separator 1	32
Recycle Valve Notch Setting in Separator 2	31
Recycle Valve Notch Setting in Separator 3	29
Recycle Valve Notch Setting in Separator 4	30
Recycle Valve Notch Setting in Separator 5	33
Recycle Valve Notch Setting in Separator 6	34

Table K2

Constraint list

1. % DNT in Crude TNT must be less than .4
2. % Dissolved Nitrobody in Spent Acid $\leq$ .5
3. % DNT in Dissolved Nitrobody $\leq$ 55.
4. Weak Nitric Concentration $\leq$ 61%
5. Fume Recovery Concentration $\leq$ 88%
6. Strong Nitric Concentration $\leq$ 99%
7. % H_2SO_4 in Oleum $\geq$ 57%
8. Wt % Actual Nitric (AN) in stages 3-6 $\leq$ 16
9. AN(3) $\geq$ 7
10. AN(4) $\geq$ 8
11. AN(5,6) $\geq$ 10
12. AN(1) $\leq$ 6
13. AN(2) $\leq$ 11
14. AN(1) $\geq$ 2.5
15. AN(2) $\geq$ 4.5
16. 20. $\leq$ [Temperature of Nitrator 1A (T1A)]
17. 20. $\leq$ T1B $\leq$ 60. °C
18. 50. $\leq$ T2 $\leq$ 70. °C
19. 60. $\leq$ T3A $\leq$ 100. °C
20. 60. $\leq$ T3B $\leq$ 100. °C
21. 70. $\leq$ T4 $\leq$ 110. °C
22. 80. $\leq$ T5 $\leq$ 115. °C
23. 90. $\leq$ T6 $\leq$ 120. °C
24. Heat Load in Nitrator 1A $\leq 2.5 \times 10^6$ BTU/hr
25. 68. $\leq$ (% Total Acidity of Spent Acid) $\leq$ 72.

Table K3

Optimum operating conditions

Basis: 59.2 tons/day production rate
10000 lb/hr oleum feed rate

Nitrator	1A	1B	2	3A	3B	4	5	6
Weak Nitric	2000		1900					
Fume Recovery Nitric	600							
Yellow Water	1000							
Strong Nitric				600	500	400	100	1100
Oleum								10000
Toluene	1763	567						
Temperature	51	33	64	83	85	90	95	110

Stage	Actual Nitric	Total Acidity
1	3.1	70.9
2	6.1	85.0
3	11.1	93.6
4	13.5	101.2
5	13.6	103.6
6	13.9	104.2

Yield = 89.2%
DNT in crude TNT = .17%
Wt % dissolved nitrobody in spent acid = .3
Wt % of dissolved nitrobody which is DNT = 19.7
Raw Material Cost = 5.45¢/lb TNT

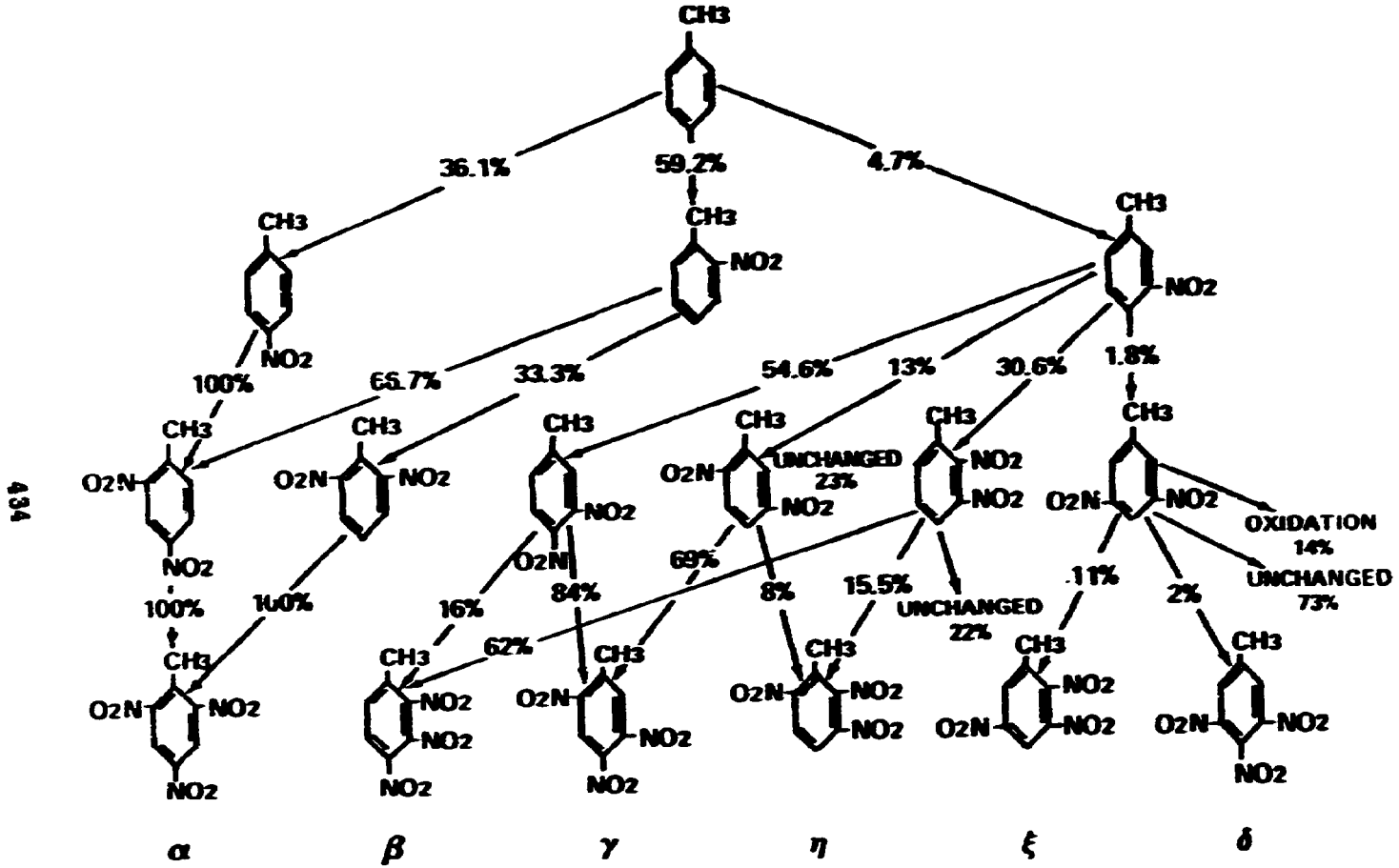


Fig 1 Isomers formed during toluene nitration

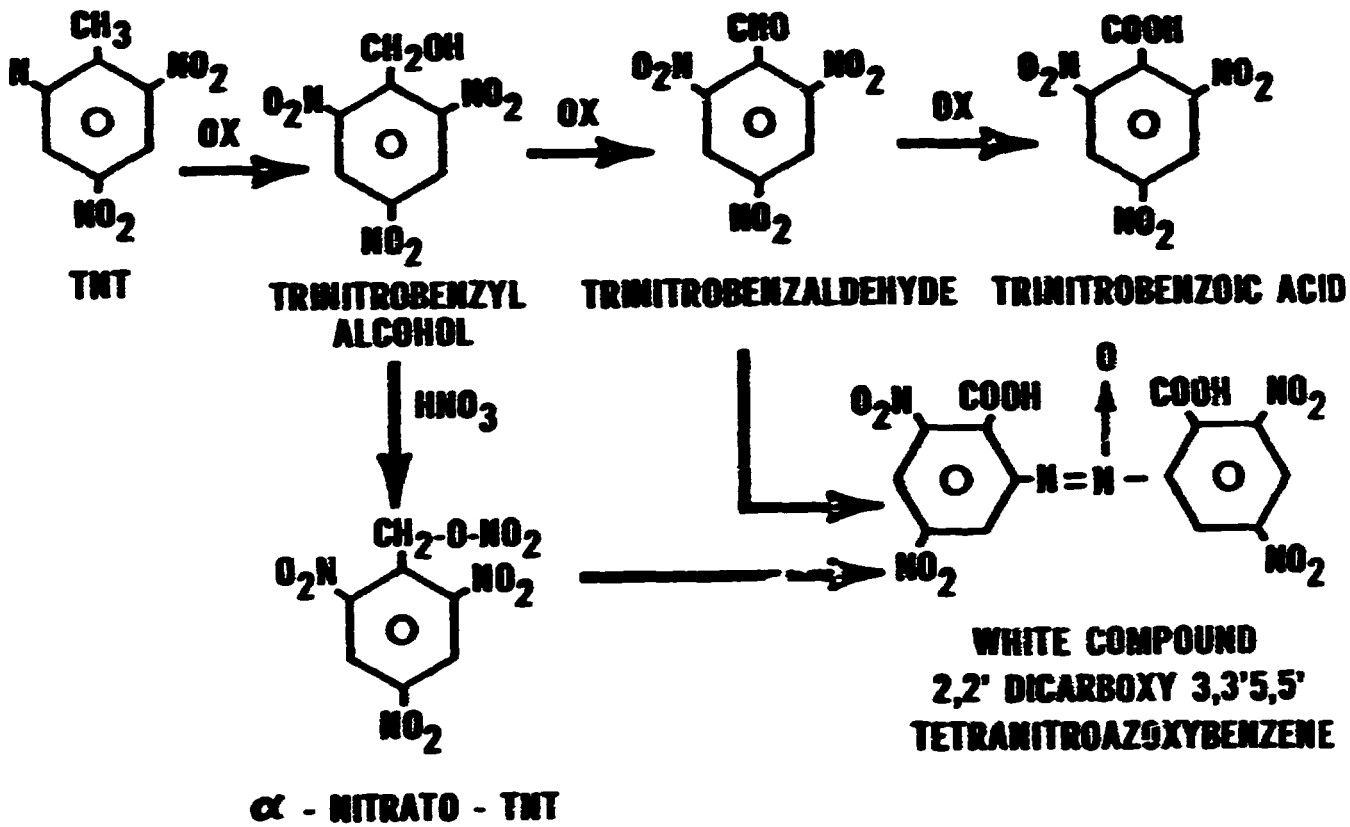


Fig 2 Oxidation of trinitrotoluene

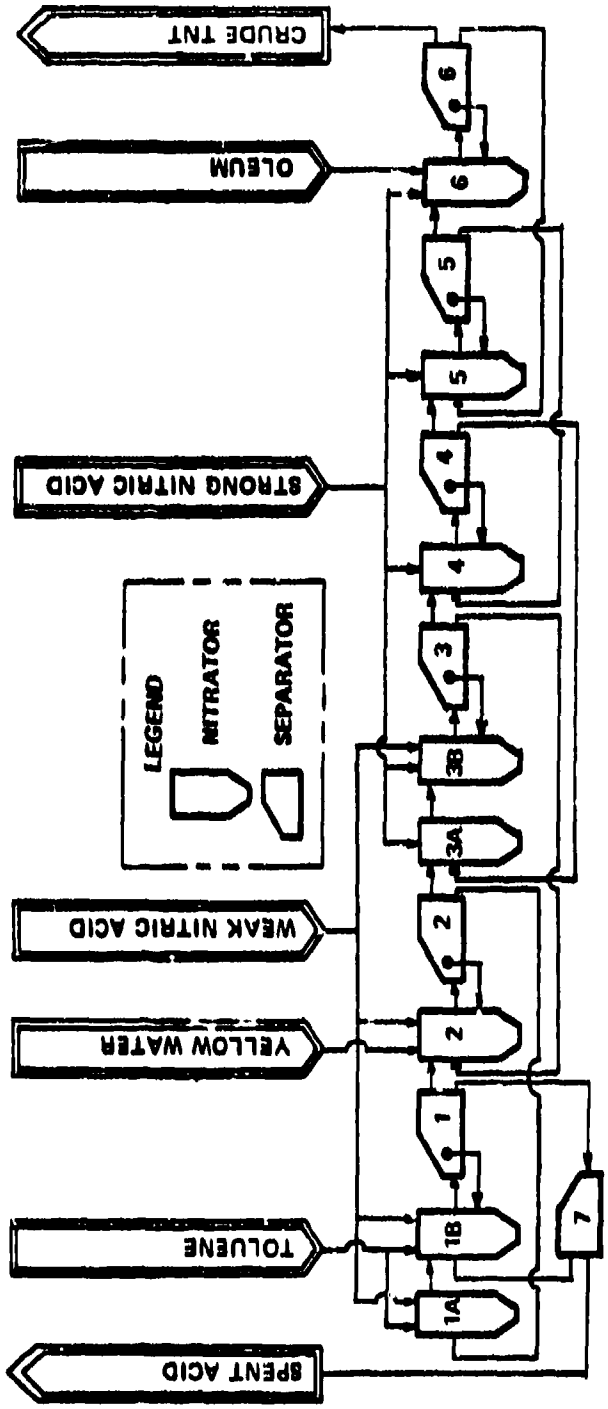


Fig 3 TNT nitration flow scheme (inter-vessel relationship)

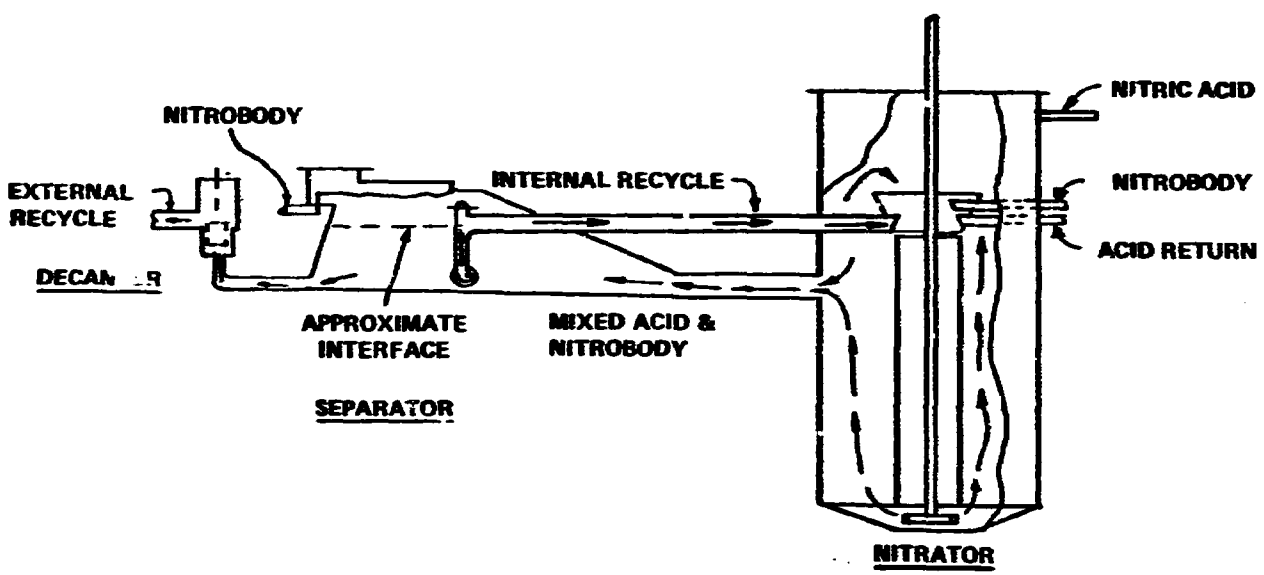
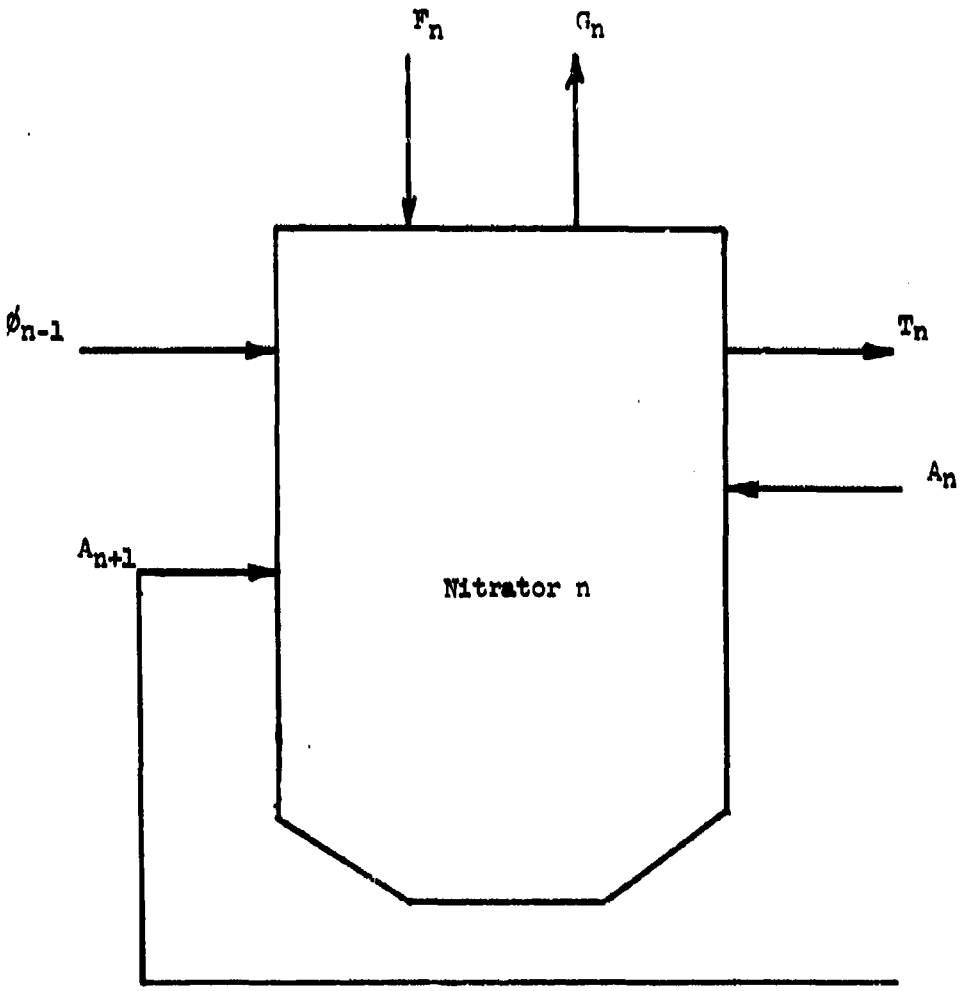


Fig 4 Nitrator-separator combination



where:

ΣF_n= sum of fresh feeds to nitrator n

ϕ_{n-1}= organic stream forward from separator n-1

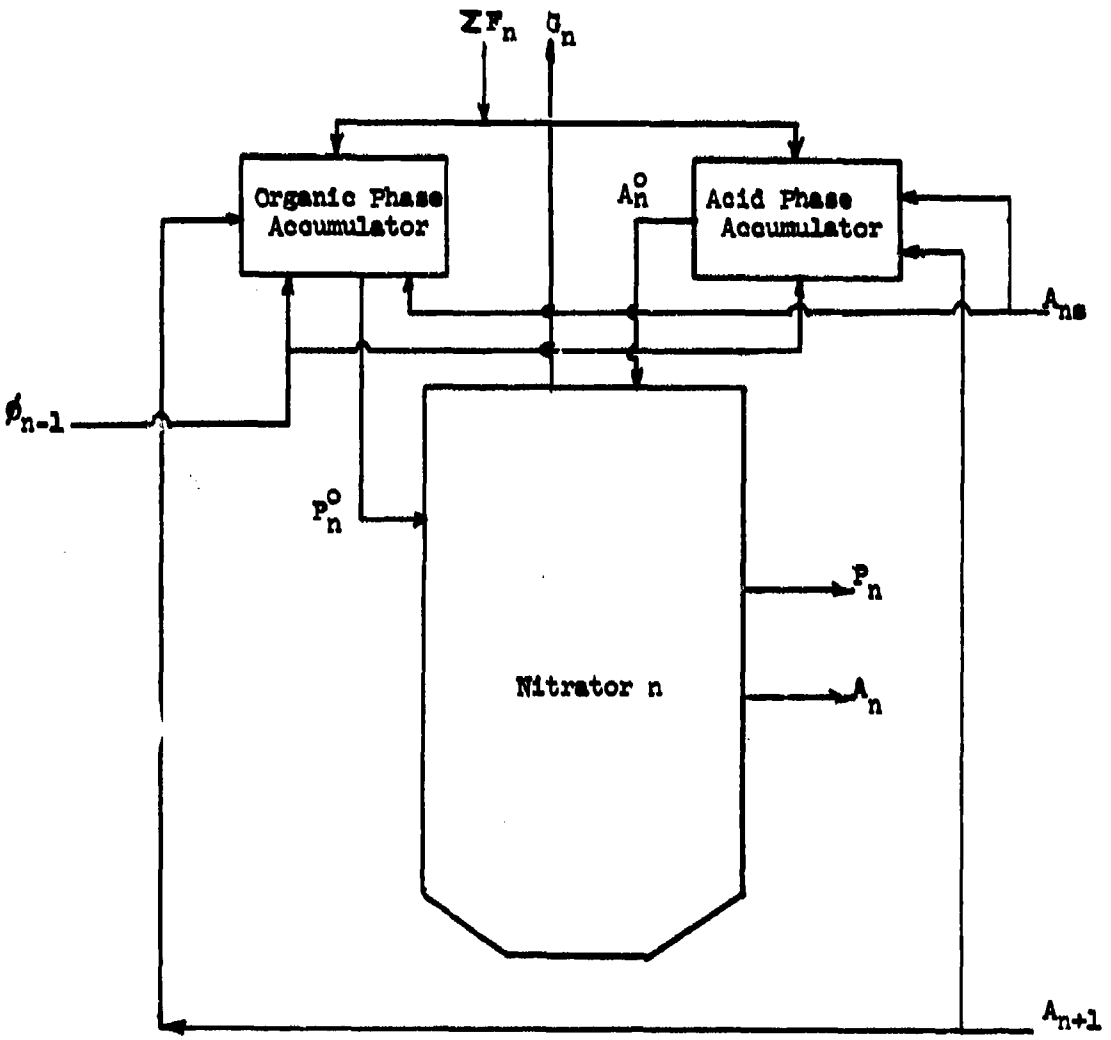
G_n= total off-gas

A_{n+1}= acid recycle stream from separator n+1

A_n= acid recycle stream from separator n

T_n= total outflow from nitrator n

Fig 5 Generalized nitrator



where:

P_n^o = total organic phase input to nitrator n

A_n^o = total acid phase input to nitrator n

P_n = total organic phase output from nitrator n

A_n = total acid phase output from nitrator n

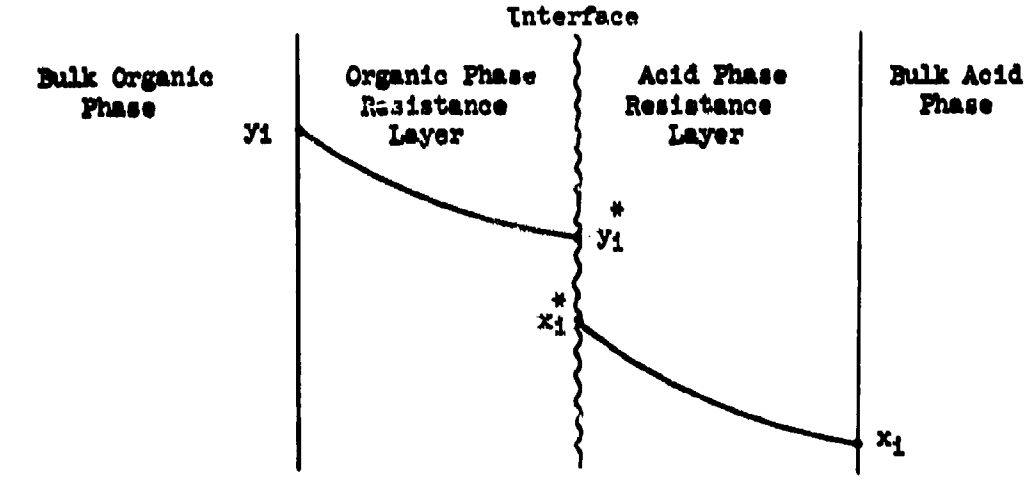
A_{ns} is equivalent to A_n in figure 5 and A_{n+1}, ϕ_{n-1}, G_n and ΣF_n are defined exactly as in figure 5

Fig 6 Simplified nitrator

CHEMICAL SPECIES CONSIDERED

ORGANIC PHASE	ACID PHASE	GAS PHASE
TOLUENE	TOLUENE	NO_x
∝– MNT	∝MNT	CO_x
M – MNT	MMNT	TNM
∝– DNT	∝DNT	
M – DNT	MDNT	
∝– TNT	∝TNT	
M – TNT	MTNT	
TNB	TNB	
TNBX	TNBX	
HNO_3	HNO_3	
	H_2SO_4	
	H_2O	
	SO_3	
	$HNOSO_4$	

Fig 7 Chemical components considered in the model



D_i - net rate of diffusion of species i into the acid phase

y_i - mole fraction species i in bulk organic phase

x_i - mole fraction species i in bulk acid phase

x_{eq}^A - equilibrium solubility of all organic species in the acid phase or mole fraction organic species in acid phase at saturation

η_ϕ - mass transfer coefficient in acid phase

η_A - mass transfer coefficient in organic phase

A_i - moles species i in acid phase

ϕ_i - moles species i in organic phase

A_T - total moles in acid phase

ϕ_T - total moles in organic phase

A_{NB} - total moles of nitrobody in acid phase

ϕ_{NB} - total moles of nitrobody in organic phase

$*$ - superscript denoting equilibrium at the interface

Fig 8 Diffusion in the nitration process

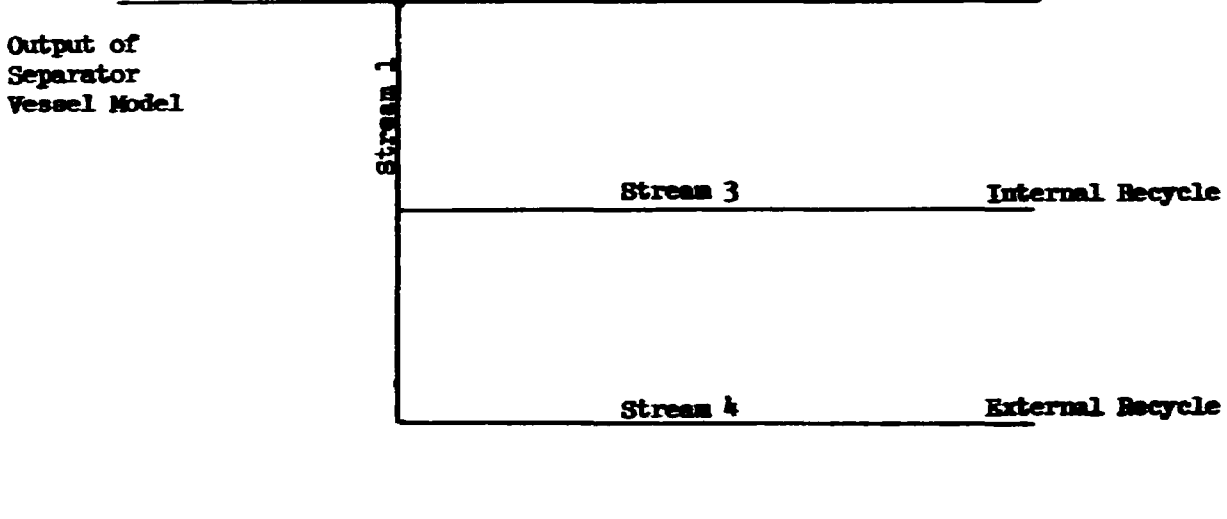


Fig 9 The separation process

LIST OF VARIABLES

Manipulated Variable	Controlled Variable
1. Water to Stage 1	Total Acidity, Stage 1
2. Weak Nitric to Stage 1	Nitric Concentration, Stage 1
3. Water to Stage 2	Total Acidity, Stage 2
4. Weak Nitric to Stage 2	Nitric Concentration, Stage 2
5. Strong Nitric to Stage 3A	Nitric to Sulfuric Ratio, Nitrator 3A
6. Strong Nitric to Stage 3B	Nitric to Sulfuric Ratio, Stage 3B
7. Strong Nitric to Stage 4	Nitric to Sulfuric Ratio, Stage 4
8. Strong Nitric to Stage 5	Nitric to Sulfuric Ratio, Stage 5
9. Strong Nitric to Stage 6	Nitric to Sulfuric Ratio, Stage 6

Fig 10 Acid concentration control--variables operated on

Block Diagram

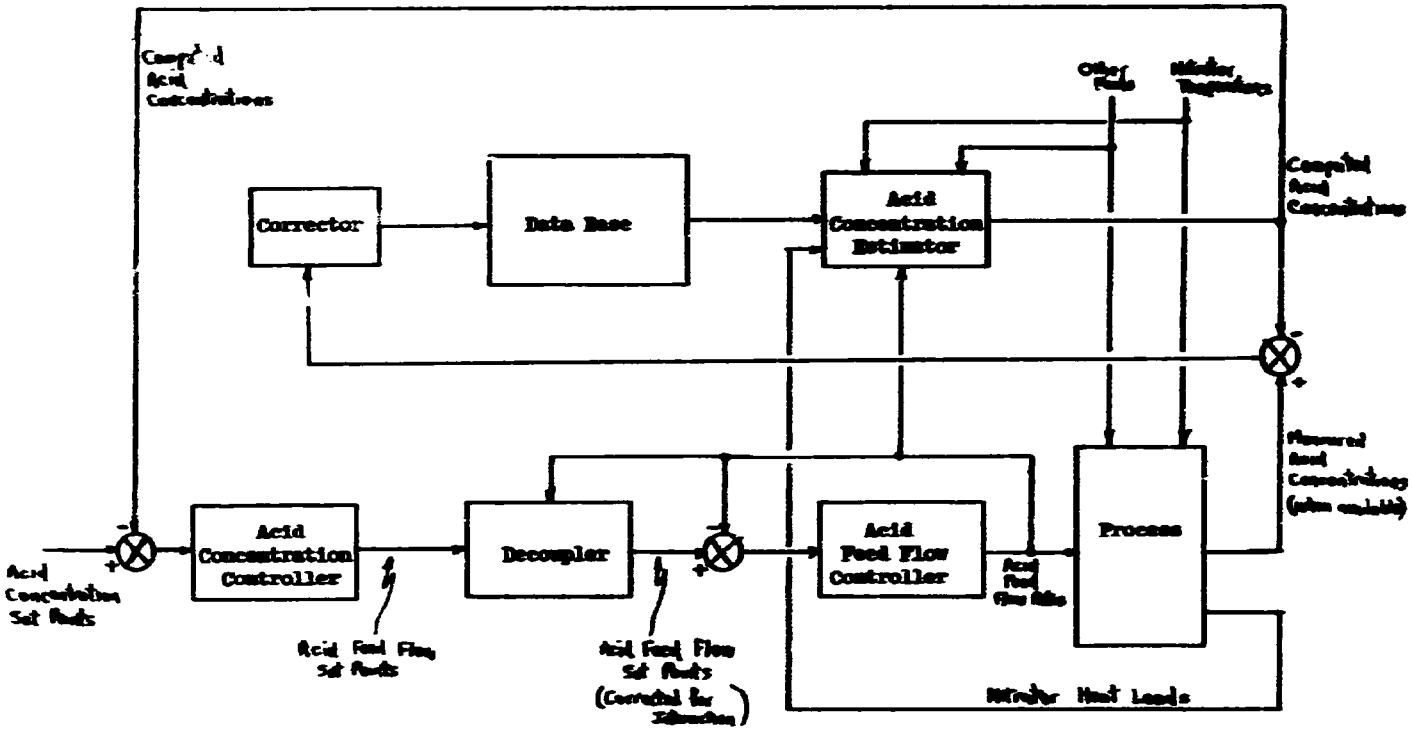


Fig 11 Acid concentration control--schematic diagram

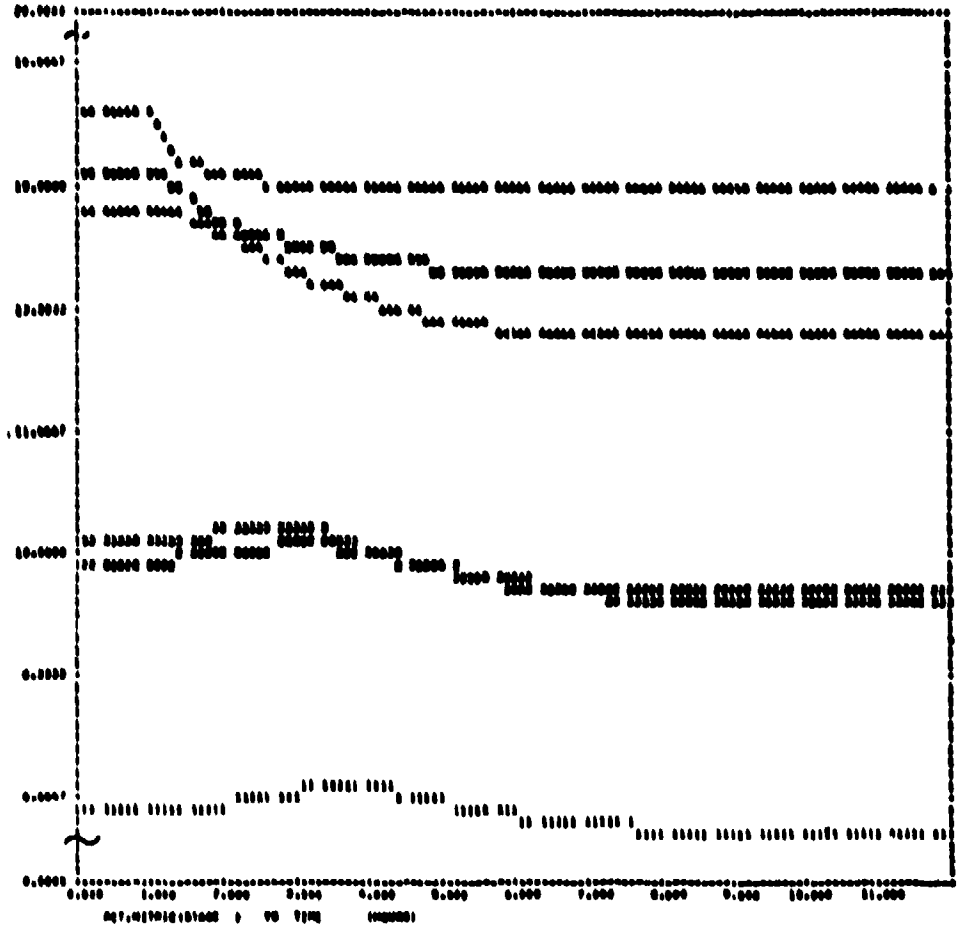


Fig 12 Open loop response of dynamic simulation

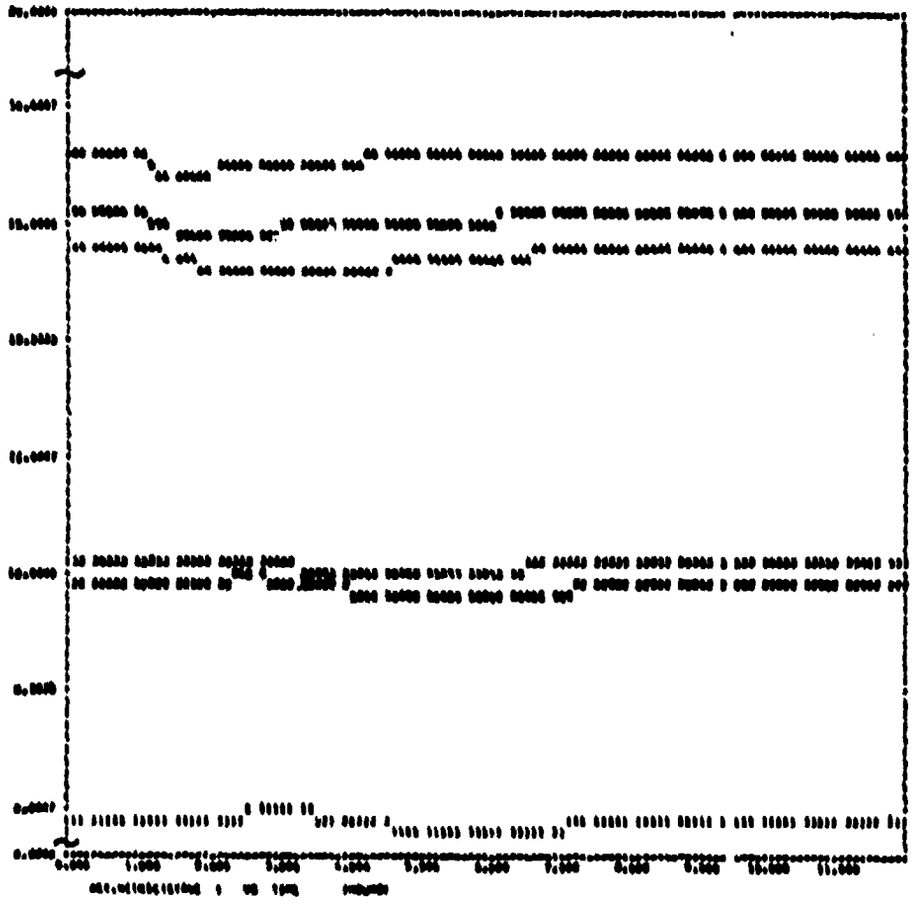


Fig 13 Response of dynamic simulation under acid concentration control