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Volume I

TWO DIMENSIONAL TRANSIENT HEATING AND SURFACE THERMOCHEMISTRY COMPUTER PROGRAM

Second Interim Technical Report
Contract F04611-67-C-0047

Prepared by
Aerotherm Corporation
Under Subcontract 2007

to

Atlantic Research Corporation
A Division of The Susquehanna Corporation
Shirley Highway at Edsall Road
Alexandria, Virginia 22314

July 5, 1968

ATLANTIC RESEARCH

185

AFRPL-TR-68-116 Volume I

TWO DIMENSIONAL TRANSIENT HEATING AND SURFACE THERMOCHEMISTRY COMPUTER PROGRAM

Second Interim Technical Report
Contract F04611-67-C-0047

Prepared by
Carl B. Moyer
Aerotherm Corporation

July 5, 1968

FOREWORD

This report was prepared by Aerotherm Corporation under subcontract to Atlantic Research Corporation under Contract F04611-67-C-0047. The work was under the direction of the Air Force Rocket Propulsion Laboratory with Mr. Robert Schoner and Lt. David Zorich as project officers.

Mr. Carl Moyer of Aerotherm prepared the report with assistance from Mr. Mitchell R. Wool and Dr. Robert M. Kendall. Mr. Eugene Olcott served as subcontract monitor for Atlantic Research.

The computer programs described in this report were used in the subsequent study of the reactions of combustion products of solid propellant rockets with pyrolytic graphite. These studies are described in Volume II, a classified report, of AFRPL-TR-68-116.

Publication of this report does not constitute Air Force approval of the report's findings or conclusions. It is published only for the exchange and stimulation of ideas.

CHARLES R. COOKE

Charles R. Cooke
Chief, Solid Rocket Division

ABSTRACT

The report describes and gives user's instructions for a computer program (ASTHMA) for predicting the in-depth temperature history and the surface recession (ablation) history of a two-dimensional, axi-symmetric, non-charring material. The in-depth solution procedure is of the conventional explicit finite-difference type. It will account for anisotropic heat conduction in the main material and allows several back-up materials. The heated surface boundary condition can have any one of three forms at each surface location at each instant:

1. Very general film-coefficient-based simultaneous heat and mass transfer type, including any number of equilibrium reactions for an environment and any ablating material, and four specific kinetically controlled reactions for carbon surfaces
2. Simplified radiation energy balance type, no ablation ("cooldown" option)
3. Specified temperature and surface recession rate.

The program was designed specifically for rocket nozzle use but has sufficient generality that it can be employed for many axi-symmetric shapes.

A User's Manual Brief Description is also presented for a computer program (ARCACE) for calculating surface thermochemical response of materials, including kinetically controlled surface reactions. This program provides for surface thermochemical boundary condition information input to the ASTHMA program. The program was designed specifically for graphitic material and solid propellant combustion products environment but can be employed for many materials and chemical systems.

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LIST OF SYMBOLS

A	area of side of nodal box	ft^2
a,b,c	nodal box side and center line lengths, Figure 7, Equation (14)	in
B'	defined as $(B'_c - \sum \dot{m}_{r_\ell}/\rho_e u_e C_M)$ thermochemical ablation parameter	---
B'_c	defined as $\dot{m}_c/\rho_e u_e C_M$, total ablation parameter	---
B'_f	defined as $\sum \dot{m}_{r_\ell}/\rho_e u_e C_M$	---
B'_g	defined as $\dot{m}_g/\rho_e u_e C_M$	---
B'_{tc}	same as B'	---
b	see a,b,c	
C	nodal capacity, Equation (16)	Btu/°F
C_H	Stanton number for heat transfer (corrected for "blowing", if necessary)	lb/ft^2 sec
C_{H_O}	Stanton number for heat transfer not corrected for blowing	lb/ft^2 sec
C_{k_i}	number of k atoms in molecule i	---
C_M	Stanton number for mass transfer	lb/ft^2 sec
c	specific heat	Btu/lb°F
c	see a,b,c	in
$\overline{D}$	constant defined by Equation (36)	ft^2/sec
$\mathcal{D}_{ij}$	binary diffusion coefficient	ft^2/sec
F	radiation view factor	---
F_i, F_j	empirical factors appearing in Equation (36)	---

LIST OF SYMBOLS (continued)

f	denotes general functional relationship	---
H_r	recovery enthalpy	Btu/lb
h	enthalpy	Btu/lb
h_c	enthalpy of ablating material at wall temperature	Btu/lb
h_w	enthalpy of gases adjacent to the wall	Btu/lb
I	total number of identifiable species	---
I	number of iteration cycles in problem	---
i,j	chemical species indices	---
K	total number of elements in system	---
K_i	mass fraction of species i	---
$\tilde{K}_k$	mass fraction of element k (regardless of molecular configuration)	---
k	thermal conductivity	Btu/ft-sec$^\circ$R
k_f	forward rate constant for kinetically controlled reaction	various
L	path lengths in a nodal box, Figure 5	ft
$\mathcal{M}$	system molecular weight $\sum x_i \mathcal{M}_i$	lb/lb mole
$\mathcal{M}_i$	molecular weight of species i	lb/lb mole
m	node corner and center row number	---
$\dot{m}$	mass flow rate per unit area from the surface, thermochemical effects only	lb/ft^2 sec
$\dot{m}_c$	total mass flow rate of "char" or main ablating material per unit surface area, all effects (thermochemical plus condensed phase mechanical removal)	lb/ft^2 sec
$\dot{m}_g$	mass flow rate of pyrolysis gas out a unit area of surface	lb/ft^2 sec

$\dot{m}_{r_\ell}$	flow rate of condensed phase ℓ mechanically removed from surface	$lb/ft^2 sec$
N	total number of nodes	---
n	node corner and center column number	---
P	total pressure	lb/ft^2
P_i	partial pressure of species i	lb/ft^2
q_{chem}	chemical energy flux term defined by Equation (36)	$Btu/ft^2 sec$
q_{cond}	rate of energy conduction into solid material at surface	$Btu/ft^2 sec$
q_{diff}	rate of energy input to solid surface by diffusional processes in the boundary layer	$Btu/ft^2 sec$
$q_{rad\ in}$	rate of energy input to the surface by radiation from the boundary layer or from outside the boundary layer, same as q_{rad}	$Btu/ft^2 sec$
$q_{rad\ out}$	rate of energy radiated away from surface	$Btu/ft^2 sec$
q_{sen}	$\triangleq \rho_e u_e C_H (H_r - h_{e_w})$	$Btu/ft^2 sec$
R	thermal resistance, see Equations (17), (18)	$sec^\circ F/Btu$
R*	contact thermal resistance	$ft^2 sec^\circ F/Btu$
r	radius	in
S	see ΔS	$^\circ R$
T	computing time	hrs
T	temperature	$^\circ R$
T_w	wall (surface) temperature, general term for $T_{s,n}$	$^\circ R$

LIST OF SYMBOLS (continued)

u_e	velocity of gases at edge of boundary layer	ft/sec
V	nodal volume	ft^3
v	gas velocity (see ρv)	ft/sec
x_i	mole fraction of species i	---
z	axial coordinate	ft
z_i^*	diffusion driving force, see Equations (33) and (34)	---

GREEK

α	heated surface absorbtivity (taken equal to ϵ_w), thermal diffusivity	---
γ	constant, empirically chosen = 2/3	---
Δ	denotes change	---
ΔS	change in surface point location during Δθ	ft
Δθ	time step in finite difference solution	sec
ε	emissivity or emittance	---
η	input multiplicative safety factor in time step calculation, Equation (20)	------
θ	time	sec
λ	constant in Equation (39)	---
μ_2	dimensionless factor defined by Equation (35)	---
ρ	density	lb/ft^3
$(\rho v)_w$	$\dot{m} + \dot{m}_g$	$lb/ft^2 sec$
$\rho_e u_e$	mass flow at boundary layer edge	$lb/ft^2 sec$

$\rho_e u_e C_H$	heat transfer convective film coefficient	$lb/ft^2 sec$
$\rho_e u_e C_M$	mass transfer convective film coefficient	$lb/ft^2 sec$
σ	Stefan-Boltzmann constant	$Btu/ft^2 sec {}^\circ R^4$
φ	parameter defined by Equation (39)	---

SUBSCRIPTS

A,B,C,D	indices for path lengths L (Fig. 5), nodal side areas A (Fig. 6) and thermal resistances R (Fig. 10)
B	see A,B,C,D
C	see A,B,C,D
CL	denotes nodal column center line
c	denotes "char" or ablating material; see $\dot{m}_c$
D	see A,B,C,D
e	denotes boundary layer outer edge, or boundary layer edge gas
g	denotes pyrolysis gas
H	see C_H
i,j	denotes any identifiable species: atom, ion, molecule
k	denotes element
ℓ	index of condensed phase species mechanically removed from surface
M	see C_M
m	node corner and center row number index
N	denotes node center

n	node corner and center column number index
p	denotes virgin plastic
r	see $\dot{m}_{r_\ell}$
s	denotes heated surface
w	denotes wall, i.e., heated surface
O	see C_{H_O}
1,2	denote "earlier" and "later"
θ,θ'	at times θ and θ', respectively

SUPERSCRIPTS

'(prime)	see B', B'_c, B'_f, B'_g, B'_{tc}
'(prime)	denotes at new time $\theta' = \theta + \Delta\theta$
T_w	enthalpy datum temperature

SPECIAL SYMBOLS

*	see Z^*_i

GLOSSARY

Some of the terms used in the text have very particular meanings. These are collected here for ready reference.

back wall	one of the four sides of the nodal mesh layout, located by convention at the bottoms of the columns; may be convectively and radiatively cooled but does not ablate
box	see "nodal box"
column	refers to one direction of the nodal mesh, heated surface is at the top of the columns
heated surface	the one surface of the four sides of the nodal mesh layout which is exposed to the hyperthermal, chemically reactive environment, located by convention at the top of the columns in the mesh; opposite side of mesh network is the back wall
mesh	assemblage of quadrilateral nodal boxes arranged in rows and columns, each row and each column having the same number of nodal boxes; encompasses all the material of interest and divides it into nodes for finite difference heat conduction analysis
nodal box	one quadrilateral zone in the mesh
nodal center, nodal point	a point within the nodal box at which all the material in the box is presumed to be lumped for the finite difference calculation, not necessarily in the center of the node
node	used for nodal box, nodal center, nodal point
null node	a nodal box in the mesh which contains no material, used for bookkeeping operations only, not involved in finite difference solution
row	refers to one direction in nodal mesh, "parallel" to heated surface
surface node	the top node in each column (excepting null nodes), that node next to (adjacent to, at) the heated surface; note that the surface nodal box is next to the heated surface and one of its four sides is exposed to the hyperthermal environment, the nodal point or nodal center however is on the side of the node farthest from the heated surface; there is a special point on the surface called the surface point which must not be confused with the surface nodal "center"

surface point	the center of the heated surface side of the top nodal box in each column (not counting null nodes); this point is distinct from the nodal point for that nodal box; the temperature of this point is determined by the surface energy balance in Options 1 and 3 or by assignment in Option 2

INTRODUCTION

AXI-SYMMETRIC TRANSIENT HEATING AND MATERIAL ABLATION PROGRAM (ASTHMA) DESCRIPTION AND USER'S MANUAL

This report presents an analysis technique and describes an associated computer program (ASTHMA) for the prediction of the thermal response and ablation of two-dimensional axi-symmetric non-charring materials. Chief applications for the computer program are rocket nozzles and entry vehicle nose tips. The in-depth temperature prediction is of the familiar explicit finite-difference type. It allows a completely general finite difference mesh layout relative to the physical r-z axes, and accounts for anisotropic heat conduction effects. The heated surface boundary condition is an unusually general thermochemical type. It accounts for three specific kinetically controlled carbon oxidation reactions, one specific kinetically controlled carbon reduction reaction, one kinetically controlled water gas shift reaction, and any number of equilibrium reactions for any combination of ablating materials and environments.

The present report has two parts. The final part is a complete, but condensed and succinct, user's manual giving explicit instructions for the preparation of input to the program and the interpretation of program output. Part I of the report presents some of the underlying analysis foundation upon which the computer program is built. Since much of the pertinent analysis work has previously been published elsewhere, these particular parts of the analysis are treated only briefly here and the reader is referenced to the previous reports for more information. The following sketch serves to clarify various physical aspects of the ablation problem treated. The

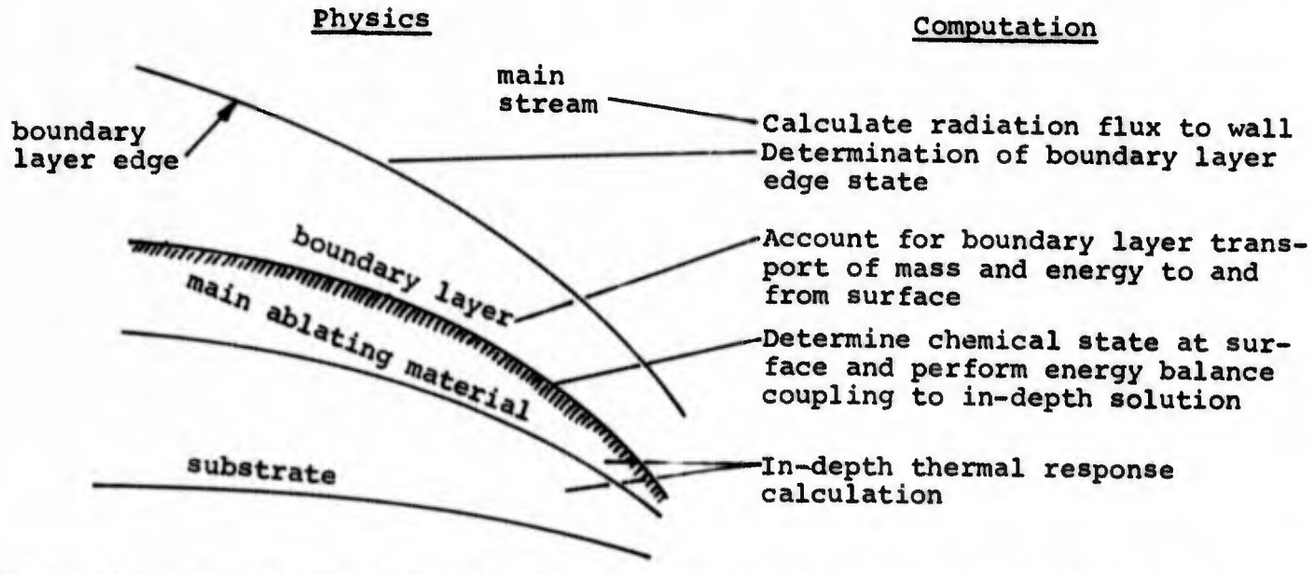

table below cites the aspects and indicates which descriptions of the analysis are to be found in the present report and which are to be found elsewhere. Note that the ASTHMA Program described in this report is usually used in

Task II - Determination of the kinetic rate constants for the reactions of H_2O, H_2, and CO_2 with pyrolytic graphite using an arc plasma generator and two-dimensional nozzle configuration

Task III - Prediction of pyrolytic coating performance in a typical nozzle configuration for several propellants and firing conditions

The results of Tasks II and III are presented in a separate report.

The author would like to express his appreciation to Mr. Mitchell R. Wool and Dr. Robert M. Kendall who prepared Appendices C and E through G.

SUMMARY OF COMPUTATIONAL TASKS

Task	Program	Where Described
1. Determine radiation flux from free stream to wall	Not computed, but accounted for by ASTHMA. User must provide as input	--
2. Determine boundary layer edge state	ACE	Ref. 9
3. Account for boundary layer transport of		
a. mass	ACE*	Refs. 1-9
b. energy	ASTHMA, but user must provide transport coefficients as input	Briefly below, also Refs.1-6
4. Surface thermochemical state	ACE*	Refs. 6-9
5. In-depth temperature	ASTHMA	Below

conjunction with another program (ACE) which handles the chemical state computations required in the heated surface boundary condition definition. The ACE program is not described in detail here; however, a user's manual, sample problems and program listing are included as appendices. The reader is referred to Reference 9 for a detailed description of the ACE program.

A complete ablation problem may be solved with the ACE and ASTHMA programs in conjunction in the following steps:

(1) Lay out nodal geometry, provide this and material properties data to ASTHMA

(2) Determine radiation flux history and $\rho_e u_e C_H$ history; provide to ASTHMA

(3) Determine chemical nature of environment and generate surface thermochemical ablation tables with ACE for input to ASTHMA

(4) Run ASTHMA, obtain temperature and surface recession histories..

The work presented herein represents Task I under Atlantic Research Corporation Subcontract 2007 (Air Force Rocket Propulsion Laboratory Prime Contract F04611-67-C-0047). The overall Aerotherm program consists of the following tasks:

Task I - Development of a two-dimensional heat conduction program appropriate to pryolytic graphite coatings on substrates

*The KCG program, Ref. 6, may alsobe used for these calculations but it has now been superceded by the ACE program.

PART I

DESCRIPTION OF ANALYSIS FOUNDATIONS FOR THE AXI-SYMMETRIC TRANSIENT HEATING AND MATERIAL ABLATION PROGRAM (ASTHMA)

This section describes much of the analysis work upon which the ASTHMA program is built. Section 1 below defines the problem treated, and Section 2 gives some description of the in-depth solution procedure. Section 3 briefly describes the heated surface boundary condition treatment.

SECTION 1

PROBLEM TREATED AND GENERAL METHOD OF SOLUTION

1.1 PROBLEM DESCRIPTION

The basic problem is to predict the surface and in-depth temperature history and surface location history of a two-dimensional, non-charring, anisotropic (but orthotropic) insulating material exposed to a chemically reactive hyperthermal environment. The chief practical examples are rocket nozzles and nose tips; the general problem is depicted schematically in Figure 1-1. Below the heated surface, the material response is characterized by

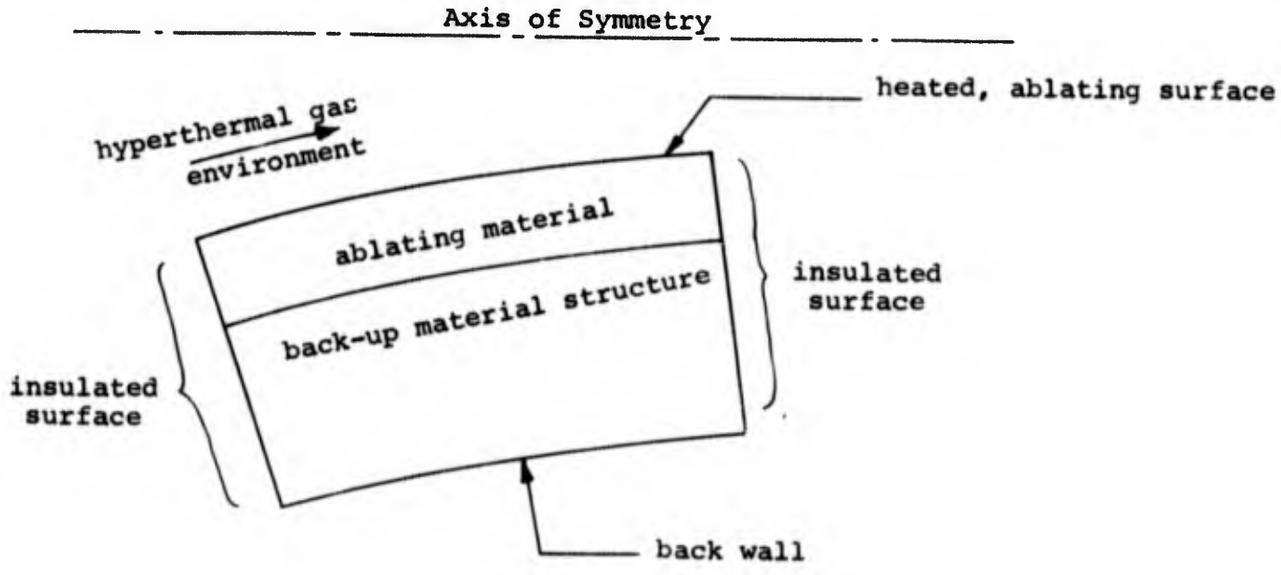

Figure 1-1. Sketch of Ablating System Considered

anisotropic heat conduction with temperature dependent thermal conductivity and specific heat. At the heated surface there is a complex boundary condition involving thermal convection from the hot gases adjacent to the surface, diffusive mass transport, and chemical corrosion. The surface chemical reactions may be in equilibrium or may be kinetically controlled in certain respects (e.g., the oxidation of carbon surfaces).

1.2 SUMMARY OF SOLUTION PROCEDURE

The solution procedure chosen for this problem is complex and is described in more detail in Sections 2 and 3 below. As a quick summary, the in-depth procedure is an explicit two-dimensional finite-difference technique. The surface response procedure solves a general energy balance and mass balance based on a film coefficient model. The ablation events are computed through consideration of the complete thermochemical response including up to four specific kinetically controlled reactions with a carbonaceous surface (all other possible chemical reactions are considered to occur in equilibrium). This approach is in contrast to more usual correlation schemes or "heat of ablation" approaches. There is no direct feedback coupling, however, between body shape change and boundary condition history; that is, the program does not include routines to compute pressure distributions and convective transfer coefficient distributions as functions of body shape (these are input a priori as functions of body location and time).

The basic computer program is called ASTHMA, for Axi-Symmetric Transient Heating and Material Ablation." It relies upon an additional program (ACE) for the calculation of thermochemical aspects of the ablation process.

1.3 COUPLING TO STRESS CALCULATIONS

The program does not include thermal stress calculations but does provide for punched card output which may be used directly as input to a separate stress program (not described here).

1.4 HISTORICAL DEVELOPMENT

The ASTHMA computer code described here constitutes a combination of parts of existing programs. Consequently there exists a large amount of background literature on certain parts of the computer code. This literature will be cited below, and the present report will abbreviate descriptions of aspects already presented elsewhere. Consequently the reader may want to consult other publications for more detailed expositions of those aspects, particularly the surface energy balance equations (Refs. 1-6) and the surface thermochemical state solution procedure (Refs. 6-9).

SECTION 2

ASPECTS OF IN-DEPTH SOLUTION

2.1 BACKGROUND REMARKS

It was the intent of the program development effort reported here not to write a new in-depth heat conduction routine since it seemed that either of two existing routines might be modified to form the basis of the new ablation program. The first such predecessor program is the One Moving Boundary Program (1MBA) reported in Reference 6. This program was originally developed for rocket nozzles and features a rather general thermochemical boundary condition. It does not allow consideration of backup materials, the effects of unequal diffusion coefficients, or mechanical removal. The chief defect of the 1MBA program for the requirements herein is the absence of a back-up material capability. A second candidate program was the Aerotherm Axi-symmetric Transient Temperature Program, AATT (Ref. 10). This program did not include ablation and therefore did not allow for receding surfaces.

It was originally intened to modify the 1MBA program for the present work since it already featured an ablation boundary condition. However further study indicated that reworking the existing back wall boundary condition treatment of the 1MBA program would involve a disproportionate amount of work.* Therefore, consideration was given to adding an ablation "package" to the existing AATT program. Such a development would avoid back-wa complexities and could incorporate without essential difficulty the latest elopments in surface ablation computation (as reported in Refs. 3, 5, and 7). However it would involve a frontal attack on a hitherto unsolved computational problem: how to construct a front node dropping scheme which would accommodate an energy-balance-determined surface temperature and recession rate without introducing oscillations in temperature and recession rate. In the front node dropping approach, the nodal network for heat conduction remains fixed with time except in the immediate vicinity of the surface. As the surface recedes due to ablation, the nodal zone adjacent to the surface shrinks. When "sufficiently" small, this node is either "dropped" from the original network or "absorbed" into the adjacent node down and computation continues. It had proven in the past to be a difficult task to design a computation scheme of the front node

*This is the classic difficulty in any scheme like the 1MBA routine which has a nodal network tied to the receding surface, so that "nodes" are dropped at the back wall of the ablating material as the heated surface moves. Such a scheme is simple in one space dimension, but two-dimensional body shape changes involve a coordinate bending as well as recession greatly complicating the back wall treatment.

ing type which is free from oscillations in surface temperature or sur-
eat flux or both. Consequently front node dropping schemes had gone
favor and had been superseded by shrinking nodal network schemes and
all node dropping schemes.

In an attempt to develop a front node dropping scheme which could be
d to the existing AATT program, the whole problem of oscillations was
ed with a special purpose one-dimensional heat conduction program.
lix A reports the details of the study; the conclusion was that a smooth
did exist although it required some sacrifice in accuracy. This scheme
upled into the existing AATT program to form the two dimensional axi-
ric ablation and heat transfer program (the ASTHMA program) described
sections below.

ODAL LAYOUT AND GEOMETRY

General Pattern

he geometric shape considered, illustrated in Figure 2-1, is imagined to
ided up into a grid pattern in the customary manner for finite differ-
omputation schemes. The area within each grid "box" will be termed a
; this is in contrast to terminology which calls each corner of the
etwork a node. The thermal capacity of each node is imagined to be
at a single point within the box; this point will be termed the nodal
. It will be convenient to assume for the moment that the nodal center
located anywhere within the nodal box. Strategies for optimizing the
on of the nodal centers will be discussed later.

or convenience, the nodes are imagined to be quadrilaterals, so that
tire nodal network is an assemblage of quadrilaterals. For bookkeeping

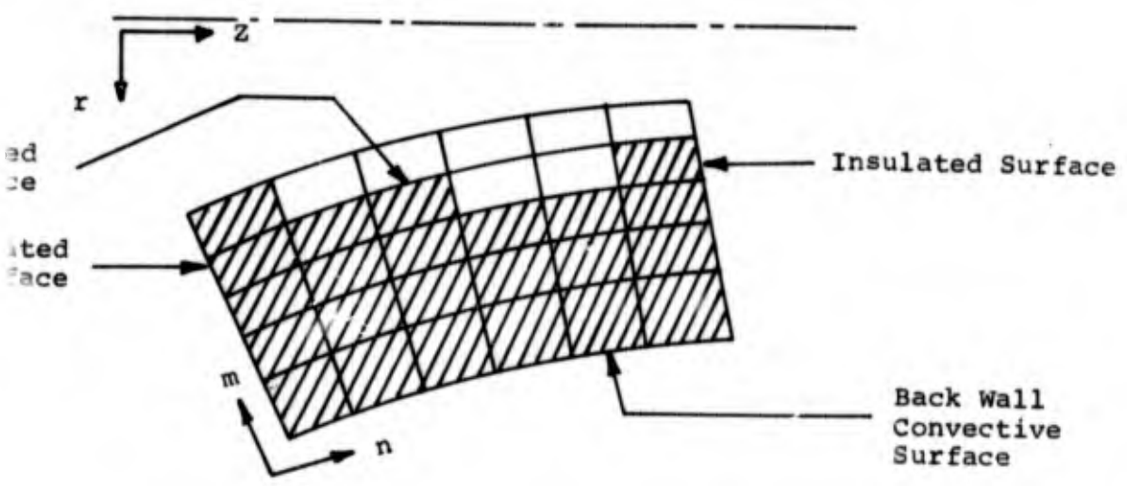

Figure 2-1. Sketch of Typical Nodal Layout

convenience, the network is imagined to be "complete", even though the shape of the material may dictate that some of the mesh boxes are empty. Both nodes (boxes or centers) and mesh corners are numbered in a row and column system which will be labeled as an m-n system, where m denotes a row and n denotes a column. The m-n mesh scheme may be oriented arbitrarily with respect to the physical r-Z coordinate scheme,* so that in general the row-column description might seem to be merely a descriptive artifice; however, in exploiting the simplicities associated with rocket nozzle geometries it has been assumed in constructing the program that the heated surface is at the top of the columns, as indicated in Figure 2-1. Thus as surface recession occurs, the boxes at the top of each column shrink; the other boxes remain fixed. This limitation that the heated surface be located at the top of each column is merely a convenience procedure exploited for the special case of the low curvature geometry of rocket nozzles. For high curvature bodies this restriction becomes inconvenient and would have to be relaxed.

The side walls of the nodal network are presumed insulated and the back wall communicates through a simple heat transfer coefficient law (plus radiation) to a "reservoir" at T_{res}. Thus the boundary condition at this face does not involve thermochemistry.

Three other "convenience limitations" have been applied to the layout of the nodal grid. First, it is assumed for the purposes of computing thermal conductances between nodal centers that the mesh scheme is nearly orthogonal, so that conductance may be taken as conductivity times side-area divided by length.** Secondly, it is presumed that only one material ablates, and that only one material is exposed to the heated surface. (These bookkeeping simplicities can easily be removed in future versions of the program.) Thirdly, it is presumed that the principal directions of thermal anisotropy are aligned with the nodal mesh. This simplifies computations and reduces input requirements. For those applications in which the heated surface intersects the principal directions of anisotropy at "difficult" angles this restriction could become a major inconvenience and more general schemes would have to be devised for those problems.

---

*That is, the nodal mesh scheme may be above or below the Z-axis line, may be oriented in any general direction, and may be "bent" or shaped in any manner convenient to the user (subject to the limitations described in the paragraphs following below).

**A suitable more general conductance calculating scheme could remove this restriction without any essential change to the program.

2.2.2 Geometry

2.2.2.1 Location of Nodal Centers

The study summarized in Appendix A showed that to obtain a smooth node dropping scheme it was necessary to avoid associating thermal capacity with the surface temperature. In terms of the conventional thermal RC network this means that a one-dimensional scheme would look like Figure 2-2. All the capacity

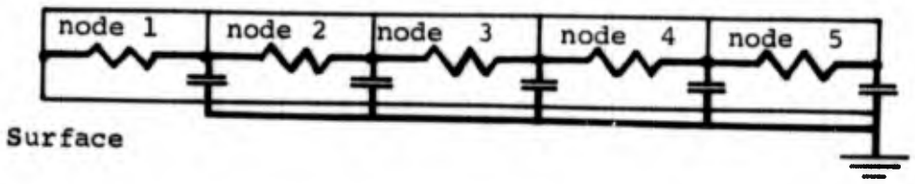

Figure 2-2. Sketch of One-Dimensional Thermal RC Network

of the surface node is located at the back of the first nodal zone, and all of the thermal resistance of this zone is interposed between the surface temperature and the temperature of the first capacity lump. Note that for m nodes or boxes the system has m+1 temperature points, in contrast to most schemes.*

In <u>two</u> dimensions, the nodal center is therefore located at the center of the "back wall" of the nodal box, that is, in the center of that side parallel to the heated surface and farthest from it. Thus for an m x n nodal network scheme, there will be m x n <u>nodal</u> temperatures (associated with thermal capacity) <u>plus</u> n <u>surface</u> temperatures (not associated with thermal capacity).

Denoting the nodal center coordinates as r_N and Z_N, the coordinates for node m, with corner coordinates m,n as shown in the sketch may be represented

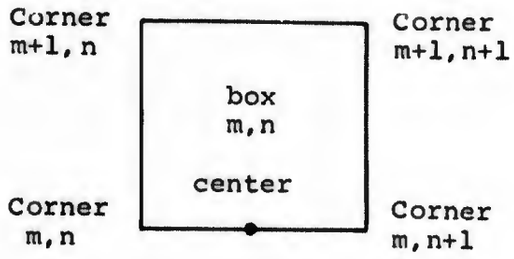

Figure 2-3. Sketch of Nodal Center Location For Ablating Material

*This scheme of course appears to be, and is, somewhat less accurate than more conventional schemes; more nodes must be taken to get accuracy comparable to that of "centered" schemes. The price paid here is compensated for by stability and smoothness of the solution at the surface.

by the following:

$$r_{N,m,n} = \frac{r_{c,m,n} + r_{c,m,n+1}}{2} \quad (1)$$

$$Z_{N,m,n} = \frac{Z_{c,m,n} + Z_{c,m,n+1}}{2} \quad (2)$$

For back-up nodes it is most desirable and common to put the nodal center in the arithmetic center of the box:

$$r_{N,m,n} = \frac{r_{c,m,n} + r_{c,m+1,n} + r_{c,m+1,n+1} + r_{c,m,n+1}}{4} \quad (3)$$

$$Z_{N,m,n} + \frac{Z_{c,m,n} + Z_{c,m+1,n} + Z_{c,m+1,n+1} + Z_{c,m,n+1}}{4} \quad (4)$$

(The ASTHMA user has the option to put back-up material nodal centers anywhere in the nodal box.)

2.2.2.2 Path Lengths for Conduction

In this and the following sections, the nodal center will have a general location $r_{N,m,n}Z_{N,m,n}$ for illustrative purposes. For computing thermal conductances, it will be necessary to have thermal path lengths between nodes. Since material properties are associated with each nodal box, first to consider path segments inside each box. In general there are four path segments of interest, as shown in Figure 2-4. The program computes the lengths $L_{m,n,B}$

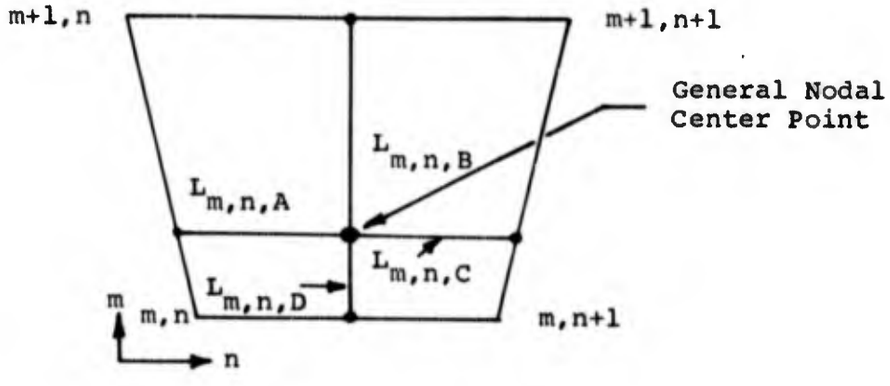

Figure 2-4. Illustration of Path Lengths

and $L_{m,n,D,}$ in the m direction, as the distances between the nodal center and the centers of the m+1 and m faces of the box. (This is because the nodal center is usually on the line joining the centers of these two faces.) Thus the paths B and D have the lengths

$$L_{m,n,B} = \left[\left(\frac{r_{c,m+1,n} + r_{c,m+1,n+1}}{2} - r_{N,m,n}\right)^2 + \left(\frac{z_{c,m+1,n} + z_{c,m+1,n+1}}{2} - z_{N,m,n}\right)^2\right]^{\frac{1}{2}} \quad (5)$$

$$L_{m,n,D} = \left[\left(\frac{r_{c,m,n+1} + r_{c,m,n}}{2} - r_{N,m,n}\right)^2 + \left(\frac{z_{c,m,n+1} + z_{c,m,n}}{2} - z_{N,m,n}\right)^2\right]^{\frac{1}{2}} \quad (6)$$

Since as noted above the nodal center is usually on the m face, however, the paths between the nodal center and the n and n+1 faces (paths A and C in the sketch) are assumed to end at points on those faces located as far down the face, proportionally, as the nodal center is located in the box. The two usual cases are the back-shifted node center on the face m, for which the paths A and C end at the corners m,n and m,n+1 respectively, and the arithmetically centered node, for which the paths A and C end at the centers of faces m and m+1 respectively. For the first case (back-shifted), we have

$$L_{m,n,A} = \left[(r_{c,m,n} - r_{N,m,n})^2 + (z_{c,m,n} - z_{N,m,n})^2\right]^{\frac{1}{2}} \quad (7)$$

$$L_{m,n,C} = \left[(r_{c,m,n+1} - r_{N,m,n})^2 + (z_{c,m,n+1} - z_{N,m,n})^2\right]^{\frac{1}{2}} \quad (8)$$

and for the second (centered) we have

$$L_{m,n,A} = \left[\left(\frac{r_{c,m,n} + r_{c,m+1,n}}{2} - r_{N,m,n}\right)^2 + \left(\frac{z_{c,m,n} + A_{c,m+1,n}}{2} - z_{N,m,n}\right)^2\right]^{\frac{1}{2}} \quad (9)$$

$$L_{m,n,C} = \left[\left(\frac{r_{c,m+1,n+1} + r_{c,m,n+1}}{2} - r_{N,m,n}\right)^2 + \left(\frac{Z_{c,m+1,n+1} + Z_{c,m,n+1}}{2} - Z_{N,m,n}\right)^2\right]^{\frac{1}{2}} \quad (10)$$

2.2.2.3 Side areas

Areas of the sides of each box are also required for thermal conductance calculations. For the sides lettered as shown in Figure 2-5, the areas are

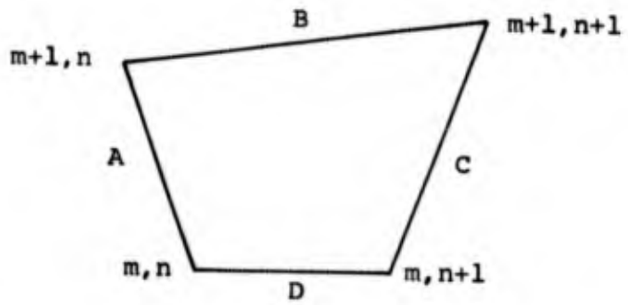

Figure 2-5. Nomenclature of Nodal Sides

given by elementary geometry (First Theorem of Pappus)

$$A_{m,n,A} = \pi(r_{c,m,n} + r_{c,m+1,n})\left[(r_{c,m+1,n} - r_{c,m,n})^2 + (Z_{c,m+1,n} - Z_{c,m,n})^2\right]^{\frac{1}{2}} \quad (11)$$

$$A_{m,n,B} = \pi(r_{c,m,n} + r_{c,m,n+1})\left[(r_{c,m,n+1} - r_{c,m,n})^2 + (Z_{c,m,n+1} - Z_{c,m,n})^2\right]^{\frac{1}{2}} \quad (12)$$

Only these two areas need to be computed for each box, since the areas on the other sides of the nodal box are identical with the areas A and B of adjacent nodes.

2.2.2.4 Volume

The volume of the elemental box is by the Second Theorem of Pappus,

$$V_{m,n} = \left[\pi/3 \left\{ Z_{c,m,n} \left[r_{c,m,n}(r_{c,m,n+1} - r_{c,m+1,n}) + r^2_{c,m,n+1} - r^2_{c,m+1,n} \right] + Z_{c,m+1,n} \left[r_{c,m+1,n} \cdot (r_{c,m,n} - r_{c,m+1,n+1}) + r^2_{c,m,n} - r^2_{c,m+1,n+1} \right] + Z_{c,m+1,n+1} \left[r_{c,m+1,n+1}(r_{c,m+1,n} - r_{c,m,n+1}) + r^2_{c,m+1,n} - r^2_{c,m,n+1} \right] + Z_{c,m,n+1} \left[r_{c,m,n+1} \cdot (r_{c,m+1,n+1} - r_{c,m,n}) + r^2_{c,m+1,n+1} - r^2_{c,m,n} \right] \right\} \right] \quad (13)$$

2.2.2.5 Geometric Effects of Surface Recession

For nodes adjacent to the heated surface, side B may move due to surface recession (ablation), This recession reduces the thermal resistance between the surface point and the adjacent nodal point, increases transverse thermal resistances (as discussed below), and reduces the thermal capacity associated with the nodal center of the nodal box adjacent to the surface. The program assumes that the surface recession occurs so as to maintain the ratios

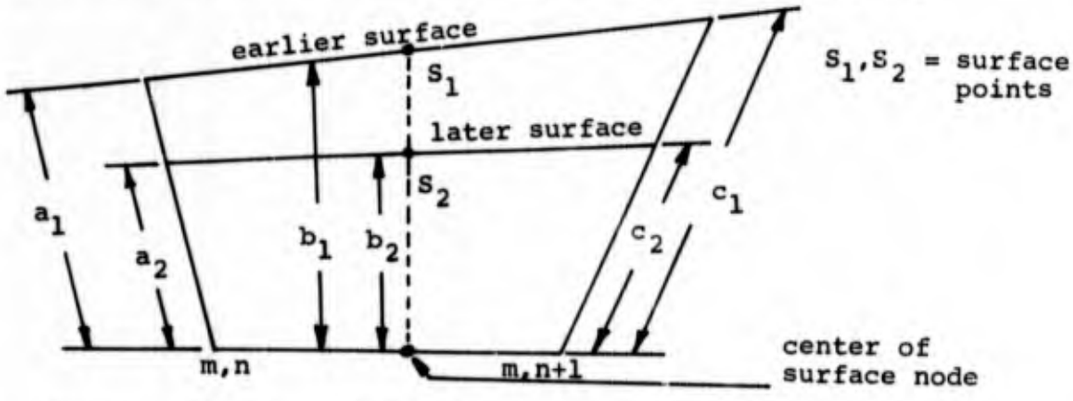

Figure 2-6. Sketch of Surface Nodal Box Undergoing Recession

$$\frac{a_2}{a_1} = \frac{b_2}{b_1} = \frac{c_2}{c_1} \quad (14)$$

as shown in Figure 2-6. The b line joins the centers of the m+1 and m planes and serves to define the location of the surface point S. The moving corners m+1,n and m+1, n+1 are located accordingly, and path lengths, areas and volumes computed as before, except that for these nodes $A_{m,n,A} \neq A_{m,n-1,c}$.

2.2.2.6 Surface Shape

As noted above and illustrated by Figure 2-7, it is most convenient to consider the surface points on the heated surface as being always located on the nodal column center line, that is, on the line joining the center points of the m+1 and m planes ("parallel" to the heated surface), where m is the row index of a nodal box at the surface and m+1 is the local corner index of the heated surface (see Fig. 2-6). The location of the surface points is all the information needed about the surface for those ablation problems with a specified, input surface recession rate as a boundary condition (the various ablation problem boundary condition options are described in Section 3 below), since for those problems, it is most convenient to specify, as input, recession history along the nodal center line. The nodal grid as input thus serves to define the various nodal column center lines, and the recession history for each column then defines the history of the surface points in a perfectly straightforward manner. However, another important heated surface boundary condition option involves not input recessions but various energy and chemistry information sufficient to calculate surface mass loss from energy balance considerations (Option 1, discussed in Section 3 below). This ablation calculation does not produce recession rates directly, of course; instead it produces rates of mass loss from the surface. It will prove convenient, nevertheless, to adhere to the concept of the surface point which moves along the column center line as recession progresses. To define the surface point motion with computed mass loss rates determined from this general energy-balance-determined option requires knowledge of the angle between the local normal to the surface and the column center line, since computed mass loss may be translated directly into recession along a normal to the surface. Recession along the normal may be projected into the nodal column center line once the angle between these two lines is known. The direction of the surface normal may conveniently be determined from the slope of the surface, that is the surface shape, and of course the direction of the column center line is known.

It is obviously not safe to use the slope of the heated (top) surface of the surface nodal box to obtain the surface slope, since in general it is neither possible nor always desirable to lay out a nodal grid which will "conform" to the "real" surface for the entire problem history. Therefore the ASTHMA program includes a special curve-fit subprogram which computes a

surface shape at each time step during one solution after examining the lay-out of the surface points. Referring to Figure 2-7, the program computes the

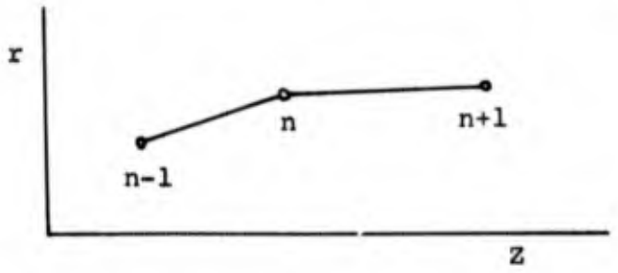

Figure 2-7. Sketch of Surface Points

slope of the surface, dr/dZ, at surface point n as the average of the slopes between surface points n-1 and n, and n and n+1. Thus

$$\left.\frac{dr}{dZ}\right|_n = \frac{1}{2}\left(\frac{r_n - r_{n-1}}{Z_n - Z_{n-1}} + \frac{r_{n+1} - r_n}{Z_{n+1} - Z_n}\right) \qquad (15)$$

Note that n-1, n, and n+1 are <u>surface</u> points, not nodal corner points. (Problems with only one nodal column have only one surface point. This requires the program to abandon the average slope scheme and to use the nodal box heated surface slope as the surface slope.)

With surface slope determined, the surface movement ΔS computed during the time step may be projected onto the nodal box center line, and then the

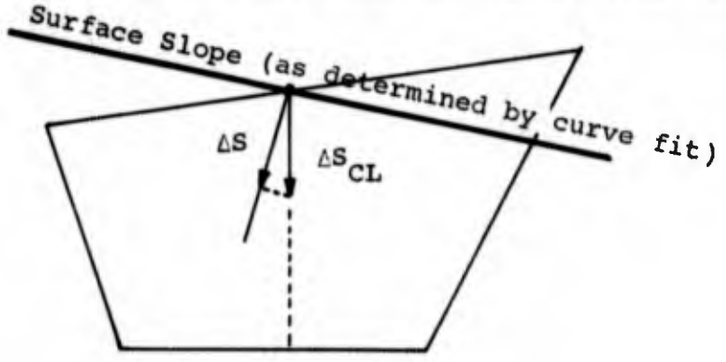

Figure 2-8. Sketch of Surface Geometrical Relationships (exaggerated)

new nodal volume computed, as indicated in the exaggerated sketch of Figure 2-8. Actual surface movement during a time step is limited to a small fraction of the nodal thickness to ensure a good approximation to the conservation of mass.

2.3 INTERNAL CONDUCTION PARAMETERS

The thermal resistances between nodes and the thermal capacity of the nodes are calculated each time interval from the material properties of the node corresponding to its temperature at that time. The material properties (density (ρ), specific heat (c), conductivity (k), and emissivity (ϵ) are input as table look up functions of temperature. Linear interpolation is employed for material property determination at temperatures intermediate to those tabulated. Constant thermal contact resistances may be specified between any or all nodes. The nodal capacities and resistances are calculated as follows:

$$C_{m,n,\theta} = \rho_{m,n,\theta} c_{m,n,\theta} V_{m,n} \tag{16}$$

$$R_{m,n,A,\theta} = \frac{1}{A_{m,n+1,A}} \left(\frac{L_{m,n,C}}{k_{m,n,\theta}} + \frac{L_{m,n+1,A}}{k_{m,n+1,\theta}} + R^*_{m,n,B} \right) \tag{17}$$

$$R_{m,n,B,\theta} = \frac{1}{A_{m+1,n,B}} \left(\frac{L_{m,n,B}}{k'_{m,n,\theta}} + \frac{L_{m+1,n,D}}{k'_{m+1,n,\theta}} + R^*_{m,n,A} \right) \tag{18}$$

Figure 2-9 shows the locations of resistances $R_{m,n,A,\theta}$ and $R_{m,n,B,\theta}$. The

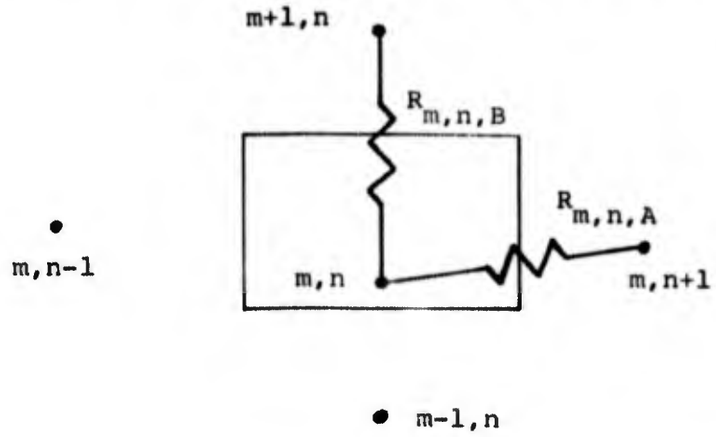

Figure 2-9. Sketch of Thermal Resistance Nomenclature

resistance on the other two sides of the nodal box are calculated when the quantities for the adjacent nodes are calculated. For nodes adjacent to the surface, however, $A_{m,n,C} \neq A_{m,n+1,A}$ generally (refer to Fig. 2-5 for area nomenclature); for these nodes

$$R_{m,n,A} = \frac{L_{m,n,C}}{A_{m,n,C} k_{m,n,\theta}} + \frac{L_{m,n+1,C}}{A_{m,n+1,A} k_{m,n+1,\theta}} + \frac{R_{m,n,B}}{A_{m,n,C}}$$

It should be noted that anisotropic thermal conductivity values k and k' are used in Equations (17) and (18), respectively.

2.4 IN-DEPTH CONDUCTION SOLUTION

The in-depth conduction solution is the explicit finite difference type often employed for transient heat conduction analysis. The temperature of node m,n at time θ' ($T_{m,n,\theta'}$) is obtained by application of the finite difference energy balance and rate equations to the nodal volume.

Solving for $T_{m,n,\theta'}$, one obtains:

$$T_{m,n,\theta'} = \left[\frac{T_{m+1,n,\theta}}{R_{m,n,B,\theta}} + \frac{T_{m,n+1,\theta}}{R_{m,n,A,\theta}} + \frac{T_{m-1,n,\theta}}{R_{m-1,n,B,\theta}} + \frac{T_{m,n-1,\theta}}{R_{m,n-1,A,\theta}} - T_{m,n,\theta} \cdot \left(\frac{1}{R_{m,n-1,A,\theta}} + \frac{1}{R_{m,n,B,\theta}} + \frac{1}{R_{m,n,A,\theta}} + \frac{1}{R_{m-1,n,B,\theta}}\right)\right] \frac{\Delta\theta}{C_{m,n,\theta}} + T_{m,n,\theta} \quad (19)$$

In the program this equation is used to obtain "new" temperatures for all nodes except those adjacent to the heated surface and for back wall nodes. Nodes adjacent to the heated surface are linked to the surface temperature implicitly and hence a special procedure is used for the temperature of these nodes, as described in the next section.

Back wall nodes include a quantity

$$hA_{m,n,D}(T_{res} - T_{m,n,\theta}) + \sigma\epsilon_{bw}A_{m,n,D}(T^4_{m,n,\theta} - T^4_{res})$$

inside the brackets of Equation (19), and have $T_{m-1,n,\theta}$ formally equal to zero.

The explicit relation (19) imposes the familiar stability restriction on the time step size $\Delta\theta = \theta' - \theta$. The ASTHMA program automatically employs a conservative stability equation for interior nodes:

$$\Delta\theta = \eta\left[\frac{C_{m,n}}{\frac{1}{R_{m,n,A}} + \frac{1}{R_{m,n,B}} + \frac{1}{R_{m,n-1,A}} + \frac{1}{R_{m-1,n,B}}}\right] \quad (20)$$

Normally for stability, the input parameter η is less than unity. Surface nodes are not considered for time interval calculation, as will be explained below; back wall nodes include the terms $A_{m,n,D}(h/2 + 4\sigma\epsilon_{bw}T^3_{m,n,\theta})$ in the denominator.

The automatic stability criterion calculation may be suppressed for any node if the user is sure that the allowed time step for that node will never be the minimum one for the system. This saves some computer time.

Alternatively, the stability criterion calculation can be suppressed entirely. If it is used, then $\Delta\theta$ must be specified. If it is used, then any or all nodes in the conduction network may be specified for time interval determination.

2.5 TEMPERATURES OF SURFACE NODES AND SURFACE POINTS

Temperatures of surface points are determined either by assignment (Option 2) or by the surface energy balance described in the next section (Options 1 and 3). The surface energy balance determines the new surface temperature of the nth column T'_{s_n} with an implicit iteration technique. Stability considerations dictate that the first node temperature also be treated implicitly, and that any transverse heat conduction link (across columns) for surface temperatures must be implicit. This latter requirement is a complex one to meet as columns recede; hence the surface temperature points are not linked transversely. Figure 2-10 shows the implicit and explicit heat conduction paths for two typical columns.

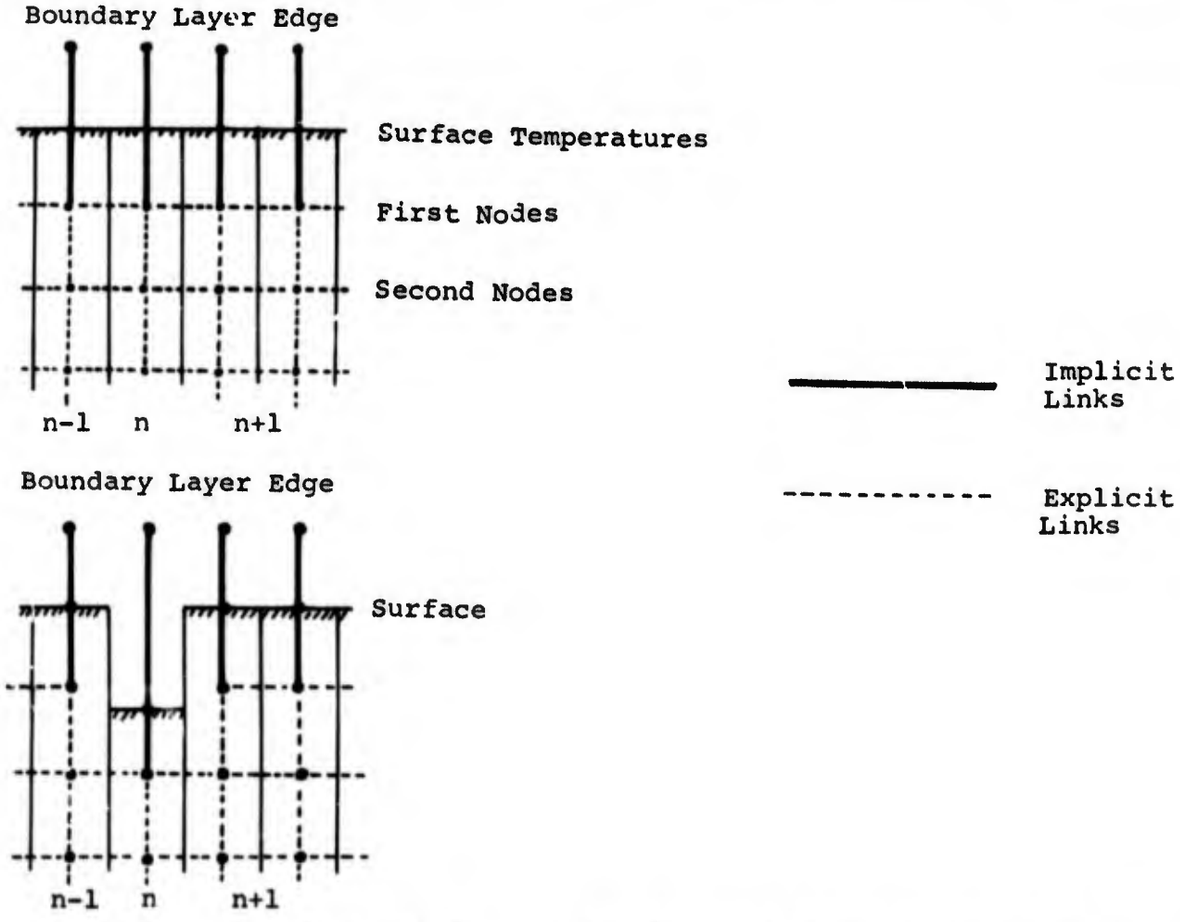

Figure 2-10. Sketch of Implicit and Explicit Temperature Links in Finite Difference Solution, for Two Typical Situations

general terms, the equation for the new temperature of a surface node (r surface point) is

$$T_{m,n,\theta'} = \left[\frac{T_{m,n+1,\theta} - T_{m,n,\theta}}{R_{m,n,A,\theta}} + \frac{T_{m,n-1,\theta} - T_{m,n,\theta}}{R_{m,n-1,A,\theta}} + \frac{T_{m-1,n,\theta} - T_{m,n,\theta}}{R_{m-1,n,B,\theta}} + \frac{T_{s,n,\theta'} - T_{m,n,\theta'}}{R_{m,n,B,\theta}} \right] \frac{\Delta\theta}{C_{m,n,\theta}} + T_{m,n,\theta} \tag{21}$$

Th s linked to the surface energy balance through the surface point temper- at $T_{S,n,\theta'}$. Formally we have a relation between the two unknowns as

$$T_{m,n,\theta'} = f(T_{S,n,\theta'}) \tag{22}$$

Th face energy balance has the general form (as described in the next se)

convection and chemical energy terms ($T_{S,n,\theta'}$)

+ radiation to wall - radiation out ($T_{s,n,\theta'}$)

$$= \frac{T_{S,n,\theta'} - T_{m,n,\theta'}}{R_{m,n,B,\theta}} = f_2(T_{m,n,\theta'}, T_{S,n,\theta'}) \tag{23}$$

wh he parentheses denote functional relationship. Relation (22) may be su uted into Equation (23) to give the non-linear surface energy balance Eq on for $T_{S,n,\theta'}$. When $T_{S,n,\theta'}$ has been found from this equation, the ne face node temperature $T_{m,n,\theta'}$ may be found from Equation (22). For su energy balance options, the method for finding $T_{S,n,\theta'}$ is described in ion 3 below. In Option 2, $T_{S,n,\theta'}$ is known immediately and Equation (2 en determines $T_{m,n,\theta'}$ at once.

SECTION 3

HEATED SURFACE BOUNDARY CONDITION ASPECTS

The ASTHMA program can account for three different types of heated surface boundary conditions:

1. Surface energy balance determined recession rate, employing general film coefficient model for boundary layer transport of energy and mass, and very general thermochemical relations at the surface (Option 1).
2. Specified surface temperature and recession rate histories (with a different history at each surface point of interest) (Option 2).
3. Simplified energy balance to determine surface temperature including only radiation terms, no recession allowed (Option 3 - "cooldown option")

Option 2 is so simple that it requires no discussion other than that given in the user's manual below. Option 1 is complex and has many interesting aspects, some of which are discussed below. A brief discussion of Option 3 follows.

3.1 GENERAL ASPECTS

The energy balance option of Surface Energy Balance Option (Option 1) of the program performs the energy balance illustrated in the sketch of Figure 3-1. The energy balance is performed for the indicated control volume fixed

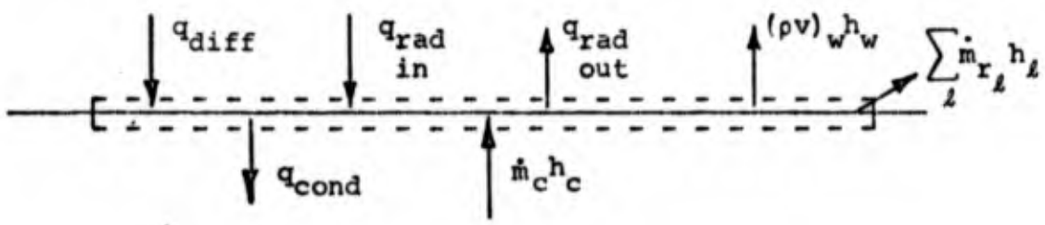

Figure 3-1. Representation of Surface Energy Terms During Ablation

to the receding surface. Energy fluxes leaving the control volume include conduction into the material, radiation away from the surface, energy in any

flow of condensed phase material such as mechanical removal,* and gross blowing at the surface. Energy inputs to the control volume include radiation in from the boundary layer and enthalpy flux due to the convection of material to the surface associated with surface recession. The final input in the sketch is denoted q_{diff}. It includes all diffusive energy fluxes from the gas phase boundary layer and the form of a correlation equation associated with the convective film coefficient model.

The computation of the surface energy balance requires from the in-depth solution a relation between the surface temperature and the rate of energy conduction into the material, q_{cond}. This relation derives naturally from the finite difference energy balance for the node just under the surface. With this information the surface energy balance considerations allow determination of the thermochemical erosion rate $\dot{m}$ and surface temperature T_w. It will be useful to keep in mind that, from this point of view, the purpose of the in-depth solution at any instant is to provide information about $q_{cond}(T_w)$. The surface energy balance equation may be written as

$$q_{diff} + \underset{in}{q_{rad}} + \dot{m}_c h_c - \underset{out}{q_{rad}} - (\rho v)_w h_w - \sum_{\ell} \dot{m}_{r_\ell} h_\ell - q_{cond} = 0 \qquad (24)$$

where

$$(\rho v)_w = \dot{m}_c - \sum_{\ell} \dot{m}_{r_\ell} \qquad (25)$$

The relation $q_{cond} = f(T_w)$ is delivered by the in-depth solution. Other dependencies of interest are

$$h_c = h_c(T_w) \qquad (26)$$

$$\underset{out}{q_{rad}} = \underset{out}{q_{rad}}(T_w) \qquad (27)$$

*The energy balance procedure has indeed been constructed to include mechanical terms but in the first version of the program failing is not allowed (in order to exploit input conveniences) since it is not usually important for rocket nozzles.

For the other terms, we may write in general

$$T_w,\ q_{diff},\ q_{\substack{rad\\in}},\ h_w,\ \sum_{\ell}\dot{m}_{r_\ell} h_\ell = \text{functions of boundary-layer-edge enthalpy, pressure, upstream events, laws for conservation of chemical elements, chemical equilibria and/or kinetic relations, } \dot{m}_c\text{, local boundary layer aerodynamics} \qquad (28)$$

Relations of the type of Equation (28) come in many forms, and may even take the form of exact solutions to boundary layer and surface chemical state routines. In the present program, the relations (28) are computed by the separate chemistry program (ACE), for use by Equation (24) in ASTHMA, based on a film coefficient model of the boundary layer transport events. The ACE program is fully described in Reference 9. Since relations (28) are obtained by a film coefficient based program (ACE), the main energy balance (24) used by the ASTHMA program is also of a film coefficient type.

When the boundary layer transport aspects of the problem are modeled by a film coefficient scheme, then both Equations (24) and (28) can be normalized in the mass transfer coefficient in the customary manner. Equation (24) becomes

$$\frac{q_{diff}}{\rho_e u_e C_M} + \frac{q_{\substack{rad\\in}} - q_{\substack{rad\\out}}}{\rho_e u_e C_M} + B'_c h_c - B' h_w - \sum_{\ell} \frac{\dot{m}_{r_\ell}}{\rho_e u_e C_M} h_\ell - \frac{q_{cond}}{\rho_e u_e C_M} = 0 \qquad (29)$$

and Equation (28) takes the general form

$$T_w,\ \frac{q_{diff}}{\rho_e u_e C_M},\ \frac{q_{\substack{rad\\in}}}{\rho_e u_e C_M},\ h_w,\ \sum_{\ell} \frac{\dot{m}_{r_\ell}}{\rho_e u_e C_M} h_\ell = \text{functions of boundary layer edge enthalpy, pressure, laws for conservation of chemical elements, chemical equilibrium and/or kinetic relations, } B'_c \qquad (30)$$

The generation of the Equation (30) relationships is the goal of the surface thermochemistry solution (ACE) as noted above. For the present it may be observed that the energy balance coupling to the in-depth solution (ASTHMA) for each time step proceeds as follows: an initial guess of the dimensionless mass removal rate B'_c is obtained in some manner. With this B'_c, the quantities $q_{diff}/\rho_e u_e C_M$, h_w, $\sum \dot{m}_{r_\ell} h_\ell / \rho_e u_e C_M$, and T_w are obtained

from the surface thermochemistry solution. The quantities h_c and $q_{rad\ out}$ are then formulated using the T_w so obtained. The surface energy balance is then computed, the q_{cond} as a function of T_w having been provided by the in-depth solution. In general, however, the sum of the terms will not equal zero but some error. An iteration procedure is then used to select successively better estimates of B'_c which drive the error to zero. Experience shows that Newton's procedure, in which the derivative of the error with respect to B'_c is used to compute the next guess for B'_c, gives good results.

3.2 COMPUTATIONAL APPROACH TO CONVECTIVE ENERGY BALANCE

3.2.1 General Description of Approach

It is evident that each iteration in the search for a surface energy balance, if performed as described above, would require a new surface chemistry solution, generally in the near neighborhood of many such previous solutions. This suggests that a tabular approach in which the surface state solutions are done beforehand for preassigned B'_c values, would offer significant computational economies. The Aerotherm CMA program (a one-dimensional, transient, charring material ablation program) has long exploited this approach with good success (Ref. 5). Since the approach used in the ASTHMA program surface energy calculations has been built on the basic CMA model, it will be useful to first describe the CMA procedures in detail and then to explain the slight changes incorporated in the ASTHMA version. For the CMA program, a complete three-dimensional table is precalculated with an entirely separate computer program* for each ablation problem. The three dimensions are $\dot{m}_c/\rho_e u_e C_M$, $\dot{m}_g/\rho_e u_e C_M = B'_g$, and another variable which effectively is the boundary layer edge state identifier, most conveniently pressure. For the problem of interest here, there is no pyrolysis gas rate $\dot{m}_g$, and the parameter B'_g instead takes on the significance of a chemical kinetics parameter k'_f, as discussed in Section 3.2.2 below. The CMA description in the following few paragraphs will continue to refer to B'_g, but there is no difference in treatment between B'_g in the CMA program and k'_f in the ASTHMA program. The physical meaning of k'_f is discussed below, in Section 3.2.2. Pressure is necessary for the surface state calculation in all cases. Specification of the boundary layer edge state implies pressure plus, say, edge enthalpy, but since only one physical location on the ablating body is involved in the one-dimensional CMA solution, the boundary layer edge state is really only a function of one variable, time. Pressure can be used instead, for convenience.

The course of a typical CMA solution might be represented as shown in Figure 3-2. As time proceeds, solutions progress through the space of the

*Applicable programs here included the Equilibrium Surface Thermochemistry Program, Version 1 (Ref. 6), and Version 2 (Ref. 8), and the ACE program (Ref. 9).

table independent variables B'_c, B'_g, and P. The dots in the picture represent solutions satisfying the surface energy balance as time progresses. Surrounding these points are a number of other points examined during the iterations to satisfy the surface energy balance. For any iteration, the solution procedure finds itself, so to speak, within a cube formed by the bracketing tabular values of B'_c, B'_g, and P. The dependent quantities T_w, $q_{diff}/\rho_e u_e C_M$, h_w and $\sum \dot{m}_{r_\ell} h_\ell / \rho_e u_e C_M$ have been precalculated for these tabular points; relevant values of these quantities for the current iteration values of B'_c, B'_g, and P can then be formed by interpolation inside the cube and the surface energy balance equation calculated. If the energy balance is not satisfied to some preselected degree of accuracy, a new value of B'_c can be selected and the process repeated.

The tabular approach was selected in general because the interpolation feature drastically reduces the number of surface state calculations while at the same time allowing sufficient accuracy.* The precalculated table approach** was chosen for the following reasons:

1. In parametric studies, tables once generated are useable for many different problems, yielding even greater economy.
2. For most problems, it is difficult to specify a priori an "adequate" array of independent tabular values B'_c, B'_g, and P. An examination of the precalculated surface tables before execution of the actual ablation-problem-plus-in-depth-solution can reveal if there are any "holes" in the tables in areas where energy terms are varying rapidly. Desirable table points can be added before the in-depth response run.
3. The surface tables are frequently of independent interest in themselves for judging the ablation effects under various conditions.
4. Finally, without the tabular approach, the occasional nonconvergent surface chemistry solution would stop the entire in-depth solution process. With the precalculated table approach, such solutions are automatically weeded out of the tables without damage to the subsequent in-depth solution.

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*For example, a typical 2000 time step problem with the usual 5 iterations per time step would require 10,000 surface state calculations, which require 1 to 3 seconds each ofr machines in the 7094 speed class. A single pressure table, on the other hand, involves only about 600 state solutions (30 char rates times 20 gas rates), a factor of 15 improvement. Multiple pressure tables reduce this advantage, but usually only a few pressure are required.

**As opposed to a direct coupling scheme in which tabular dependent entries were only calculated as needed.

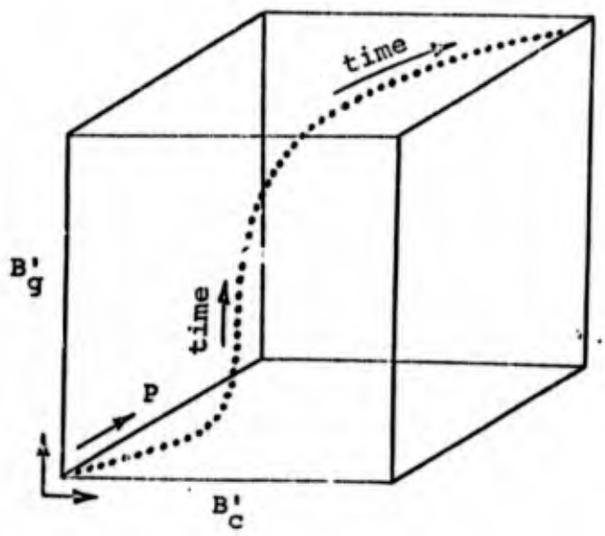

Figure 3-2. Representation of Course of Independent Variables in Surface History

On the other side of the ledger, some disadvantages in the precalculated table approach are evident however:

1. Figure 3-2, which is a realistic schematic view of a typical calculation history, indicates that most of the laboriously calculated and assembled surface state points in the table are never used in the course of a given solution.

2. The "mechanical" linkage between the surface state solution and the in-depth solution, i.e., the transfer of punched card surface state output to input of the in-depth program, leads to computing delays and occasionally to gross input blunders (wrong decks, missing parts of decks, etc.).

3. Significant storage is required by the large precalculated table.

These disadvantages are usually outweighed by the advantages of the precalculated table approach, however. Hence this same well tested apprcach has been adopted for the ASTHMA program. The char ablation rate parameter B'_c and the pressure (or edge state) parameter P retain their original (CMA) significance, but the gas rate parameter B'_g is dropped and is replaced by a kinetics paramter $k_f/\rho_e u_e C_M = k'_f$. This substitution, however, has brought in a number of new aspects discussed in the following subsection. Further information on this topic of kinetics can be found in Reference 9.

3.2.2 Treatment of Kinetics Parameters

The new surface state program ACE (Ref. 9) differs from earlier Aerotherm surface state programs by allowing certain chemical reactions to be rate controlled, rather than requiring complete equilibrium. In consequence, the ASTHMA program, which uses as input the output of the ACE program, is able to account for chemical kinetics. It does this through a "kinetics parameter" of the form $k_f/\rho_e u_e C_M$ which replaces the pyrolysis gas rate parameter B'_g of the charring material program noted above. This kinetics parameter is explained in detail in Reference 9; it is a measure of the relative importance of chemical surface kinetics for those reactions considered by the state program to be kinetically controlled.

The program user inputs to the ASTHMA program the forward rate coefficient of one particular kinetically controlled reaction used by the chemistry state solution program (ACE) in its solution. The chemistry program will identify this reaction both on its printed output and on certain cards in the punched output.

This odd and somewhat inconvenient kinetics link between the surface state program (ACE) and the in-depth program (ASTHMA) derives from the generality of the ACE program. Reference 9 explains how, in the mass balances

and chemistry relations used in ACE, kinetic rate equations always appear divided by $\rho_e u_e C_M$. Thus, since any forward rate coefficients used in ACE are used in the form $k_f/\rho_e u_e C_M$, the ACE user inputs parametric array values of $k_f/\rho_e u_e C_M$ for all kinetically controlled reactions. The ASTHMA user, however, is forced by the nature of his problem to deal with both the set of k_f's and $\rho_e u_e C_M$ as separate entities. Therefore he must specify both $\rho_e u_e C_M$ and the specific values of the k_f's. Regardless of the number of k_f's used in the ACE solution (i.e., the number of kinetically controlled reactions), after the surface state solution is completed the relationship between these coefficients is fixed and cannot be changed. Thus the ASTHMA user only needs to communicate with ACE through a single "kinetics number," and hence the ACE program punches as its output card one specific value $k_f/\rho_e u_e C_M$ rather than the complete set of values representing all kinetically controlled reactions. The ASTHMA user inputs to ASTHMA values for $\rho_e u_e C_M$ and whatever value of k_f he wishes for the single "flag" reaction used by the ACE program in its output. Unfortunately, a single output card for each surface state point (fixed B_c', k_f', and P) has insufficient space even to identify the flag reaction, let alone to identify the complete set of kinetically controlled reactions employed. Therefore the ASTHMA user will have to excercise great caution to ensure that all cards in his surface state "deck" (see Section 1.8 in the User's Manual below) were constructed with the same set of kinetically controlled reactions, the same set of values of kinetic coefficients, and have the same "flag" reaction identification.

3.2.3 Change in Treatment of Pressure

One further change was made from the CMA pattern of solution. Since the ASTHMA program was designed primarily for rocket nozzle applications where the range of pressures is small, the interpolation in the pressure direction was dropped. Instead, each surface column is flagged to one specific pressure (or edge state) in the set of tables. No interpolation is done.

3.3 FORMS OF THE FILM COEFFICIENT MODEL SURFACE ENERGY BALANCE EQUATION USED IN OPTION ∴

In making the surface energy balance calculation described in Section 3.2 above, the ASTHMA program uses a variety of surface energy balance equations of the general form of Equation (29). The basic equation, derived in Reference 1 with analogy arguments, is

$$\rho_e u_e C_H (H_r - h_w)_{\substack{\text{edge}\\ \text{gas}}} + \rho_e u_e C_M \left[\sum_i (K_{i_e} - K_{i_w}) h_i^{T_w} + B_c' h_c + B_g' h_g - B' h_w \right]$$

$$+ \alpha_w q_{rad} - F\sigma\epsilon T_w^4 - q_{cond} = 0 \qquad (31)$$

It should be noted that, like all film coefficient expressions, this equation is not a universally valid one. It is well established for frozen boundary layer, catalytic wall problems with no net mass transfer (Refs. 11, 12). It is presumed accurate for reactive boundary layers as well (see a discussion of similar considerations in Ref. 13). For problems with net mass transfer (ablation), which are of interest here, the equation is less well established, but

1. Has been derived with "respectable" analogy arguments (Ref. 1)
2. Compares well with similar results derived by Lees (Ref. 12)
3. Has given good predictions when compared to some experimental data and to results of "exact" boundary layer solutions.
4. Gives results independent of the choice of enthalpy datum state (an important criterion)
5. Reduces, for $C_M = C_H$, to a widely accepted energy balance law (Refs. 14, 15) for simultaneous heat and mass transfer

Equation (31) has been generalized in Reference 2 to the case of <u>unequal</u> mass diffusion coefficients, again by analogy arguments. The result is

$$\rho_e u_e C_H (H_r - h_w)_{\substack{\text{edge}\\ \text{gas}}} + \rho_e u_e C_M \left[\sum_i (Z_{i_e}^* - Z_{i_w}^*) h_i^{T_w} + B_c' h_c + B_g' h_g - B' h_w \right]$$

$$+ \alpha_w q_{rad} - F\sigma\epsilon T_w^4 - q_{cond} = 0 \qquad (32)$$

where

$$Z_i^* \triangleq \frac{A_i^\gamma K_i^{1-\gamma}}{\sum_j^I Z_j^\gamma k_j^{1-\gamma}} \qquad (33)$$

$$Z_i \triangleq \frac{m_i x_i}{F_i \mu_a} = \frac{m K_i}{F_i \mu_a} \quad \text{since} \quad m_i x_i = m K_i \qquad (34)$$

and

$$\mu_a \triangleq \sum_i \frac{m_i x_i}{F_i} = m \sum \frac{K_i}{F_i} \qquad (35)$$

The factors F_i in these equations derive from the particular relation between the binary diffusion coefficients which must hold if the governing differential equations are to reduce to the forms from which Relation (32) can be inferred. This relation is

$$\mathcal{D}_{ij} = \frac{\bar{D}}{F_i F_j} \tag{36}$$

and can be regarded as an accurate correlation of experimental data for the binary diffusion coefficient $\mathcal{D}_{ij}$. The quantity $\bar{D}$ is a constant for a given pressure. The constants F_i depend weakly on temperature.

Equation (32) is somewhat less well founded than the corresponding Equation (31) but does have plausibility. Furthermore, the equation reduces to Equation (31) for equal diffusion coefficients, as it should, and Equation (32) can be shown to be independent of the enthalpy datum state and thus fulfills a basic physical requirement.

The ACE program provides to the ASTHMA program the four dependent quantities $h_{w_{edge\ gas}}(T_w,p)$, $T_w(B'_c,p)$, $\sum_i z_{i_e} h_i^{T_w}(B'_c,p)$ and $\sum_i z^*_{i_w} h_i^{T_w}(B'_c,p)$ for a given value of k'_f. With the quantity $h_{w_{edge\ gas}}(T_w,p)$ stored in one table with independent variables T_w and p, and the other three dependent quantities stored in a table with independent variables B'_c, k'_f, and p, the ASTHMA program may find surface energy balances at any surface point and time (i.e., given pressure and $\rho_e u_e C_M$) by (1) selecting the correct p table, (2) finding $k'_f = k_f/\rho_e u_e C_M$, (3) finding the dependent quantities in the two tables at k'_f values bracketing the actual k'_f and for some B'_c, (4) interpolating on k'_f, (5) forming the energy balance equation (32) and noting the error or departure from zero, (6) selecting a new B'_c for another try. The Newton-Raphson method is used for selecting the next guess of B'_c in step (6). When that B'_c yielding an energy balance is determined, the new T_w is known as a dependent quantity; thus the new surface temperature is determined.

3.4 Cooldown Energy Balance Option

For representing radiation controlled situations, such as cooldown after exposure to convective heating, it is useful to have a surface energy balance option which has only radiation terms. Such an option is built into the ASTHMA program and is termed "Option 3". The energy balance for this case is simply

$$\alpha_w q_{rad} - F\sigma\epsilon T_w^4 - q_{cond} = 0 \tag{37}$$

3.5 INPUT AND CORRECTION OF HEAT TRANSFER COEFFICIENT

To employ the film coefficient formulation just described, the program user must provide the program with values of the heat transfer coefficient $\rho_e u_e C_H$ as functions of time. Two practical problems must be settled in this respect:

1. How is C_M related to C_H?
2. Can both C_M and C_H be specified as functions of edge conditions (i.e., of time) independent of the subsequent problem solution (i.e., mass transfer rates and body shape)?

In answer to the first question it may be stated that within the present formulation it is adequate to take the ratio C_M/C_H as a constant. The value of this constant is a measure of the ratio of the mean mass transfer aspects of the boundary layer to the mean heat transfer aspects. For equal mass diffusion coefficients, a vast amount of experimental data (as summarized, for example, in Ref. 15) suggest the correlation $C_M/C_H = Le^{\gamma}$. It may be hypothesized that for unequal mass diffusion coefficients the same procedure may be employed with the Lewis Number, Le, defined by the procedure set forth in Reference 2 involving $\overline{D}$. Thus, the input to the program consists of a time table of values for $\rho_e u_e C_H$ and the constant factor C_M/C_H.

In answer to question 2., changes of C_H with body shape are not usually of interest for rocket nozzle problems and hence are not accounted for in the ASTHMA program. A more important problem concerns the dependence of C_H on the actual rate of mass transfer. This problem has been ignored up to now, the implication being that C_H is determined by the boundary layer edge aerodynamics alone. This is known to be incorrect. The value of C_H depends fairly strongly on $\dot{m}$. If we denote the C_H with $\dot{m} = 0$ as C_{H_O}, this dependence is shown by both data and analysis to be accurately represented by

$$\frac{C_H}{C_{H_O}} = \frac{\varphi}{e^{\varphi}-1} \tag{38}$$

where

$$\varphi \triangleq \frac{2\lambda \dot{m}}{\rho_e u_e C_{H_O}} \tag{39}$$

This correction is built into the program.

PART II

USER'S MANUAL
ASTHMA PROGRAM

his section of the report summarizes the input requirements of the program in a form convenient for user of the program and provides c instructions for program operation.

SECTION 1

DESCRIPTION OF INPUT

e input to the Axi-Symmetric Transient Heating and Material Ablation can conveniently be considered as having eight parts. All eight portf the deck must be present for each run (with the exception of the -equilibrium data in the case of surface-boundary conditions Options Option 3 in conjunction with Option 3). These individual parts are ed in the following subsections.

1. TLE AND HEADING INFORMATI N

e first three cards of the data deck are used to transmit title and information to the output. The first 72 columns of each of these ay be used for the title, the alphameric information in columns 61 72 of the third card being used as a page heading on all pages after st.

1. NERAL PROBLEM CONSTANTS

e card provides the program with certain general constants.

Co	Format	Data	Units
1	I3	Largest m index in nodal network, number of rows of boxes (not corners)	---
4	I3	Largest n index in nodal network, number of columns of boxes (not corners)	---
7	E6.4	Initial value of problem time	sec
13	E6.4	Final value of problem time	sec
19	E6.4	Output time interval	sec
25	E6.4	Computation time increment. If entered, this interval is always used and stability considerations are suppressed. If blank, stability limited time step will be calculated by program	sec

Column	Format	Data	Units
31-36	E6.4	Safety factor multiplying stability time step limit, see Equation (20)	---
37-42	E6.4	Heat of formation of ablating material at 536°R (298°K)	Btu/lb
43-48	E6.4	Blowing reduction parameter λ of Equation (35); this value may alternatively be inserted as a function of time in the time tables (Section 1.7 below); blank values in time table will be filled with this constant value*	---
49-54	E6.4	Back wall heat transfer coefficient	Btu/ft-sec°R
55-60	E6.4	Back wall emittance	---
61-66	E6.4	Reservoir temperature communicating with back wall	°R
67	I1	KASE, flag for stacked problems; +1 denotes another case to follow, 0 denotes last problem	---
68	I1	KSTRP, calls for punched nodal output compatible with thermal stress programs; 1 calls for punched output at all print times, 2 calls for punched output at special times given on following card	

1.3 SPECIAL PUNCHED TEMPERATURE OUTPUT SPECIFICATION (OPTIONAL)

If KSTRP on the previous card is 2, up to eight special output times are to be provided for the punched output on a single card. See output description for further information.

Column	Format	Data	Units
1-10	8F10.0	Up to eight output times for punched output data	sec
11-20			
21-30...			

1.4 NODAL NET CORNER COORDINATE CARDS

This set of cards provides the nodal box corner coordinates and certain nodal center locations to the program. For m rows and n columns, there will be (m+1) (n+1) corner coordinate cards. It is advisable to run the corner coordinate cards through any convenient plot program to check the nodal layout before any heat transfer calculations are made.

*Recommended values are 0.5 for laminar flow, 0.4 for turbulent.

Corner cards must be entered in order beginning at m=1, n=1 and continuing up the first column of corners (n=1) for all m's until column is completed, returning to bottom of next column m=1, n=2, and so on.

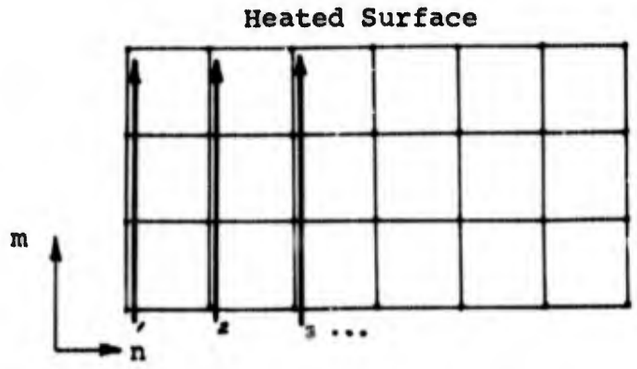

Figure 1-1. Sketch of Nodal Corner Input Order

Corners m, n representing boxes m, n which have no material (null nodes entered to complete the mesh lattice) may be blank entries, but a card must always be included. There must be (m+1)(n+1) corner cards.

Nodal center specifications must be blank for the main material. The program will automatically locate these nodal points. Nodal centers for back up materials may be entered or may be left blank. If blank, the program will compute a centered nodal location for these nodes.

Present dimensions allow 300 nodal boxes, with a maximum of 40 columns.

Column	Format	Data	Units
1-7	E7.5	Corner radius, r_c	inches
8-14	E7.5	Corner axial location, Z_c	inches
15-21	E7.5	Nodal center radius coordinate r_N, must be blank for main ablating material, may be blank for back-ups	inches
22-28	E7.5	Nodal center axial coordinate Z_N, must be blank for main ablating material, may be blank for back-ups	inches

1.5 NODAL DATA CARDS

This set of cards identifies the materials in the nodal boxes, flags the time tables and surface thermochemistry tables to be associated with the nodes, and specifies radiation view factors. For an m by n mesh network mn cards must appear, blank cards being entered for null (no material) nodes. Cards begin at 1,1 and proceed to m,1, followed by 1,2 to m,2, and so on.

Column	Format	Data	Units
1	I1	Material number of material in this box, refers to numbered material properties tables. Blank for null node	---
2	I1	Enter 1 if used for stability limit calculation of time step. Leave blank if this node can safely be omitted from stability considerations (economy measure)	---
3	I1	Enter 1 if this node is at the heated surface, otherwise blank	---
4	I1	Enter number of surface thermochemistry table which is to be used for energy balance calculations on this node if it is or becomes a surface node (see Section 1.8.3 below)	---
5-6	I2	Enter number of time-function table which is to be used for boundary conditions for this node if it is or becomes a surface node (see Section 1.7 below)	---
7-12	E6.4	Leave blank (reserved for future use)	---
13-18	F6.4	Initial temperature of this node	$^{\circ}R$
19-24	E6.4	Interface (contact) resistance at top of node (m+1 plane)	$ft^2 sec^{\circ}R/Btu$
25-30	E6.4	Interface (contact) resistance at right side of node (n+1 plane)	$ft^2 sec^{\circ}R/Btu$
31-36	E6.4	Option 1 radiation view factor for this node if it is or becomes a surface node	---
37-42	E6.4	Option 3 radiation view factor for this node if it is or becomes a surface node	---

1.6 MATERIALS PROPERTIES TABLES

One table of temperature dependent material properties is input for each material appearing in the nodal network. A lead card gives the total number of materials used. The tables are not numbered and are presumed to be encountered in ascending numerical order, beginning at one and including no gaps or omitted table numbers. The main ablating material must have material number and table number one. There must be at least two temperature entries in each table. Present dimensions allow six material property tables, with 15 temperature entries in each table.

First Card

Column	Format	Data	Units
1-2	I2	Total number of materials	---

Tabular Entry Cards

Column	Format	Data	Units
1-2	I2	Flag. Last entry in table has -1; blank for other cards	---
3-8	E6.4	Temperature	$^{\circ}R$
9-14	E6.4	Density. Enter in first card only; will not be a function of temperature	lb/ft^3
15-20	E6.4	Specific heat C_p	$Btu/lb^{\circ}R$
21-26	E6.4	Thermal conductivity along rows (n-direction)	$Btu/ft\text{-}sec^{\circ}R$
27-32	E6.4	Emissivity (emittance)	---
33-38	E6.4	Thermal conductivity along columns (m-direction), if blank will be taken as equal to n-direction conductivity	$Btu/ft\text{-}sec^{\circ}R$

1.7 FUNCTIONS-OF-TIME TABLES ("HEATING" TABLES)

A series of tables provides heated surface boundary condition information as functions of time. The various time tables are independent, and each nodal box in the in-depth layout has been given the number of a time-table for use if and when that node becomes a surface node.

Three general types of boundary condition sets are available, referred to here as Options 1, 2, and 3. Section 3 of Part I above provides further description.

The three options are:

Option 1 - General convection-radiation heating with coupled mass transfer, including the effects of unequal heat and mass transfer coefficients (non-unity Lewis number) and unequal mass diffusion coefficients.

Option 2 - Specified surface temperature and surface recession rate.

Option 3 - Specified radiation view factor and incident radiation flux, as functions of time, for a stationary surface ("cooldown" option).

Options 1 and 3 are surface energy balance options; Option 2 does not, of course, use an energy balance.

Each time table may have a sequence of heating options; thus it is convenient to think of each time table as consisting of a number of sub-tables, each sub-table representing one option. The switch from one option to another requires a repeated time entry, the first card representing the last entry of the earlier table and the second card representing the start of the next table.

The total number of time values in each time-table is limited to 25. Each sub-table must have at least 2 entries, hence the number of sub-tables in a table cannot exceed 12. (The most common problem has only 2, representing an Option 1 or Option 2 calculation followed by cooldown, Option 3). Time entries must be in increasing order.

The tables are presumed to be numbered sequentially beginning with table number 1. There may be ten different time tables. The format for the time-tables is as follows:

Columns	Format	Data	Units
1	I2	Flag, nominally blank, punched to indicate the last card of each time table. Punch +1 for last card of last time table, -1 for last card of any preceding time tables	---
3-10	F8.2	Time (independent variable)	sec
11-20	F10.5	Option 1: Recovery enthalpy, relative to the same chemical-base state as used with the heats of formation	Btu/lb
		Option 2: Surface temperature	$^{\circ}R$
		Option 3: Blank	
21-30	F10.5	Option 1: Radiant energy flux to the surface	Btu/ft^2-sec
		Option 2: Surface-recession measured along nodal column center lines	mil
		Option 3: Radiant energy flux to the surface	Btu/ft^2-sec
31-40	F10.5	Option 1: Heat transfer coefficient	lb/ft^2-sec
		Option 2: Blank	
		Option 3: <u>Must</u> be blank	
41-50	F10.5	Option 1: Pressure (not used, information only)	atm
		Option 2: ad lib	
		Option 3: ad lib	
51-60	F10.5	Blowing rate parameter λ (see Section 1.2)	---

1.8 SURFACE THERMOCHEMISTRY DATA (OPTION 1 ONLY)

1.8.1 Introduction

Problems involving use of the surface thermochemistry option (Option 1) require the input of an array of surface mass and energy data particular to the option and the material being analyzed. These data include the specification of the ratio of mass transfer coefficient to heat transfer coefficient, the kinetic parameter radiation view factor, and surface thermochemical data. The cards containing this input are described below. Problems not involving Option 1 calculations do not need the surface equilibrium data deck. The program can be instructed to use the surface tables from the preceding problem (if any), in which case additional surface tables are not provided. The "surface tables" then consist of only the "lead card" described below.

1.8.2 Ratio of Mass to Heat Transfer Coefficient and Kinetics Parameter

A single card serves to specify the ratio of the convective mass transfer coefficient to the convective heat transfer coefficient (C_M/C_H) and flag kinetics parameter k_f.

Column	Format	Data	Units
1-10	F10.0	C_M/C_H	---
11-20	F10.0	Kinetics parameter k_f, forward rate coefficient of one kinetically controlled reaction in surface state solution; the particular reaction is identified in the surface state program output (see Section 3.2 in Part I above)	various
21-39	19X	Blank	---
40	I1	One punch means to use surface state tables of preceding job for this job. Blank means to read data on following thermochemistry surface deck.	---

1.8.3 Surface Thermochemistry Table

1.8.3.1 Introduction

This table supplies the necessary input data for the surface energy balance computations in Option 1. (This energy balance is discussed in Section 3 of Part I above.)

Most commonly the deck of cards which make up the surface thermochemistry table is generated by the Aerotherm Chemical Equilibrium Program (ACE). The user's manual for the ACE program describes this table in complete detail (Ref. 9). On occasion the user may desire to construct his own surface

thermochemistry table, and so the following sections include brief descriptions of the organization and format of these tables. The main emphasis however will be on the communication between the ACE program and the ASTHMA program, since this is of the most general interest.

1.8.3.2 Edge Enthalpy Data

Equations (31) and (32) of Section .3, Part I, above, indicate that if diffusion coefficients are not equal or if the ratio C_M/C_H is not unity, then the surface energy balance requires data about the edge gases of the boundary layer. These data are provided in special "edge tables" which precede each pressure section of the surface tables (the various sections of the surface tables are described in Section 1.8.3.3 below). The independent variables for an edge table are pressure and temperature. Dependent variables are h_{ew} and the sum $\sum z_{ie} h_i^{T_w}$.

The edge enthalpy data are entered on the cards as follows:

Column	Format	Data	Units
1-6	E6.4	Pressure	atm
7-26		Blank	---
27-30	F4.2	Unequal diffusion exponent* $1-\gamma$	---
31-37	E7.5	Temperature	°K (°R if negative, in which case enthalpies below are Btu/lb)
38-43	E6.4	$B_f' = \sum \dot{m}_{r_\ell} / \rho_e u_e C_M$ (not used in present version of ASTHMA program)	---
44-51	E8.5	Summation $\sum z_{ie}^* h_i^{T_w}$	Cal/gr (Btu/lb if temperature is entered with minus sign)
52-59	E8.5	h_{ew}	Cal/gr (Btu/lb if temperature is entered with minus sign)
60-65	A6	Unused	---
66	I1	0 (flag signifying that this card is part of the edge gas table)	---
67-78	2A6	Problem identification (not read)	---
79-80	I2	Page number on ACE output listing containing the data punched on this card (not read)	---

*This quantity is discussed in the user's manual for the ACE program (Ref. 9) and also in Refs. 1-6.

Note that although the ACE program will provide a data deck using °K and cal/gr, in those rare cases in which a user wishes to supply his own deck and prefers to work in °R and Btu/lb, he may do so simply by introducing a minus sign as a flag in front of the temperature entries.

The table length is limited to 5 pressure sets (it may have only 1 pressure set) with not more than 25 nor less than 3 temperature entries in each set. The series of temperature values may be different for the edge table at each pressure set. The table is organized as a series of sections, each representing one pressure and each preceding the corresponding pressure group of the surface thermochemistry deck as described below. The temperature entries within each section must be ordered, either ascending or descending. Similarly the pressures must be ordered either ascending or descending. (Decks generated by the ACE program will have been automatically ordered properly.)

1.8.3.3 Surface Thermochemistry Tables

This table is comprised of a series of sections. Each section represents one pressure* and one kinetics parameter value. Each section consists of two subsections. The second represents surface temperatures too low for ablation; in this subsection surface temperature is the independent variable. The first subsection contains the ablating cases; here the ablation rate is the third independent variable and the surface temperature is a dependent variable.

Thus one table has three independent variables: pressure, kinetics parameter k_f', and either surface temperature or ablation rate, depending on whether the surface temperature is high enough for ablation.

The table has either two or three dependent variables, according to whether the surface temperature is high enough for ablation. Two dependent variables always present are the summation $\sum z_{iw}^* h_i^{T_w}$ and h_w, the enthalpy of the wall gases. The third dependent variable is the surface temperature, but it is dependent only in those cases for which the surface temperature is high enough for ablation. (Otherwise, the surface temperature functions as an independent variable.)

The ACE program generates separate groups for each pressure, one at a time. These groups must be ordered on pressure (either ascending or descending)

*Remember that the word "pressure" is used as a handy edge state parameter. In general, of course, there are two independent edge state variables, which are properly accounted for by the ACE program in its chemistry solution. The ASTHMA program needs only to be given some "flag" to distinguish edge states. Pressure is chosen for this purpose, and hence the word "pressure" is used here as shorthand for "edge state."

by the user to make up the surface thermochemistry deck. Within each pressure group the kinetics parameters k'_f will be ordered in descending order. Within each kinetics section, non-zero ablation rate entries will be grouped ahead of the zero ablation rate entries. The non-zero ablation rate entries will not be ordered in any particular way on the ablation rates; any necessary ordering is made automatically by the ASTHMA Program as it reads in the data. The zero ablation rate entries are ordered with descending temperatures.

(Users providing their own thermochemistry decks must ensure that the pressures and kinetic parameters are ordered, but the ordering may be either ascending or descending in each case. Within each kinetics section, the non-zero ablation rate entries and the zero ablation rate entries may be shuffled together but the zero ablation rate entries must be encountered in order of descending temperature during the reading process. Non-zero (ablating) ablation entries need not be ordered. The ablation rate for non-ablating (zero ablation rate) entries need not actually be zero, but may not exceed an ablation rate in the ablation section. These cards are identified as zero ablation rate cards by a unity flag in column 66, as described in the format specification below.

The number of pressure groups may not exceed 5 (and may be only 1); the number of kinetic parameters in each pressure group may not exceed 8 and may not be less than 2. The sequence of kinetics parameter values need not be the same in the different pressure sections. Within each kinetics section the number of ablation rate entries, including the zero ablation rate (independent surface temperature) cards, may not exceed 24 and may not be less than 2. The series of ablation values B'_c may be unique for each section.

The $^{\circ}$R-Btu/lb option described for the edge tables in Section 1.8.3.2 may be used for these tables also.)

The card format for the surface equilibrium data is as follows:

Column	Format	Data	Units
1-6	E6.4	Pressure	atm
7-14	E8.5	Ablation rate $\dot{m}_c/\rho_e u_e C_M = B'_c$	---
15-20	E6.4	Gas rate $\dot{m}_g/\rho_e u_e C_M = B'_g$ (not used by ASTHMA)	---
21-26	E6.4	Kinetics parameter $k_f/\rho_e u_e C_M$	various
27-30	F4.2	Unequal diffusion exponent*	---

*This quantity is discussed in the user's manual for the ACE program (Ref. 9) and also in Refs. 1-6.

Column	Format	Data	Units
31-37	E7.5	Surface temperature	^{o}K (^{o}R if negative in which case enthalpies below are Btu/lb)
38-43	E6.4	$B'_f = \sum \dot{m}_{r_\ell} / \rho_e u_e C_M$ (not used in present version of ASTHMA program)	---
44-51	E8.5	Summation $\sum Z^{*}_{iw} h_i^{T_w}$	Cal/gr (Btu/lb if temperature is entered with minus sign)
52-59	E8.5	Enthalpy of wall gases h_w	Cal/gr (Btu/lb if temperature is en entered with minus sign)
60-65	A6	Chemical symbol of surface species. (ACE program prints such symbols arranged alphabetically and truncated from right end if necessary	
66	I1	1 for assigned-temperature entries in the equilibrium program (no ablation); > 1 for surface thermochemistry with ablation (temperature is dependent	---
67-78	2A6	Problem identification (not read)	---
79-86	I2	Page number on ACE output listing containing the data punched on this card (not read)	---

1.8.3.4 Termination Card

The surface equilibrium data deck must be terminated by a single blank card. Output decks of the ACE program may not have such a card, in which case the user must supply it.

1.8.3.5 Assembled Thermochemical Deck

Figure 1-2 shows a picture of an assembled thermochemical data deck for several pressures.

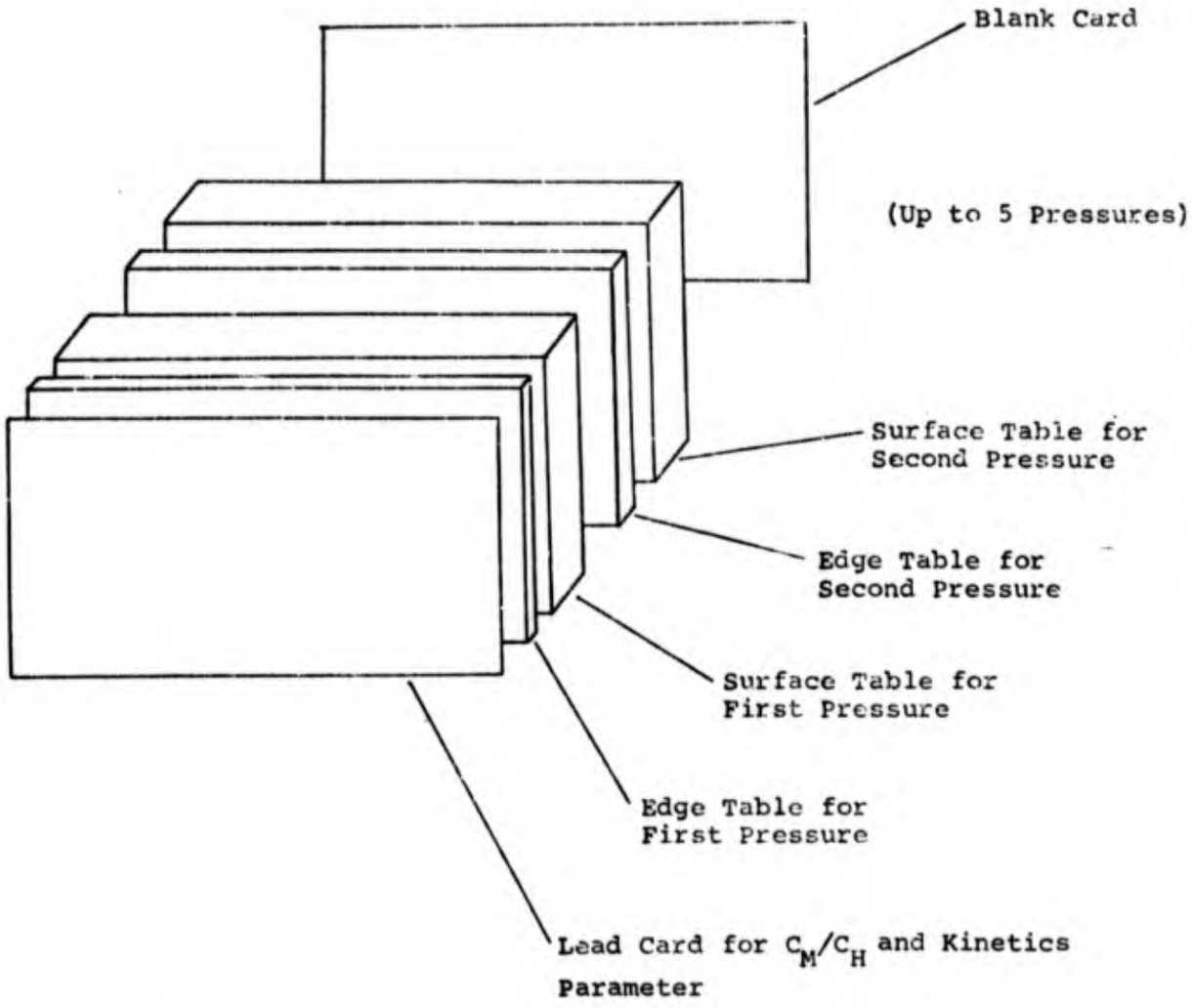

Figure 1-2. Sketch of Surface Thermochemistry Table Make-Up

SECTION 2

PROGRAM OUTPUT

2.1 INPUT DATA (EXCEPT SURFACE THERMOCHEMICAL TABLES)

Program output begins with an output of the input title and heading information, output interval specifications and general program constants, nodal data (including any computed nodal center locations), material property tables, and time dependent boundary conditions table.

All this output is fully labeled and is printed exactly as input by the user.

2.2 SURFACE THERMOCHEMISTRY TABLES

2.2.1 Edge Enthalpy Table

If there is an edge enthalpy table, it is output exactly as input.

2.2.2 Surface Thermochemistry Table

This table is output re-ordered with increasing ablation rates in each section and with a new computed term in place of the input enthalpy terms. For each entry in the surface thermochemistry tables the program computes the quantity

$$\left[\sum_i (Z^*_{ie} - Z_{iw}) h_i^{T_w} - B' h_w + \frac{\dot{m}_c h_c}{\rho_e u_e C_M} + \frac{\dot{m}_g h_g}{\rho_e u_e C_M}\right] = \frac{q_{chem}}{\rho_e u_e C_M} = \text{Chem prod} \quad (36)$$

and then outputs it as the dependent variable of interest in the output surface equilibrium table.* This term occurs directly in the surface energy balance (Eqs. (31) and (32) of Section 3.3, Part I above) and is a useful diagnostic quantity. In the output, this quantity is labeled CHEM PROD. It has the units (Btu/ft^2-sec)/(lb/ft^2-sec) = Btu/lb and can be loosely thought of as the chemical energy release per pound of $\rho_e u_e C_M$, where $\rho_e u_e C_M$ can be thought of as the "scrubbing flux" or "Reynolds flux."

In the output table, the quantity $\rho_e u_e C_M$ is abbreviated to CM.

---

*If edge tables are omitted, only the last three terms on the left are included. The mechanical removal energy term has been omitted from this equation since it is not presently considered by ASTHMA.

2.3 REGULAR OUTPUT

2.3.1 Introduction

At each output interval, as specified by the user, the program prints out the current values of ablation rates, nodal temperatures, and other supplementary information, as described below.

2.3.2 General Information

The first line of output gives the current problem time. The second line shows the current values of a number of miscellaneous quantities:

Heading	
QTOT, SUR	Total energy input to the surface $\iint q_{cond} dA d\theta$, Btu
QTOT, INT	Total energy rise of subsurface materials, Btu
CNSV FNER	Conservation of energy check, ratio QTOT,SUR/QTOT,INT
CRNODE	m, n indices of node yielding smallest stability limited time step
ITER	Total number of computational cycles (steps) required to reach the indicated value of output time. Note that the initial time is numbered as 1.
NODE D-TIME	Stability limited time step for critical node, sec
ACT D-TIME	Actual current time step; may be smaller than stability time step due to high surface recession or output matching

2.3.3 Miscellaneous Surface Data

A single line gives a set of data for each point on the heated surface. Each line presents the following data:

Heading	
ROW	Row number of node below this surface point (remember that surface points are distinct from nodal points)
COL	Column number of this surface point
OPTN	Current problem (heating) option at this surface point (1, 2, or 3)

Heading	
SURF ITER	Number of iterations required for the surface energy balance during the previous cycle
SURF TEMP(R)	Surface point temperature in degrees Rankine
H EDGE	The input edge enthalpy as determined by linear interpolation in the functions-of-time table
H WALL	Option 1: Enthalpy of edge gases at the wall temperature, h_{ew} Option 2: Blank Option 3: Blank
B PRIME TOT	Parameter $B'/\rho_e u_e C_M = (B'_f + B'_{tc})/\rho_e u_e C_M$ (current version of ASTHMA requires $B'_f = 0$)
HEAT COEFF	The current value of the convective heat transfer coefficient $\rho_e u_e C_H$ as linearly interpolated in the functions-of-time table and corrected for the effec of transpiration (blowing) according to $C_H/C_{H_O} = \zeta/(e^{\zeta}-1)$ where $\zeta = 2\lambda\dot{m}/C_{H_O}$ and C_{H_O} is the heat transfer coefficient before being corrected for blowing
CH/CHO	The ratio C_H/C_{H_O}, indicating the amount of blowing correction
PRESSURE	Current value of pressure for this column is interpolated in functions-of-time tables
RADIUS	Current radial coordinate of this surface point (inches)
Z	Current axial location of this surface point (inches)

2.3.4 Surface Rate Quantities

A series of lines, one for each surface point, gives the current recession rates, mass loss (ablation) rates, and surface energy flux rates.

Heading	
ROW	Low number of node below this surface point

COL	Column number of this surface point
RECESSION RATES- CENTER LINE	Rate of movement of surface point down column center line of surface nodal box (mils/sec)
NORMAL	Rate of movement of surface in direction normal to tangent to surface at this surface point (mils/sec)
MASS RATES MDOT TOTAL	$\dot{m}_{tc} + \sum \dot{m}_{r_\ell}$, total local mass loss rate (ablation), lb/ft^2 sec

SURFACE ENERGY FLUX RATES

This group of terms all appear in the surface energy balance, Equation (32), and have the units Btu/ft^2 sec

CONVECTED IN	$q_{sen} = \rho_e u_e C_H (H_r - h_{e_w})$
RADIATED IN	$q_{rad} = \alpha_w q_{rad}$
RADIATED OUT	$q_{\substack{rad \\ out}} = F\epsilon_w \sigma T_w^4$
CHENICAL GENERATION	$q_{chem} = \rho_e u_e C_M$(chem prod)
CONDUCTION AWAY	q_{cond}

2.3.5 Surface Time Integrated Quantities

These lines correspond exactly to the line of surface rate quantities described above. Here the quantities are integrated over time and the column surface area, so that the units of these quantities are "Btu for this column n" or Btu/col, so to speak. The area integration is done since the surface area of a column varies with time and there is no generally preferred area upon which to base the time integrated flux terms.

2.3.6 In-Depth Data

This block of data gives the current temperatures (degrees Rankine) of the subsurface nodal points. The m,n index coordinates of the points are included for convenience.

2.3.7 Optional Punched Card Output

Optional output called for by the KSTRP flag of Section 1.2 above provides punched card temperature input for various thermal stress codes. These cards are punched for all nodal and surface point temperatures for either special punch times or for all regular output times. The card format is:

Column	Format	Data	Units
1-10	F10.3	Point radius r	in
11-20	F10.3	point axial coordinate Z	in
21-30	F10.3	point temperature	^{o}R
31-38	8H	Units ININDEGR	---
39-41	I3	Point row index m (blank if a surface point	---
42-45	IH/,I3	Point column index	---
46-48	3H	Title MAT (material)	---
49-50	I2	Material number at this point	---
51-57	F7.2	time	sec
58-59	2H	Sb, units of time	---
60-71	2A6	Problem identification of columns 61-72 of third title card (Section 1.1)	---
72	1X		---
73-75	I3	Card number	---
76-77	2H	OF	---
78-80	I3	Total number of cards punched for this time	---

2.4 DUMPS

2.4.1 Introduction

To prevent the execution of computations that are wasteful or probably erroneous, the program provides certain emergency stops with dumps of diagnostic information.

2.4.2 Too-Small-Time-Step Dump

A dump occurs if the program selects a time step as small as 10^{-6} seconds. Computation ceases and the program prints out the current surface column number. Then the program sets the final problem time equal to the current time, and thus forces an output of all the current values of the standard output quantities, followed by a termination of computation.

2.4.3 Too-Many-Surface-Iterations Dump

The program allows 51 iterations to find an acceptable surface energy balance at any column point. If a balance has not been obtained after 51 iterations, the program writes the diagnostic message "Iteration Stop" and a block of diagnostic data. Since stops of this kind are complex in nature, and generally involve the surface thermochemistry data deck, the dump data must often be communicated to the program authors for analysis.

Iteration stops are almost always due to "unfortunate" variations in the tabular energy quantities making up the surface energy balance. Hence the iteration stop dump contains the 51 sets of paired values of the independent variable (either temperature or $\ell n\ B'_c$) and the surface energy balance error generated during the search for a surface energy balance. The program then dumps the surface energy balance equation error (departure from zero) at each tabular B'_c (or temperature if failure occurred in nonablating section), in the two tables bracketing the current value of kinetics parameter, properly interpolated at the current value of the kinetics parameter, for current values of CH, $q_{rad\ in}$, and in-depth conduction data. This information, plus the iteration history, permits a rather complete picture of the surface energy balance error function shape, and this in turn should usually allow an accurate assessment of the particular feature of the function currently hindering convergence.

2.4.4 Unacceptable-Surface-Thermochemistry-Table Stop

A series of checks built into the input routine serve to detect common errors in the make-up of the surface thermochemistry tables. Discovery of an error stops the reading process and the program prints out a single line:

Bad Surface Equilibrium Table of Type ---

Five error types are detected as follows:

Type	
0	Current section of independent temperature entries (no ablation) is not in descending order in temperature
1	Mass rate in no-ablation subsection has been set greater than a mass rate in the ablation subsection. Although the "zero-mass-rate" can differ from zero, they must not exceed an actual ablation rate entry.
2	Edge table has been omitted even though the diffusion coefficients are not equal (unequal diffusion exponent $\neq$ 0).

Type	
3	Edge table has been omitted even though $C_M/C_H \neq 1$
4	Inconsistent unequal diffusion exponent (this must be uniform for all tables)

2.4.5 Sense Switch Dumps

Sense Switch 1 calls for output every time step, Sense Switch 2 generates extra diagnostic dumps at every output, and Sense Switch 3 dumps some additional surface table information just prior to execution of the main program iteration loop.

SECTION 3
MISCELLANEOUS

3.1 RUNNING TIME

At present, the ASTHMA program has only been run on the Philco 2000-212, for which the execution time is well approximated by

$$T(\text{hrs}) = 5 \times 10^{-7}\ NI \qquad \pm 25\% \tag{41}$$

where N = number of nodes and I = number of iterations, provided that the number of iterations per output page exceeds about 3 (otherwise output time begins to be appreciable). Iterations I may be estimated from

$$I = \frac{\text{problem time}}{\text{time step limit}} \tag{42}$$

and the time step limit may usually be estimated fairly closely from a small number of obvious candidate nodes:

$$\text{time step limit} \approx \frac{\ell^2}{4\alpha}$$

for square nodes of side ℓ, and

$$\text{time step limit} \approx \frac{\ell^2}{2\alpha}$$

for "thin" nodes of minimum side ℓ.

Estimates for other machines were made using empirical speed ratios based upon similar Fortran programs for jobs of roughly 10 minutes duration. If we write T = ANI, then we have

Machine	A (hrs)	Estimated Error
Philco 2000-212	5×10^{-7}	±25%
CDC 3800	5×10^{-7}	±50%
CDC 6600	3×10^{-7}	±50%
Univac 1108	3×10^{-7}	±50%
IBM 7094	12×10^{-7}	±50%
360/40	50×10^{-7}	±50%
360/44	25×10^{-7}	±50%
360/50	25×10^{-7}	±50%
360/65	5×10^{-7}	±50%

3.2 STORAGE REQUIREMENTS

The ASTHMA program itself requires only about 5200_{10} word of storage. Associated subroutines require about 1000_{10} words. Most storage requirement is for dimensioned variables in various commons. With present dimensions, these require about $15,600_{10}$ words. Thus the program is a tight fit in a 32,000 word machine, with present dimension values.

3.3 TAPE REQUIREMENTS

The program uses no scratch tapes. It uses logical unit number 5 for input and 6 for printed output, and uses a punch tape through a PUNCH statement.

3.4 FORTRAN DECK MAKE-UP

The ASTHMA program is in Fortran IV and consists of the following units:

(1) Main Program

(2) Subroutine SURFB
Surface energy balance procedures

(3) Subroutine LCOUNT
Counts lines, turns and numbers pages

(4) Subroutine LOOK
Table look-up with linear interpolation

(5) Subroutine SLOPQ
Quadratic curve fit and slope finder

(6) Subroutine OGLE
Table look-up with cubic curve fit

(7) Subroutine ORDERD
Ordering routine

(8) Subroutine SEQUA

Orders according to results of ORDERD

(9) Subroutine SLOPL

Linear curve fit and slope finder

(10) Subroutine VCOS

Evaluates cosine of angle between surface normal and nodal center line

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APPENDIX A

STUDY OF FRONT NODE DROPPING SCHEMES

APPENDIX A

STUDY OF ALTERNATIVE FRONT NODE DROPPING SCHEMES FOR TRANSIENT ABLATION CALCULATIONS

A-1 GENERAL REMARKS

Finite difference calculations of the subsurface temperature response and the surface recession history of ablating materials have employed three general types of nodal bookkeeping schemes

1. nodal mesh fixed in the material, with any node dropping required by surface recession occurring at the front (heated) surface
2. nodal mesh fixed to receding surface, with node dropping taking place at back wall
3. nodal mesh fixed at both front and back walls, with all nodes shrinking as recession occurs.

The first scheme, although offering an appealing simplicity, proved to suffer from irritating oscillations in predicted heated surface temperature, recession rate, and heat flux. Experiences such as those reported by Brogan (Refs. A-1, A-2) encouraged investigators to consider back-surface node dropping (type 2 above) and shrinking coordinate systems (type 3 above) with excellent success for problems with one space dimension.

Consequently, interest in front node dropping schemes waned, even though occasional papers on the technique appeared from time to time (e.g., Refs. A-3 and A-4). Ablation problems with two or three dimensions usually do not lend themselves to simple treatments with receding nodal grids or shrinking grids, due to the many tedious bookkeeping aspects of recording the nodal positions in moving grids, and attempts to construct multidimensional computer programs with moving or shrinking nodes have proven discouragingly complex and unreliable (Refs. A-5 to A-8). Therefore, in the course of the present work front node dropping schemes appeared to deserve some reconsideration, and several alternative front node dropping schemes were examined for stability and smoothness of predicted surface temperature using a special-purpose, one-dimensional computer program. Section A-2 below describes the schemes considered.

A-2 METHODS EXAMINED

The schemes considered differ from each other in two aspects:

1. the location of the finite difference thermal capacity lumps relative to the thermal resistance links, and

2. the temperature at which the ablating material is injected into the surface control volume for the surface energy balance calculation.

Under point (1), the three arrangements shown in Figure A-1 were examined.

In Figure A-1 the small arrows indicate which zone thermal capacity is lumped into each capacitor in the R-C network. Note that Scheme (1) never has any capacitance associated with the surface temperature, while Scheme (2) always has capacitance associated with the surface temperature. Scheme (3) has no capacitance at the surface in mode (1), but does have capacitance at the surface in mode (2).

The three capacitance distribution schemes constituted one computational aspect tested; the second aspect concerned the surface energy balance. The surface energy balance equation, Equation (32) in the main text above, simplified to the familiar relation for Le = 1 and $C_M/C_H = 1$ is

$$\rho_e u_e C_H \left[H_r - (1 + B')h_w \right] + \dot{m}_c h_c - F\sigma\varepsilon T_w^4 - q_{cond} = 0 \qquad \text{(A-1)}$$

In this equation the term $\dot{m}_c h_c$ represents the energy injected in the surface control volume (see Figure 12 of the main text) with the subsurface material. A study of the finite difference networks of Figure A-1 reveals a choice of enthalpies to use in this term:

1. the enthalpy of the material in the top-most (shrinking) capacitance
2. the enthalpy corresponding to the heated surface temperature.

Choices (1) and (2) lead to different results in both Scheme (1) and in Mode (1) of Scheme (3) since in these cases the shrinking capacitance does not have the temperature of the surface. Enthalpy choice (1) gives an appealing consistency with the in-depth solution, since from the in-depth point of view energy is definitely being convected away at the temperature of the shrinking capacitance. Choice (2) on the other hand seems more accurate from the point of view of the surface energy balance.

A conventional explicit finite difference computer program was written to test numerically the three capacitance distribution schemes with both choices of injection enthalpy, since no amount of refined general analysis could be expected to answer the crucial question of surface temperature smoothness. The test problem was a 0.9-inch slab of graphite, insulated on the back wall, exposed to a step recovery enthalpy in air of 2600 Btu/lb at 65 atm, with $\rho_e u_e C_H = 1.76$ lb/ft^{2}sec. For computation, the slab was divided into a crude network of nine 0.10-inch nodes in order to exaggerate any oscillations.

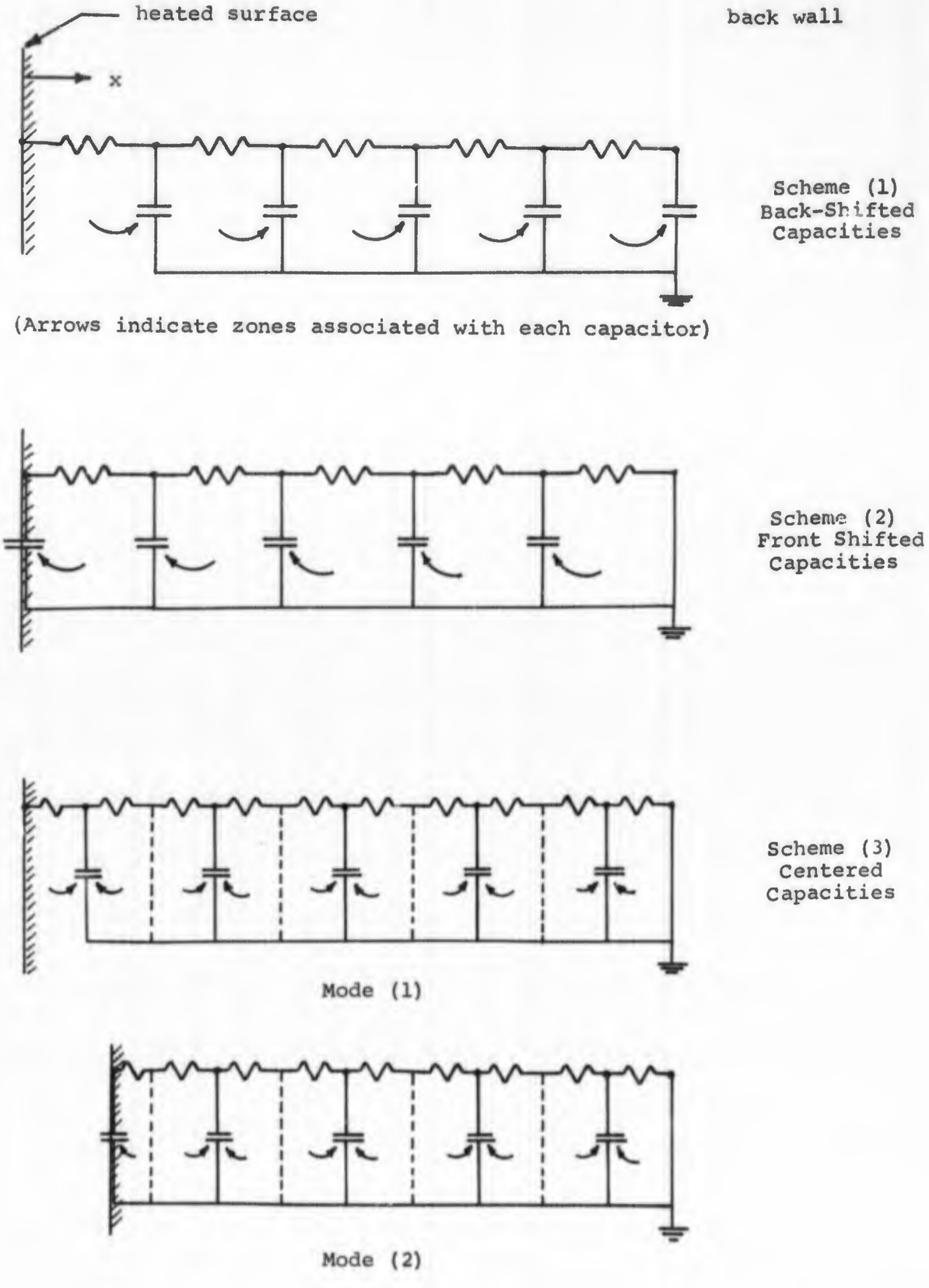

Figure A-1. Thermal R-C Network Representation of Three Alternative Schemes for Front Node Dropping

Figure A-2 shows the results for the three schemes with enthalpy choice (1), top capacitance injection. All three capacitance distributions produce surface temperature predictions which oscillate around the exact result (obtained from the well verified CMA program with small nodes). The back-shifted and centered schemes produce drastic temperature jumps whenever a node is dropped. These jumps are apparently a consequence of the sudden shift in injection temperature which occurs as a node is dropped for these two schemes. (Note that the front shifted scheme, which is inherently a front surface injection scheme, is smoother.)

Figure A-3 confirms this suspicion. It displays results for the same three capacitance arrangements as Figure A-2 but with front surface enthalpy used for the $\dot{m}_c h_c$ injection term. The front shifted scheme is unchanged, of course, and the back shifted and centered capacitance scheme predictions have lost their saw-toothed appearance. The back-shifted scheme, in fact, has produced a very acceptably smooth temperature prediction. The prediction is too high, however, an error due evidently to the obvious failure to account for energy absorbtion of the injected (ablated) material between the time it figuratively leaves the in-depth scheme at the top capacitance temperature and the time it enters the boundary layer at the higher front surface temperature. This conclusion is confirmed by top-capacitance injection results of Figure A-2, since this energy absorption is accounted for in that injection scheme. The average predicted result in Figure A-2 for the back-shifted capacity scheme is closer to the exact answer than the result shown in Figure A-3 exactly because the absorption is accounted for. The fact that the finite difference scheme applies the absorption correction in a saw-toothed manner (as the top capacitance temperature gradually approaches the heated surface and then abruptly recedes to the next nodal point down as a node is dropped) is what gives the saw-toothed appearance to the temperature prediction of Figure A-2.

This suggests that a preferable accuracy improvement could be made in the smooth prediction of the back-shifted scheme plus surface injection by adding during each time step some smooth correction for the missing absorption quantity instead of the saw-toothed absorption implied by top-capacitance injection. A candidate correction energy absorption rate might be

$$\text{surface energy balance correction term} = \dot{m}_{avg} c_p (T_w - T_1)_{avg} \qquad \text{(A-2)}$$

where "avg" denotes average during the ablation of a surface node and T_1 is the temperature of the first capacitance lump. This would still be inherently saw-toothed but would usually have less drastic jumps than the top capacitance

injection scheme. It is, of course, impractical to use this correction since during a transient problem both $\dot{m}_{avg}$ and $(T_w - T_i)_{avg}$ only become known after the node has ablated away and its entire past history is available. A more workable correction would have the form

$$\text{surface energy balance correction term} = \dot{m}C_p \left(-\frac{\partial t}{\partial x}\right)_s \frac{\delta_{1_o}}{2} \qquad \text{(A-3)}$$

where δ_{1_o} denotes the <u>initial</u> thickness of the current top node. This correction has all virtues and no defects except possible lack of accuracy. It involves current quantities and, hence, can be calculated at every time step, and since it involves $\left(-\frac{\partial t}{\partial x}\right) = \frac{q_{cond}}{k}$ it can be directly inserted into the surface energy balance, equation (A-1), without difficulty. Thus, the surface energy balance equation becomes

$$\rho_e u_e C_H \left[H_r - (1+B')h_w\right] + \dot{m}_c h_{c_1} - F\sigma\varepsilon T_w^4 - q_{cond}\left(1 + \frac{\dot{m}_c C_p}{2k}\delta_{1_o}\right) = 0 \qquad \text{(A-4)}$$

(for back-shifted capacities, Scheme (1)).

This modification was applied to the back-shifted capacitance scheme and Figure A-4 shows the improvement effected by the convection correction factor $(\dot{m}_c C_p/2k)\delta_{1_o}$ applied to q_{cond}. The solution rapidly approaches the exact solution. The inaccuracy in early time (< 2 seconds) may be seen to be due to the crude nodal size; reducing the nodes to 0.025 inch instead of 0.10 inch results in the generally improved prediction also shown in Figure A-4.

CONCLUSIONS

The back-shifted capacity scheme with solids injected into the surface energy balance at the surface temperature provides the smoothest temperature prediction of the six methods tested. The accuracy of this method is not good unless some correction is made for the inconsistency resulting from material removal from the in-depth solution at the shrinking capacitor temperature, which is usually different from the surface temperature. A simple, smooth correction (Equation A-3) for this effect provided excellent accuracy. The back-shifted capacity scheme with front surface injection plus the simple correction has been incorporated into the two-dimensional axi-symmetric heat conduction routine (ASTHMA) described in the main text above.

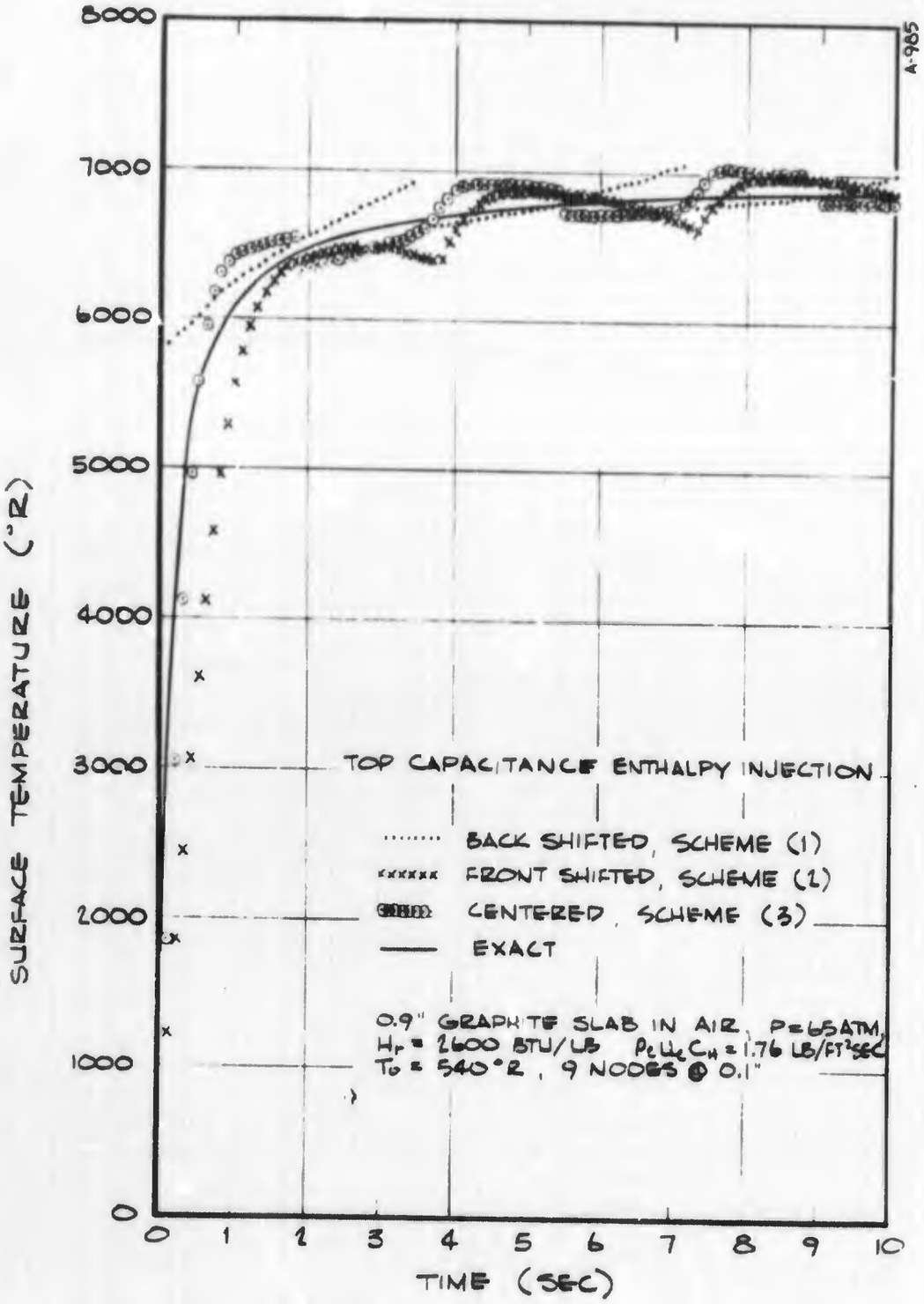

FIGURE A-2 COMPARISON OF RESULTS OF THREE CAPACITANCE DISTRIBUTION SCHEMES.

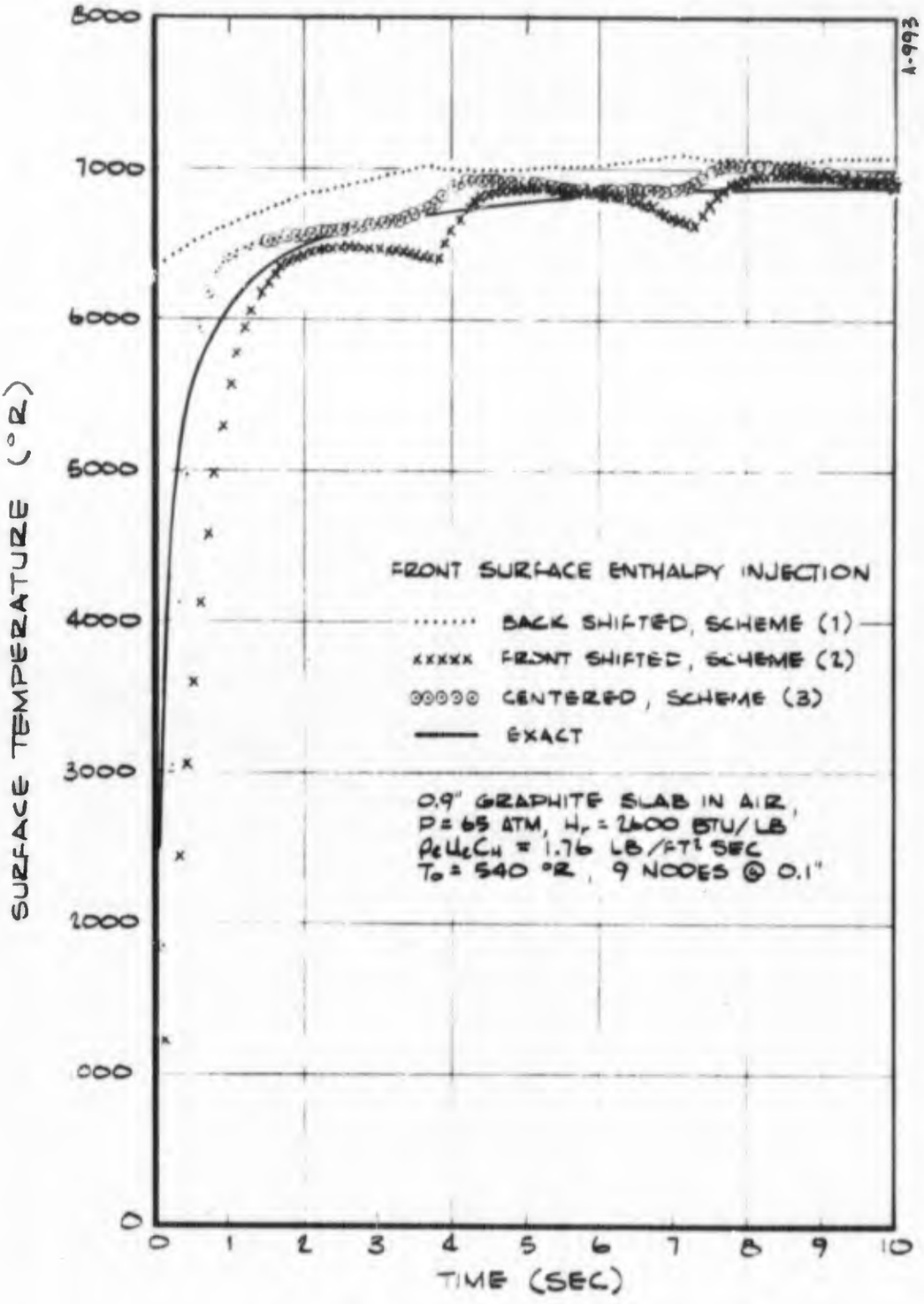

FIGURE A-3 COMPARISON OF RESULTS OF THREE CAPACITANCE DISTRIBUTION SCHEMES.

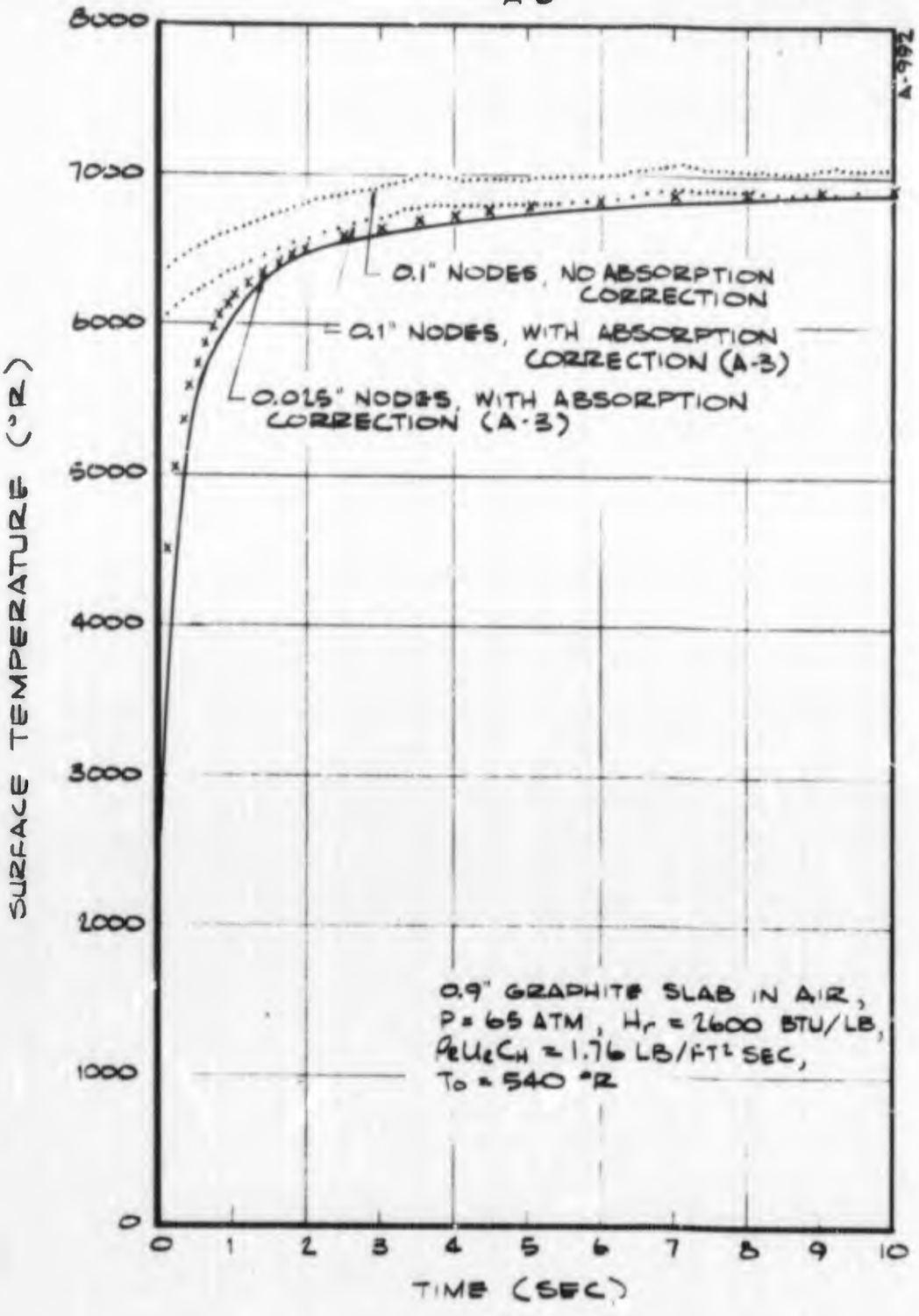

FIGURE A-4 TEMPERATURE PREDICTIONS FOR BACK SHIFTED CAPACITANCE SCHEME PLUS FRONT SURFACE INJECTION, BOTH WITH AND WITHOUT ABSORPTION CORRECTION

APPENDIX A

REFERENCES

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APPENDIX B

RECENT CHANGES IN ASTHMA

APPENDIX B
RECENT CHANGES IN ASTHMA

After the conclusion of the ASTHMA program work presented in the main text, further use of the program demonstrated the desireability of some modifications and additions. These changes have been incorporated in the program deck actually delivered under this subcontract and are presented in this Appendix (written some months after the main report above). Program users may find it helpful to note the new input features described here in the User's Manual portion of the main report above.

B-1 VARIABLE OUTPUT INTERVAL OPTION

Provision has been added to ASTHMA for changing standard output print intervals during a problem (generally similar to the capability of the CMA program described in reference B-1). In the earlier versions of ASTHMA, a single output time interval was provided on the first data card (following the three title cards). In the new version, this scheme has been retained but it has been supplemented with the variable output interval option. This option is called into play by a zero entry for the output increment in the first data card. With this number zero, a new card is introduced, following this first data card, with the following information:

Column	Format	Data	Units
1-10	F10.0	First output time interval, applied at initial time	(sec)
11-20	F10.0	Transition time between first output time interval and second output time interval	(sec)
21-30	F10.0	Second output time interval	(sec)
31-40	F10.0	Transition time between second output time interval and third output time interval	(sec)
41-50	F10.0	Third output time interval	(sec)
51-60	F10.0	Transition time between third output time interval and fourth output time interval	(sec)
61-70	F10.0	Fourth output time interval	
71-80	F10.0	Not used	

It will be noted that up to four output time intervals may be used. Output intervals are changed during the problem at the "transition times." A smaller number may be used by leaving the unneeded output intervals and transition times blank. In general, a blank or zero output interval will stop the problem at the immediately preceding transition time. Blank or zero transition times will be automatically set to the final time. The transition times should be entered in ascending order; no automatic ordering is done.

This optional output interval card precedes the optional card giving special punched output times (see p. 29 above).

B-2 CHANGE IN SURFACE ENERGY BALANCE LINKAGE

The linkage between the surface energy balance and the subsurface solution as described in Section 2.5 above proved to be unstable in certain circumstances.

Consequently, two new linkage procedures were devised, and the program now allows the user a choice of three linkage options. The first option is the procedure described in Section 2.5 above. The second is unconditionally stable but does not conserve energy in the sense that all energy conducted into the surface does not appear in $\rho C_p \partial T/\partial \theta$ terms. This non-conservation version, although theoretically objectionable, has been tested for a wide range of problems and has worked very well. The third option ties the second node below the surface implicitly to the surface node (in each column) in a consistent manner (i.e. so as to conserve energy) and should be the preferred option as it is both stable and energy-conservative. However, it has received little testing as yet.

The user choice among these options is indicated by a 0 (or blank), 1, or 2 punch in column 69 of the first data card of the data deck (after the three title cards). Refer to page 29 above for a description of this card. The punches designate the options as follows:

Linkage Option No.	Description	Remarks
0	As described in ASTHMA manual, surface) to-first node (of a column) implicit	Inherently unstable if nodes are dropped. Although usually successful, this scheme is not recommended if ablation is sufficient to cause any nodes to be dropped.
1	Surface-to-first-node link implicit, first-to-second node 1/4 implicit	Stable, but theoretically objectionable because it does not conserve energy, Has worked well in practice.
2	Surface-to-first-node link implicit, first-to-second node half implicit	Stable. Conserves energy. Should be best all round procedure but has received little testing.

B-3 SURFACE SHAPE CURVE FIT OPTION

The surface shape curve fit routine described on pages 11 and 12 above has been supplemented with another routine. The user designates which curve fit procedure shall be used during the calculation with a punch in column 70 of the first data card of the data deck (see page 29 of the manual). A zero or blank

calls for the linear slope averaging routine described on pages 11-12 of the manual. A one punch calls for a quadratic curve fit slope averaging routine known as SLØPQ described in Reference B-2. This routine gives better results for relatively smooth and flat (small dr/dz) shapes common to rocket nozzles; it usually performs poorly if surface points are closely spaced in the z direction (large dr/dz) and gives meaningless answers for double valued r(z) shapes. For these latter shapes, the linear fit routine should be used.

B-4 MULTIPLE ABLATING MATERIALS

The ASTHMA program has been modified so that any substrate material may appear in a nodal box at the heated surface. (Previously, as described in the User's Manual above, the ablating material had to be material number one.) Options 2 and 3 boundary conditions may be applied to any surface material without restriction. Option 1 type surface thermochemical boundary conditions may be applied to any number of exposed surface materials simultaneously, but only with a tight restriction; this restriction derives from the program feature that in computing surface energy balance ablation quantities it needs the enthalpy of the substrate material at the wall temperature. In obtaining this it refers only the heat of formation of material number 1 and the specific heat function for material number 1. Therefore, although the ablating substrate materials may carry different material identifications, they must (for Option 1 calculations) have identical enthalpy-temperature relations. This limits the multimaterial capability for Option 1 to materials of different densities, emissivities, and thermal conductivities.

Since in Options 2 and 3 surface thermochemistry tables are not used, the identical enthalpy-temperature limitation does not apply for these options. Any materials with any thermal properties may appear at the surface. (It was really for this application that the multimaterial capability was added.)*

---

*An additional restriction applies to the pressure-interpolation version of ASTHMA mentioned in Section 6 which is generally not used for rocket nozzle applications. In that version, the program chooses surface thermochemistry tables during the solution only on the basis of pressure. If the pressure range for one exposed material overlaps that of another, an artificial device must be used to distinguish the sets of pressures appropriate to each material. The most convenient device is to repunch false flag pressures in the surface tables appropriate to the additional exposed materials, and to enter appropriate pressure histories in the relevant time (heating) tables to cause the right selection of pressure tables to be made.

This restriction does not apply to the no-interpolation version of ASTHMA described in the main report above, since specific surface tables may be flagged to any node.

B-5 SURFACE THERMOCHEMISTRY TABLE FORMAT OPTION

The surface thermochemistry tables input to the ASTHMA program may be generated by a number of different surface state programs with different punched card output formats. Consequently a format option punch has been added to the ASTHMA program; the user may thus designate the format of the surface thermochemistry tables in the data deck as presented below.

B-5.1 Lead Card

There are four format choices, designated by a 0 (or blank), 1, 2, or 3 punch in column 50 of the lead card for the table (see page 34 above):

Column	Format	Data	Units
1-40		As on p. 34	Various
41-49	9X	Blank	---
50	I1	Format flag;	
		0 or blank ____	New standard format
		1 ____	Format on p. 34
		2 ____	"Anderson format"
		3 ____	CMA format

The first three formats vary only in Columns 1-20. Columns 21-80 remain as described on pages 37-38 of the manual. (We describe here only the surface tables; edge tables have the same formats as the surface tables in each case.) The fourth format is the older CMA format used in the Aerotherm Charring Material Thermal Response and Material Ablation Program (Ref. B-1).

B-5.2 New Standard Format (0 Punch)

The format cited on page 37 above was not that originally intended. The ultimate standard card output by the ACE program will follow this plan:

Column	Format	Data	Units
1-6	E6.4	Pressure	atm
7-12	E6.4	Gas rate $\dot{m}_g/\rho_e u_e C_M = B'_g$ (not used by ASTHMA)	---
13-20	E8.5	Ablation rate $\dot{m}_c/\rho_e u_e C_M = B'_c$	---
21-80		As on pp. 37-38, User's Manual	

This is the card output format of the ACE program described in Appendix C.

B-5.3 ASTHMA Manual Format (1 Punch)

This format is cited on pages 37 and 38 above but will probably not become an output option of ACE

B-5.4 "Anderson Format"

This format has been used to date for output by the ACE program and a number of tables have been generated with it. It has, however, an inconvenient format field for the ablation rate (due to a programming slip) and will be abandoned soon. This format is as follows:

Column	Format	Data	Units
1-6	E6.4	Pressure	atm
7-14	E8.4	Gas rate $\dot{m}_g/\rho_e u_e C_M = B_g'$ (not used by ASTHMA)	---
15-20	E8.5	Ablation rate $\dot{m}_c/\rho_e u_e C_M = B_c'$	---
21-80		As on pp. 37-38, User's Manual	

B-5.5 CMA Format

This is an optional ACE output format intended for use with the CMA program. Since so many graphite-in-air surface tables already exist with this format, it is useful to have it as an ASTHMA input format also. In this format the kinetics parameter is assumed by ASTHMA to be in what is the B_g' slot of the CMA input. An ACE problem with kinetics output in the CMA card format will lose the kinetics information, however, since there is no provision for it in the ACE output statement. Hence, this format will probably not be used for problems with kinetic control, and the kinetic parameters entered in the B_g' slot will be fake numbers. This format is as follows:

Column	Format	Data	Units
1-8	F8.5	Pressure	atm
9-16	F8.5	Gas rate $\dot{m}_g/\rho_e u_e C_M$	---
17-24	F8.5	Char rate $\dot{m}_c/\rho_e u_e C_M$	---
25-33	F9.4	Surface temperature	^oK (^oR if negative in which case enthalpies below are Btu/lb)

Column	Format	Data	Units
34-38	F5.3	Unequal diffusion exponent	---
39-47	F9.3	Summation $\sum z^*_{iw} h_i^o$	Cal/gr (Btu/lb if temperature is entered with minus sign)
48-56	F9.3	Enthalpy of wall gases h_w	Cal/gr (Btu/lb if temperature is entered with minus sign
57-58	I2	0 for assigned-temperature entries in the equilibrium program (no ablation); >0 for equilibrium surface thermochemistry with ablation (temperature is dependent)	---
59-60	2X	Blank	---
61-66	A6	Chemical symbol of surface species. (EST* program prints such symbols arranged alphabetically and truncated from right end if necessary.)	---
67-78	2A6	Problem identification (not read)	---
79-80	I2	Page number on EST output listing containing the data punched on this card (not read)	

B-6 CHANGES IN ASTHMA PROGRAM TO INTERPOLATE ON PRESSURE

The ASTHMA program was designed primarily for two dimensional axisymmetric rocket nozzle ablation analysis. Since pressure varies axially in rocket nozzles, but usually does not vary significantly with time, the program exploited the simplifications possible in the direct assignment of particular pressure tables to given surface points. This allowed a kind of coupled time-dependent pressure effect since different pressures could be assigned to different nodes in a column; thus as the surface receded, a time varying pressure would be imposed on a given column of nodes according to the recession history.

This scheme is not very satisfactory for other bodies such as nose-tips, however, since large pressure changes may take place over a period of time, independent of body shape change effects, due to the time varying nature of the flow field. Therefore, appropriate modifications have been made in the surface energy balance routine of the ASTHMA program to allow time dependent pressures, with appropriate interpolation or pressure, for a given nodal column.

---

*or ACE

Thus there are now two alternative versions of the ASTHMA program, each useful for a given class of problems.

The only physical change needed to convert ASTHMA to the pressure-interpolation version described here is the substitution of the subroutine SURFB. This subroutine is called by ASTHMA and hence has retained its name, but the Fortran decks of the two versions of this subroutine are appropriately distinguished with comment cards.

Since the pressure interpolation version of ASTHMA is of minimal utility for rocket nozzle work, this version is not further described here and is not the version of the program deck provided under this subcontract.

APPENDIX B

References

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B-2 Aerotherm Corporation, Palo Alto, Calif.: Fortran Variable Names, Aerotherm Charring Material Ablation Program, Version 2. February 1966.

APPENDIX C

ASTHMA PROGRAM SAMPLE PROBLEM

MITCHELL R. WOOL

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ASTHMA INPUT DECK

```
APG 112D 800 PSIA CHAMBER PRESSURE, BASELINE CASE 6032,03, PLUS COOLDOWN
AFTER 6.0 SECONDS, PYROLYTIC GRAPHITE SURFACE, USING 6 NODAL COLUMNS AND
6 THERMOCHEMISTRY TABLES ASSIGNED BY NODE.                    112,800,COOL
 12  6 0.    60.   1.          .90   0.    .4    .001  .85   530.  111   1
2.618  0.000
1.998  0.000
1.557  0.000
1.204  0.000
1.059  0.000
0.985  0.000
0.911  0.000
0.850  0.000
0.838  0.000
0.826  0.000
0.814  0.000
0.802  0.000
0.790  0.000
2.618  0.200
1.998  0.200
1.557  0.200
1.204  0.200
1.020  0.193
0.918  0.185
0.825  0.170
0.763  0.159
0.752  0.157
0.741  0.154
0.730  0.152
0.719  0.149
0.708  0.146
2.618  0.419
1.998  0.419
1.557  0.400
1.204  0.400
1.004  0.397
0.868  0.388
0.749  0.370
0.681  0.356
0.669  0.353
0.656  0.350
0.644  0.347
0.631  0.344
0.618  0.341

1.998  0.600
1.557  0.600
1.204  0.600
1.003  0.600
0.845  0.597
0.708  0.592
0.638  0.588
0.623  0.586
```

```
  0.608   0.585
  0.593   0.583
  0.578   0.582
  0.562   0.580

  1.998   0.800
  1.557   0.800
  1.204   0.800
  1.002   0.800
  0.841   0.801
  0.706   0.806
  0.643   0.809
  0.627   0.810
  0.611   0.811
  0.595   0.812
  0.580   0.814
  0.564   0.818

  1.998   1.000
  1.557   1.000
  1.204   1.000
  1.002   1.000
  0.850   1.006
  0.730   1.020
  0.677   1.029
  0.664   1.031
  0.651   1.034
  0.638   1.036
  0.625   1.039
  0.612   1.042

  1.998   1.185
  1.557   1.185
  1.204   1.185
  1.010   1.185
  0.876   1.185
  0.759   1.185
  0.708   1.185
  0.696   1.185
  0.684   1.185
  0.672   1.185
  0.660   1.185
  0.648   1.185
  3               530.
  3               530.
  2               530.
  2               530.
  2               530.
  2               530.
  2               530.
  11 1 1          530.                .97
  11 1 1          530.                .97
```

11 1 1	530.	.97	
11 1 1	530.	.97	
1111 1	530.	.97	
3	530.		
3	530.		
2	530.		
2	530.		
2	530.		
2	530.		
2	530.		
11 1 2	530.	.97	
11 1 2	530.	.97	
11 1 2	530.	.97	
11 1 2	530.	.97	
1111 2	530.	.97	
3	530.		
2	530.		
2	530.		
2	530.		
2	530.		
2	530.		
11 2 3	530.	.97	.058
11 2 3	530.	.97	.058
11 2 3	530.	.97	.058
11 2 3	530.	.97	.058
1112 3	530.	.97	.058
3	530.		
2	530.		
2	530.		
2	530.		
2	530.		
2	530.		
11 2 4	530.	.97	.17
11 2 4	530.	.97	.17
11 2 4	530.	.97	.17
11 2 4	530.	.97	.17
1112 4	530.	.97	.17
3	530.		
2	530.		
2	530.		
2	530.		
2	530.		
2	530.		
110305	530.	.97	.174
110305	530.	.97	.174
110305	530.	.97	.174
110305	530.	.97	.174
111305	530.	.97	.174

```
  3              530.
  2              530.
  2              530.
  2              530.
  2              530.
  2              530.
  11 3 6         530.                    .97    .176
  11 3 6         530.                    .97    .176
  11 3 6         530.                    .97    .176
  11 3 6         530.                    .97    .176
  1113 6         530.                    .97    .176
    3
     0525. 137.   .240  5000-1 .90  3610-3
     0780.        .276  5000-1 .90  2820-3
     1060.        .313  4470-1 .90  2635-3
     1390.        .357  3333-1 .90  2305-3
     1850.        .409  4450-1 .90  2000-3
     2190.        .445  2015-1 .90  1835-3
     2650.        .480  1736-1 .90  1778-3
     3060.        .498  1611-1 .90  1835-3
     4460.        .520  1418-1 .90  2222-3
     7460.        .520  1388-1 .90  2890-3
   -19999.        .520  1388-1 .90  2890-3
      525.  74.3  .240  3380-2 .90
      780.        .276  3380-2 .90
     1030.        .313  3380-2 .90
     1390.        .357  3380-2 .90
     1850.        .409  3380-2 .90
     2190.        .445  3380-2 .90
     2650.        .480  3380-2 .90
     3060.        .498  3380-2 .90
     4460.        .520  3380-2 .90
     7460.        .520  3380-2 .90
   -19999.        .520  3380-2 .90
      525.  111.  .230  5560-4 .90
      960.        .310  5560-4 .90
     1460.        .500  5560-4 .90
     1960.        .530  5560-4 .90
     2460.        .560  5560-4 .90
     3460.        .600  5560-4 .90
     4460.        .610  5560-4 .90
     5460.        .620  5560-4 .90
     6460.        .630  5560-4 .90
     7460.        .640  5560-4 .90
   -19999.        .640  5560-4 .90
      0.0        2020.     785.       0.875      50.6       0.4
      4.0        2020.     785.       0.875      50.6       0.4
      4.0
   -1 60.0                                                   0.4
      0.0        2006.     785.       1.053      47.5       0.4
      4.0        2006.     785.       1.053      47.5       0.4
      4.0
```

```
-1 60.0                                                   0.4
   0.0       1984.     785.      1.262      41.0          0.4
   4.0       1984.     785.      1.262      41.0          0.4
   4.0
-1 60.0                                                   0.4
   0.0       1937.     785.      1.310      31.5          0.4
   4.0       1937.     785.      1.310      31.5          0.4
   4.0
-1 60.0                                                   0.4
   0.0       1787.     785.      1.070      17.8          0.4
   4.0       1787.     785.      1.070      17.8          0.4
   4.0
-1 60.0                                                   0.4
   0.0       1761.     785.      1.010      16.0          0.4
   4.0       1761.     785.      1.010      16.0          0.4
   4.0
+1 60.0                                                   0.4
 0.603       3.04E04
```

SURFACE THERMOCHEMISTRY TABLE (ARCACE OUTPUT) ↓

```
 4800+2  0+0       0+0   0+0    040000+4    0+0 11422+4 11422+40000000    EDGE TABLE
 4800+2  0+0       0+0   0+0    035000+4    0+0 90000+3 90000+30000000    EDGE TABLE
 4800+2  0+0       0+0   0+0    030000+4    0+0 66155+3 66155+30000000    EDGE TABLE
 4800+2  0+0       0+0   0+0    025000+4    0+0 42725+3 42725+30000000    EDGE TABLE
 4800+2  0+0       0+0   0+0    020000+4    0+0 19922+3 19922+30000000    EDGE TABLE
 4800+2  0+0       0+0   0+0    015000+4    0+0-20967+2-20967+20000000    EDGE TABLE
 4800+2  0+0       0+0   0+0    010000+4    0+0-22858+3-22858+30000000    EDGE TABLE
 4800+2  0+0       0+0   0+0    050000+3    0+0-39996+3-39996+30000000    EDGE TABLE
 4800+2  C+0-23283-95200+5      010000+4    0+0-11811+4-11811+4C*     2
 4800+2  0+0 35308-65200+5      015000+4    0+0-63673+3-63673+3C*     2   INLET SURF
 4800+2  0+0 47822-35200+5      020000+4    0+0-34919+3-34919+3C*     2   INLET SURF
 4800+2  0+0 56405-25200+5      022500+4    0+0-19715+3-19715+3C*     2   INLET SURF
 4800+2  0+0 71152-15200+5      025000+4    0+0 16105+3 16105+3C*     2   INLET SURF
 4800+2  0+0 12888+05200+5      027500+4    0+0 46588+3 46588+3C*     2   INLET SURF
 4800+2  0+0 16613+05200+5      030000+4    0+0 71992+3 71992+3C*     2   INLET SURF
 4800+2  0+0 23266+05200+5      032500+4    0+0 10674+4 10674+4C*     2   INLET SURF
 4800+2  0+0 36859+05200+5      035000+4    0+0 15899+4 15899+4C*     2   INLET SURF
 4800+2  0+0 11560+15200+5      040000+4    0+0 31598+4 31598+4C*     2   INLET SURF
 4800+2  0+0-23283-9            010000+4    0+0-11811+4-11811+4C*     2
 4800+2  0+0 35308-6            015000+4    0+0-63673+3-63673+3C*     2   INLET SURF
 4800+2  0+C 47822-3            020000+4    0+0-34919+3-34919+3C*     2   INLET SURF
 4800+2  0+0 56405-2            022500+4    0+0-19715+3-19715+3C*     2   INLET SURF
 4800+2  0+0 71152-1            025000+4    0+0 16105+3 16105+3C*     2   INLET SURF
 4800+2  0+0 12888+0            027500+4    0+0 46588+3 46588+3C*     2   INLET SURF
 4800+2  0+0 16613+0            030000+4    0+0 71992+3 71992+3C*     2   INLET SURF
 4800+2  0+0 23266+0            032500+4    0+0 10674+4 10674+4C*     2   INLET SURF
 4800+2  0+0 36859+0            035000+4    0+0 15899+4 15899+4C*     2   INLET SURF
 4800+2  0+0 11560+1            040000+4    0+0 31598+4 31598+4C*     2   INLET SURF
 3140+2  0+0     0+05200+5      040000+4    0+0 11444+4 11444+40000000    EDGE TABLE
 3140+2  0+0     0+05200+5      035000+4    0+0 89993+3 89993+30000000    EDGE TABLE
 3140+2  0+0     0+05200+5      030000+4    0+0 65925+3 65925+30000000    EDGE TABLE
 3140+2  0+0     0+05200+5      025000+4    0+0 42279+3 42279+30000000    EDGE TABLE
 3140+2  0+0     0+05200+5      020000+4    0+0 19269+3 19269+30000000    EDGE TABLE
 3140+2  0+0     0+05200+5      015000+4    0+0-29435+2-29435+20000000    EDGE TABLE
```

```
3140+2   0+0      0+05200+5   010000+4   0+0-23881+3-23881+30000000     EDGE TABLE
3140+2   0+0      0+05200+5   050000+3   0+0-41146+3-41146+30000000     EDGE TABLE
3140+2   0+0-11641-93850+5     010000+4   0+0-11193+4-11193+4C*     2    THROAT
3140+2   0+0 24342-63850+5     015000+4   0+0-60297+3-60297+3C*     2
3140+2   0+0 32759-33850+5     020000+4   0+0-31587+3-31587+3C*     2    THROAT
3140+2   0+0 37943-23850+5     022500+4   0+0-16971+3-16971+3C*     2    THROAT
3140+2   0+0 41234-13850+5     025000+4   0+0 96459+2 96459+2C*     2    THROAT
3140+2   0+0 12241+03850+5     027500+4   0+0 48444+3 48444+3C*     2    THROAT
3140+2   0+0 16256+03850+5     030000+4   0+0 75382+3 75382+3C*     2    THROAT
3140+2   0+0 23485+03850+5     032500+4   0+0 11295+4 11295+4C*     2    THROAT
3140+2   0+0 38959+03850+5     035000+4   0+0 17079+4 17079+4C*     2    THROAT
3140+2   0+0 12878+13850+5     040000+4   0+0 33563+4 33563+4C*     2    THROAT
3140+2   0+0-11641-9           010000+4   0+0-11193+4-11193+4C*     2    THROAT
3140+2   0+0 24342-6           015000+4   0+0-60297+3-60297+3C*     2
3140+2   0+0 32759-3           020000+4   0+0-31587+3-31587+3C*     2    THROAT
3140+2   0+0 37943-2           022500+4   0+0-16971+3-16971+3C*     2    THROAT
3140+2   0+0 41234-1           025000+4   0+0 96459+2 96459+2C*     2    THROAT
3140+2   0+0 12241+0           027500+4   0+0 48444+3 48444+3C*     2    THROAT
3140+2   0+0 16256+0           030000+4   0+0 75382+3 75382+3C*     2    THROAT
3140+2   0+0 23485+0           032500+4   0+0 11295+4 11295+4C*     2    THROAT
3140+2   0+0 38959+0           035000+4   0+0 17079+4 17079+4C*     2    THROAT
3140+2   0+0 12878+1           040000+4   0+0 33563+4 33563+4C*     2    THROAT
1600+2   0+0      0+03850+5   040000+4   0+0 11447+4 11447+40000000     EDGE TABLE
1600+2   0+0      0+03850+5   035000+4   0+0 89673+3 89673+30000000     EDGE TABLE
1600+2   0+0      0+03850+5   030000+4   0+0 65275+3 65275+30000000     EDGE TABLE
1600+2   0+0      0+03850+5   025000+4   0+0 41309+3 41309+30000000     EDGE TABLE
1600+2   0+0      0+03850+5   020000+4   0+0 17996+3 17996+30000000     EDGE TABLE
1600+2   0+0      0+03850+5   015000+4   0+0-45024+2-45024+20000000     EDGE TABLE
1600+2   0+0      0+03850+5   010000+4   0+0-25696+3-25696+30000000     EDGE TABLE
1600+2   0+0      0+03850+5   050000+3   0+0-43140+3-43140+30000000     EDGE TABLE
1600+2   0+0-23283-94820+5     010000+4   0+0-10165+4-10165+4C*     2    EXIT SURF
1600+2   0+0 27345-64820+5     015000+4   0+0-54530+3-54530+3C*     2    EXIT SURF.
1600+2   0+0 36186-34820+5     020000+4   0+0-26271+3-26271+3C*     2    EXIT SURF.
1600+2   0+0 39897-24820+5     022500+4   0+0-11622+3-11622+3C*     2    EXIT SURF.
1600+2   0+0 33106-14820+5     025000+4   0+0 12309+3 12309+3C*     2    EXIT SURF.
1600+2   0+0 11389+04820+5     027500+4   0+0 51930+3 51930+3C*     2    EXIT SURF.
1600+2   0+0 15822+04820+5     030000+4   0+0 81611+3 81611+3C*     2    EXIT SURF.
1600+2   0+0 24217+04820+5     032500+4   0+0 12485+4 12485+4C*     2    EXIT SURF.
1600+2   0+0 43538+04820+5     035000+4   0+0 19317+4 19317+4C*     2    EXIT SURF.
1600+2   0+0 15255+14820+5     040000+4   0+0 36698+4 36698+4C*     2    EXIT SURF.
1600+2   0+0-23283-9           010000+4   0+0-10165+4-10165+4C*     2    EXIT SURF
1600+2   0+0 27345-6           015000+4   0+0-54530+3-54530+3C*     2    EXIT SURF.
1600+2   0+0 36186-3           020000+4   0+0-26271+3-26271+3C*     2    EXIT SURF.
1600+2   0+0 39897-2           022500+4   0+0-11622+3-11622+3C*     2    EXIT SURF.
1600+2   0+0 33106-1           025000+4   0+0 12309+3 12309+3C*     2    EXIT SURF.
1600+2   0+0 11389+0           027500+4   0+0 51930+3 51930+3C*     2    EXIT SURF.
1600+2   0+0 15822+0           030000+4   0+0 81611+3 81611+3C*     2    EXIT SURF.
1600+2   0+0 24217+0           032500+4   0+0 12485+4 12485+4C*     2    EXIT SURF.
1600+2   0+0 43538+0           035000+4   0+0 19317+4 19317+4C*     2    EXIT SURF.
1600+2   0+0 15255+1           040000+4   0+0 36698+4 36698+4C*     2    EXIT SURF.
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CARD COUNT - 311

ASTHMA OUTPUT

ABBOTT-ERM AXI-SYMMETRIC TRANSIENT HEATING AND MATERIAL ABLATION PROGRAM

APG 112C 800 PSIA CHAMBER PRESSURE; BASELINE CASE 4032.03, PLUS COOLDOWN
AFTER 4.0 SECONDS, PYROLYTIC GRAPHITE SURFACE, USING A NODAL COLUMNS AS
A TABLE OF CHEMISTRY TABLES ASSIGNED BY NODE. 112,800,COOL

INPUT DATA

DIMENSIONS OF INPUT DATA

TIME	SEC	TEMPERATURE	DEG R	DENSITY	LB PER CUBIC FT
SPECIFIC HEAT	BTU PER LB DEG R	CONDUCTIVITY	BTU PER FT SEC DEG R	EMISSIVITY	DIMENSIONLESS
HEAT COEFFICIENT	LB PER SQ FT SEC	ENTHALPY	BTU PER LB	NODAL COORDINATES	INCHES
RESISTANCES	SQ FT SEC DEG R PER BTU				

PROBLEM CONSTANTS

MMAX	NMAX	INIT TIME	FINL TIME	PRNT TIME	TIME INCR	TIME CNST	VKIN
42	6	0.	0.4000+002	0.1000+001	0.	0.9000+002	0.

BACK WALL CONVECTION COEF BTU/FTSC-SEC-DEG R	BACK WALL EMISSIVITY	RESERVOIR TEMPERATURE
0.0010	0.850	530.00

ACROTHERM AXI-SYMMETRIC TRANSIENT HEATING AND MATERIAL ABLATION PROGRAM

NODAL DATA

MATL	THTI	SIDE	ENTB	HTTB	HEAT CNST	INIT TEMP	CONT RES A	CONT RES B	VF1	VF3
3	0	0	0	0	0.	0.5300+003	0.	0.	0.	0.
3	0	0	0	0	0.	0.5300+003	0.	0.	0.	0.
2	0	0	0	0	0.	0.5300+003	0.	0.	0.	0.
2	0	0	0	0	0.	0.5300+003	0.	0.	0.	0.
2	0	0	0	0	0.	0.5300+003	0.	0.	0.	0.
2	0	0	0	0	0.	0.5300+003	0.	0.	0.	0.
2	0	0	0	0	0.	0.5300+003	0.	0.	0.	0.
1	1	0	1	1	0.	0.5300+003	0.	0.	0.9700+000	0.
1	1	0	1	1	0.	0.5300+003	0.	0.	0.9700+000	0.
1	1	0	1	1	0.	0.5300+003	0.	0.	0.9700+000	0.
1	1	0	1	1	0.	0.5300+003	0.	0.	0.9700+000	0.
1	1	1	1	1	0.	0.5300+003	0.	0.	0.9700+000	0.
3	0	0	0	0	0.	0.5300+003	0.	0.	0.	0.
3	0	0	0	0	0.	0.5300+003	0.	0.	0.	0.
2	0	0	0	0	0.	0.5300+003	0.	0.	0.	0.
2	0	0	0	0	0.	0.5300+003	0.	0.	0.	0.
2	0	0	0	0	0.	0.5300+003	0.	0.	0.	0.
2	0	0	0	0	0.	0.5300+003	0.	0.	0.	0.
1	1	0	1	2	0.	0.5300+003	0.	0.	0.9700+000	0.
1	1	0	1	2	0.	0.5300+003	0.	0.	0.9700+000	0.
1	1	0	1	2	0.	0.5300+003	0.	0.	0.9700+000	0.
1	1	0	1	2	0.	0.5300+003	0.	0.	0.9700+000	0.
1	1	1	1	2	0.	0.5300+003	0.	0.	0.9700+000	0.
0	0	0	0	0	0.	0.	0.	0.	0.	0.
3	0	0	0	0	0.	0.5300+003	0.	0.	0.	0.

```
2   0   0   0   0   0.      0.5300+003  0.      0.      0.      0.
2   0   0   0   0   0.      0.5300+003  0.      0.      0.      0.
2   0   0   0   0   0.      0.5300+003  0.      0.      0.      0.
2   0   0   0   0   0.      0.5300+003  0.      0.      0.      0.
1   1   0   2   3   0.      0.5300+003  0.      0.      0.9700+000  0.5800-001
1   1   0   2   3   0.      0.5300+003  0.      0.      0.9700+000  0.5800-001

1   1   0   2   3   0.      0.5300+003  0.      0.      0.9700+000  0.5800-001
1   1   0   2   3   0.      0.5300+003  0.      0.      0.9700+000  0.5800-001
1   1   0   2   3   0.      0.5300+003  0.      0.      0.9700+000  0.5800-001
0   0   0   0   0   0.      0.          0.      0.      0.          0.
0   0   0   0   0   0.      0.5300+003  0.      0.      0.          0.
2   0   0   0   0   0.      0.5300+003  0.      0.      0.          0.
2   0   0   0   0   0.      0.5300+003  0.      0.      0.          0.
2   0   0   0   0   0.      0.5300+003  0.      0.      0.          0.
2   0   0   0   0   0.      0.5300+003  0.      0.      0.          0.
2   0   0   0   0   0.      0.5300+003  0.      0.      0.          0.
1   1   0   2   4   0.      0.5300+003  0.      0.      0.9700+000  0.1700+000
1   1   0   2   4   0.      0.5300+003  0.      0.      0.9700+000  0.1700+000
1   1   0   2   4   0.      0.5300+003  0.      0.      0.9700+000  0.1700+000
1   1   0   2   4   0.      0.5300+003  0.      0.      0.9700+000  0.1700+000
1   1   0   2   4   0.      0.5300+003  0.      0.      0.9700+000  0.1700+000
0   0   0   0   0   0.      0.          0.      0.      0.          0.
2   0   0   0   0   0.      0.5300+003  0.      0.      0.          0.
2   0   0   0   0   0.      0.5300+003  0.      0.      0.          0.
2   0   0   0   0   0.      0.5300+003  0.      0.      0.          0.
2   0   0   0   0   0.      0.5300+003  0.      0.      0.          0.
2   0   0   0   0   0.      0.5300+003  0.      0.      0.          0.
```

2	0	0	0	0	0.	0.5300+003	0.	0.	0.	0.	
1	1	0	3	5	0.	0.5300+003	0.	0.	0.9700+000	0.1740+000	
1	1	0	3	5	0.	0.5300+003	0.	0.	0.9700+000	0.1740+000	
1	1	0	3	5	0.	0.5300+003	0.	0.	0.9700+000	0.1740+000	
1	1	0	3	5	0.	0.5300+003	0.	0.	0.9700+000	0.1740+000	
1	1	1	3	5	0.	0.5300+003	0.	0.	0.9700+000	0.1740+000	
0	0	0	0	0	0.	0.	0.	0.	0.	0.	
3	0	0	0	0	0.	0.5300+003	0.	0.	0.	0.	
2	0	0	0	0	0.	0.5300+003	0.	0.	0.	0.	
2	0	0	0	0	0.	0.5300+003	0.	0.	0.	0.	
2	0	0	0	0	0.	0.5300+003	0.	0.	0.	0.	
2	0	0	0	0	0.	0.5300+003	0.	0.	0.	0.	
2	0	0	0	0	0.	0.5300+003	0.	0.	0.	0.	
1	1	0	3	6	0.	0.5300+003	0.	0.	0.9700+000	0.1760+000	
1	1	0	3	6	0.	0.5300+003	0.	0.	0.9700+000	0.1760+000	
1	1	0	3	6	0.	0.5300+003	0.	0.	0.9700+000	0.1760+000	
1	1	0	3	6	0.	0.5300+003	0.	0.	0.9700+000	0.1760+000	
1	1	1	3	6	0.	0.5300+003	0.	0.	0.9700+000	0.1760+000	

MATERIAL PROPERTIES TABLES
MATERIAL NO. 1

TEMP	DENSITY	SPEC HEAT	CONDUCT	EMISSIV	CONDUCT2
0.5250+003	0.1370+003	0.2400+000	0.5000-001	0.9000+000	0.3610-003
0.7800+003	0.1370+003	0.2760+000	0.5000-001	0.9000+000	0.2820-003
0.1040+004	0.1370+003	0.3150+000	0.4470-001	0.9000+000	0.2635-003
0.1300+004	0.1370+003	0.3570+000	0.3333-001	0.9000+000	0.2305-003
0.1560+004	0.1370+003	0.4090+000	0.4450-001	0.9000+000	0.2000-003
0.2190+004	0.1370+003	0.4450+000	0.3015-001	0.9000+000	0.1835-003
0.2650+004	0.1370+003	0.4870+000	0.1736-001	0.9000+000	0.1778-003
0.3000+004	0.1370+003	0.4980+000	0.1491-001	0.9000+000	0.1835-003
0.4440+004	0.1370+003	0.5210+000	0.1418-001	0.9000+000	0.2222-003
0.7440+004	0.1370+003	0.5270+000	0.1388-001	0.9000+000	0.2890-003
0.9990+004	0.1370+003	0.5270+000	0.1386-001	0.9000+000	0.2896-003

MATERIAL NO. 2

TEMP	DENSITY	SPEC HEAT	CONDUCT	EMISSIV	CONDUCT2
0.5250+003	0.7430+002	0.2400+000	0.3380-002	0.9000+000	0.
0.7800+003	0.7430+002	0.2760+000	0.3380-002	0.9000+000	0.
0.1040+004	0.7430+002	0.3150+000	0.3380-002	0.9000+000	0.

0.1300+004	0.7430+002	0.3570+000	0.3380-002	0.9000+000	0.
0.1800+004	0.7430+002	0.4090+000	0.3380-002	0.9000+000	0.
0.2300+004	0.7430+002	0.4450+000	0.3380-002	0.9000+000	0.
0.2650+004	0.7430+002	0.4800+000	0.3380-002	0.9000+000	0.
0.3040+004	0.7430+002	0.4980+000	0.3380-002	0.9000+000	0.
0.4440+004	0.7430+002	0.5200+000	0.3380-002	0.9000+000	0.
0.9440+004	0.7430+002	0.5200+000	0.3380-002	0.9000+000	0.
0.9999+004	0.7430+002	0.5200+000	0.3380-002	0.9000+000	0.

MATERIAL NO. 3

TEMP	DENSITY	SPEC HEAT	CONDUCT	EMISSIV	CONDUCT2
0.5550+003	0.1110+003	0.2300+000	0.5560-004	0.9000+000	0.
0.9600+003	0.1110+003	0.3100+000	0.5560-004	0.9000+000	0.
0.1440+004	0.1110+003	0.5000+000	0.5560-004	0.9000+000	0.
0.1960+004	0.1110+003	0.5300+000	0.5560-004	0.9000+000	0.
0.2440+004	0.1110+003	0.5600+000	0.5560-004	0.9000+000	0.
0.3440+004	0.1110+003	0.6000+000	0.5560-004	0.9000+000	0.
0.4460+004	0.1110+003	0.6100+000	0.5560-004	0.9000+000	0.
0.5440+004	0.1110+003	0.6200+000	0.5560-004	0.9000+000	0.
0.6440+004	0.1110+003	0.6300+000	0.5560-004	0.9000+000	0.
0.7440+004	0.1110+003	0.6400+000	0.5560-004	0.9000+000	0.
0.9999+004	0.1110+003	0.6400+000	0.5560-004	0.9000+000	0.

---TIME DEPENDENT BOUNDARY CONDITIONS---

TIME TABLE NUMBER 1

TIME (SEC)	PROB OPTN	RECOVERY ENTHALPY (BTU/LB)	RADIATION HEAT RATE (BTU/SQ FT-SECOND)	HEAT COEFF (LB/SQ FT-SECOND)	PRESSURE (ATM)	BLOWING REDUCTION PARAMETER
0.	1	2020.00	785.00	0.8750	50.00000	0.400
4.00	1	2020.00	785.00	0.8750	50.00000	0.400

TIME (SEC)	PROB OPTN	VIEW FACTOR	RADIATION HEAT RATE (BTU/SQ FT-SECOND)
4.00	3	0.	0.
60.00	3	0.	0.

TIME TABLE NUMBER 2

TIME (SEC)	PROB OPTN	RECOVERY ENTHALPY (BTU/LB)	RADIATION HEAT RATE (BTU/SQ FT-SECOND)	HEAT COEFF (LB/SQ FT-SECOND)	PRESSURE (ATM)	BLOWING REDUCTION PARAMETER
0.	1	2000.00	785.00	1.0530	47.50000	0.400
4.00	1	2000.00	785.00	1.0530	47.50000	0.400

TIME (SEC)	PROB OPTN	VIEW FACTOR	RADIATION HEAT RATE (BTU/SQ FT-SECOND)
4.00	3	0.	0.
60.00	3	0.	0.

TIME TABLE NUMBER 3

TIME (SEC)	PROB OPTN	RECOVERY ENTHALPY (BTU/LB)	RADIATION HEAT RATE (BTU/SQ FT-SECOND)	HEAT COEFF (LB/SQ FT-SECOND)	PRESSURE (ATM)	BLOWING REDUCTION PARAMETER
0.	1	1944.00	785.00	1.2420	41.00000	0.400
4.00	1	1944.00	785.00	1.2420	41.00000	0.400
TIME (SEC)	PROB OPTN	VIEW FACTOR	RADIATION HEAT RATE (BTU/SQ FT-SECOND)			
4.00	3	0.	0.			
60.00	3	0.	0.			

TIME TABLE NUMBER 4

TIME (SEC)	PROB OPTN	RECOVERY ENTHALPY (BTU/LB)	RADIATION HEAT RATE (BTU/SQ FT-SECOND)	HEAT COEFF (LB/SQ FT-SECOND)	PRESSURE (ATM)	BLOWING REDUCTION PARAMETER
0.	1	1937.00	785.00	1.3100	31.50000	0.400
4.00	1	1937.00	785.00	1.3100	31.50000	0.400
TIME (SEC)	PROB OPTN	VIEW FACTOR	RADIATION HEAT RATE (BTU/SQ FT-SECOND)			
4.00	3	0.	0.			
60.00	3	0.	0.			

TIME TABLE NUMBER 5

TIME (SEC)	PROB OPTN	RECOVERY ENTHALPY (BTU/LB)	RADIATION HEAT RATE (BTU/SQ FT-SECOND)	HEAT COEFF (LB/SQ FT-SECOND)	PRESSURE (ATM)	BLOWING REDUCTION PARAMETER
0.	1	1787.00	785.00	1.0700	17.00000	0.400
4.00	1	1787.00	785.00	1.0700	17.00000	0.400
TIME (SEC)	PROB OPTN	VIEW FACTOR	RADIATION HEAT RATE (BTU/SQ FT-SECOND)			
4.00	3	0.	0.			
60.00	3	0.	0.			

TIME TABLE NUMBER 6

TIME (SEC)	PROB OPTN	RECOVERY ENTHALPY (BTU/LB)	RADIATION HEAT RATE (BTU/SQ FT-SECOND)	HEAT COEFF (LB/SQ FT-SECOND)	PRESSURE (ATM)	BLOWING REDUCTION PARAMETER
0.	1	1701.00	785.00	1.0100	16.00000	0.400
4.00	1	1701.00	785.00	1.0100	16.00000	0.400
TIME (SEC)	PROB OPTN	VIEW FACTOR	RADIATION HEAT RATE (BTU/SQ FT-SECOND)			
4.00	3	0.	0.			
60.00	3	0.	0.			

CH/CHO = PHI/(EXP(PHI)-1.) WHERE PHI = 2.*BP* RDOT/CHO.. BRP IN TABLE

---SURFACE EQUILIBRIUM DATA---

RATIO OF MASS TO HEAT TRANSFER COEFFICIENTS = 0.845
EQUIL DIFFUSION EXPONENT = 0.
NO RADIUS CORRECTION ON C-

P = 28.0000 ATM

TEMPERATURE (DEG R)	EDGE ENTH AT T-WALL	TEMPERATURE (DEG R)	EDGE ENTH AT T-WALL	TEMPERATURE (DEG R)	EDGE ENTH AT T-WALL
7200.00	2055.96	4500.00	749.05	1800.00	-441.44
6300.00	1620.00	3600.00	458.40	900.00	-743.93
5400.00	1190.79	2700.00	167.74		

KINETICS PRM = 0.520+005 PRESSURE = 48.0000 ATM

TEMP (DEG R)	M-DOT- CHAR/CM	CHEM,PROD (BTU/LB)	SURFACE SPECIES	TEMP (DEG R)	M-DOT- CM/R/CM	CHEM,PROD (BTU/LB)	SURFACE SPECIES
1800.00	-0.0000	1714.54	C•	4950.00	0.1280	984.44	C•
2700.00	0.0000	1108.37	C•	5400.00	0.1661	43.88	C•
3600.00	0.0005	988.04	C•	5850.00	0.2327	-399.36	C•
4050.00	0.0056	927.61	C•	6300.00	0.3684	-1316.22	C•
4500.00	0.0712	581.2	C•	7200.00	1.1560	-4590.67	C•

KINETICS PRM = 0. PRESSURE = 48.0000 ATM

TEMP (DEG R)	M-DOT- CHAR/CM	CHEM,PROD (BTU/LB)	SURFACE SPECIES	TEMP (DEG R)	M-DOT- CM/R/CM	CHEM,PROD (BTU/LB)	SURFACE SPECIES
1800.00	-0.0000	1714.54	C•	4950.00	0.1280	984.44	C•
2700.00	0.0000	1108.37	C•	5400.00	0.1661	43.88	C•
3600.00	0.0005	988.04	C•	5850.00	0.2327	-399.36	C•
4050.00	0.0056	927.61	C•	6300.00	0.3684	-1316.22	C•
4500.00	0.0712	581.2	C•	7200.00	1.1560	-4590.67	C•

P = 21.4000 ATM

TEMPERATURE (DEG R)	EDGE ENTH AT T-WALL	TEMPERATURE (DEG R)	EDGE ENTH AT T-WALL	TEMPERATURE (DEG R)	EDGE ENTH AT T-WALL
7200.00	2059.92	4500.00	741.02	1800.00	-453.84
6300.00	1619.87	3600.00	446.24	900.00	-743.63
5400.00	1186.85	2700.00	152.96		

ABNOTHERM AXI-SYMMETRIC TRANSIENT HEATING AND MATERIAL ABLATION PROGRAM

KINETICS PRM = 0,385+005 PRESSURE = 31,400 ATM

TEMP (DEG R)	M-DOT- CHAR/CM	CHEM,PROD (BTU/LB)	SURFACE SPECIES	TEMP (DEG R)	M-DOT- CHAR/CM	CHEM,PROD (BTU/LB)	SURFACE SPECIES
1800.00	-0.0000	1584.85	C*	4950.00	0.1224	933.62	C*
2700.00	0.0000	1032.36	C*	5400.00	0.1626	-34.47	C*
3400.00	0.0003	916.01	C*	5850.00	0.2349	-538.43	C*
4050.00	0.0038	864.73	C*	6300.00	0.3894	-1415.74	C*
4500.00	0.0412	651.32	C*	7200.00	1.2878	-7733.27	C*

KINETICS PRM = 0, PRESSURE = 31,400 ATM

TEMP (DEG R)	M-DOT- CHAR/CM	CHEM,PROD (BTU/LB)	SURFACE SPECIES	TEMP (DEG R)	M-DOT- CHAR/CM	CHEM,PROD (BTU/LB)	SURFACE SPECIES
1800.00	-0.0000	1584.85	C*	4950.00	0.1224	933.62	C*
2700.00	0.0000	1032.36	C*	5400.00	0.1626	-34.47	C*
3400.00	0.0003	916.01	C*	5850.00	0.2349	-538.43	C*
4050.00	0.0038	864.73	C*	6300.00	0.3894	-1415.74	C*
4500.00	0.0412	651.32	C*	7200.00	1.2878	-7733.27	C*

P = 76.0000 ATM

TEMPERATURE (DEG R)	EDGE ENTH AT T-WALL	TEMPERATURE (DEG R)	EDGE ENTH AT T-WALL	TEMPERATURE (DEG R)	EDGE ENTH AT T-WALL
7200.00	2060.46	4500.00	743.56	1800.00	-442.53
6300.00	1614.11	3600.00	323.63	900.00	-776.59
5400.00	1174.95	2700.00	-81.04		

KINETICS PRM = 0,482+005 PRESSURE = 14,0000 ATM

TEMP (DEG R)	M-DOT- CHAR/CM	CHEM,PROD (BTU/LB)	SURFACE SPECIES	TEMP (DEG R)	M-DOT- CHAR/CM	CHEM,PROD (BTU/LB)	SURFACE SPECIES
1800.00	-0.0000	1367.17	C*	4950.00	0.1139	139.87	C*
2700.00	0.0000	900.51	C*	5400.00	0.1582	-179.64	C*
3400.00	0.0004	797.44	C*	5850.00	0.2422	-810.38	C*
4050.00	0.0040	748.14	C*	6300.00	0.4354	-2218.69	C*
4500.00	0.0331	571.74	C*	7200.00	1.5255	-9850.38	C*

KINETICS PRM = 0, PRESSURE = 14,000 ATM

TEMP (DEG R)	M-DOT- CHAR/CM	CHEM,PROD (BTU/LB)	SURFACE SPECIES	TEMP (DEG R)	M-DOT- CHAR/CM	CHEM,PROD (BTU/LB)	SURFACE SPECIES
1800.00	-0.0000	1367.17	C*	4950.00	0.1139	139.87	C*
2700.00	0.0000	900.5	C*	5400.00	0.1582	-179.64	C*
3400.00	0.0004	797.4	C*	5850.00	0.2422	-810.38	C*
4050.00	0.0040	748.1	C*	6300.00	0.4354	-2218.69	C*
4500.00	0.0331	571.7	C*	7200.00	1.5255	-9850.38	C*

GRID COORDINATES

I	J	RC(IN)	ZC(IN)	RN(IN)	ZN(IN)
1	1	0.26180+001	0.	0.261[illegible]+001	0.10000+000
2	1	0.19980+001	0.	0.199[illegible]+001	0.10000+000
3	1	0.15570+001	0.	0.1557[illegible]+001	0.10000+000
4	1	0.12040+001	0.	0.1204[illegible]+001	0.10000+000
5	1	0.10590+001	0.	0.10395+001	0.96500-001
6	1	0.98500+000	0.	0.9515[illegible]+000	0.92500-001
7	1	0.91100+000	0.	0.8680[illegible]+000	0.85000-001
8	1	0.85000+000	0.	0.8065[illegible]+000	0.79500-001
9	1	0.83800+000	0.	0.7950[illegible]+000	0.78500-001
10	1	0.82400+000	0.	0.7835[illegible]+000	0.77000-001
11	1	0.81400+000	0.	0.7720[illegible]+000	0.76000-001
12	1	0.80200+000	0.	0.7605[illegible]+000	0.74500-001
13	1	0.79000+000	0.		
1	2	0.26180+001	0.20000+000	0.261[illegible]+001	0.30950+000
2	2	0.19980+001	0.20000+000	0.199[illegible]+001	0.30950+000
3	2	0.15570+001	0.20000+000	0.1557[illegible]+001	0.30000+000
4	2	0.12040+001	0.20000+000	0.1204[illegible]+001	0.30000+000
5	2	0.10200+001	0.17000+000	0.1012[illegible]+001	0.29500+000
6	2	0.91[illegible]0+000	0.14500+000	0.8930[illegible]+000	0.28650+000
7	2	0.82500+000	0.17000+000	0.7870[illegible]+000	0.27000+000
8	2	0.76300+000	0.15900+000	0.7220[illegible]+000	0.25750+000
9	2	0.75200+000	0.13700+000	0.7105[illegible]+000	0.25500+000
10	2	0.74100+000	0.13400+000	0.6985[illegible]+000	0.25200+000
11	2	0.73000+000	0.13200+000	0.6870[illegible]+000	0.24950+000
12	2	0.71900+000	0.14900+000	0.6750[illegible]+000	0.24650+000
13	2	0.70800+000	0.14600+000		
1	3	0.26180+001	0.41900+000	0.1309[illegible]+001	0.20950+000
2	3	0.19980+001	0.41900+000	0.199[illegible]+001	0.50950+000
3	3	0.15570+001	0.42000+000	0.1557[illegible]+001	0.50000+000
4	3	0.12040+001	0.42000+000	0.1204[illegible]+001	0.50000+000
5	3	0.10040+001	0.39700+000	0.10035+001	0.49850+000
6	3	0.86800+000	0.36800+000	0.8565[illegible]+000	0.49250+000
7	3	0.74900+000	0.37000+000	0.7285[illegible]+000	0.48100+000
8	3	0.68100+000	0.35000+000	0.6595[illegible]+000	0.47200+000
9	3	0.66900+000	0.33300+000	0.6460[illegible]+000	0.46950+000
10	3	0.65600+000	0.35000+000	0.6320[illegible]+000	0.46750+000
11	3	0.64400+000	0.34700+000	0.6185[illegible]+000	0.46500+000
12	3	0.63100+000	0.34400+000	0.6045[illegible]+000	0.46300+000
13	3	0.61900+000	0.34100+000		
1	4	0.	0.	0.	0.
2	4	0.19980+001	0.60[illegible]000+000	0.199[illegible]+001	0.70000+000
3	4	0.15570+001	0.60[illegible]000+000	0.1557[illegible]+001	0.70000+000
4	4	0.12040+001	0.60[illegible]000+000	0.1204[illegible]+001	0.70000+000
5	4	0.10030+001	0.60[illegible]000+000	0.10025+001	0.70000+000
6	4	0.84500+000	0.59700+000	0.8430[illegible]+000	0.69900+000
7	4	0.70800+000	0.59200+000	0.7070[illegible]+000	0.69900+000
8	4	0.63400+000	0.58[illegible]800+000	0.6405[illegible]+000	0.69850+000
9	4	0.62400+000	0.58[illegible]600+000	0.6220[illegible]+000	0.69800+000

10	4	0.60800+000	0.59300+000	0.60950+000	0.69800+000
11	4	0.59300+000	0.59300+000	0.59400+000	0.69750+000

12	4	0.57800+000	0.57200+000	0.57900+000	0.69800+000
13	4	0.56200+000	0.57000+000		
1	5	0.	0.	0.	0.
2	5	0.19980+001	0.80000+000	0.19980+001	0.90000+000
3	5	0.15570+001	0.80000+000	0.15570+001	0.90000+000
4	5	0.12040+001	0.80000+000	0.12040+001	0.90000+000
5	5	0.10020+001	0.80000+000	0.10020+001	0.90000+000
6	5	0.84100+000	0.81000+000	0.84550+000	0.90350+000
7	5	0.70600+000	0.81600+000	0.71800+000	0.91300+000
8	5	0.64300+000	0.81900+000	0.66000+000	0.91900+000
9	5	0.62700+000	0.81000+000	0.64550+000	0.92050+000
10	5	0.61100+000	0.81100+000	0.63100+000	0.92250+000
11	5	0.59500+000	0.81200+000	0.61650+000	0.92400+000
12	5	0.58000+000	0.81400+000	0.60250+000	0.92650+000
13	5	0.56400+000	0.81800+000		
1	6	0.	0.	0.	0.
2	6	0.19980+001	0.13000+001	0.19980+001	0.10925+001
3	6	0.15570+001	0.13000+001	0.15570+001	0.10925+001
4	6	0.12040+001	0.13000+001	0.12040+001	0.10925+001
5	6	0.10020+001	0.13000+001	0.10020+001	0.10925+001
6	6	0.85000+000	0.13060+001	0.86500+000	0.10955+001
7	6	0.73000+000	0.13200+001	0.74450+000	0.11025+001
8	6	0.67700+000	0.13290+001	0.69250+000	0.11070+001
9	6	0.66400+000	0.13310+001	0.68000+000	0.11080+001
10	6	0.65100+000	0.13340+001	0.66750+000	0.11095+001
11	6	0.63800+000	0.13360+001	0.65500+000	0.11105+001
12	6	0.62500+000	0.13390+001	0.64250+000	0.11120+001
13	6	0.61200+000	0.13420+001		
1	7	0.	0.		
2	7	0.19980+001	0.11850+001		
3	7	0.15570+001	0.11850+001		
4	7	0.12040+001	0.11850+001		
5	7	0.10100+001	0.11850+001		
6	7	0.87600+000	0.11850+001		
7	7	0.75900+000	0.11850+001		
8	7	0.71000+000	0.11850+001		
9	7	0.69600+000	0.11850+001		
10	7	0.68200+000	0.11850+001		
11	7	0.67200+000	0.11850+001		
12	7	0.66200+000	0.11850+001		
13	7	0.64800+000	0.11850+001		

OPTION 1 - ABLATION CALCULATION

********** 2.00 SECONDS **********

GENERAL

TIME	QTOT,SUR	QTOT,VAT	CASV ERER	#NODE	ITER	NODE D-TIME	ACT D-TIME
0.2000+001	0.5449+002	0.3321+002	0.1039+001	8	6	74	0.54724+001	0.51309-002

HEATED SURFACE

-------VISCELLANEOUS SURFACE DATA-------

RO.	COL	ORTN	SURF ITER	SURF TEMP(R)	H EDGE (BTU/LB)	H WALL (BTU/LB)	M PRIME TOT	MASS COEFF (LB/FT2-SEC)	CH/CH*	PRESSURE (ATM)	RADIUS (IN)	Z
11	1	1	3	5907.6	2020.00	1432.01	0.2468	0.49868	0.94499	0.506+002	0.770+000	0.758+000
12	2	1	3	5917.4	2006.00	1434.71	0.2493	0.50979	0.94462	0.475+002	0.687+000	0.250+000
13	3	1	3	5892.2	1984.00	1422.74	0.2463	0.71900	0.94485	0.410+002	0.619+000	0.465+000
14	4	1	4	5881.3	1937.00	1417.48	0.2433	0.74708	0.94576	0.315+002	0.593+000	0.698+000
15	5	1	3	5717.9	1787.00	1329.27	0.2137	0.61411	0.95188	0.178+002	0.609+000	0.925+000
16	6	1	3	5671.8	1761.00	1304.87	0.2048	0.58+84	0.95472	0.163+002	0.650+000	0.111+001

--------SURFACE RATE QUANTITIES--------

LOCATION		--RECESSION RATES-- (MILS/SEC)		--MASS RATES-- (LB/FT2-SEC)		--SURFACE ENERGY FLUX RATES-- (BTU/FT2-SEC)				
RO.	COL	CENTER LINE	NORMAL	MDOT TOTAL	MDOT THERM	CONVECTED TA	CHEMICAL GENERATION	RADIATION ABSORBED	RADIATION EMITTED	CONDUCTION AWAY
11	1	11.343938	10.767409	0.123+000	0.123+000	0.486+003	-0.258+003	0.707+003	0.511+003	0.424+003
12	2	12.977984	13.095376	0.150+000	0.150+000	0.588+003	-0.322+003	0.707+003	0.515+003	0.438+003
13	3	15.515767	15.510116	0.177+000	0.177+000	0.669+003	-0.448+003	0.707+003	0.506+003	0.410+003
14	4	15.942111	15.918972	0.182+000	0.182+000	0.684+003	-0.458+003	0.707+003	0.502+003	0.389+003
15	5	11.502214	11.495982	0.131+000	0.131+000	0.488+003	-0.384+003	0.707+003	0.449+003	0.348+003
16	6	10.458619	10.410010	0.119+000	0.119+000	0.437+003	-0.328+003	0.707+003	0.435+003	0.384+003

------SURFACE TIME INTEGRATED QUANTITIES------

		--RECESSION TOTALS-- (MILS)		--MASS ABLATION TOTALS-- (LB/COL)		--SURFACE ENERGY FLUX TOTALS-- (BTU/COL)				
RO.	COL	CENTER LINE	NORMAL	MDOT TOTAL	MDOT THERM	CONVECTED TA	CHEMICAL GENERATION	RADIATION ABSORBED	RADIATION EMITTED	CONDUCTION AWAY
11	1	21.5773	21.5173	0.131+002	0.131+002	0.528+001	-0.241+001	0.797+001	0.554+001	0.579+001
12	2	25.7447	25.8057	0.179+002	0.179+002	0.748+001	-0.484+001	0.890+001	0.626+001	0.672+001
13	3	29.5792	29.5742	0.217+002	0.217+002	0.895+001	-0.619+001	0.907+001	0.631+001	0.652+001
14	4	30.3612	30.3612	0.223+002	0.223+002	0.921+001	-0.647+001	0.931+001	0.572+001	0.577+001
15	5	21.7449	21.7449	0.149+002	0.149+002	0.594+001	-0.483+001	0.845+001	0.516+001	0.528+001
16	6	20.0804	20.0814	0.465+002	0.465+002	0.195+002	-0.154+002	0.238+002	0.162+002	0.449+001

IN-DEPTH DATA

NODE		TEMP	NODE		TEMP	NODE		TEMP	NODE		TEMP	NODE		TEMP
1	1	0.5300+003	2	1	0.5300+003	3	1	0.5351+003	4	1	0.5919+003	5	1	0.7252+003
6	1	0.8717+003	7	1	0.1119+004	8	1	0.1395+004	9	1	0.2273+004	10	1	0.3752+004
11	1	0.5627+004	12	1	0.	1	2	0.5300+003	2	2	0.5300+003	3	2	0.5334+003
4	2	0.5691+003	5	2	0.6497+003	6	2	0.8224+003	7	2	0.1101+004	8	2	0.1375+004
9	2	0.2229+004	10	2	0.3811+004	11	2	0.	12	2	0.	1	3	0.
2	3	0.5300+003	3	3	0.5322+003	4	3	0.5539+003	5	3	0.6228+003	6	3	0.7647+003
7	3	0.1041+004	8	3	0.1261+004	9	3	0.2070+004	10	3	0.3557+004	11	3	0.
12	3	0.	1	4	0.	2	4	0.5300+003	3	4	0.5314+003	4	4	0.5476+003
5	4	0.6030+003	6	4	0.7364+003	7	4	0.1000+004	8	4	0.1204+004	9	4	0.1934+004
10	4	0.3240+004	11	4	0.5741+004	12	4	0.	1	5	0.	2	5	0.5300+003
3	5	0.5313+003	4	5	0.5475+003	5	5	0.6056+003	6	5	0.7467+003	7	5	0.1014+004
8	5	0.1194+004	9	5	0.1887+004	10	5	0.2988+004	11	5	0.4764+004	12	5	0.
1	6	0.	2	6	0.5300+003	3	6	0.5315+003	4	6	0.5494+003	5	6	0.6138+003
6	6	0.7578+003	7	6	0.1039+004	8	6	0.1221+004	9	6	0.1934+004	10	6	0.3131+004
11	6	0.4933+004	12	6	0.									

OPTION 3 - COOLDOWN CALCULATION

** 5.00 SECONDS **

GENERAL

TIME	QTOT,SUR	QTOT,TAT	CNSV ENER	CHNODE	ITER	NODE D-TIME	ACT D-TIME
0.5000+001	0.4664+002	0.6529+002	0.1021+001	8 1	154	0.4246?-001	0.10000-001

HEATED SURFACE

--------MISCELLANEOUS SURFACE DATA--------

ROW	CEL	OPTN	SURF ITER	SURF TEMP(R)	H EDGE (BTU/LB)	H WALL (BTU/LB)	B PRIME TOT	MASS COEFF (LB/FT2-SEC)	CH/CHO	PRESSURE (ATM)	RADIUS (IN)	Z
[illegible]	1	3	4	1779.6	0.	0.	0.	0.	0.	0.100-005	0.793+000	0.782-001
[illegible]	2	3	4	1753.0	0.	0.	0.	0.	0.	0.100-005	0.712+000	0.255+000
[illegible]	3	3	4	1741.9	0.	0.	0.	0.	0.	0.100-005	0.649+000	0.470+000
[illegible]	4	3	4	1776.2	0.	0.	0.	0.	0.	0.100-005	0.624+000	0.698+000
[illegible]	5	3	3	2133.6	0.	0.	0.	0.	0.	0.100-005	0.632+000	0.922+000
[illegible]	6	3	3	2324.2	0.	0.	0.	0.	0.	0.100-005	0.671+000	0.111+001

AEROTHERM AXI-SYMMETRIC TRANSIENT HEATING AND MATERIAL ABLATION PROGRAM

--------SURFACE RATE QUANTITIES--------

-LOCATION-		--RECESSION RATES-- (MILS/SEC)		--MASS RATES-- (LB/FT2-SEC)			--SURFACE ENERGY FLUX RATES-- (BTU/FT2-SEC)			
ROW	COL	CENTER LINE	NORMAL	MDOT TOTAL	MDOT TCHEM	CONVECTED IN	CHEMICAL GENERATION	RADIATION ABSORBED	RADIATION EMITTED	CONDUCTION AWAY
9	1	0.	0.	0.	0.	0.	0.	0.	0.	0.591-007
9	2	0.	0.	0.	0.	0.	0.	0.	0.	0.147-007
9	3	0.	0.	0.	0.	0.	0.	0.	0.231+000	-0.231+000
9	4	0.	0.	0.	0.	0.	0.	0.	0.733+000	-0.733+000
9	5	0.	0.	0.	0.	0.	0.	0.	0.156+001	-0.156+001
9	6	0.	0.	0.	0.	0.	0.	0.	0.126+001	-0.126+001

-----SURFACE TIME INTEGRATED QUANTITIES-----

		--RECESSION TOTALS-- (MILS)		--MASS ABLATION TOTALS-- (LB/COL)			--SURFACE ENERGY FLUX TOTALS-- (BTU/COL)			
ROW	COL	CENTER LINE	NORMAL	MDOT TOTAL	MDOT TCHEM	CONVECTED IN	CHEMICAL GENERATION	RADIATION ABSORBED	RADIATION EMITTED	CONDUCTION AWAY
9	1	43.8677	43.8677	0.276-002	0.276-002	0.117+002	-0.529+001	0.164+002	0.116+002	0.112+002
9	2	50.6111	50.6111	0.367-002	0.367-002	0.151+002	-0.708+001	0.181+002	0.128+002	0.133+002
9	3	59.6862	59.6862	0.445-002	0.445-002	0.180+002	-0.107+002	0.184+002	0.129+002	0.129+002
9	4	61.4642	61.4642	0.417-002	0.417-002	0.166+002	-0.982+001	0.168+002	0.117+002	0.111+002
9	5	44.8436	44.8436	0.312-002	0.312-002	0.116+002	-0.886+001	0.172+002	0.108+002	0.916+001
9	6	41.4957	41.6957	0.195-001	0.195-001	0.482+002	-0.683+002	0.967+002	0.675+002	0.903+001

IN-DEPTH DATA

NODE		TEMP	NODE		TEMP	NODE		TEMP	NODE		TEMP	NODE		TEMP
1	1	0.5350+003	2	1	0.5302+003	3	1	0.6231+003	4	1	0.9705+003	5	1	0.1319+004
6	1	0.1556+004	7	1	0.1693+004	8	1	0.1739+004	9	1	0.1760+004	10	1	0.
11	1	0.	12	1	0.	1	2	0.5300+003	2	2	0.5301+003	3	2	0.6058+003
4	2	0.5737+003	5	2	0.1221+004	6	2	0.1515+004	7	2	0.1714+004	8	2	0.1753+004
9	2	0.	10	2	0.	11	2	0.	12	2	0.	1	3	0.
2	3	0.5501+003	3	3	0.5947+003	4	3	0.6037+003	5	3	0.1112+004	6	3	0.1451+004
7	3	0.1698+004	8	3	0.1744+004	9	3	0.	10	3	0.	11	3	0.
12	3	0.	1	4	0.	2	4	0.5301+003	3	4	0.5843+003	4	4	0.7611+003
5	4	0.1934+004	6	4	0.1385+004	7	4	0.1666+004	8	4	0.1738+004	9	4	0.1776+004
10	4	0.	11	4	0.	12	4	0.	1	5	0.	2	5	0.5301+003
3	5	0.5796+003	4	5	0.7474+003	5	5	0.1029+004	6	5	0.1386+004	7	5	0.1713+004
8	5	0.1810+004	9	5	0.2144+004	10	5	0.	11	5	0.	12	5	0.
1	6	0.	2	6	0.5300+003	3	6	0.5784+003	4	6	0.7494+003	5	6	0.1028+004
6	6	0.1572+004	7	6	0.1688+004	8	6	0.1763+004	9	6	0.2027+004	10	6	0.
11	6	0.	12	6	0.									

APPENDIX D

FORTRAN IV LISTING OF ASTHMA COMPUTER PROGRAM

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      CASTHMA
C-----MODIFICATION OF AATT TO ACCOUNT FOR RECEDING SURFACES
C-----DIMENSIONED AS CORNERS
      COMMON CR(402),CZ(402),AA(402),AB(402),AC(402),AD(402)
C-----DIMENSIONED AS NODES
      COMMON MATL(200),KTH(200),KSH(200),KWE(200),KTU(200),CON(200),
     1TA(200),TB(200),CRA(200),CRB(200),PLA(200),PLB(200),PLC(200),
     2PLD(200),VOL(200),RA(200),RB(200),CAP(200),ENT(200),QNP(200),
     3VF1(200),VF3(200)
C-----DIMENSIONED AS SURFACE NODES (NUMBER OF COLUMNS)
      COMMON KSUR(40),TS(40),DSDT(40),DSDTS(40),DS(40),DST(40),U(40)
      COMMON PLBS(40),DSTT(40),QCONDT(40),QCNV(40),QCNVT(40),QCHM(40),
     1QCHMT(40),QRAB(40),QRABT(40),QRAD(40),QRADT(40),DSDTBN(40),DSN(40)
      COMMON CMDOT(40),HEDG(40),CMT(40),HAL(40),G(40),GZ(40),PR(40)
      COMMON II(40),SZ(40),SR(40),EMN(40),ITSR(40)
      COMMON IABLS(40),KDROP(40)
C-----DIMENSIONED AS PROPERTY TABLES, ENTRIES X MATERIALS
      COMMON TT(15,6),RT(15,6),CPT(15,6),CNT(15,6),CNT2(15,6),
     1EPT(15,6),TTMX(6)
      DIMENSION THZ(15)
C-----DIMENSIONED AS TIME TABLES, ENTRIES X TABLE NO
      COMMON THT(25,10),CHT(25,10),RET(25,10),TQR(25,10),TPI(25,10),
     1TBRP(25,10)
      DIMENSION IOPT(25)
C-----MISCELLANEOUS QUANTITIES
      COMMON RECORD(36),TMPR(5),MPR(5),NNPR(5)
      COMMON VITER(51),EITER(51),IAB,RO
      COMMON VKIN,CMH,CM,CH
      COMMON TH,DTH,PRT,THI,THF,DLTH,ETA,ITS,DTHS
      COMMON FV,FT,PIB,ZRO,KQOP,MX,NN,NAT,NHT,GNTS,QSUM,SIG
      COMMON KRESC,KSLOP
      COMMON/ENRGY/TPR(5),NMG(5),TMG(8,5),NLO(8,5),NHI(8,5),
     1KHI(8,5),TTSEN(25,5),THSEN(25,5),TCPSEN(25,5),
     2TLMC(25,8,5),ISEN(5),TTS(25,8,5),TCHEM(25,8,5),
     3NPR
      DIMENSION TASEN(25,5),TCASEN(25,5),TSURF(25),TSEN(25),IZ(25)
      COMMON/LK/KOUT,IEX,DEN,VK,IHI(40),ILO(40),IR(40)
      DIMENSION TPN(8)
      DIMENSION PRTI(4),TPTCG(4)
      DATA BLANK/6H      /
  300 FORMAT(2I3,1PE6.4,4I1)
  301 FORMAT(4E7.5)                                                    AN  0012
  302 FORMAT(4I1,I2,6E6.4)
  303 FORMAT(I2,F8.2,5F10.5)
 3030 FORMAT(I2,6E6.4)
  304 FORMAT(1H1,25X,71HAEROTHERM AXI-SYMMETRIC TRANSIENT HEATING AND MA
     1TERIAL ABLATION PROGRAM/113X,4HPAGE,I3//)
  305 FORMAT(12A6)                                                     AN  0016
  306 FORMAT(//11H INPUT DATA//27H   DIMENSIONS OF INPUT DATA//114H   TIAN  0017
     1ME              SEC                TEMPERATURE   DEG R          AN  0018
     2        DENSITY              LB PER CUBIC FT/112H   SPECIFIC HEAT  AN  0019
     3   BTU PER LB DEG R   CONDUCTIVITY  BTU PER FT SEC DEG R      EMISAN  0020
     4IVITY         DIMENSIONLESS/15H   HEAT COEFFICIENT  LB PER SQ FTAN  0021
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     5 SEC   ENTHALPY      BTU PER LB                    NODAL COORDINATES  AN  0022
     6INCHES/44H   RESISTANCES      SQ FT SEC DEG R PER BTU///20H   PROAN  0023
     7BLEM CONSTANTS//85H   HMAX HMAX      INIT TIME   FINL TIME   PRNT AN  0024
     8TIME   TIME INCR   TIME CNST      VKIN/)
  307 FORMAT(//20H   NODAL COORDINATES//5X,1HI,5X,1HJ,5X,6HRC(IN),7X,6HZ
     1C(IN),7X,6HRN(IN),7X,6HZN(IN)/)
  308 FORMAT(13H   NODAL DATA//97H   MATL THTA SIDE ENTB HTTB   HEAT CNSAN  0028
     1T   INIT TEMP   CONT RES A  CONT RES B      VF1          VF3/)
  309 FORMAT(29H   MATERIAL PROPERTIES TABLES/)                          AN  0030
  310 FORMAT(15H   MATERIAL NO.I3//73H      TEMP       DENSITY    SPEC HAN* 0031
     1EAT    CONDUCT     EMISSIV     CONDUCT2/)
  311 FORMAT(//25H   HEATING TABLES, OPTION12/)                          AN  0033
  312 FORMAT(17H   HEAT TABLE NO.I3//50H      TIME     HEAT COEFF  RECOVAN  0034
     1 ENTH   RAD FACTOR/)
  313 FORMAT(//22H   WALL ENTHALPY TABLE//34H      TEMP      ENTH 1     AN  0036
     1 ENTH 2/)                                                          AN  0037
  314 FORMAT(1X,2I5,5X,6(E11.4,1X)//)
  315 FORMAT(1X,6E12.4)                                                  AN* 0039
  316 FORMAT(1X,5I5,2X,6(E11.4,1X)//)
  317 FORMAT(17H   HEAT TABLE NO.I3//37H      TIME         TEMP      RECOVAN  0041
     1 ENTH/)                                                            AN  0042
  318 FORMAT(3X,I3,3X,I3,1X,4E13.5)
  319 FORMAT(///12H OUTPUT DATA//28H   DIMENSIONS OF OUTPUT DATA//118H  AN  0044
     1 TIME        SEC                    QTOT,SUR,INT    BTU          AN  0045
     2          CONVECTIVE HEAT COEFF  LB PER SQ FT SEC/115H   TEMPERATAN  0046
     3URE  DEG R                    QNET AND QCONV  BTU PER SQ FT SEC   AN  0047
     4  QTOT                  BTU PER SQ FT//)                           AN  0048
  320  FORMAT(2I6)
  321 FORMAT(I2,10E7.5)
  322 FORMAT(//30H H VS  TEMPERATURE, TABLE NO. I2/3X4HTEMP9X1HH8X4HTEMP
     19X1HH8X4HTEMP9X1HH8X4HTEMP9X1HH8X4HTEMP9X1HH)
  323 FORMAT(//23H H VS  TIME, TABLE NO. I2/3X4HTIME9X1HH8X4HTIME9X1HH8X
     14HTIME9X1HH8X4HTIME9X1HH8X4HTIME9X1HH)
  324 FORMAT(10E11.3)
  332 FORMAT(/ 111H              NODE      TEMP       NODE      TEMP     AN  0054
     1  NODE      TEMP       NODE      TEMP       NODE      TEMP/)      AN  0055
  333 FORMAT(10X,5(I5,I4,E12.4))                                         AN  0056
  334 FORMAT(16X,
     1        72H   TIME       QTOT,SUR    QTOT,INT   CNSV ENER  CRNODEAN  0057
     2 ITER  NODE D-TIME,2X,11H ACT D-TIME/)
  335 FORMAT(16X,4(E11.4,1X),2I3,I5,2E13.5/)
  337 FORMAT(//11X,2I4,5E12.4)
  534 FORMAT (1H //23X40H---TIME DEPENDENT BOUNDARY CONDITIONS---/1H )    0790
  535 FORMAT (9X,4HTIME,8X,4HPROB,3X,8HRECOVERY,3X,9HRADIATION,4X,4HHEAT
     15X,8HPRESSURE,3X,7HBLOWING/9X,5H(SEC),7X,4HOPTN,3X,8HENTHALPY,3X,
     29HHEAT RATE,4X,5HCOEFF,14X,9HREDUCTION/28X,8H(BTU/LB),2X,11H(BTU/S
     3Q FT-,1X,10H(LB/SQ FT-,3X,5H(ATM),3X,9HPARAMETER /40X,7HSECOND),
     44X,7HSECOND))
  536 FORMAT (6X,F8.2,8X,I2,4X,2(F8.2,3X),F8.4,3X,F8.5,3X,F8.3)
  537 FORMAT (1H /9X,69HCH/CHO = PHI/(EXP(PHI)-1.) WHERE PHI = 2.*BRP*M
     1DOT/CHO. BRP IN TABLE)
  538 FORMAT(//27X34H---SURFACE EQUILIBRIUM DATA---)                     0850
  552 FORMAT (9X,4HTIME,5X,4HPROB,3X,7HSURFACE,4X,7HSURFACE/9X,5H(SEC),
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     17X,4HOPTN,5X,4HTEMP,5X,9HRECESSION/28X,7H(DEG R),5X,6H(MILS))
 556 FORMAT (9X,4HTIME,8X,4HPROB,5X,4HVIEW,5X,9HRADIATION/9X,5H(SEC),
     17X,4HOPTN,4X,6HFACTOR,4X,9HHEAT RATE/38X,11H(BTU/SQ FT-/40X,
     27HSECOND))
5780 FORMAT(E6.4,6X,E8.5,E6.4,F4.2,E7.5,6X,2E8.5,A6,I1)
5781 FORMAT(E6.4,E8.5,6X,E6.4,F4.2,E7.5,6X,2E8.5,A6,I1)
5782 FORMAT(E6.4,8X,E6.4,E6.4,F4.2,E7.5,6X,2E8.5,A6,I1)
5789 FORMAT(//6X,14HKINETICS PRM =E10.3,8X,10HPRESSURE =,F9.4,4H ATM//
     17X,2(4HTEMP,5X,26HM-DOT-  CHEM.PROD  SURFACE,3X)/6X,2(36H(DEG R)
     2CHAR/CM   (BTU/LB)  SPECIES,2X))
5790 FORMAT (6X,26HNO RADIUS CORRECTION ON CH)
5791 FORMAT(3F8.5,F9.4,F5.3,2F9.3,I2,A6)
5792 FORMAT(//6X,3HP =,F9.4,4H ATM//6X,3(25HTEMPERATURE  EDGE ENTH   )/
     16X,3(25H  (DEG R)    AT T-WALL   ))
5793 FORMAT (//6X,37HBAD SURFACE EQUILIBRIUM TABLE OF TYPE,I2)
5794 FORMAT (//6X,74HEQUAL MASS AND HEAT TRANSFER COEFFICIENTS AND EQUA
     1L DIFFUSION COEFFICIENTS)
5795 FORMAT(5X,F8.2,2X,F7.4,2X,F8.2,4A,A6,1X,F8.2,2X,F7.4,2X,F8.2,4A,A6
     1)
5796 FORMAT(2F10.3,3(9X,I1))
5797 FORMAT(//6X,45HRATIO OF MASS TO HEAT TRANSFER COEFFICIENTS =,F6.3/
     1 6X,28HUNEQUAL DIFFUSION EXPONENT =,F6.3)
5798 FORMAT                          (6X,F9.2,4X,F9.2,3X,F9.2,4X,F9.
     22,3X,F9.2,4X,F9.2)
5799 FORMAT (6X,66HHEAT TRANSFER COEFFICIENT MULTIPLIED BY (R INITIAL/R
     : CURRENT)**1.8)
 581 FORMAT(/34X,2HBACK WALL CONVECTION,6X,9HBACK WALL,10X,9HRESERVOIR/
     132X,23HCOEF BTU/FTSQ-SEC-DEG R,8X,1CHEMISSIVITY,8X,11HTEMPERATURE/
     237XF10.4,18XF6.3,10XF10.2)
 819 FORMAT(25H1OUT OF RANGE OF H TABLES/5X7H TEMP= E9.4,10X6HTIME= E9.
     14)
 820 FORMAT(54H IS LARGER THAN THE LAST ENTRY IN THE WALL ENTH. TABLE)
 821 FORMAT(55H IS SMALLER THAN THE FIRST ENTRY IN THE WALL ENTH.TABLE)
 822 FORMAT(24HOTHE TEMPERATURE OF NODE2I4)                          AN  0049
 823 FORMAT(49H IS LARGER THAN THE LAST ENTRY IN MATL. PROP. TAB.I3)  AN  0050
 824 FORMAT(51H IS SMALLER THAN THE FIRST ENTRY IN MATL. PROP. TAB.I3) AN 0051
     CALL DEFIO(5,5,8)
     CALL DEFIO(6,6,5)
C----GENERAL CONSTANTS
     FV=.5                                                          AN  0063
     FT=.083333333                                                  AN  0064
     RANK = 459.688
     ZRO=0.0                                                        AN  0065
     PIE=.021816616                                                 AN  0066
     INCH=5
     INPUT=5
     KOUT=6
     SIG=.481E-12
     NPG=1
C----MAIN INPUT BLOCK INCLUDING OUTPUT LISTING OF INPUT
 225 WRITE (6,304)        NPG                                       AN  0067
     READ (5,305)            (RECORD(I),I=1,36)
     WRITE (6,305)           (RECORD(I),I=1,36)                     AN  0069
```

```
      WRITE (6,306)                                                    AN  0070
      READ (5,303) MM,NN,THI,THF,THP,DLTH,ETA,DM2,ERP,HCONV,EPSW,TRES,
     1KASE,KSTRP,KRESC,KSLOP
      KSLOP=KSLOP+1
      KRESC=KRESC+1
      IF(ETA) 2253,2253,2254
 2253 ETA=0.75
 2254 CONTINUE
      WRITE(6,314) MM,NN,THI,THF,THP,DLTH,ETA,VKIN
      WRITE(KOUT,581) HCONV,EPSW,TRES
      IF(THP) 2255,2255,2267
 2267 TPTCG(1)=1.E+30
      GO TO 2256
 2255 READ(INPUT,2252) (PRTI(I),TPTCG(I),I=1,4)
      TPTCG(4)=THF
      DO 2257 I=1,3
      IF(TPTCG(I)) 2258,2255,2257
 2258 TPTCG(I)=THF
 2257 CONTINUE
      CALL LCOUNT (5,LCT,NPG,RECORD(35))
      WRITE (KOUT,2259)
 2259 FORMAT(//49X,21HOUTPUT TIME INTERVALS)
      WRITE(KOUT,2260) PRTI(1),THI,TPTCG(1)
 2260 FORMAT(/21X,17HOUTPUT INTERVAL =,F7.4,13H SECONDS FROM,F9.4,
     114H SECONDS UNTIL,F9.4,8H SECONDS)
      IF(TPTCG(1)-THF) 2261,2263,2263
 2261 DO 2262 I=2,4
      IF(TPTCG(I)-THF) 2266,2264,2264
 2264 CALL LCOUNT(1,LCT,NPG,RECORD(35))
      WRITE(KOUT,2265) PRTI(I),TPTCG(I-1)
 2265 FORMAT(21X,17HOUTPUT INTERVAL =, F7.4,13H SECONDS FROM,
     1F9.4,25H SECONDS UNTIL FINAL TIME//)
      GO TO 2263
 2266 CALL LCOUNT (1,LCT,NPG,RECORD(35))
 2262 WRITE(KOUT,2260) PRTI(I),TPTCG(I-1),TPTCG(I)
 2263 THP=PRTI(1)
      IF(THP) 2268,2268,2256
 2268 THF=THI
 2256 CONTINUE
      IF(KSTRP-2) 2250,2251,2251
 2251 READ (5,2252) (TPN(I),I=1,6)
 2252 FORMAT (6F10.0)
 2250 CONTINUE
      N=NN+1                                                           AN  0073
      M=MM+1                                                           AN  0074
      K=0                                                              AN  0075
      DO 200 J=1,N                                                     AN  0076
      DO 200 I=1,M                                                     AN  0077
      K=K+1                                                            AN  0078
      READ (5,301)  AA(K),AB(K),AC(K),AD(K)
      CR(K)=AB(K)
  200 CZ(K)=AD(K)
      CALL LCOUNT(-2*M*N-3,LCT,NPG,RECORD(35))
```

```
      WRITE (6,308)                                                    AN  0080
      K=0                                                              AN  0081
      DO 201 J=1,NN                                                    AN  0082
      DO 201 I=1,MM                                                    AN  0083
      K=K+1                                                            AN  0084
      READ (5,302)          MATL(K),KTH(K),KSH(K),KWE(K),KTU(K),CON(K)
     1,TA(K),CRA(K),CRB(K),VF1(K),VF3(K)
  201 WRITE (6,316)              MATL(K),KTH(K),KSH(K),KWE(K),KTU(K),CONAN  0087
     1(K),TA(K),CRA(K),CRB(K),VF1(K),VF3(K)
      CALL LCOUNT(4,LCT,NPG,RECORD(35))
      WRITE (6,309)                                                    AN  0089
      READ (5,303)          NMT
      J=0                                                              AN  0091
  202 J=J+1                                                            AN  0092
      WRITE (6,310)             J                                      AN  0093
      I=1                                                              AN  0094
  203 READ(5,3030) NC,TT(I,J),RT(I,J),CPT(I,J),CNT(I,J),EPT(I,J),CNT2(I,
     1J)
      RT(I,J)=RT(1,J)
      CALL LCOUNT(1,LCT,NPG,RECORD(35))
      WRITE (6,315)          TT(I,J),RT(I,J),CPT(I,J),CNT(I,J),EPT(IAN  0097
     1,J),CNT2(I,J)
      IF (NC) 205,204,205                                              AN  0099
  204 I=I+1                                                            AN  0100
      GO TO 203                                                        AN  0101
  205 TTMX(J)=TT(I,J)                                                  AN  0102
      ILO(J)=1
      IHI(J)=I
      IR(J)=1
      IF(J-1) 2053,2050,2053
 2050 THZ(1)=0.
      ILO(19)=1
      IHI(19)=I
      IR(19)=1
      DO 2051 L=2,I
 2051 THZ(L)=THZ(L-1)+(CPT(L,1)+CPT(L-1,1))/2.*(TT(L,1)-TT(L-1,1))
      TZ=536.
      CALL LOOK(1,TZ,TT(1,1),THZ(1),0,0,0,HSH,HA,1)
      DO 2052 L=1,I
 2052 THZ(L)=THZ(L)-HSH
 2053 CONTINUE
      IF(J-NMT)202,206,206
C-----TIME (HEATING) TABLES
  206 CALL LCOUNT(4,LCT,NPG,RECORD(35))
      WRITE(6,534)
      J=0
      KNN=0
  207 J=J+1
      NTH=0
      IS=0
      KN=0
      NOPT=0
  371 NTH=NTH+1
```

```
      READ(5,303) NC,THT(NTH,J),RET(NTH,J),TQR(NTH,J),CHT(NTH,J),
     1TPI(NTH,J),TBRP(NTH,J)
      IF(TBRP(NTH,J)) 374,375,374
  375 TBRP(NTH,J)=BKP
  374 IJ=1
      IF(CHT(NTH,J)) 342,342,343
  342 IJ=2
      IF(RET(NTH,J)-2.) 344,344,343
  344 IJ=3
  343 IOPT(NTH)=IJ
      IF(IJ-IS) 345,346,345
  345 NOPT=NOPT+1
      IS=IJ
  346 IF(NC) 372,371,372
  372 ILO(J+20)=1
      IHI(J+20)=NTH
      IR(J+20)=1
      CALL LCOUNT(2+NTH+NOPT+3,LCT,NPG,RECORD(35))
      WRITE(6,5380) J
 5380 FORMAT(15X,18HTIME TABLE NUMBER ,I2/)
      IS=0
      DO 3476 I=1,NTH
      IJ=IOPT(I)
      IF(IJ-IS) 347,349,347
  347 IS=IJ
      GO TO (3471,3472,3473),IJ
 3471 WRITE(KOUT,535)
      KN=1
      GO TO 3474
 3472 WRITE(KOUT,552)
      GO TO 3475
 3473 WRITE(KOUT,556)
      GO TO 3475
  349 GO TO (3474,3475,3475),IJ
 3474 WRITE(6,536) THT(I,J),IJ,RET(I,J),TQR(I,J),CHT(I,J),
     1TPI(I,J),TBRP(I,J)
      GO TO 3476
 3475 WRITE(6,536) THT(I,J),IJ,RET(I,J),TQR(I,J)
 3476 CONTINUE
      NHT=J
      IF(KN) 3732,3732,373
  373 DO 3731 I=1,NTH
 3731 TPI(I,J)=ALOG(AMAX1(TPI(I,J),.000001))
      KNN=1
 3732 IF(NC) 207,207,3733
 3733 IF(KNN) 1390,1390,328
  328 CALL LCOUNT(2,LCT,NPG,RECORD(35))
      WRITE(6,537)
C-----SURFACE THERMOCHEMISTRY TABLES
      READ(INPUT,5796) CMHS,VFZ,NR,NST,KTCTB
      KTCTB=KTCTB+1
      VKIN=VFZ
      IF(NST) 290.,290,29.1
```

```
      2900 CMH=CMHS
           GO TO 2902
      2901 IF(KNST-777) 2909,2903,2909
      2903 IF(CMH-CMHS) 2907,2905,2907
      2905 CALL LCOUNT(4,LCT,NPG,RECORD(35))
           WRITE(KOUT,2906)
      2906 FORMAT(//10X,54HSURFACE TABLES ARE THE SAME AS IN PREVIOUS PROBLEM
          1//)
           GO TO 1390
      2907 CALL LCOUNT(4,LCT,NPG,RECORD(35))
           WRITE(KOUT,2908)
      2908 FORMAT(//10X,72HPREVIOUS SURFACE TABLES CALLED FOR BUT CM/CH RATIO
          1 HAS CHANGED, QUIT JOB//)
           STOP
      2909 CALL LCOUNT(4,LCT,NPG,RECORD(35))
           WRITE(KOUT,2910)
      2910 FORMAT(//10X,70HPREVIOUS SURFACE TABLES CALLED FOR BUT THIS IS FIR
          1ST PROBLEM, QUIT JOB//)
           STOP
      2902 KNST=777
           IF (RSV) 3280,3280,3281
      3280 NR=0
      3281 CONTINUE
           WLS=-1
           NSEN=-1
           IP=1
           IPN=1
           I=1
           IN=1
           J=0
      2800 J=J+1
           GO TO (2911,2912,2913,2914),KTCTB
      2911 READ(INCH,5780) PSV,TLMC(J,I,IP),DMS,WLQ,TTS(J,I,IP),TCHEM(J,I,IP)
          1,TSEN(J),TSURF(J),JNG
           GO TO 2916
      2912 READ(INCH,5781) PSV,TLMC(J,I,IP),DMS,WLQ,TTS(J,I,IP),TCHEM(J,I,IP)
          1,TSEN(J),TSURF(J),JNG
           GO TO 2916
      2913 READ(INCH,5782) PSV,TLMC(J,I,IP),DMS,WLQ,TTS(J,I,IP),TCHEM(J,I,IP)
          1,TSEN(J),TSURF(J),JNG
      2916 JNG=JNG-1
           GO TO 2915
      2914 READ(INCH,5791) PSV,DMS,TLMC(J,I,IP),TTS(J,I,IP),WLQ,TCHEM(J,I,IP)
          1,TSEN(J),JNG,TSURF(J)
      2915 CONTINUE
           IF(JNG) 2817,2817,2821
      2817 TSURF(J)=BLANK
      2821 CONTINUE
           IF(TTS(J,I,IP)) 2803,2802,2801
      2801 TTS(J,I,IP)=TTS(J,I,IP)*1.8
           TCHEM(J,I,IP)=TCHEM(J,I,IP)*1.8
           TSEN(J)=TSEN(J)*1.8
           GO TO 2805
```

```
      2803 TTS(J,I,IP)=-TTS(J,I,IP)
      2805 IF(WLS) 2809,2807,2807
      2807 IX=4
           IF(WLS-WLQ) 2824,2811,2824
      2809 WLS=WLQ
      2811 IF(NSEN) 2802,2828,2828
      2802 IF(JNG) 2805,2804,2804
      2804 NSEN=J-1
           ISEN(IP)=NSEN
           IF (NSEN-1) 8806,7806,7806
      7806 DO 2806 L=1,NSEN
           TTSEN(L,IP)=TTS(L,1,IP)
           TZSEN(L,IP)=TCHEM(L,1,IP)
      2806 THSEN(L,IP)=ISEN(L)
      8806 CONTINUE
           IF(NSEN-1) 2820,2820,2808
      2808 CALL SLOPQ(NSEN,TTSEN(1,IP),THSEN(1,IP),TCPSEN(1,IP))
           CALL SLOPQ(NSEN,TTSEN(1,IP),TZSEN(1,IP),TCZSEN(1,IP))
           LLL=(NSEN-1)/3+1
           IF(IP-1) 2815,2813,2815
      2813 CALL LCOUNT(9,LCT,NPG,RECORD(35))
           WRITE (KOUT,538)
           WRITE (KOUT,5797) CMH,WLQ
           IF (NR) 2816,2816,2816
      2816 WRITE (KOUT,5799)
           GO TO 2815
      2818 WRITE (KOUT,5790)
      2815 CALL LCOUNT(LLL+6          ,LCT,NPG,RECORD(35))
           WRITE(KOUT,5792)PSV
           IF (LLL-1) 9819,8819,8819
      8819 DO 2819 LL=1,LLL
           IF (NSEN-LL) 7819,6819,6819
      6819 INT=(NSEN-LL)/LLL
           M2=LL+INT*LLL
           WRITE(KOUT,5798) (TTSEN(L,IP),THSEN(L,IP),L=LL,M2   ,LLL)
      7819 CONTINUE
      2819 CONTINUE
      9819 CONTINUE
           GO TO 2862
      2820 NSEN=0
           IX=3
           IF(CMH-1.) 2824,2822,2824
      2822 IX=2
           IF(WLQ) 2824,2826,2824
      2824 WRITE (KOUT,5793) IX
C                                                          TIXE LLAC
           STOP                                                        C
      2826 IF(IP-1) 2862,2861,2862
      2828 IF(TTS(J,I,IP)) 2829,2832,2829
      2829 IF(PSV-TPR(IP)) 2832,2830,2832
      2830 IF(DMS-TMG(I,IP)) 2834,2832,2834
      2832 IPN=IP+1
           NMG(IP)=I
```

```
      IN=0
      NSEN=-NSEN
 2834 IN=IN+1
      NHI(I,IP)=J-1
      NMC=J-1
      IX=5
      IF(NMC-1) 2824,2824,4852
 4852 CONTINUE
      CALL ORDERD(NMC,TLMC(1,I,IP),IZ)
      CALL SEQUA(NMC,IZ,TTS(1,I,IP),TCHEM(1,I,IP),TSEN(1),TSURF(1))
      IX=0
      IG=1
      BPG=0.
      HGA=0.
      NLO(I,IP)=1
      KHI(I,IP)=1
 2852 DO 2852 K=1,NMC
      BP=BPG+TLMC(K,I,IP)
      CALL LOOK(1,TTS(K,I,IP),TT(1,1),TH2(1),0,0,0,HCH,CT2,1)
      HCH=HCH+DH2
      IF(NSEN) 2838,2836,2838
 2836 TCHEM(K,I,IP)=BPG*HGA+TLMC(K,I,IP)*HCH-BP*TSEN(K)
      GO TO 2840
 2838 CALL OGLE(1,TTS(K,I,IP),HZ,ISEN(IP),TTSEN(1,IP),TZSEN(1,IP),TCZSEN
     1(1,IP))
      CALL OGLE(1,TTS(K,I,IP),HE,ISEN(IP),TTSEN(1,IP),THSEN(1,IP),TCPSEN
     1(1,IP))
      TCHEM(K,I,IP)=BPG*HGA+TLMC(K,I,IP)*HCH-BP*TSEN(K)+HZ-TCHEM(K,I,IP)
      TSEN(K)=HE
 2840 IF(TSURF(K)-BLANK) 2844,2842,2844
 2842 NLO(I,IP)=K+1
      IF(IG+IX-1) 2846,2846,2824
 2844 IX=1
 2846 IF(K-IG) 2852,2852,2848
 2848 IF(TTS(K,I,IP)-TTS(K-1,I,IP)) 2850,2850,2851
 2850 IG=NMC
      GO TO 2852
 2851 KHI(I,IP)=K
 2852 CONTINUE
      LLL=(NMC-1)/2+1
      CALL LCOUNT(LLL+6          ,LCT,NPG,RECORD(35))
      IF (LLL-1) 6010,6009,6009
 6009 WRITE(KOUT,5789) TMG(I,IP),TPR(IP)
      DO 6006 LL=1,LLL
      IF (NMC-LL) 6008,6007,6007
 6007 INT=(NMC-LL)/LLL
      M2=LL+INT*LLL
      WRITE(KOUT,5795)                          (TTS(L,I,IP),TLMC(L,I,IP),TCHEM
     1(L,I,IP),TSURF(L),L=LL,M2,LLL)
 6008 CONTINUE
 6006 CONTINUE
 6010 CONTINUE
      IF (NMC-1) 4856,3856,3856
```

```
 2856 DO 2656 K=1,NMC
      TCHEM(K,I,IP)=CMH*TCHEM(K,I,IP)-TSEN(K)
      IF(K-NLO(I,IP)) 2856,2854,2854
 2854 VK=K
      TLMC(K,I,IP)=ALOG(AMAX1(TLMC(K,I,IP),VK*1.E-10))
 2856 CONTINUE
 4856 CONTINUE
      CALL SSWTCH(3,JJ)
      GO TO (710,711),JJ
  710 CALL LCOUNT(LLL+6,LCT,NPG,RECORD(35))
      IF (LLL-1) 6015,6014,6014
 6014 WRITE(KOUT,5787)
 5787 FORMAT(///3X,39H---DUMPED VERSION OF PRECEDING TABLE---//)
      WRITE(KOUT,5789) TMG(I,IP),TPR(IP)
      DO 6011 LL=1,LLL
      IF (NMC-LL) 6013,6012,6012
 6012 INT=(NMC-LL)/LLL
      M2=LL+INT*LLL
      WRITE(KOUT,5788)                              (TTS(L,I,IP),TLMC(L,I,IP),TCHEM
     1(L,I,IP),TSEN(L) ,L=LL,M2 ,LLL)
 5788 FORMAT(5X,F8.2,2X,F7.4,2X,F8.2,2X,F8.2,1X,F8.2,2X,F7.4,2X,F8.2,2X,
     1F8.2)
 6013 CONTINUE
 6011 CONTINUE
 6015 CONTINUE
  711 CONTINUE
      IF(TTS(J,I,IP)) 2862,2870,2862
 2861 CALL LCOUNT(8                ,LCT,NPG,RECORD(35))
      WRITE (KOUT,538)
      WRITE(KOUT,5794)
      IF (NR) 2863,2863,2864
 2864 WRITE (KOUT,5799)
      GO TO 2862
 2863 WRITE (KOUT,5790)
 2862 TPR(IPN)=PSV
      TMG(IN,IPN)=DMS
      TLMC(1,IN,IPN)=TLMC(J,I,IP)
      TTS (1,IN,IPN)=TTS (J,I,IP)
      TCHEM(1,IN,IPN)=TCHEM(J,I,IP)
      TSURF(1)=TSURF(J)
      TSEN(1)=TSEN(J)
      J=1
      I=IN
      IP=IPN
      GO TO 2800
 2870 NPR=IP
      IR(12)=1
      ILO(12)=1
      IHI(12)=I
      DO 2872 I=1,IP
 2872 TPR(I)=ALOG(TPR(I))
      IR(13)=1
      IHI(13)=NPR
```

```
      ILO(13)=1
      CALL SSWTCH(3,KSSW)
      GO TO (700,1390),KSSW
  700 CALL LCOUNT(3,LCT,NPG,RECORD(35))
      WRITE(KOUT,703)
  703 FORMAT(//10X,48HDUMP OF TABLE INDICES NLO(I,J),NHI(I,J),KHI(I,J))
      DO 701 J=1,NPR
      CALL LCOUNT(3,LCT,NPG,RECORD(35))
      WRITE(KOUT,704) J
  704 FORMAT(/15X,6HIPR = ,I2/1H )
      L=NMG(J)
      CALL LCOUNT(L,LCT,NPG,RECORD(35))
      WRITE(KOUT,702) (NLO(I,J),NHI(I,J),KHI(I,J),I=1,L)
  701 CONTINUE
  702 FORMAT(20X,3(2X,I2))
 1390 CONTINUE
C-----INITIALIZATIONS
      TH=THI                                                    AN  0128
      PRT=THI+THP                                               AN  0129
      QNTS=ZRO                                                  AN  0130
      QNTI=ZRO                                                  AN  0131
      DTHM = 100.0
      KK=MM*NN                                                  AN  0133
      IAB=0
      RO=RT(1,1)
      CMD=0.
C-----NOTE TABLE II GIVES K IN M DIRECTION
      DO 216  I = 1 , NMT
      IF (CNT2(1,I) .NE. 0.0)  GO TO 216
      DO 215  J = 1,15
      CNT2(J,I) = CNT(J,I)
  215 CONTINUE
  216 CONTINUE
      DO 825 I=1,NN
      DSDT(I)=0.0
      DSDTB(I)=0.0
      DS(I)=0.0
      DST(I)=0.0
      DSTT(I)=0.0
      QCONDT(I)=0.
      DSDTSN(I)=0.
      DSN(I)=0.
      QCNV(I)=0.
      QCNVT(I)=0.
      IABLS(I)=0
      QCHM(I)=0.
      QCHMT(I)=0.
      QRAB(I)=0.
      QRABT(I)=0.
      QRAD(I)=0.
      QRADT(I)=0.
      CMDOT(I)=0.
      CMT(I)=0.
```

```
      KDROP(I)=0
  825 TS(I)=0.0
C-----SURFACE IDENTIFICATION AND CHECKING
      M=0
      K=0
      DO 828 J=1,NN
      L=-1
      KT=0
      DO 826 I=1,MM
      K=K+1
      KTS=KT
      KT=MATL(K)
      IF(KT) 827,827,826
  827 IF(KTS) 826,826,829
  829 L=L+1
      KCAN=K-1
  826 CONTINUE
      IF(KT) 8291,8261,8260
 8260 L=L+1
      KCAN=K
 8261 IF(L) 8291,8262,8291
 8262 KSUR(J)=KCAN
      MATL(KCAN)=-MATL(KCAN)
      TS(J)=TA(KCAN)
      KSH(KCAN)=1
      GO TO 828
 8291 CALL LCOUNT(2,LCT,NPG,RECORD(35))
      WRITE(6,8292) J
 8292 FORMAT(/10X,33HERRONEOUS NODAL LAYOUT IN COLUMN ,I3/)
      M=M+1
  828 CONTINUE
      IF(M) 8281,8281,8280
 8280 TH=THF
      GO TO 468
 8281 CONTINUE
      IFIN = 1
      CALL LCOUNT(5,LCT,NPG,RECORD(35))
      WRITE (6,307)
C-----GEOMETRY CALCULATIONS
      DO 8283 I=1,NN
      K=KSUR(I)
      J=K+I
      L=J+MM+1
      SR(I)=(CR(J)+CR(L))/2.
 8283 SZ(I)=(CZ(J)+CZ(L))/2.
      K=0                                                    AN  0136
      L=MM+1                                                 AN  0137
      N=L
      M=0                                                    AN  0138
      DO 1 J=1,NN                                            AN  0139
      DO 2 I=1,MM                                            AN  0140
      K=K+1                                                  AN  0141
      L=L+1                                                  AN  0142
```

```
      M=M+1                                                          AN  0143
      IF (AC(K)) 4,3,4                                               AN  0144
C-----PATH LENGTHS FOR BACKSHIFTED BUT SIDEWAYS CENTERED NODES
    3 AC(K)=-.5*(AA(K)+AA(L))
    4 IF (AD(K)) 6,5,6                                               AN  0146
    5 AD(K)=-.5*(AB(K)+AB(L))
    6 CALL LCOUNT(1,LCT,NPG,RECORD(35))
      WRITE(6,318) I,J,AA(K),AB(K),AC(K),AD(K)
      HA=AA(K)-AC(K)
      HB=AB(K)-AD(K)
      HC=HA*HA+HB*HB                                                 AN  0151
      PLA(M)=FT*SQRT (HC)
      HA=FV*(AA(K+1)+AA(L+1))-AC(K)                                  AN  0153
      HB=FV*(AB(K+1)+AB(L+1))-AD(K)                                  AN  0154
      HC=HA*HA+HB*HB                                                 AN  0155
      PLB(M)=FT*SQRT (HC)
      HA=AA(L)-AC(K)
      HB=AB(L)-AD(K)
      HC=HA*HA+HB*HB                                                 AN  0159
      PLC(M)=FT*SQRT (HC)
      PLD(M)=ZRO
      HA=AA(K)*AA(K)                                                 AN  0165
      HB=AA(K)*AA(K+1)                                               AN  0166
      HC=AA(K)*AA(L)                                                 AN  0167
      HD=AA(K+1)*AA(K+1)                                             AN  0168
      HE=AA(K+1)*AA(L+1)                                             AN  0169
      HF=AA(L)*AA(L)                                                 AN  0170
      HG=AA(L)*AA(L+1)                                               AN  0171
      HH=AA(L+1)*AA(L+1)                                             AN  0172
      HS=ZRO                                                         AN  0173
      HS=HS+AB(K)*(HC-HB+HF-HD)                                      AN  0174
      HS=HS+AB(K+1)*(HB-HE+HA-HH)                                    AN  0175
      HS=HS+AB(L)*(HG-HC+HH-HA)                                      AN  0176
      HS=HS+AB(L+1)*(HE-HG+HD-HF)                                    AN  0177
      VOL(M)=6.060171E-04*ABS (HS)
      HA=AA(K+1)-AA(K)                                               AN  0179
      HB=AB(K+1)-AB(K)                                               AN  0180
      HC=HA*HA+HB*HB                                                 AN  0181
      HD=SQRT (HC)
      HE=PIB*HD*(AA(K)+AA(K+1))                                      AN  0183
      HA=AA(L)-AA(K)                                                 AN  0184
      HB=AB(L)-AB(K)                                                 AN  0185
      HC=HA*HA+HB*HB                                                 AN  0186
      HD=SQRT (HC)
      HF=PIB*HD*(AA(K)+AA(L))                                        AN  0188
      AA(M)=HE                                                       AN  0189
    2 AB(M)=HF                                                       AN  0190
      K=K+1                                                          AN  0191
      L=L+1                                                          AN  0192
    7 HA=AA(L)-AA(K)                                                 AN  0196
      HB=AB(L)-AB(K)                                                 AN  0197
      HC=HA*HA+HB*HB                                                 AN  0198
      HD=SQRT (HC)
```

```
      AC(M)=PIP*HD*(AA(K)+AA(L))                                    AN  0200
      CALL LCOUNT(1,LCT,NPG,RECORD(35))
      WRITE(6,318) N,J,AA(K),AS(K)
    1 CONTINUE                                                      AN  0201
      LU=MM+1
      LL=NN+1
      DO 12 I=1,LU
      K=K+1
      CALL LCOUNT(1,LCT,NPG,RECORD(35))
   12 WRITE(6,318) I,LL,AA(K),AB(K)
      M=M-MM                                                        AN  0202
      DO 8 I=1,MM                                                   AN  0203
      K=K+1                                                         AN  0204
      M=M+1                                                         AN  0205
    9 HA=AA(K+1)-AA(K)                                              AN  0209
      HB=AB(K+1)-AB(K)                                              AN  0210
      HC=HA*HA+HB*HB                                                AN  0211
      HD=SQRT (HC)
      AD(M)=PIB*HD*(AA(K)+AA(K+1))                                  AN  0213
    8 CONTINUE                                                      AN  0214
      M=0                                                           AN  0215
      L=MM                                                          AN  0216
      K=MM-1                                                        AN  0217
      N=NN-1                                                        AN  0218
      DO 10 J=1,N                                                   AN  0219
      DO 11 I=1,K                                                   AN  0220
      M=M+1                                                         AN  0221
      L=L+1                                                         AN  0222
   13 AC(M)=AB(M+1)                                                 AN  0226
   14 AD(M)=AA(L)                                                   AN  0228
   11 CONTINUE                                                      AN  0229
      M=M+1                                                         AN  0230
      L=L+1                                                         AN  0231
   18 AD(M)=AA(L)                                                   AN  0235
   10 CONTINUE                                                      AN  0236
      DO 1000 J=1,NN
      K=KSUR(J)
 1000 PLBS(J)=PLB(K)
      CALL LCOUNT(-10,LCT,NPG,RECORD(35))
      WRITE (6,319)                                                 AN  0237
      ITER=0                                                        AN  0238
C-----MAIN ITERATION LOOP
   30 IF (DLTH) 31,31,32                                            AN  0239
   31 DTH=100.                                                      AN  0240
      GO TO 33                                                      AN  0241
   32 DTH=DLTH                                                      AN  0242
   33 ITER=ITER+1                                                   AN  0243
C-----MATERIAL PROPERTIES,NODAL RESISTANCES AND CAPACITIES
      I=0                                                           AN  0244
      L=MM                                                          AN  0245
      DO 39 JJ=1,NN                                                 AN  0246
      DO 40 III=1,MM
      I=I+1                                                         AN  0248
```

```
      L=L+1                                                          AN  0249
      IF(MATL(I)) 42,41,42
   41 RA(I)=ZRO                                                      AN  0251
      RB(I)=ZRO                                                      AN  0252
      GO TO 40                                                       AN  0253
   42 KT=IABS(MATL(I))
      IF (TTMX(KT)-TA(I)) 43,43,44                                   AN  0255
   43 HB=TA(I)                                                       AN  0256
      GO TO 500                                                      AN  0257
   44 IF (TA(I)-TT(1,KT)) 45,46,46                                   AN  0258
   45 HB=TA(I)                                                       AN  0259
      GO TO 501                                                      AN  0260
   46 IT=1                                                           AN  0261
   47 IF (TT(IT,KT)-TA(I)) 48,48,49                                  AN  0262
   48 IT=IT+1                                                        AN  0263
      GO TO 47                                                       AN  0264
   49 JT=IT-1                                                        AN  0265
      HC=(TA(I)-TT(JT,KT))/(TT(IT,KT)-TT(JT,KT))                     AN  0266
      HD=CNT(JT,KT)+HC*(CNT(IT,KT)-CNT(JT,KT))                       AN  0267
      HA=CRB(I)+PLC(I)/HD                                            AN  0268
      HM = CNT2(JT,KT) + HC * (CNT2(IT,KT) - CNT2(JT,KT) )
      HB = CRA(I) + PLB(I) / HM
      HE=RT(JT,KT)+HC*(RT(IT,KT)-RT(JT,KT))                          AN  0270
      HF=CPT(JT,KT)+HC*(CPT(IT,KT)-CPT(JT,KT))                       AN  0271
      CAP(I)=VOL(I)*HE*HF                                            AN  0272
   35 IF(MATL(I)+1) 50,50,51
   50 U(JJ)=AC(I)/HB
      RB(I)=0.0
      GO TO 61
   51 KT=IABS(MATL(I+1))
      IF(KT) 53,52,53
   52 WRITE(6,831)
  831 FORMAT (10X,27HERRONEOUS NODAL ARRANGEMENT)
      TH=THF
      GO TO 468
   53 IF (TTMX(KT)-TA(I+1)) 54,54,55                                 AN  0282
   54 HB=TA(I+1)                                                     AN  0283
      GO TO 500                                                      AN  0284
   55 IF (TA(I+1)-TT(1,KT)) 56,57,57                                 AN  0285
   56 HB=TA(I+1)                                                     AN  0286
      GO TO 501                                                      AN  0287
   57 IT=1                                                           AN  0288
   58 IF (TT(IT,KT)-TA(I+1)) 59,59,60                                AN  0289
   59 IT=IT+1                                                        AN  0290
      GO TO 58                                                       AN  0291
   60 JT=IT-1                                                        AN  0292
      HC=(TA(I+1)-TT(JT,KT))/(TT(IT,KT)-TT(JT,KT))                   AN  0293
      HM = CNT2(JT,KT) + HC * (CNT2(IT,KT) - CNT2(JT,KT) )
      HB = HB + PLD(I+1) / HM
      RB(I)=AB(I+1)/HB                                               AN  0296
   61 IF (JJ-NN) 63,62,63                                            AN  0297
   62 RA(I)=ZRO                                                      AN  0298
      GO TO 40                                                       AN  0299
```

```
      63 KT=IABS(MATL(L))
         IF (KT) 65,64,65                                          AN  0301
      64 RA(I)=ZRO                                                 AN  0302
         GO TO 40                                                  AN  0303
      65 IF (TTMX(KT)-TA(L)) 66,66,67                              AN  0304
      66 HB=TA(L)                                                  AN  0305
         GO TO 500                                                 AN  0306
      67 IF (TA(L)-TT(1,KT)) 68,69,69                              AN  0307
      68 HB=TA(L)                                                  AN  0308
         GO TO 501                                                 AN  0309
      69 IT=1                                                      AN  0310
      70 IF (TT(IT,KT)-TA(L)) 71,71,72                             AN  0311
      71 IT=IT+1                                                   AN  0312
         GO TO 70                                                  AN  0313
      72 JT=IT-1                                                   AN  0314
         HC=(TA(L)-TT(JT,KT))/(TT(IT,KT)-TT(JT,KT))                AN  0315
         HD=CNT(JT,KT)+HC*(CNT(IT,KT)-CNT(JT,KT))                  AN  0316
         IF(MATL(I)+IABS(MATL(I))) 7200,7202,7200
    7200 IF(KT+MATL(L)) 7201,7202,7201
    7202 HA=HA/(AD(I)+.00000001)+PLA(L)/(HD*(AA(L)+.00000001))
         RA(I)=1./HA
         GO TO 40
    7201 CONTINUE
         HA=HA+PLA(L)/HD                                           AN  0317
         RA(I)=AA(L)/HA                                            AN  0318
      40 CONTINUE                                                  AN  0319
      39 CONTINUE                                                  AN  0320
C-----HEAT FLUX LOOP
     221 QSUM=ZRO                                                  AN  0321
         KK=MM*NN                                                  AN  0322
         I=0                                                       AN  0323
         J=1                                                       AN  0324
         K=-1                                                      AN  0325
         L=MM                                                      AN  0326
         M=-MM                                                     AN  0327
         DO 75 JJ=1,NN                                             AN  0328
         DO 76 III=1,MM
         I=I+1                                                     AN  0330
         J=J+1                                                     AN  0331
         K=K+1                                                     AN  0332
         L=L+1                                                     AN  0333
         M=M+1                                                     AN  0334
         IF (MATL(I)) 114,115,114                                  AN  0335
     115 TB(I)=ZRO                                                 AN  0336
         GO TO 76                                                  AN  0337
     114 HA=ZRO                                                    AN  0338
         HB=ZRO                                                    AN  0339
         IF (K) 78,78,77                                           AN  0340
      77 HA=HA+TA(K)*RB(K)                                         AN  0341
         HB=HB+R3(K)                                               AN  0342
      78 IF (J-KK) 79,79,80                                        AN  0343
      79 HA=HA+TA(J)*RB(I)                                         AN  0344
         HB=HB+RB(I)                                               AN  0345
```

```
      80 IF (L-KK) 81,81,82                                          AN 0346
      81 HA=HA+TA(L)*RA(I)                                           AN 0347
         HB=HB+RA(I)                                                 AN 0348
      82 IF (M) 84,84,83                                             AN 0349
      83 HA=HA+TA(M)*RA(M)                                           AN 0350
         HB=HB+RA(M)                                                 AN 0351
      84 IF (CAP(I)) 85,86,85                                        AN 0352
      86 TB(I)=HA/HB                                                 AN 0353
         GO TO 76                                                    AN 0354
      85 DEN=HB                                                      AN 0355
      97 TB(I)=HA-TA(I)*HB                                           AN 0407
      98 IF (DLTH) 76,99,76                                          AN 0408
      99 IF (KTH(I)) 76,76,1001
    1001 IF(MATL(I)) 76,76,100
     100 HC=ETA*CAP(I)/DEN                                           AN 0410
         IF (HC-DTH) 101,76,76                                       AN 0411
     101 DTH=HC                                                      AN 0412
         MCRIT=III
         NCRIT=JJ                                                    AN 0414
      76 CONTINUE                                                    AN 0415
      75 CONTINUE                                                    AN 0416
C
C-----GO TO SURFACE ENERGY BALANCE PACKAGE
      CALL SURFB
C
C-----NEW TEMPERATURES LOOP
     107 K=0                                                         AN 0422
         DO 120 J=1,NN                                               AN 0423
         DO 121 I=1,MM                                               AN 0424
         K=K+1                                                       AN 0425
         IF (MATL(K)) 121,121,136                                    AN 0426
     136 IF(CAP(K)) 122,121,123
     122 WRITE(6,127) K
     127 FORMAT(//10X,26HNEGATIVE CAPACITY AT NODE ,I3//)
         THF=TH
         GO TO 468
     123 IF (KSH(K)) 124,124,125                                     AN 0429
     125 WRITE(6,126)  K
     126 FORMAT(//10X,34HNODAL BLUNDER AT 123, HEATED NODE ,I3,38H HAS MATE
        1RIAL NUMBER GREATER THAN ZERO//)
         THF=TH
         GO TO 468
     124 IF(MATL(K+1)) 1240,1242,1243
    1240 IF(KRESC-3) 1243,1241,1243
    1241 IF(KDROP(J)) 1242,1242,1243
    1242 TB(K)=(TB(K)+RB(K)*(TB(K+1)-TA(K+1)))*DTH/CAP(K)+TA(K)
         GO TO 121
    1243 HA=TB(K)*DTH/CAP(K)+TA(K)
         TB(K)=HA                                                    AN 0460
     121 CONTINUE                                                    AN 0461
     120 CONTINUE                                                    AN 0462
         KK=MM*NN                                                    AN 0463
     466 DO 467 I=1,KK                                               AN 0627
```

```
      QNTI=QNTI+CAP(I)*(TB(I)-TA(I))                                    AN  0628
  467 TA(I)=TB(I)                                                       AN  0629
      IF((DTH .LT. DTHM) .AND. (TH .NE. PRT)) DTHM = DTH
      CALL SSWTCH(5,KSSW)
      GO TO (4671,4672),KSSW
 4671 IF(ITER-3347) 4672,4672,4673
 4673 IF(ITER-3450) 468,468,4672
 4672 CONTINUE
      CALL SSWTCH(1,KSSW)
      GO TO (468,4674),KSSW
 4674 IF(TH-PRT) 4674,468,4674
 4674 IF(TH-THF) 472,468,468
C-----OUTPUT BLOCK
  468 CEC=QNTS/QNTI                                                     AN  0631
      CALL LCOUNT(17+NN,LCT,NPG,RECORD(35))
      WRITE(6,3364) TH
 3364 FORMAT(//1X,51(1H*),F7.2,8H SECONDS,53(1H*)//52X,13H***GENERAL***)
      WRITE (6,334)                                                     AN  0632
      WRITE(6,335) TH,QNTS,QNTI,CEC,MCRIT,NCRIT,ITER,DTHS,DTHM
      WRITE (6,336)
  336 FORMAT(//49X,22H***HEATED SURFACE***///40X,40H-------MISCELLANEOUS
     1 SURFACE DATA-------//2X,25HROW COL OPTN  SURF   SURF,6X,6HM EDGE,
     25X,6HM WALL,3X,4OHE PRIME  MASS COEFF    CH/CHO   PRESSURE,4X,6HRA
     3DIUS,1OX,1H2/16X,57HITER  TEMP(R)   (BTU/LB)   (BTU/LB)    TOT   (
     4LB/FT2-SEC),14X,5H(ATM),6X,4H(IN))
      K=0
      DO 949 J=1,NN
      DO 949 I=1,MM
      K=K+1
      IF(KSH(K)) 949,949,950
  950 BP=CMDOT(J)/G(J)
      BR=G(J)/G2(J)
      R=SR(J)
      Z=SZ(J)
      ITS=ITSR(J)
      WRITE(6,3370) I,J,II(J),ITS,TS(J),HEDG(J),HWL(J),BP,G(J),BR,PR(J),
     1R,Z
 3370 FORMAT(2X,I3,1X,I3,3X,I1,2X,I5,2X,F7.1,2(2X,F9.2),2X,F7.4,3X,
     1F9.5,3X,F7.5,3(2X,E10.3))
  949 CONTINUE
      CALL LCOUNT(8+NN,LCT,NPG,RECORD(35))
      WRITE(6,3360)
 3360 FORMAT(//40X,39H--------SURFACE RATE QUANTITIES--------//1X,
     1  31H-LOCATION-  --RECESSION RATES--,8X,14H--MASS RATES--,20X,
     229H--SURFACE ENERGY FLUX RATES--/18X,10H(MILS/SEC),13X,
     312H(LB/FT2-SEC),29X,13H(BTU/FT2-SEC))
      WRITE(6,3361)
 3361 FORMAT(60X,9HCONVECTED,4X,8HCHEMICAL,4X,9HRADIATION,3X,9HRADIATION
     1,2X,10HCONDUCTION/2X,56HROW COL   CENTER LINE  NORMAL      MDOT TOT
     2AL  MDOT TCHEM,6X,2HIN,6X,21HGENERATION   ABSORBED,5X,7HEMITTED,
     36X,4HAWAY)
      K=0
      DO 951 J=1,NN
```

```
      DO 9510 I=1,MM
      K=K+1
      IF(KSH(K)) 9510,9510,9511
 9511 HA=DSDTB(J)*12000.
      HB=DSDTBN(J)*12000.
      WRITE(6,3362) I,J,HA,HB,CMDOT(J),CMDOT(J),QCNV(J),
     1QCHM(J),QRAB(J),QRAD(J),QNP(K)
 3362 FORMAT(2X,I3,1X,I3,3X,2(F10.6,1X),2X,7(E10.3,2X))
 9510 CONTINUE
      CALL LCOUNT(8+NN,LCT,NPG,RECORD(35))
      WRITE(6,3363)
 3363 FORMAT(//38X,44H-----SURFACE TIME INTEGRATED QUANTITIES-----//
     113X,46H--RECESSION TOTALS--  --MASS ABLATION TOTALS--,
     215X,30H--SURFACE ENERGY FLUX TOTALS--/20X,6H(NILS),17X,
     38H(LB/COL),23X,9H(BTU/COL))
      WRITE(6,3361)
      K=0
      DO 9512 J=1,NN
      DO 9512 I=1,MM
      K=K+1
      IF(KSH(K)) 9512,9512,9513
 9513 HA=DSTT(J)*12000.
      HB=HA
      WRITE(6,3366) I,J,HA,HB,CMT(J),CMT(J),QCNVT(J),
     1QCHMT(J),QRABT(J),QRADT(J),QCONDT(J)
 3366 FORMAT(2X,I3,1X,I3,3X,2(F10.4,1X),2X,7(E10.3,2X))
 9512 CONTINUE
      CALL SSWTCH(4,KSSW)
      GO TO (9496,9497),KSSW
 9496 CALL LCOUNT(5+2*NN,LCT,NPG,RECORD(35))
      WRITE(6,9493)
 9493 FORMAT(//2X,10HEXTRA DUMP/2X,44HI,J,U,VOL,RA,RB,CAP,AA,AB,AC,AD,PL
     1B,PLBS,EMN//)
      K=0
      DO 9490 J=1,NN
      DO 9490 I=1,MM
      K=K+1
      IF(KSH(K)) 9490,9490,9491
 9491 WRITE(6,9492) I,J,U(J),VOL(K),RA(K),RB(K),CAP(K),AA(K),AB(K),AC(K)
     1,AD(K),PLB(K),PLBS(J),EMN(J)
 9492 FORMAT(2X,I3,2X,I3,1PE11.3/10X,2E11.3)
 9490 CONTINUE
      CALL LCOUNT(3+NN,LCT,NPG,RECORD(39))
      WRITE(6,9503)
 9503 FORMAT(//2X,40HI,J,DSDT,DSDTB,DS,DST,DSTT,MATL,KSH,KSUR/)
      K=0
      DO 9500 J=1,NN
      DO 9500 I=1,MM
      K=K+1
      IF(KSH(K)) 9500,9500,9501
 9501 WRITE(6,9502) I,J,DSDT(J),DSDTB(J),DS(J),DST(J),DSTT(J),MATL(K),
     1KSH(K),KSUR(J)
 9502 FORMAT(2X,2I4,5E12.3,3I4)
```

```
 9500 CONTINUE
      CALL LCOUNT(4,LCT,NPG,RECORD(35))
      WRITE(6,9494) PRT,THI,THF,DLTH,ETA,FV,FT,PIE,ZRO,KJOP,MM,NN,KK,
     1NMT,NHT
 9494 FORMAT(///2X,36HPRT,THI,THF,DLTH,ETA,FV,FT,PIE,ZRO,KJOP,MM,NN,KK,NM
     1T,NHT/2X,9E11.3,I2,2I4,3I3///)
 9497 CONTINUE
      IF(KSTRP-1) 849,842,8421
 8421 DO 8422 I=1,8
      IF(ABS(TH-TPN(I))-.0000001) 842,842,8422
 8422 CONTINUE
      GO TO 849
  842 K=0
      NS=0
      DO 840 J=1,NN
      DO 840 I=1,MM
      K=K+1
      IF(MATL(K)) 8420,840,841
 8420 NS=NS+1
  841 NS=NS+1
  840 CONTINUE
      K=0
      N=0
      LL=0
      LR=MM+1
      DO 843 J=1,NN
      DO 844 I=1,MM
      K=K+1
      LL=LL+1
      LR=LR+1
      IF(MATL(K)) 845,844,845
  845 N=N+1
      Z=(CZ(LL)+CZ(LR))/2.0
      R=(CR(LL)+CR(LR))/2.0
      PUNCH 846, R,Z,TA(K),I,J,MATL(K),TH,RECORD(35),RECORD(36),N,NS
  846 FORMAT (3F10.3,8HININDEGR,I3,1H/,I3,3HMAT,I2,F7.2,2HS ,2A6,1X,I3,
     12HOF,I3)
      IF(MATL(K)) 847,844,844
  847 N=N+1
      LL=LL+1
      LR=LR+1
      RAT=PLB(K)/PLB(J)
      R=R+RAT*((CR(LL)+CR(LR))/2.0-R)
      Z=Z+RAT*((CZ(LL)+CZ(LR))/2.0-Z)
      MOUT=-MATL(K)
      PUNCH 848, R,Z,TS(J),J,MOUT,TH,RECORD(35),RECORD(36),N,NS
  848 FORMAT (3F10.3,8HININDEGR,3A,1H/,I3,3HMAT,I2,F7.2,2HS ,2A6,1X,I3,
     12HOF,I3)
  844 CONTINUE
  843 CONTINUE
  849 CONTINUE
      CALL LCOUNT(KK/5+6,LCT,NPG,RECORD(35))
      WRITE(6,9365)
```

```
 3365 FORMAT(//49X,19H***IN-DEPTH DATA***/)
      WRITE (6,332)
      KPR=0                                                        AN 0643
      K=0                                                          AN 0644
      DO 240 J=1,NN                                                AN 0645
      DO 240 I=1,MM                                                AN 0646
      K=K+1                                                        AN 0647
      KPR=KPR+1                                                    AN 0648
      IF(MATL(K)) 952,951,952
  951 TMPR(KPR)=TA(K)
      GO TO 953
  952 TMPR(KPR) = TA(K)
  953 MPR(KPR)=I
      NNPR(KPR)=J
      IF (KPR-5) 240,241,240                                       AN 0652
  241 WRITE(6,333)  (MPR(L),NNPR(L),TMPR(L),L=1,5)
      KPR=0                                                        AN 0654
  240 CONTINUE                                                     AN 0655
      IF (KPR) 469,469,242                                         AN 0656
  242 WRITE(6,333)  (MPR(L),NNPR(L),TMPR(L),L=1,KPR)
  469 IF(TH-THF) 472,470,470
  470 IF(KASE) 471,471,225
  471 STOP
  472 IF(TH-PRT) 30,4721,4721
 4721 IF(TH-TPTCG(1)+.000001) 473,474,474
  473 PRT=AMIN1(PRT+THP,TPTCG(1))
      DTHM=100.
      GO TO 30
  474 IF(PRTI(2)) 476,476,475
  476 CALL LCOUNT(5,LCT,NPG,RECORD(35))
      WRITE (KOUT,477)
  477 FORMAT(//10X,62HHAVE ENCOUNTERED A ZERO OUTPUT INTERVAL, AM QUITTI
     1ING THIS JOB//)
      GO TO 470
  475 THP=PRTI(2)
      DO 478 I=1,3
      TPTCG(I)=TPTCG(I+1)
  478 PRTI(I)=PRTI(I+1)
      GO TO 473
  500 WRITE(6,822) III,JJ
      WRITE (6,823)              KT
      THF=TH                                                       AN 0664
      GO TO 468                                                    AN 0665
  501 WRITE(6,822) III,JJ
      WRITE (6,824)              KT
      THF=TH                                                       AN 0668
      GO TO 468                                                    AN 0669
  505 WRITE (6,819)              TA(I),TH
      THF=TH
      GO TO 468
      END
```

```
      SUBROUTINE SURFR
C-----DIMENSIONED AS CORNERS
      COMMON CR(402),CZ(402),AA(402),AB(402),AC(402),AD(402)
C-----DIMENSIONED AS NODES
      COMMON MATL(200),KTH(200),KSM(200),KSE(200),KTU(200),CON(200),
     1TA(200),TR(200),CRA(200),CRR(200),PLA(200),PLB(200),PLC(200),
     2PLD(200),VOL(200),RA(200),RP(200),CAP(200),ENT(200),QNP(200),
     3VF1(200),VF3(200)
C-----DIMENSIONED AS SURFACE NODES (NUMBER OF COLUMNS)
      COMMON KSUR(40),TS(40),HSDT(40),QSDTS(40),DS(40),DST(40),J(40)
      COMMON PLRS(40),DSTT(40),QCONDT(40),QCNV(40),QCNVT(40),QCHM(40),
     1QCHMT(40),QRAB(40),QRADT(40),QRAD(40),QRADT(40),QSDTRN(40),DSN(40)
      COMMON CVDOT(40),HEDG(40),CNT(40),HAL(40),G(40),GZ(40),PR(40)
      COMMON II(40),SZ(40),SR(40),EMN(40)
      COMMON ITSR(40)
      COMMON IABLS(40),KGROP(40)
      DIMENSION FMS(40),BPSV(40)
C-----DIMENSIONED AS PROPERTY TABLES, ENTRIES X MATERIALS
      COMMON TT(15,6),RT(15,6),CPT(15,6),CNT(15,6),CNT2(15,6),
     1EPT(15,6),TTMX(6)
C-----DIMENSIONED AS TIME TABLES, ENTRIES X TABLE NO
      COMMON THT(25,10),CHT(25,10),RET(25,10),TQR(25,10),TPI(25,10),
     1TSRP(25,10)
C-----MISCELLANEOUS QUANTITIES
      COMMON RECORD(36),TMPR(5),KPR(5),NNPR(5)
      COMMON VITER(51),EITER(51),IAS,RO
      COMMON VKIN,CMM,CV,CH
      COMMON TH,DTH,PRT,THI,THF,DLTH,ETA,ITS,DTHS
      COMMON FV,FT,PIR,ZRO,KQOP,MN,NN,NNT,NHT,QNTS,QSUM,SIG
      COMMON KRESC,KSLOP
      DIMENSION Y2(8)
      COMMON/ENRGY/TPR(5),NMG(5),TMG(8,5),ALO(8,5),NHI(8,5),
     1KHI(8,5),TTSEN(25,5),THSEN(25,5),TCPSEA(25,5),
     2TLMC(25,8,5),ISEN(5),TTS(25,8,5),TCHEM(25,8,5),
     3NPR
      COMMON/LC/KOUT,IEX,DEN,VR,IHI(40),ILO(40),IR(40)
      DATA BLANK/6H      /
C-----ADJUSTMENT OF TIME STEP ACCORDING TO LIMITATIONS OF TIME TABLES
      DTHS=DTH
      TH=TH+DTH
      DO 290 J=1,NN
      K=KSUR(J)
      KT=KTU(K)
      IF(KT) 290,290,296
  296 NTT=KT+20
      I=IR(NTT)
  291 IF(THT(I+1,KT)-TH+.00001) 294,294,292
  294 IF(I+1-IHI(NTT)) 292,290,290
  292 I=I+1
      IF(THT(I+1,KT)-THT(I,KT)) 291,293,291
  293 TH=TH-DTH
      THOS=THT(I,KT)-.01
      DTH=AMAX1(.1,THT(I,KT)-TH)
```

```
      TH=TH+DTH
      GO TO 291
  290 IR(NTT)=1
C-----DEFINE ALLOWABLE TIME STEP
      K=C
      TH=TH-DTH
      DO 2 I=1,NN
      DSDT(I)=DSDTB(I)
      K=KSUR(I)
      DTH=AMIN1(DTH,PLBS(I)/(1.+DSDT(I)+.000001)*(PLBS(I)/500.+PLB(K))/
     1(DSDT(I)+.000001))
      IF(DTH-1.0E-12) 106,106,107
  106 WRITE (6,108)
  108 FORMAT(10X,19HTOO SMALL TIME STEP//)
      WRITE(6,109)  I
  109 FORMAT(10X,6HCOLUMN,I3//)
      THF=TH
      RETURN
  107 CONTINUE
    2 CONTINUE
      HA=TH+DTH
      IF(HA-PRT) 105,105,104
  104 DTH=PRT-TH
      TH=PRT
      GO TO 4
  105 TH=TH+DTH
    4 CONTINUE
C-----GET SLOPES NOW PENDING REARRANGEMENT OF THIS SECTION
      GO TO (2904,2905),KSLOP
 2904 CALL SLOPL(MX,NN,SZ,SR,EMS,EMN)
      GO TO 2903
 2905 CONTINUE
      IF(NN-1) 2901,2901,2902
 2901 EMN(1)=1.E+30
      GO TO 2903
 2902 CALL SLOPQ(NN,SZ,SR,EMN)
      DO 2900 J=1,NN
 2900 EMN(J)=-1./(EMN(J)+1.E-30)
 2903 CONTINUE
C-----MAIN COLUMN LOOP FOR SURFACE OPERATIONS
C
      DO 7 I=1,NN
C
C-----INTERPOLATE IN TIME TABLES AND IDENTIFY OPTION
C
      K=KSUR(I)
      KT=KTU(K)
      IF(KT) 20,20,21
   20 HA=TB(K)*DTH/CAP(K)+TA(K)
      TB(K)=HA
      TS(I)=TB(K)
      DSDTB(I)=0.
      DSDTBN(I)=0.
```

```
      QNP(K)=0.
      GO TO 7
   21 CONTINUE
      ITL=13
      ITS=1
      KT=IABS(MATL(K))
      NTT=KT+20
      J=IR(NTT)
      DEN=(TH-THT(J,KT))/(THT(J+1,KT)-THT(J,KT))
      IF(THT(J+1,KT)-THT(J,KT)) 2940,2940,295
 2940 DEN=0.
  295 CH=CHT(J,KT)+DEN*(CHT(J+1,KT)-CHT(J,KT))
      QRA=TQR(J,KT)+DEN*(TQR(J+1,KT)-TQR(J,KT))
      HE=HET(J,KT)+DEN*(HET(J+1,KT)-HET(J,KT))
      BRP=TBRP(J,KT)+DEN*(TBRP(J+1,KT)-TBRP(J,KT))
      PRES=TPI(J,KT)+DEN*(TPI(J+1,KT)-TPI(J,KT))
      FACT=DTH/CAP(K)
      KOOP=1
      IF(CH) 297,297,2970
  297 KOOP=2
      CH=0.0
      IF(HE-2.0) 298,298,299
  298 KOOP=3
      HE=0.
      GO TO 2990
C-----OPTION 2 PREPARATIONS
  299 TS(I)=HE
      ST=HE
      SA=QRA/12000.
      DS(I)=SA-DSTT(I)-PLBS(I)+PLB(K)+DST(I)
      DSDTB(I)=DS(I)/DTH
      HA=VCOS(K,I,MM,CR,CZ,SZ,SR,EMN,PLB,PLBS,DST)
      IF(HA-.1) 2991,2991,2992
 2991 WRITE(6,2993) I,KOOP
 2993 FORMAT(//10X,28HBAD SURFACE SHAPE AT COLUMN ,I2,58H.  AM RETURNING
     1 TO MAIN PROGRAM WITH THF = TH.  OPTION IS ,I2,1H.//)
      WRITE(KOUT,2994) (J,EMS(J),EMN(J), J=1,MM)
 2994 FORMAT(10X,15HI,EMS(I),EMN(I)//(1X,I2,2E12.3))
      THF=TH
      RETURN
 2992 CONTINUE
      DSN(I)=DS(I)*HA
      DSDTBN(I)=DSDTB(I)*HA
      CMD=DSDTB(I)*RO
      QCHEM=0.
      QCONV=0.
      QRA=0.
      RAD=0.
      CM=0.
      CMZ=0.
      SR=0.
      HW=0.
      HE=0.
```

```
      ITS=0
      GO TO 265
C-----OPTION 3 CALCULATIONS
 2990 TABC=90000.
      DSDTB(I)=0.
      DS(I)=0.
      DSDTBN(I)=0.
      DSN(I)=0.
      CMD=0.
      CM=0.
      CHZ=0.
      HW=0.
      GO TO (2995,2996,2996),KRESC
 2995 A=U(I)/(AC(K)*(1.+FACT*U(I))
      B=-A*(FACT*TB(K)+TA(K))
      GO TO 2997
 2996 A=U(I)/AC(K)*(1.+FACT*RB(K-1))/(1.+FACT*(U(I)+RB(K-1)))
      B=-A*(TA(K)+FACT*TB(K)/(1.+FACT*RB(K-1)))
 2997 CONTINUE
      ERFX=-B
      QCHEM=0.
      QCONV=0.
      VF=VF3(K)
      GO TO 240
C-----OPTION 1 PREPARATIONS
 3070 BF=CMDOT(I)/CH
      VF=VF1(K)
      CHZ=CH
      PHI=2.*BRP*BF
      IF(PHI-.01) 2071,2071,2072
 2071 CH=CH*(1.-.5*PHI)
      GO TO 2073
 2072 CH=CH/(EXP(PHI)-1.)*PHI
 2073 CM=CH*CMH
      GO TO (2076,2077,2077),KRESC
 2076 A=U(I)/(AC(K)*(1.+FACT*U(I))
      B=-A*(FACT*TB(K)+TA(K))
 2077 A=U(I)/AC(K)*(1.+FACT*RB(K-1))/(1.+FACT*(U(I)+RB(K-1)))
      B=-A*(TA(K)+FACT*TB(K)/(1.+FACT*RB(K-1)))
 2078 CONTINUE
      CMOL=BPSV(I)
      IAB=IABLS(I)
      ERFX=CH*HE-B
      IPR=KWE(K)
      ILO(12)=1
      IHI(12)=NMG(IPR)
      BPG=VKIN/CM
      CALL LOOK(12,BPG,TMG(1,IPR),0,0,0,0,Y2(1),Y2(2),1)
      IMG=IR(12)
      VRM=VR
      ILO(14)=NLO(IMG,IPR)
      IHI(14)=NHI(IMG,IPR)
      ILO(15)=NLO(IMG+1,IPR)
```

```
      IHI(15)=NHI(IMG+1,IPR)
      I1=ILO(14)
      I2=ILO(15)
      IF(IHI(14)-I1) 240,240,203
  203 IF(IHI(15)-I2) 240,240,204
  204 TARC=TTS(I1,IMG,IPR)+VRM*(TTS(I2,IMG+1,IPR)-TTS(I1,IMG,IPR))
      IF(TS(I)-TARC) 240,240,205
C-----ABLATING SURFACE
  205 IF(IAB) 206,206,207
  206 CMDL=TLMC(I1,IMG,IPR)-VRM*(TLMC(I1,IMG,IPR)-TLMC(I2,IMG+1,IPR))
      CMD=EXP(CMDL)*CM
      IAB=1
  207 CALL LOOK(14,CMDL,TLMC(1,IMG,IPR),TTS(1,IMG,IPR),
     1TCHEM(1,IMG,IPR),0.0,Y2(1),Y2(3),2)
      IRA=IR(14)
      CALL LOOK(15,CMDL,TLMC(1,IMG+1,IPR),TTS(1,IMG+1,IPR),
     1TCHEM(1,IMG+1,IPR),0.0,Y2(5),Y2(7),2)
      IRB=IR(15)
      DO 208 J=1,4
  208 Y2(J)=Y2(J)+VRM*(Y2(J+4)-Y2(J))
      ST=Y2(1)
      CALL LOOK(19,ST,TT(1,MT),EPT(1,MT),0.0,0.0,EMIV,DMIV,1)
      TSSQ=ST*ST
      RAD=SIG*EMIV*TSSQ*TSSQ*VF
      ERR=CH*Y2(2)+EMIV*QRA-RAD-A*ST+ERFX
C-----CONVECTION CORRECTION TO BE ADDED
      DERR=CH*Y2(4)+((QRA-RAD/EMIV)*DMIV-4./ST*RAD-A)*Y2(3)
      ERRC=ERR/DERR
      VITER(ITS)=CMDL
      EITER(ITS)=ERR
      CMDL=CMDL-ERRC
      IF(ILO(14)-IRA) 210,211,211
  210 IF(ILO(15)-IRB) 212,211,211
  212 CMMI=AMAX1(TLMC(IRA,IMG,IPR)+TLMC(IRA-1,IMG,IPR),
     1TLMC(IRB,IMG+1,IPR)+TLMC(IRB-1,IMG+1,IPR))/2.
      CMDL=AMAX1(CMDL,CMMI)
  211 IF(IHI(14)-IRA-1) 220,220,213
  213 IF(IHI(15)-IRB-1) 220,220,214
  214 CMMA=AMIN1(TLMC(IRA+1,IMG,IPR)+TLMC(IRA+2,IMG,IPR),
     1TLMC(IRB+1,IMG+1,IPR)+TLMC(IRB+2,IMG+1,IPR))/2.
      CMDL=AMIN1(CMDL,CMMA)
      IF(ITS-ITL-1) 220,215,216
  215 ERRS=ERR
      CMDL=CMMA
      GO TO 222
  216 IF(ERR*ERRS) 218,222,217
  217 CMDL=CMMA
      GO TO 222
  218 ITL=55
      IF(ERRC) 219,222,222
  219 CMDL=CMMI
      GO TO 222
  220 IF(ITS-ITL) 222,221,222
```

```
  221 CMDL=AMIN1(TLMC(I1,IMG,IPR),TLMC(I2,IMG+1,IPR))
  222 CMD=EXP(CMDL)*CM
      IF(ITS-50) 223,223,224
  223 ITS=ITS+1
      IF(ABS(ERR1-1.) 262,262, 207
  224 WRITE(6,225)(VITER(J),EITER(J),J=1,51)
  225 FORMAT(10X,37HSURFACE ENERGY BALANCE ITERATION STOP//12X,26HVARIAB
     1LE AND ERROR HISTORY//(15X,1PE14.3))
 2264 WRITE(6,226) TH,DTH,VRM,ERFX,HE,ST,TASC,EMIV,DMIV,
     1RAD,QRA,A,B,CH,CM,CMH,Y2(1),Y2(2),
     2Y2(3),Y2(4),ST,TS(I),IAB,I,K,I1,I2/55HILO(14
     3)=ILO(15),IHI(14),IHI(15),IRA,IRB,ITS,ITL,IMG,IPR
  226 FORMAT(//10X,105HTH,DTH,VRM,ERFX,HE,ST,TASC,EMIV,DMIV,RAD,QRA,A,B,
     1CH,CM,CMH,Y2(1),Y2(2),Y2(3),Y2(4),ST,TS(I),IAB,I,K,I1,I2/55HILO(14
     2)=ILO(15),IHI(14),IHI(15),IRA,IRB,ITS,ITL,IMG,IPR//10X,9E12.3/10X,
     39E12.3/10X,4E12.3,15I4/)
      WRITE(6,2262) VF,CHZ,BRP,PHI,FACT,U(I),AC(K),VRP,EMN(I),PLBS(I),
     1PLB(K),CAP(K),VOL(K),TB(K)
 2262 FORMAT(//10X,76HVF,CHZ,BRP,PHI,FACT,U(I),AC(K),VRP,EMN(I),PLBS(I),
     1PLB(K),CAP(K),VOL(K),TB(K)//10X,9E12.3/10X,5E12.3)
      L=K-MM
      IH=K+MM
      WRITE(6,2263) MATL(L),MATL(K),MATL(IH  ),MATL(K-1),RA(K),RB(K),RA(
     1L),RB(K-1),DST(I),DSTT(I),AA(K),AB(K),AD(K),AD(L),AA(IH  ),PLA(K),
     2PLD(K),PLC(K),PLC(L),PLB(K-1),PLA(IH  )
 2263 FORMAT(//10X,1H,1HMATL(L),MATL(K),MATL(K+MM),MATL(K-1),RA(K),RB(K),
     1RA(L),RB(K-1),DST(I),DSTT(I),AA(K),AB(K),AD(K),AD(L)/10X,55HAA(K+M
     2M),PLA(K),PLD(K),PLC(K),PLC(L),PLB(K-1),PLA(K+MM)//10X,4I5,7E12.3/
     310X,7E12.3/3.X,3E12.3//)
      IF(IAB) 2266,2266,2267
 2266 RETURN
 2267 CONTINUE
      L=0
      IR(19)=1
      IL=ILO(14)
      IH=IHI(14)
      DO 227 J=IL,IH
      L=L+1
      CALL LOOK(15,TLMC(J,IMG,IPR),TLMC(1,IMG+1,IPR),TTS(1,IMG+1,IPR),
     1TCHEM(1,IMG+1,IPR),0.0,0.0,Y2(1),Y2(3),2)
      Y2(1)=TTS(J,IMG,IPR)+VRM*(Y2(1)-TTS(J,IMG,IPR))
      Y2(2)=TCHEM(J,IMG,IPR)+VRM*(Y2(2)-TCHEM(J,IMG,IPR))
      ST=Y2(1)
      TSSQ=ST*ST
      CALL LOOK(19,ST,TT(1,MT),EPT(1,MT),0.0,0.0,EMIV,DMIV,1)
      RAD=SIG*EMIV*TSSQ*TSSQ*VF
      ERR=CH*Y2(2)+EMIV*QRA-RAD-A*ST+ERFX
      EITER(L)=ERR
  227 VITER(L)=TLMC(J,IMG,IPR)
      WRITE(6,228) IMG
  228 FORMAT(///10X,92HCOMPLETE SURFACE TABLE FOR ANALYSIS, COMPUTED USIN
     1G CURRENT VALUES OF CH,QRA,HE,A,P, AND VRM//12X,6HIMG = ,I2//)
      WRITE(6,229) (VITER(J),EITER(J),J=1,L)
```

```
  229 FORMAT(20X,8HLN ERROR,10X,24HENERGY BALANCE ERROR/41X,
     114H(BTU/SQFT-SEC)//(19X,E10.3,14X,E10.3))
      L=0
      IL=ILO(15)
      IH=IHI(15)
      DO 230 J=IL,IH
      L=L+1
      CALL LOOK(14,TLMC(J,IMG+1,IPR),TLMC(1,IMG,IPR),
     1TTS(1,IMG,IPR),TCHEM(1,IMG,IPR),0,0,Y2(1),Y2(3),2)
      Y2(1)=Y2(1)+(TTS(J,IMG+1,IPR)-Y2(1))*VRM
      Y2(2)=Y2(2)+(TCHEM(J,IMG+1,IPR)-Y2(2))*VRM
      ST=Y2(1)
      TSSQ=ST*ST
      RAD=SIG*EMIV*TSSQ*TSSQ*VF
      CALL LOOK(19,ST,TT(1,MT),EPT(1,MT),0,0,0,EMIV,DMIV,1)
      ERR=CH*Y2(2)+EMIV*QRA-RAD-A*ST+ERFX
      EITER(L)=ERR
  230 VITER(L)=TLMC(J,IMG,IPR)
      IMG=IMG+1
      WRITE(6,231) IMG
  231 FORMAT(/12X,6HIMG = ,I2//)
      WRITE(6,229) (VITER(J),EITER(J),J=1,L)
      THF=TH
      RETURN
C-----NON-ABLATING SURFACE
C
  240 IAB=0
      CMD=0.
      IF(KOOP-3) 2400,2491,2491
 2400 ILO(16)=1
      IHI(16)=KHI(IMG,IPR)
      ILO(17)=1
      IHI(17)=KHI(IMG+1,IPR)
      ST=TS(1)
  249 CALL LOOK(16,ST,TTS(1,IMG,IPR),TCHEM(1,IMG,IPR),0,0,0,
     1Y2(1),Y2(2),1)
      CALL LOOK(17,ST,TTS(1,IMG+1,IPR),TCHEM(1,IMG+1,IPR),
     10,0,0,Y2(3),Y2(4),1)
      DO 241 J=1,2
  241 Y2(J)=Y2(J)+VRM*(Y2(J+2)-Y2(J))
 2491 CONTINUE
      TSSQ=ST*ST
 2401 CALL LOOK(19,ST,TT(1,MT),EPT(1,MT),0,0,0,EMIV,DMIV,1)
      RAD=SIG*EMIV*TSSQ*TSSQ*VF
      ERR=CH*Y2(1)+EMIV*QRA-RAD-A*ST+ERFX
      DERR=CH*Y2(2)+ (QRA-RAD/EMIV)*DMIV-4./ST*RAD-A
      ERRC=ERR/DERR
      VITER(ITS)=ST
      EITER(ITS)=ERR
      ST=ST-ERRC
      IRA=IR(16)
      IRB=IR(17)
      IF(ILO(16)-IRA) 242,244,244
```

```
  242 IF(ILO(17)-IRB) 243,244,244
  243 TSMI=AMAX1(TTS(IRB,IMG+1,IPR)+TTS(IRB-1,IMG+1,IPR),
     1TTS(IRA,IMG,IPR)+TTS(IRA-1,IMG,IPR))/2.
      ST=AMAX1(ST,TSMI)
  244 IF(IHI(16)-IRA-1) 247,247,245
  245 IF(IHI(17)-IRB-1) 247,247,246
  246 TSMA=AMIN1(TTS(IRB+1,IMG+1,IPR)+TTS(IRB+2,IMG+1,IPR),
     1TTS(IRA+1,IMG,IPR)+TTS(IRA+2,IMG,IPR))/2.
      ST=AMIN1(ST,TSMA)
  247 IF(ITS-50) 248,248,250
  248 ITS=ITS+1
      IF(ABS(ERR)-1.) 260,260, 249
  250 WRITE(6,225)(VITER(J),EITER(J),J=1,51)
      WRITE(6,251) TH,DTH,VRM,ERFX,HE,ST,TABC,EMIV,DMIV,
     1RAD,QRA,A,B,CH,CM,CMH,Y2(1),Y2(2),
     2Y2(3),Y2(4),TS(I),DSDT(I),DSDTB(I),
     3CMD,PLB(K),PLBS(I),I,K,IPR,IMG,
     4ILO(16),IHI(16),ILO(17),IHI(17),IR(16),
     5IR(17),IRA,IRB,ITS,ITL,MT
  251 FORMAT(10X,10HTH,DTH,VRM,ERFX,HE,ST,TABC,EMIV,DMIV,RAD,QRA,A,B,CH
     1,CM,CMH,Y2(1),Y2(2),Y2(3),Y2(4),TS(I),DSDT(I),DSDTB(I)/10X,9HCMD
     2,PLB(K),PLBS(I),I,K,IPR,IMG,ILO(16),IHI(16),ILO(17),IHI(17),IR(16)
     3,IR(17),IRA,IRB,ITS,ITL,MT//10X,9E12.3/10X,8E12.3/10X,8E12.3/15I3/
     4)
      L=0
      IL=ILO(16)
      IH=IHI(16)
      DO 252 J=IL,IH
      L=L+1
      CALL LOOK(17,TTS(J,IMG,IPR),TTS(1,IMG+1,IPR),TCHEM(1,IMG+1,IPR),0.
     1,0.,Y2(3),Y2(4),1)
      Y2(1)=TCHEM(J,IMG,IPR)+VRM*(Y2(3)-TCHEM(J,IMG,IPR))
      ST=TTS(J,IMG,IPR)
      CALL LOOK(19,ST,TT(1,MT),EPT(1,MT),0.,0.,0.,EMIV,DMIV,1)
      ISSQ=ST*ST
      RAD=SIG*EMIV*TSSQ*TSSQ*VF
      ERR=CH*Y2(1)+EMIV*QRA-RAD-A*ST+ERFX
      EITER(L)=ERR
  252 VITER(L)=ST
      WRITE(6,228) IMG
      WRITE(6,253) (VITER(J),EITER(J),J=1,L)
  253 FORMAT(20X,9HSURF TEMP,10X,20HENERGY BALANCE ERROR/
     121X,7H(DEG R),14X,14H(BTU/SQFT-SEC)//(19X,E10.3,15X,E10.3))
      L=0
      IL=ILO(17)
      IH=IHI(17)
      DO 254 J=IL,IH
      L=L+1
      CALL LOOK(16,TTS(J,IMG+1,IPR),TTS(1,IMG,IPR),TCHEM(1,IMG,IPR),
     10.,0.,Y2(3),Y2(4),1)
      Y2(1)=Y2(3)+VRM*(TCHEM(J,IMG+1,IPR)-Y2(3))
      ST=TTS(J,IMG+1,IPR)
      CALL LOOK(19,ST,TT(1,MT),EPT(1,MT),0.,0.,0.,EMIV,DMIV,1)
```

```
      TSSQ=ST*ST
      RAD=SIG*EMIV*TSSQ*TSSQ*VF
      ERR=CH*Y2(1)+EMIV*QRA-RAD-A*ST+ERFX
      EITER(L)=ERR
  254 VITER(L)=ST
      IMG=IMG+1
      WRITE(6,231) IMG
      WRITE(6,253) (VITER(J),EITER(J),J=1,L)
      THF=TH
      GO TO 2264
C-----POST ITERATION
C
  260 IF(KOOP-2) 261,261,2650
  261 Y2(2)=Y2(1)
  262 QCHEM=Y2(2)
      IF(ISEN(1)) 263,264,263
  264 QCONV=0.
      GO TO 266
  263 CALL OGLE(1,ST,QCONV,ISEN(IPR),TTSEN(1,IPR),THSEN(1,IPR),
     1TCPSEN(1,IPR))
  266 QCHEM=(QCHEM+QCONV)*CH
      HW=QCONV
      QCONV=CH*(HE-QCONV)
      DSDTBN(I)=CMD/RO
      HA=VCOS(K,I,MM,CR,CZ,SZ,SR,EMN,PL5,PL55,DST)
      IF(HA-.1) 2991,2991,2660
 2660 CONTINUE
      BPSV(I)=CMDL
      DSDTB(I)=DSDTBN(I)/HA
      DS(I)=DSDTB(I)*DTH
      DSN(I)=DS(I)*HA
 2650 TS(I)=ST
  265 GO TO (2651,2652,2652),KREFC
 2651 TB(K)=(FACT*(TB(K)+U(I)*TS(I))+TA(K))/(1.+FACT*U(I))
      GO TO 267
 2652 TB(K)=(FACT*(TB(K)+U(I)*ST)+(1.+FACT*RB(K-1))*TA(K))/(1.+FACT*
     1(U(I)+RB(K-1)))
  267 PL8(K)=PL5(K)-DS(I)
      QN=(TS(I)-TB(K))*U(I)
      QCONDT(I)=QCONDT(I)+QN*DTH
      QSUM=QSUM+QN
      QNP(K)=QN/AC(K)
      QCNV(I)=QCONV
      QCNVT(I)=QCONV*AC(K)*DTH+QCNVT(I)
      QCHM(I)=QCHEM
      QCHMT(I)=QCHMT(I)+QCHEM*DTH*AC(K)
      QRP=EMIV*QRA
      QRAB(I)=QRP
      QRABT(I)=QRABT(I)+QRP*DTH*AC(K)
      QRAD(I)=RAD
      QRADT(I)=QRADT(I)+RAD*DTH*AC(K)
      CMDOT(I)=CMD
      HEDG(I)=HE
```

```
      CMT(I)=CMT(I)+CMD*AC(K)*DTH
      I1(I)=KOOP
      ITSR(I)=ITS
      IABLS(I)=IAB
      HWL(I)=HW
      G(I)=CM
      GZ(I)=CHZ*CMH
      PR(I)=EXP(PRES)
C-----NODE DROPPING PACKAGE
      IF(PLB(K)) 1,,10,11
   10 IF(K-(I-1)*MM-1) 13,13,12
   12 IF(MATL(K-1)) 15,15,1200
 1200 IF(MATL(K-1)-MT) 13,14,13
   14 DS(I)=PLB(K)+DS(I)
      DSTT(I)=DSTT(I)+PLBS(I)-DST(I)
      PLB(K)=0.0
      MATL(K)=0
      MATL(K-1)=-MATL(K-1)
      KSUR(I)=K-1
      KDROP(I)=1
      CAP(K)=0.
      KSH(K)=0
      KSH(K-1)=1
      PLBS(I)=PLB(K-1)
      DST(I)=0.0
      QNP(K-1)=QNP(K)
      GO TO (1200,1200,1201),KRESC
 1201 TB(K-1)=(TB(K-1)+RB(K-1)*(TB(K)-TA(K)))*DTH/CAP(K-1)+TA(K-1)
      GO TO 1202
 1200 TB(K-1)=TB(K-1)*DTH/CAP(K-1)+TA(K-1)
 1202 CONTINUE
      GO TO 7
   13 WRITE(6,16) I,K
   16 FORMAT (//10X,23HRUN THROUGH IN COLUMN ,I3,9H AT NODE ,I3//)
      THF=TH
      GO TO 17
   15 WRITE(6,18) I,K
   18 FORMAT(//10X,35HIMPROPER NODAL NUMBERING IN COLUMN ,I3,9H AT NODE
     1,I3//)
      THF=TH
      GO TO 17
   11 KDROP(I)=0
      IF((PLBS(I)-PLB(K)-DST(I))/PLBS(I)-.001) 7,7,1100
 1100 HA=PLBS(I)-PLB(K)-DST(I)
      DST(I)=DST(I)+HA
      DSTT(I)=DSTT(I)+HA
C-----NEW AREAS AND NEW VOLUME
      RAT=1.-DST(I)/PLBS(I)
      J=K+I-1
      CRL=CR(J)+RAT*(CR(J+1)-CR(J))
      CZL=CZ(J)+RAT*(CZ(J+1)-CZ(J))
      HA=CRL-CR(J)
      HB=CZL-CZ(J)
```

```
      HC=HA*HA+HB*HB
      HD=SQRT(HC)
      HE=PIB*HD*(CR(J)+CRL)
      AA(K)=HE
      L=J+MM+1
      CRR=CR(L)+RAT*(CR(L+1)-CR(L))
      CZR=CZ(L)+RAT*(CZ(L+1)-CZ(L))
      HA=CRR-CR(L)
      HB=CZR-CZ(L)
      HC=HA*HA+HB*HB
      HD=SQRT(HC)
      HF=PIB*HD*(CRR+CR(L))
      AD(K)=HE
      HA=CRR-CRL
      HB=CZR-CZL
      HC=HA*HA+HB*HB
      HD=SQRT(HC)
      AC(K)=PIB*HD*(CRR+CRL)
      HA=CR(J)*CR(J)
      HB=CR(J)*CRL
      HC=CR(J)*CR(L)
      HD=CRL*CRL
      HE=CRL*CRR
      HF=CR(L)*CR(L)
      HG=CR(L)*CRR
      HH=CRR*CRR
      HS=ZRO
      HS=HS+CZ(J)*(HC-HB+HF-HD)
      HS=HS+CZ(L)*(HG-HC+HB-HA)
      HS=HS+CZL*(HB-HE+HA-HH)
      HS=HS+CZR*(HE-HG+HC-HF)
      VOL(K)=6.J6171E-04*ABS(HS)
      SR(I)=(CRL+CRR)/2.
      SZ(I)=(CZL+CZR)/2.
    7 CONTINUE
      QNTS=QNTS+QSUM*DTH
   17 RETURN
      END
```

```
      SUBROUTINE ORDERD (NX,X1,I1)
      DIMENSION X1(1),I1(1)
      DIMENSION LS(20)
      NM=IABS(NX)
      LS(1)=1
      LS(2)=1
      LS(3)=2
      LI=3
      I1(1)=1
      DO 1 N=2,NM
      I1(N)=N
      L=LS(LI)
      LA=LI
      J=N
      X1C=X1(J)
      I1C=I1(J)
      J=J-L
      IF(J) 31,31,34
   34 LI=LI+1
      LS(LI)=L+L
      GO TO 29
   33 LA=LA-1
      L=LS(LA)
      IF(L) 3,3,41
   41 J=J-L
   32 IF(J) 31,31,29
   31 LA=LA-1
      L=LS(LA)
      J=J+L
      IF(L) 4,4,32
   30 LA=LA-1
      L=LS(LA)
      IF(L) 4,4,42
   42 J=J+L
   29 IF(NX) 229,129,129
  229 IF(X1C-X1(J)) 30,53,33
  129 IF(X1(J)-X1C) 30,53,33
   53 J=1
      GO TO 3
    4 J=J+1
    3 M=N-1
      MM=M
      DO 2 K=J,MM
      X1(M+1)=X1(M)
      I1(M+1)=I1(M)
    2 M=M-1
      I1(J)=I1C
    1 X1(J)=X1C
      RETURN
      END
      SUBROUTINE SEQUA(N,L,A,B,C,D)
      DIMENSION A(1),B(1),C(1),D(1),L(1)
      IS=J
```

```
      IF (N-1) 2030,1030,1030
 1030 DO 30 II=1,N
      I=II
   21 J=L(I)
      L(I)=I
      IF(J-1) 22,30,22
   22 IF(IS) 25,23,25
   23 SA=A(I)
      SB=B(I)
      SC=C(I)
      SD=D(I)
      IS=I
   26 A(I)=A(J)
      B(I)=B(J)
      C(I)=C(J)
      D(I)=D(J)
      I=J
      GO TO 21
   25 IF(IS-J) 26,28,26
   28 IS=0
      A(I)=SA
      B(I)=SB
      C(I)=SC
      D(I)=SD
   30 CONTINUE
 2030 CONTINUE
      RETURN
      END
      SUBROUTINE LOOK(II,XL,X,A,B,C,E,Y,D,IDN)                    CMA 1001
      COMMON/LK/KOUT,IEX,DEN,VR,IHI(40),ILO(40),IR(40)
      DIMENSION  X(1),Y(1),D(1)
      DIMENSION A(1),B(1),C(1),E(1)
      IH=IHI(II)                                                  CMA 1004
      IL=ILO(II)                                                  CMA 1005
      IEX=0
      IF(X(IH)-X(IL)) 30,30,29
   30 IEX=1
      IF (XL-X(IH)) 3,2,31
   31 IF (XL-X(IL)) 6,5,4
   29 IF(XL-X(IH))1,2,3                                           CMA 1006
    1 IF(XL-X(IL))4,5,6                                           CMA 1007
    6 I=IR(II)                                                    CMA 1008
      I=MIN0(I,IH)
      I=MAX0(I,IL)
      IS=1                                                        CMA 1009
      IT=1                                                        CMA 1010
      GO TO 8                                                     CMA 1011
   11 I=I+1                                                       CMA 1012
      IS=0                                                        CMA 1013
    8 IF(IEX) 28,28,38
   28 IF(XL-X(I)) 7,10,9                                          CMA 1014
   38 IF(XL-X(I)) 9,10,7
    7 I=I-1                                                       CMA 1015
```

```
      IT=J                                                          CMA 1016
      IF(IS)10,10,8                                                 CMA 1017
    9 IF(IT)10,10,11                                                CMA 1018
    3 IEX=3                                                         CMA 1019
    2 I=IH-1                                                        CMA 1020
      GO TO 10                                                      CMA 1021
    4 IEX=2                                                         CMA 1022
    5 I=IL                                                          CMA 1023
   10 DEN=X(I+1)-X(I)                                               CMA 1024
      IR(II)=I                                                      CMA 1025
      VR=XL-X(I)
      IF(IDN) 13,13,14                                              CMA 1027
   14 GO TO (21,22,23,24),IDN
   24 Y(4)=E(I)
      D(4)=E(I+1)-E(I)
   23 Y(3)=C(I)
      D(3)=C(I+1)-C(I)
   22 Y(2)=B(I)
      D(2)=B(I+1)-B(I)
   21 Y(1)=A(I)
      D(1)=A(I+1)-A(I)                                              CMA 102
      DO 12  J=1,IDN
   20 D(J)=D(J)/DEN
   12 Y(J)=Y(J)+D(J)*VR
   13 VR=VR/DEN
      CALL SSWTCH(2,JJ)
      GO TO (200,2-1),JJ
  200 IF (IDN-2) 2-2,2-2,204
  204 IF(II-1) 201,202,201
  202 WRITE (KOUT,2-3) II,IL,IH,XL,IR(II),VR,DEN,IEX,IDN
  203 FORMAT (3(2X,I2),2X,E1-.3,2X,I2,F1-.4,2X,E1-.3,2(2X,I2))
      IF (IDN-1) 2-25,1025,1025
 1025 WRITE(KOUT,205)(Y(K),D(K),K=1,IDN)
  205 FORMAT(4(2X,E1-.3))
 2025 CONTINUE
  201 CONTINUE
      RETURN                                                        CMA 1035
      END
      SUBROUTINE SLOPQ(NUMX,X,P,EM)                                 01M
C     SLOPE EVALUATION ROUTINE
C
      DIMENSION X(1), P(1), EM(1), Z(1)                             02M
   30 EM(2) = ( P(2) - P(1) ) / ( X(2) - X(1) )                     02Q
      EM(1) = EM(2)
      Z(1)=0.0                                                      025
      QC = EM(1)                                                    02U
      DO 36 I = 1 , NUMX                                            02W
      IPO = I + 1                                                   02Y
      IPT = I + 2                                                   03A
      IT = IPO - NUMX                                               03C
      IF (IT) 33 , 31 , 32
   31 QB=QC
      GO TO 41
```

```
   32 GO TO 40                                                          035
   33 XOT = X(I) - X(IPO)                                               03S
      XTT = X(IPO) - X(IPT)                                             03W
      XTO = X(IPT) - X(I)                                               03Y
      AA = P(I) / ( XOT * XTO )
      XOTT=XOT*XTT
   37 AB=P(I+1)/XOTT
      AC = P(IPT) / ( XTT * XTO )                                       04C
      AAA = AA * XTT                                                    04E
      ABB = AB * XTO                                                    04G
      ACC = AC * XOT                                                    04I
      QA = QC                                                           04K
      QB = EM(I)                                                        04M
      QC = EM (IPO)                                                     04O
      EM(IPO) = AA * (XOT - XTT) + ACC - AAA                            04Q
      EM(IPT) = AC * (XTT - XTO) + AAA - ABB                            04U
      EM(I)=   AA * (XTO - XOT) + ABB - ACC                             04Y
   34 QE = EM(I)
      IF(I-2) 36,41,35
   35 EM(I) = ( QE + QA ) /2.
   41 EM(I) = (EM(I) + QB ) /2.
   40 XD=X(I)-X(I-1)
   36 CONTINUE
      RETURN
      END
      SUBROUTINE OGLE(N,XAM,PRM,NUMX,X,P,EM)
      DIMENSION XAM(1),X(1),P(1),EM(1),PRM(1),DPDIM(1)
      XDIF=X(NUMX)-X(1)
      IS=1
    2 DO 600 J=1,N
      XA=XAM(J)
   59 IO=1
      IT=1
   61 IF(XDIF) 72,60,71
   71 IF(XA-X(IS)) 62,63,64
   72 IF(X(IS)-XA) 62,63,64
   62 IF(IS-1)671,671,68
   68 IS=IS-1
      IT=2
      GO TO (61,66),IO
  672 IS=NUMX
  671 I=IS
      H=0.
      DPDI=EM(I)
      GO TO 67
   63 PR=P(IS)
      DPDI=EM(IS)
      GO TO 601
   64 IS=IS+1
      IF(IS-NUMX)69,69 ,672
   69 IO=2
      GO TO (61,65),IT
   65 IS=IS-1
```

```
   66 I=IS
      G=(((PLI+1)-P(I))/(X(I+1)-X(I)))-EM(I))/(X(I+1)-X(I))
      F=(((EM(I+1)-EM(I))/(X(I+1)-X(I)))-2.*G)/(X(I+1)-X(I))
      H=(F*(XA-X(I+1))+G)*(XA-X(I))
      DPDI=(H+H+EM(I))*(XA-X(I))*(XA-X(I))
   67 PR=(H+EM(I))*(XA-X(I))+P(I)
  601 CONTINUE
      PRM(J1=PR
  600 CONTINUE
   60 CONTINUE
    4 RETURN
      END
      SUBROUTINE SLOPL(M,N,X,Y,EMS,EMN)
      COMMON CR(402),CZ(402),AA(402),AB(402),AC(402),AD(402)
C-----DIMENSIONED AS NODES
      COMMON MATL(200),KTH(200),KSH(200),KWE(200),KTU(200),CON(200),
     1IA(200),IB(200),CRA(200),CRB(200),PLA(200),PLB(200),PLC(200),
     2PLD(200),VOL(200),RA(200),RB(200),CAP(200),ENT(200),QNP(200),
     3VF1(200),VF3(200)
C-----DIMENSIONED AS SURFACE NODES (NUMBER OF COLUMNS)
      COMMON KSUR(40),TS(40),DSDT(40),DSDTB(40),DS(40),DST(40),U(40)
      COMMON PLBS(40)
      DIMENSION X(1),Y(1),EMS(1),EMN(1)
      IF(N-1) 100,100,101
  100 J=M
      RAT=1.-DST(1)/PLBS(1)
      CRL=CR(J)+RAT*(CR(J+1)-CR(J))
      CZL=CZ(J)+RAT*(CZ(J+1)-CZ(J))
      L=J+M+1
      CRR=CR(L)+RAT*(CR(L+1)-CR(L))
      CZR=CZ(L)+RAT*(CZ(L+1)-CZ(L))
      DZ=CZR-CZL
      DR=CRR-CRL
      IF(DZ) 151,150,151
  150 S1=1.E+30
      GO TO 152
  151 IF(DR) 153,154,153
  154 S1=1.E-30
      GO TO 152
  153 S1=DR/DZ
  152 S2=-1./S1
      EMS(1)=S1
      EMN(1)=S2
      RETURN
  101 S1=0.
      S2=0.
      NS=0
      DXS=X(2)-X(1)
      K=N-1
      DO 200 I=1,K
      DX=X(I+1)-X(I)
      DY=Y(I+1)-Y(I)
      IF(DX) 302,300,302
```

```
      IF(DY) 301,320,301
  320 NS=NS+1
      GO TO 200
  301 S2=2.E+30/ABS(DY)*DY
      GO TO 303
  302 S2=DY/DX
      IF(DX*DXS) 304,305,303
  304 IF(S1+S2) 307,306,307
  306 EMS(I)=1.0E+30
      GO TO 305
  307 EMS(I)=2.*S1*S2/(S1+S2)
      GO TO 305
  303 EMS(I)=(S1+S2)/2.
  305 DXS=DX
      IF(NS) 200,200,321
  321 LL=I-NS
      LU=I-1
      NS=0
      DO 323 J=LL,LU
  323 EMS(J)=EMS(I)
  200 S1=S2
      EMS(1)=2.*EMS(1)
      EMS(N)=S2
      DO 310 I=1,N
      IF(EMS(I)) 311,312,311
  312 EMN(I)=1.0E+30
      GO TO 310
  311 EMN(I)=-1./EMS(I)
  310 CONTINUE
      RETURN
  500 FORMAT(2I5)
      END
      SUBROUTINE LCOUNT (I,LCT,NPG,R)
C-----PHILCO/ASTHMA VERSION
      COMMON/LK/KOUT,IEX,DEN,VR,IHI(40),ILO(40),IR(40)
      DIMENSION R(2)
  551 FORMAT(1H1,25X,71HAEROTHERM AXI-SYMMETRIC TRANSIENT HEATING AND MA
     1TERIAL ABLATION PROGRAM/113X,4HPAGE,I3/106X,2A6)
  552 FORMAT(1H1,25X,71HAEROTHERM AXI-SYMMETRIC TRANSIENT HEATING AND MA
     1TERIAL ABLATION PROGRAM/111X6HPAGES ,I3/109X,8HTHROUGH ,I3/108X,
     22A6)
      IJK=I
      IF (IJK) 2,2,3
    2 IJK=-IJK
      GO TO 4
    3 LCT=LCT-IJK
      IF (LCT) 4,5,5
    4 NPG=NPG+1
      LCT=55-IJK
      IF(LCT) 6,7,7
    6 NEX=(IJK-1)/55
      LCT=(NEX+1)*55-IJK
      N=NPG
```

```
      NPG=NPG+NEX
      WRITE(KOUT,552) N,NPG,R
      GO TO 5
    7 CONTINUE
      WRITE (KOUT,551) NPG,R
    5 RETURN
      END
      FUNCTION VCOS(K,I,MM,CR,CZ,SZ,SR,EMN,PLB,PLBS,DST)
C-----SPECIAL ANDERSON/SCHAEFER/ARC RESTRICTED VERSION
      DIMENSION CR(1),CZ(1),SZ(1),SR(1),EMN(1),PLB(1)
      DIMENSION PLBS(1),DST(1)
      J=K+I-1
      L=J+MM+1
      R1=(CR(J)+CR(L))/2.
      Z1=(CZ(J)+CZ(L))/2.
      DZ=SZ(I)-Z1+1.E-30
      DIST=PLBS(I)-DST(I)
      EMNA=ABS(EMN(I))
      VCOS=DZ/(DIST  *SQRT(1.+EMNA**2))*(EMN(I)/EMNA+(SR(I)-R1)/DZ*EMNA)
     1/12.0
      VCOS=ABS(VCOS)
      RETURN
      END
```

APPENDIX E

ARCACE COMPUTER PROGRAM USER'S MANUAL

MITCHELL R. WOOL

ROBERT M. KENDALL

CARD SET 1 - CONTROL CARD (1 CARD)

Field 1 (Columns 1-10, 10I1) Control Variable, KR(10).
KR is used to control the various program options.

Column 1 - State Option

0	Assigned temperature
1	Surface equilibrium with kinetics at assigned temperature
2	Assigned enthalpy
3	Constant entropy expansion from previous chamber calculation
8	Stop

Column 2 - Elemental Composition

0	Accept resident values (same as input to a previous solution)
≥1	Input new elemental composition data for the system components (see card set 2)

Column 3 - Molecular Data

0	Accept resident values for molecular data
1,2,3,4	Read from cards JANAF data (card set 3)
3,4	Store all molecular data read from cards on tape
5,6	Read all molecular data from tape as last stored
2, 4, 6	Output JANAF data for selected set of molecules

Column 4 - Unused

Column 5 - Unused

Column 6 - Unused

Column 7 - Diagnostic Control

0	No diagnostic output
1	Single line of diagnostics per iteration
j(>1)	For 5(j-1) iterations full diagnostics will be output and for subsequent iterations the single line will be output

Column 8 - Unused

Column 9 - Kinetics Input Option, If KR(1) = 1, (Col. 1)

0	Use previously input kinetic reaction data
1	Input kinetic reaction data (see card set 4)

Column 10 - Card Output Option

0	No card output
1	Output single card per convergent solution of data appropriate to ASTHMA input

Field 2 (Columns 11-20, F10.5) State Variable, Z.

For non-zero Z, Z is assigned to T (temperature, $^{\circ}K$) for KR(1) of 0 or 1, to HIP (enthalpy, cal/gm) for KR(1) of 2, and to SIP (entropy, cal/gm $^{\circ}K$) for KR(1) of 3.

A negative temperature entry results in a frozen composition of the system (as previously obtained) and the calculation of properties of this system at the absolute value of the assigned temperature.

If Z is zero resident values of temperature, enthalpy or entropy will be used in the solution specification consistent with the KR(1) assignment.

Field 3 (Columns 21-30, F10.5) Pressure Variable, PR.

For non-zero PR, PR is assigned as system pressure, P (atmospheres). For zero PR, P is unaltered (=1. before first solution).

Field 4 (Columns 71-80, 2A4,A2) Job Name, TILE(3)

This will appear on printed and punched output.

CARD SET 2 - ELEMENTAL COMPOSITION DATA (IS+1 CARDS)

Card 1

Field 1 (Columns 1-3, I3) Number of Elements in the System, IS

Cards 2,3,.., IS+1. One Card for Each Element

Field 1 (Columns 1-3, I3) Atomic Number of an Element, KAT(99 is not allowable).

Field 2 (Columns 4-15, 3A4) Name of Element (in three parts), ATA, ATB and ATC.

For output identification only.

Field 3 (Columns 16-25, F10.5) Atomic Weight of Element, WAT.

Field 4 (Columns 26-55, 3F10.5) Relative Elemental Composition, TK

Relative amounts of element in components 1, 2 and 3 (edge gas, pyrolysis gas and char, respectively for surface mass balances). Positive values are in relative gram-atomic-weights (or moles) and negative values are in relative gram-mass units. For example, consider component 2 containing 50. mass percent of C and 50. mass percent of SiO_2 or equivalently 60.06 grams of C for each 60.06 grams of SiO_2 (1 mole of SiO_2) or

finally 60.06 gm of carbon for each 1. gram-atomic-weight of Si and 2 gram-atomic-weights of O. For this example it would be most convenient to input in columns 36-45 of the cards for C,O and Si: - 60.06, 2., and 1., respectively.

CARD SET 3 - THERMOCHEMICAL EQUILIBRIUM DATA (3 CARDS PER SPECIES)

Cards 1,4,7, etc. One for each species, whether molecular, atomic, or condensed. This card describes the element composition of the species and establishes its name designation.

Fields 1,3,5, ...,13 (Columns 1-3, 7-9, 13-15, ..., 37-39, each F3.0) Number of Atoms, ALPT

Fields 2,4,6, ...,14 (Columns 4-6, 10-12, 16-18, ..., 40-42, each I3) Atomic Number, JAT

The field sets, 1-2, 3-4, 5-6, ..., 13-14, represent the number of atoms, ALPT, of atomic number, JAT, contained in this species. One field set for each element of the species. For example, NO_2 is described in fields 1 through 4 as bb1bb7bb2bb8; that is, one atom of Nitrogen (atomic number 7) and two atoms of Oxygen (atomic number 8).

If field 1 is zero this card is presumed to represent the end of the card set.

Field 15 (Columns 43-72, 7A4A2) Thermochemical Data Source Identification, SØRCE.

Used for output only.

Field 16 (Columns 73-80, 2A4) Species Name Designation, AMØA and AMØB.

This variable is used for output.

Cards 2,5,8,... One for Each Species

Field 1 (Columns 1-9, E9.6) Heat of Formation, RA.

Species heat of formation at 298°K from JANAF base state (elements in natural form at 290°K), cal/mol.

Fields 2,3,4, 5, and 6 (Columns 10-54, 5E9.6) Curve Fit Constants, RB, RC, RD, RE and RF.

Constants appropriate to lower temperature range of thermodynamic data. The thermochemical curve fits are as follows with T in °K.

Heat Capacity

$$C_p = R_C + R_D T + R_E/T^2 \quad , \quad \text{cal/mol °K}$$

Enthalpy

$$h - h_{298°K} = R_B + \left[R_C T + \frac{1}{2} R_D T^2 - R_E/T\right]_{3,000°K}^{T} \quad , \text{ cal/mol}$$

Entropy

$$S = R_F + \left[R_C \ln T + R_D T - \frac{1}{2} R_E/T^2\right]_{3,000°K}^{T} \quad , \quad \text{cal/mol °K}$$

Field 7 (Columns 61-66, F6.0) Upper Limit of Lower Temperature Range, TU in °K

Field 8 (Columns o7, I1) Phase Specification for Lower Temperature Range, KPHA.

KPHA equals 1, 2 or 3 for gas, solid or liquid, respectively.

Cards 3,6,9 ... One for Each Molecule. Same as cards 2,5,8 ..., except for upper temperature range of thermochemical data.

The arrangement of these three card sets is, mathematically, unimportant for equilibrium solutions. In fact, if no condensed phase species exist within the system, the convergence path should be identical. Numerically this is not always true. A single species can dominate more than one mass equation and singular arrays may result. Such a situation can be avoided by placing these dominant species at the front of the thermochemical data deck.

The program automatically selects as base species the first set of species satisfying the requirement that 1) all other species may be formed from this base species set and 2) that no balanced reaction can be written

involving only base species. One base species may be considered to represent each element. In the numerics of the program, the base species actually become the "elements" of the mass balances. The means of establishing whether one species may be formed from another are the specifications given in fields 1 to 14 of cards 1,4,7,..., etc. of card set 3. Any reaction which can occur based on these specifications will be considered equilibrated in the system under study. To suppress equilibrium, it is thus required to change names (i.e., atomic numbers) of certain elements and to introduce new "elements."

The last card of this set is blank and serves as the data sentinel for card set 3. Three card data sets have been generated at Aerotherm for over 500 species mostly based on the JANAF thermochemical data. The data format of these cards is the same as that described in NAVWEPS Report 7043.

CARD SET 4 - REACTION RATE INFORMATION

Card 1

Field 1 (Column 1-3, I3) Number of Kinetically Controlled Reactions to be Considered, MT.

Defines the number of 3 card subsets containing reaction rate data, reactant coefficients, and product coefficients, respectively; one subset for each reaction.

Cards 2,5,8,... Forward Rate Data

Field 1 (Columns 1-10, E10.4) Pre-exponential Factor Divided by $\rho_e u_e C_M$, FKF.

The units of the input parameter, FKF, are mols of reaction per unit mass per unit driving potential (in atmosphere units).

Field 2 (Columns 11-20, E10.4) Activation Energy for the Forward Reaction, EAK, cal/gram.

Field 3 (Columns 21-30, E10.4) Reaction Exponent, EXK.

The driving potential as obtained from the reaction stoichiometry is raised to this power in evaluating the reaction rate.

Cards 3,6,9,... Reactant Coefficients

Fields 1,2,3,... (Columns 1-10, 11-20, 21-30, ..., 8E10.4) One for Each Base Species

The stoichiometric coefficients on the reactants. In the present formulation only base species may

be used as reactants. Thus some care must be used in establishing the order of card set 3 and thus fixing a priori the set of base species.

Cards 4,7,10,... Product Coefficients

Fields 1,2,3... (Columns 1-10, 11-20, 21-30, ..., 8E10.4) One for Each Base Species

The stoichiometric coefficients on the products or their equilibrium base species equivalents if they are not base species. For example, if the base species are CO, H_2O, H_2, C* for a system where C* is the only isolated (nonequilibrium) species a reaction written as

$$H_2 + 2C^* \rightarrow C_2H_2$$

could equivalently be written

$$H_2 + 2C^* \rightarrow 2CO + 3H_2 - 2H_2O$$

and this is the manner in which the product stoichiometric coefficients would be input.

APPENDIX F

ARCACE PROGRAM SAMPLE PROBLEMS

MITCHELL P. WOOL

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ISENTROPIC EXPANSION CALCULATION INPUT DECK

```
011   0 003901.      68.                                                    APG 1120
  6
  1 HYDROGEN     1.008     3.2219
  6 CARBON      12.011     0.5649
  7 NITROGEN    14.008     0.5366
  8 OXYGEN      16.000     2.2486
 13 ALUMINUM    26.970     1.0130
 17 CHLORINE    35.457     0.5369
  1  6  1  8  0  0  0  0  0  0  0  0  0  OJANAF 03/61                          CO
-264170+5 223570+5 865040+1 117021-3-898211+6 653700+2  500. 3000.1   0.CO
-264170+5 223570+5 115496+2-424139-3-131563+8 653700+2 3000. 5000.1   0.CO
  2  1  0  0  0  0  0  0  0  0  0  0  0  OJANAF 03/61                          H2
 000000-0 212100+5 711963+1 621950-3-71269+6 484650+2  500. 3000.1   0.H2
 000000-0 212100+5 681794+1 589854-3 265106+7 484650+2 3000. 5000.1   0.H2
  1  6  2  8        0  0  0  0  0  0  0  0  0  OJANAF 03/61                    CO2
-940540+5 365350+5 144559+2 210386-3-182392+7 798480+2  500. 3000.1   0.CO2
-940540+5 365350+5 156451+2-381561-4-602768+7 798480+2 3000. 5000.1   0.CO2
  2  1  1  8  0  0  0  0  0  0  0  0  0  OJANAF 03/61                          H2O
-577980+5 302010+5 112254+2 811397-3-260800+7 684210+2  500. 3000.1   0.H2O
-577980+5 302010+5 157278+2-191548-3-173599+8 684210+2 3000. 5000.1   0.H2O
  1  6     0  0  0  0  0  0  0  0  0  0  0  OJANAF 03/61                       C*
 000000-0 144120+5 586075+1 953976-4-766621+6 121290+2  500. 3000.2 100.C*
 000000-0 144120+5 485134+1 291605-3 307202+7 121290+2 3000. 5000.2 100.C*
  1 13  0  0  0  0  0  0  0  0  0  0  0  OJANAF 03/61                       AL*
 240000+4 189130+5 696390+1 125221-4 347759+5 251963+2  500. 3000.3  10.AL*
 240000+4 189130+5 744466+1-758263-4-210774+7 251963+2 3000. 5000.3  10.AL*
  1  8  1 13  1 17  0  0  0  0  0  0  0  OJANAF 03/64                    ALCLO*
-189599+6 520567+5 190512+2 572817-3-702975+6 550490+2  500. 1500.2   0.ALCLO*
-189599+6 514899+5 205116+2-165920-3-149571+7 548210+2 1500. 3000.2   0.ALCLO*
  1 13  3 17  0  0  0  0  0  0  0  0  0  OJANAF 03/64                    ALCL3*
-168579+6 101100+6 185370+2 114499-1-169000-1 100183+3  300.  460.2   0.ALCL3*
-160559+6 720036+5 274254+2-331897-3-164863+6 104630+3  460. 3000.3   0.ALCL3*
  1  7  1 13  0  0  0  0  0  0  0  0  0  OJANAF 12/62                       ALN*
-760000+5 312665+5 122768+2-178828-4-673685+6 299013+2  500. 2790.2 100.ALN*
-760000+5 314405+5 408674+2-915846-4-230400+9 299601+2 2790. 5000.2 100.ALN*
  1  4  4  8  2 13  0  0  0  0  0  0  0  OJANAF 09/64                 AL2BEO4*
-544999+6 126706+6 349699+2 797503-2-109209+7 112014+3  500. 2000.2   0.AL2BEO4*
-544999+6 126469+6 421930+2 570773-2-118459+8 111929+3 2000. 3000.2   0.AL2BEO4*
  3  8  2 13  0  0  0  0  0  0  0  0  0  OJANAF 09/61                    AL2O3*
-400400+6 811817+5 319699+2 120451-4-217514+7 772577+2  500. 2318.2 100.AL2O3*
-366770+6 759318+5 351153+2-192777-4-555942+6 893107+2 2318. 5000.3 100.AL2O3*
  1  4  0  0  0  0  0  0  0  0  0  0  0  OJANAF 09/61                       BE*
 C00000-0 193025+5 828125+1-288958-5-173046+7 170595+2  500. 1556.2 100.BE*
 288100+4 182708+5 769547+1-257476-5-213324+7 184265+2 1556. 5000.3 100.BE*
  1  4  2 17  0  0  0  0  0  0  0  0  0  OJANAF 06/65                    BECL2*
-118599+6 625645+5 160605+2 445380-2-220604+6 659883+2  300.  682.2   0.BECL2*
-117399+6 763159+5 290199+2       0+0 686422-2 804288+2  682. 2000.3   0.BECL2*
  1  4  2  9  0  0  0  0  0  0  0  0  0  OJANAF 12/63                    BEF2*
-241957+6 546211+5 207446+2-139307-4 558937+6 583302+2  500. 2000.2  10.BEF2*
-241957+6 548613+5 210844+2 256246-5-533447+6 584292+2 2000. 5000.2  10.BEF2*
  1  4  1  8  0  0  0  0  0  0  0  0  0  OJANAF 09/63                       BEO*
-143100+6 337038+5 160771+2-434631-3-593740+7 291887+2  500. 2820.2  10.BEO*
```

SPECIES SET TO BE USED FOR EXPANSION OR EQUILIBRIUM CALCULATIONS ONLY

GENERAL GAS PHASE SPECIES SET PRESENTED IN SURFACE THERMOCHEMISTRY SAMPLE PROBLEM, WHICH FOLLOWS, GOES HERE

CONDENSED SPECIES SET FOR EXPANSION OR EQUILIBRIUM CALCULATIONS ONLY

```
-129562+6 359122+5 153149+2 182960-3-190747+6 347723+2 2820. 5000.3  10.BE0*
  2  4  1  6  0  0  0  0  0  0  0  0  0  0 OJANAF 03/62                 BE2C*
-222000+5 519028+5 229814+2-271974-5-635112+7 430672+2  500. 2401.2 100.BE2C*
-653500+4 526826+5 195224+2 723914-5-483551+6 499909+2 2401. 5000.3 100.BE2C*
  3  4  2  7  C  0  0  0  C  0  0  0  0  0 OJANAF 03/63                 BE3N2*
-137800+6 863645+5 386258+2-227477-3-117238+8 776686+2  500. 2473.2  10.BE3N2*
-110735+6 916598+5 288203+2-194536-3 779046+8 907280+2 2473. 5000.3  10.BE3N2*
  1  1  1  5  2  8  0  0  0  0  0  0  0  0 OJANAF 12/64                 BH02*
-191869+6 849683+5 943587+1 133656-1-323428+5 692658+2  300.  900.2   0.BH02*
-191869+6 573189+5 276870+2-207617-2-355870+7 568310+2  900. 1500.2   0.BH02*
  1  5  1  7  0  0  0  0  0  0  0  0  0  0 OJANAF 9/63                  BN*
-595100+5 291896+5 119161+2 239906-4-89106?+6 257049+2  500. 2500.2  10.BN*
-595100+5 290739+5 117157+2 257181-5-24002?+6 256618+2 2500. 5000.2  10.BN*
  4  1  2  5  4  8  0  0  0  0  0  0  0  0 OJANAF 03/66                 B2H4O4*
-337099+6 199911+6 287825+2 279798-1-837893+6 167294+3  300.  900.2   0.B2H4O4*
-337099+6 164343+6 580007+2 572414-2-828021+7 151554+3  900. 1500.2   0.B2H4O4*
  2  5  3  8  0  0  0  0  0  0  0  0  0  0 OJANAF 12/60                 B2O3*
-300978+6 811530+5 299659+2 700906-3-130981+7 828910+2  500. 3000.2 100.B2O3*
-300978+6 811530+5 288865+2 659184-3 884491+7 828910+2 3000. 5000.2 100.B2O3*
  3  5  3  8  3  9  0  0  0  0  0  0  0  0 OJANAF 03/65                 B3F3O3*
-586499+6 190799+6 286473+2 258435-1-572281+6 184615+3  300.  900.2   0.B3F3O3*
-586499+6 142747+6 679396+2-414850-2-105348+8 163343+3  900. 1500.2   0.B3F3O3*
  3  1  3  5  3  8  0  0  0  0  0  0  0  0 OJANAF 03/65                 B3H3O3*
-301699+6 167244+6 311184+2 194520-1-123978+7 157175+3  300. 1200.2   0.B3H3O3*
-301699+6 139716+6 581678+2-647494-5-656656+7 145381+3 1200. 2000.2   0.B3H3O3*
  4  5  1  6  0  0  0  0  0  0  0  0  0  0 OJANAF 12/65                 CB4*
-929999+4 829591+5 230566+2 537468-2-105961+7 681801+2  500. 2743.2   0.CB4*
 180999+5 790399+5 325000+2-160344-8-237919+2 767634+2 2743. 3500.3   0.CB4*
  3  6  4 13  0  0  0  0  0  0  0  0  0  0 OJANAF 06/63                 C3AL4*
-489999+5 117824+6 411943+2 249972-2-159504+7 114878+3  500. 1500.2   0.C3AL4*
-489999+5 116642+6 454353+2 560830-3-459367+7 114410+3 1500. 3000.2   0.C3AL4*
  4  1  1  7  1 17  0  0  0  0  0  0  0  0 OJANAF 12/60                 CLH4N*
-753799+5 877759+5 239667+2 525476-2-392315+6 910481+2  300. 1200.2   0.CLH4N*
-753799+5 789689+5 300000+2-152997-9-247332-0 872322+2 1200. 2000.2   0.CLH4N*
  4  1  1  7  4  8  1 17  0  0  0  0  0  0 OJANAF 12/62                 CLH4NO4*
-706900+5 27531?+6 145787+2 523599-1 302440+5 224155+3  300.  900.2   0.CLH4NO4*
-706900+5 231364+6 623232+2 200088-1-150588+8 205225+3  900. 1500.2   0.CLH4NO4*
200    0 00          54.4                                            112D,CHMBR
300    0 00          48.0                                            COLS. 3-4
300    0 00          31.4                                            COLS. 3-4
300    0 00          16.0                                            COLS. 5-6
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CONDENSED SPECIES SET (CONCLUDED)

ISENTROPIC EXPANSION CALCULATION OUTPUT

AEROTHERM CHEMICAL EQUILIBRIUM JOB APG 112D 0110000000*

RELATIVE ELEMENTAL COMPOSITIONS, ATOMIC WTS/UNIT MASS

AT.NO.	ELEMENT	ATOMIC WT	COMPONENT 1	COMPONENT 2	COMPONENT 3
1	HYDROGEN	1.00800	0.032561	0.	0.
6	CARBON	12.01100	0.056555	0.	0.
7	NITROGEN	14.00800	0.053729	0.	0.
8	OXYGEN	16.00000	0.022512	0.	0.
13	ALUMINUM	26.97000	0.101417	0.	0.
17	CHLORINE	35.45700	0.053759	0.	0.

ELEMENT	HYDROGEN	CARBON	NITROGEN	OXYGEN	ALUMINUM	CHLORINE
BASE SP	H2	CO	N2	H2O	ALCL	CLH

I 3

AEROTHERM CHEMICAL EQUILIBRIUM (ACE) SOLUTION

CHAMBER [illegible] 3?? K [illegible] ATM

PRESSURE	SP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
0.42201+[illegible]	0.12269+004	0.77964+000	[illegible].46084-001	0.11174+001

PROPERTY ROUTINE OUTPUT IN LB-MASS,FT,SEC,BTU,AND DEG-R

TEMP	VISC	COND	PRAP	PR	SC
0.7021-+004	0.48226-004	0.96149-004	0.24480-003	0.30156+000	0.74434+000

MU*	MU2	MOL.WT	UTIL	CPTIL
0.71004+000	0.19881+002	0.33488+002	0.67447+004	0.96935+000

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER ; ; ; ;

1	6	7	8	13	17
0.39514-001	0.67929-001	0.75254-001	0.36019+000	0.27352+000	0.19059+000
0.14910+000	0.11353+000	0.12672+000	0.29140+000	0.53756-001	0.24615+000

TEMP = 3901.0003 DEG-K PRES = 68.0000 ATM MOL WT = 33.4873827

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
H2O	0.10749+000	CO	0.18209+000	H2	0.32904+000
H2	0.89369-001	CLH	0.92891-001	ALCL	0.29109-001
CO2	0.70553-002	C	0.27779-002	O2	0.35578-00[illegible]
C3-	0.10946-012	C2H	0.40117-008	CH4	0.29596-007
H	0.59032-007	C2H2	0.19274-008	[illegible]	0.92515-001
HO	0.17836-001	NO	0.15723-002	CHO	0.21393-00[illegible]
CL	0.17359-001	CL2	0.20242-004	CHN	0.15641-004
ALO2	0.16469-006	ALCL2	0.19951-001	ALHO2	0.28544-002
AL	0.38102-002	ALC	0.90577-012	ALCLO	0.16249-00[illegible]
AL-	0.53849-003	ALN	0.46628-005	ALCL3	0.16672-00[illegible]
AL-O	0.48563-004	ALO	0.15205-002	AL2CL6	0.17218-01[illegible]
AL2O	0.12916-002	AL2O2	0.29294-004	CCL	0.77240-00[illegible]
CCLN	0.45443-007	CCLO	0.11026-004	CCL2	0.88056-011
CCL2O	0.11322-008	CCL3	0.44424-014	CCL4	0.15408-01[illegible]
CH	0.37204-007	CHCL3	0.47310-013	CHNO	0.11231-005
CH2	0.11735-007	CH2CL2	0.49089-011	CH2O	0.22418-005
CH3	0.16229-006	CH3CL	0.52216-009	CN	0.40669-006
C2	0.87831-011	C2H3	0.46762-011	C2H4	0.14325-011
C2-4O	0.37399-013	C2H6	0.40178-015	C2N2	0.13471-01[illegible]
C3	0.26715-014	C3H2	0.94525-014	C3H3	0.14401-014
C3-4	0.59053-016	C3H6	0.26018-015	C3O2	0.90918-013
CL-O	0.17341-004	CLNO	0.18713-006	CLNO2	0.11572-011
CLO	0.18617-004	CLO2	0.46735-009	CL2O	0.25107-00[illegible]
CN	0.69832-004	HNO	0.36812-005	HNO2	0.29049-007
HNO3	0.11759-011	HO2	0.92575-005	H2N	0.33705-004
H3	0.16978-004	H4N2	0.47649-011	N	0.44040-004
N03	0.36912-012	N2O	0.23673-006	N2O3	0.76465-014
N2O4	0.82932-019	N2O5	0.23666-022	O3	0.20621-007
C4	0.89171-020	C4H	0.17060-014	C4H2	0.21259-017
C4-3	0.50499-019	C4H4	0.44064-020	C4N2	0.24047-0[illegible]
AL*	0.	ALCL3*	0.	ALCL3*	0.
AL2*	0.	AL2O3*	0.13941+00[illegible]	C3ALA4*	0.
CL-4N*	0.	CLH4NO4*	0.	C*	0.

ENTHALPY =-0.46299940+003 CAL/GM ENTROPY = 0.20874+001 CAL/GM-DEG K
DENSITY = 0.444041+000 LB/CU.FT. MASS CONDENSED/MASS GAS = 0.73722+000 B-PRIME = 0.
VEL = 0. FT/SEC MACH = 0. AREA = 0. SQFT/LB/SEC
H-GAS= 0.19277+004 BTU/LB H-KINETIC = 0. BTU/LB

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AEROTHERM CHEMICAL EQUILIBRIUM JOB 1170,CHMBR      2000000000

  CP-FROZEN     CP-EQUIL    DLNM/DLNT    DLNM/DLNP      GAMMA
 0.42480+000 0.12760+001 0.81997+000 -0.50097-001 0.11146+001

PROPERTY ROUTINE OUTPUT IN LB-MASS,FT,SEC,BTU,AND DEG-R
   VISC        VISC        COND        GBAR        PR          SC
0.67427+004 0.47835-004 0.95570-004 0.30429-005 0.30135+000 0.74389+000
   MU          MU2         MOL,WT      MUIL        CPTIL
0.72864+000 0.19837+002 0.33348+002 0.68985+004 0.98928+000
ELEMENTAL X AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . .
     1           6           7           8          13          17
0.32914-001 0.67929-001 0.75254-001 0.36019+000 0.27352+000 0.19059+000
0.14829+000 0.11331+000 0.12647+000 0.29130+000 0.54054-001 0.24653+000

     TEMP = 3866,0809 DEG-K     PRES = 54,4000 ATM     MOL WT = 33,3474749
```

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
H2O	0.10617+009	CO	0.18136+000	H2	0.32587+000
N2	0.88491-001	CLH	0.92547-001	ALCL	0.29614-001
CO2	0.70336-002	O	0.10278-002	O2	0.38794-005
CS-	0.60021-013	C2H	0.67750-009	CH4	0.13617-007
C	0.50529-007	C2H2	0.12256-008	H	0.96873-001
HO	0.18352-001	NO	0.15988-002	CHO	0.18494-003
CL	0.18298-001	CL2	0.19280-004	CHN	0.12381-004
NO2	0.15856-006	ALCL2	0.19053-001	ALHO2	0.28627-002
AL	0.40177-002	ALC	0.46565-011	ALCLO	0.16130-003
ALH	0.51500-003	ALN	0.42837-005	ALCL3	0.14810-005
AL-O	0.46435-004	ALO	0.15950-002	AL2CL6	0.11039-010
AL2O	0.13218-002	AL2O2	0.99892-004	CCL	0.60434-009
CCLN	0.35253-007	CCLO	0.94559-005	CCL2	0.64004-011
CCL2O	0.87955-009	CCL3	0.42501-014	CCL4	0.94370-017
CH	0.29343-007	CHCL3	0.10831-013	CHNO	0.88680-006
CH2	0.88149-008	CH2CL2	0.31312-011	CH2O	0.17691-005
CH3	0.11433-004	CH3CL	0.33972-009	CN	0.33282-006
C2	0.60403-011	C2H3	0.26228-011	C2H4	0.75685-012
C2H4O	0.18882-015	C2H6	0.17394-015	C2N2	0.84143-011
C3	0.15379-014	C3H2	0.46744-014	C3H3	0.65836-015
C3H4	0.24559-016	C3H5	0.08427-016	C3O2	0.56150-015
CL-O	0.16135-004	CLNO	0.16713-004	CLNO2	0.96992-012
CLO	0.18457-004	CLO2	0.43137-009	CL2O	0.21955-009
HN	0.63583-004	HNO	0.83257-005	HNO2	0.25551-007
HNO3	0.97614-012	HO2	0.21793-005	H2N	0.28647-004
H3N	0.13521-004	H4N2	0.28824-011	N	0.43264-004
NO3	0.32666-012	N2O	0.21443-006	N2O3	0.60146-014
N2O4	0.61549-019	N2O5	0.16378-022	N3	0.29146-009
C4	0.37934-023	C4H	0.74010-017	C4H2	0.86299-018
C4H3	0.18521-019	C4H4	0.44800-020	C4N2	0.96325-022
AL*	0.	ALCLO*	0.	ALCL3*	0.
AL2*	0.	AL2O3*	0.13874+000	C3AL4*	0.
CL-4N*	0.	CLH4NO4*	0.	C*	0.

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     ENTHALPY =-0,4629940+003 CAL/GM     ENTROPY = 0,21008+001 CAL/GM-DEG K
     DENSITY = 0,356761+000 LB/CU,FT.     MASS CONDENSED/MASS GAS = 0,73446+000  B-PRIME = 0.
  VEL = 0,          FT/SEC    MACH = 0,          AREA = 0,          SQFT/LB/SEC
H-GAS= 0.19398+004 BTU/LB    H-KINETIC = 0,          BTU/LB
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CHAMBER CONDITIONS
P = 54.4 ATM, H. DEFINED FROM
PREVIOUS SOLUTION)

E-5

ISENTROPIC EXPANSIONS FROM ABOVE CHAMBER CONDITIONS

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AEROTHERM CHEMICAL EQUILIBRIUM JOB COLS. 1-4      3000000000

     CP-FROZEN     CP-EQUIL    DLNV/DLNT   DLNP/DLNT    GAMMA
   0.42588+000 0.12620+001 0.80119+000 0.46457-001 0.11162+001

PROPERTY ROUTINE OUTPUT IN LB-MASS,FT,SEC,BTU,AND DEG-R
     VISC        VIST        COND        CRAR          PR          SC
 0.44-0?+004 0.47384-004 0.95155-004 0.33884-005 0.30?8?+000 0.74446+000
                 MU?        MOL,WT      WTIL        CPTIL
 0.7?734+000 0.19605+002 0.33429+002 0.47504+004 0.99122+000
ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER ; , , ,
                             7           8          1X           17
 0.32514-001 0.67929+001 0.75254-001 0.34019+000 0.27352+000 0.19059+000
 0.14910+000 0.11377+000 0.12698+000 0.28965+000 0.52273-001 0.24872+000

      TEMP = 3827,2934 DEG-K      PRES = 48,0000 ATM      MOL WT = 33,4282843

  SPECIES    MOLE FR,          SPECIES    MOLE FR,          SPECIES    MOLE FR,
  H2O       0.10527+000        CO         0.48189+000       H2         0.32830+000
  H2        0.88948+001        CLH        0.94237-001       ALCL       0.28873-001
  CO2       0.69754-002        O          0.28493-002       C2         0.35880-003
  C3-       0.44454-013        C2H        0.54342-009       CH4        0.11759-007
  C         0.42366-007        C2H2       0.10060-008       N          0.25856-001
  HO        0.17540-001        NO         0.44970-007       CHO        0.16939-003
  CL        0.18338-001        CL2        0.48605-004       CHN        0.11142-004
  AO?       0.13681-006        ALCL2      0.38791-001       ALHO2      0.26623-002
  AL        0.37451-002        ALC        0.80126-011       ALCLO      0.15032-001
  ALH       0.46265-003        ALN        0.36189-005       ALCL3      0.14618-003
  ALHO      0.41224-004        ALO        0.14566-002       AL2CL6     0.96672-011
  AL2O      0.11918-002        AL2O2      0.26520-005       CCL        0.49546-009
  CCLN      0.31075-007        CCLO       0.86013-005       CCL2       0.52584-011
  CCL2O     0.77370-009        CCL3       0.33738-014       CCL4       0.74734-017
  CH        0.24232-007        CHCL3      0.87844-014       CHNO       0.78692-006
  CH2       0.73184-008        CH2CL2     0.25940-011       CH2O       0.15774-005
  CH3       0.97682-007        CH3CL      0.28765-009       CN         0.28643-004
  C2        0.45867-011        C2H3       0.20064-011       C2H4       0.58645-012
  C2H4O     0.13642-015        C2H6       0.12502-015       C2N2       0.66775-011
  C3        0.11125-014        C3H2       0.33346-014       C3H3       0.46450-015
  C3H4      0.17248-016        C3H5       0.45230-014       C3O2       0.43358-013
  CLHO      0.14879-004        CLNO       0.14554-008       CLNO2      0.76945-012
  CLO       0.16884-004        CLO2       0.35527-009       CL2O       0.18691-009
  HN        0.57229-004        HNO        0.29284-005       HNO2       0.21483-007
  HNO3      0.75332-012        HO2        0.48973-005       N2         0.25748-004
  H3N       0.12269-004        H4N2       0.21927-011       N          0.39270-004
  NO2       0.25221-012        N2O        0.48844-008       N2O3       0.43101-014
  N2O4      0.40489-019        N2O5       0.97367-023       O3         0.16096-003
  C4        0.25151-029        C4H        0.49723-017       C4H2       0.57443-014
  C4H3      0.11814-019        C4H4       0.82270-021       C4N2       0.62185-009
  AL*       0.                 ALCLO*     0.                ALCL3*     0.
  AL2O*     0.                 AL2O3*     0.14013+000       C3AL4*     0.
  CLH4NO*   0.                 CLH4NO4*   0.                C*         0.
      ENTHALPY =-0,491651?+003 CAL/GM      ENTROPY = 0.21008+001 CAL/GM-DEG K
      DENSITY = 0,124925+000 LB/CU,FT,        MASS CONDENSED/MASS GAS = 0.74419+000  BURNING = 1.
  VE  = 0,161+004 FT/SEC    MACH = 0,675+000    AREA = 0,195-002 SQFT/LB/SEC
 H-MASS; 0,19052+004 BTU/LB    H-KINETIC = 0,51254+002 BTU/LB
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AEROTHERM CHEMICAL EQUILIBRIUM JOB COLS, 3-4   3000000000

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
0.42489+000	0.12149+001	0.74290+000	0.44003+001	0.11152+001

PROPERTY ROUTINE OUTPUT IN LB-MASS,FT,SEC,BTU,AND DEG-R

VISC	VISC	COND	PRAR	PR	SC
0.4465-+001	0.45943-004	0.93696-004	0.48799-003	0.29921+000	0.74442+000

MU	M/2	MOL.WT	HTIL	CPTIL
0.74486+000	0.19705+002	0.33700+002	0.64739+004	0.69763+000

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER : . . .

1	6	7	8	13	17
0.32514-001	0.67929-001	0.75254-001	0.36019+000	0.27352+000	0.19059+000
0.17149+000	0.11539+000	0.12864+000	0.28414+000	0.46348-001	0.25389+000

TEMP = 3692.1133 DEG-K   PRES = 31.4000 ATM   MOL WT = 33.6904124

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
H2O	0.10209+000	CO	0.48367+000	H2	0.33654+000
N2	0.89875-001	CLH	0.40022+000	ALCL	0.26263-001
CO2	0.67763-002	O	0.22877-002	O2	0.27344-001
C3H	0.16088-013	C2H	0.95667-009	CH4	0.71953-008
C	0.23025-007	C2H2	0.51712-009	H	0.91976-001
HO	0.14915-001	NO	0.11859-002	CHO	0.12542-003
CL	0.18359-001	CL2	0.16436-004	CHN	0.78645-005
NO2	0.81656-007	ALCL2	0.17855-001	ALHO2	0.20560-002
AL	0.28873-002	ALC	0.16908-011	ALCLO	0.11695-004
ALH	0.31702-003	ALN	0.23048-005	ALCL3	0.13947-003
ALHO	0.27054-004	ALO	0.10519-002	AL2CL6	0.61872-011
AL2O	0.82177-003	AL2O2	0.47293-004	CCL	0.25081-009
CCLN	0.20249-007	CCL2	0.42182-005	CCL2	0.26383-011
CCL2O	0.50031-009	CCL3	0.15354-014	CCL4	0.33885-017
CH	0.12543-007	CHCL3	0.43266-014	CHNO	0.52444-006
CH2	0.38751-008	CH2CL2	0.13748-011	CH2O	0.10689-005
CH3	0.57341-007	CH3CL	0.16445-009	CN	0.17115-006
C2	0.17840-011	C2H3	0.81113-017	C2H4	0.24898-012
C2H4O	0.45441-016	C2H6	0.41292-014	C2N2	0.30542-011
C3	0.36999-015	C3H2	0.10649-014	C3H3	0.14376-015
C3H4	0.50491-017	C3H5	0.16345-016	C3O2	0.18049-013
CLHO	0.11223-004	CLNO	0.00899-007	CLNO2	0.34522-007
CLO	0.12336-004	CLO2	0.18205-009	CL2O	0.10591-009
HN	0.39760-004	HNO	0.18844-005	HNO2	0.11774-007
HNO3	0.30694-012	HO2	0.11675-005	H2N	0.17852-004
H3N	0.88344-005	H4N2	0.86515-012	N	0.27955-004
NO3	0.98881-013	N2O	0.12041-008	N2O3	0.13584-014
N2O4	0.95001-020	N2O5	0.15074-023	O3	0.73289-010
C4	0.52167-021	C4H	0.12602-017	C4H2	0.14583-014
C4H3	0.25939-023	C4H4	0.18804-021	C4N2	0.14185-020
AL*	0.	ALCLO*	0.	ALCL3*	0.
AL2O*	0.	AL2O3*	0.44469+000	C3AL4*	0.
CLH4NO*	0.	CLH4NO4*	0.	C*	0.

ENTHALPY = -0.5869944+003 CAL/GM   ENTROPY = 0.21008+001 CAL/GM-DEG K

DENSITY = 0.21816+000 LB/CU.FT.   MASS CONDENSED/MASS GAS = 0.77534+000   B-PRIME = 0.

VEL = 0.333+004 FT/SEC   MACH = 0.100+001   AREA = 0.138-002 SQFT/LB/SEC

H-GAS= 0.17891+004 BTU/LB   H-KINETIC = 0.22158+003 BTU/LB

AFRPT-EHM CHEMICAL EQUILIBRIUM JOB COLS, 5-6 300000000

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
0.42474+000	0.11418+001	-0.65294+000	-0.37279-001	0.11137+001

PROPERTY ROUTINE OUTPUT IN LB-MASS,FT,SEC,BTU,AND DEG-R

VISC	COND	PRAR	PR	SC
0.43815-004	0.91222+004	0.87140-003	0.29713+000	0.74949+000

M.W.	MOL.WT	ETIL	CETIL
0.19512+002	0.34117+002	0.60012+004	0.10042+001

ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER : : : :

1	6	7	8	13	17
0.32514-001	0.67929-001	0.75254-001	0.34819+000	0.27352+000	0.19059+000
0.17529+000	0.11752+000	0.13107+000	0.27561+000	0.37719-001	0.24280+000

TEMP = 3487.8712 DEG-K PRES = 16.0000 ATM MOL WT = 34.1171122

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
H2O	0.96631-001	CO	0.15641+000	H2	0.34949+000
N2	0.91217-001	CLH	0.11049+000	ALCL	0.21940-001
CO2	0.64543-002	O	0.15419-002	O2	0.14883-004
C3H	0.32178-014	C2H	0.77359-010	CH4	0.33710-008
C	0.83811-008	C2H2	0.18226-009	H	0.84532-001
HO	0.11196-001	NO	0.79201-003	CHO	0.77105-004
CL	0.18067-001	CL2	0.13794-004	CHN	0.45334-005
NO2	0.34957-007	ALCL2	0.16905-001	ALHO2	0.13080-002
AL	0.18137-002	ALC	0.97684-012	ALCLO	0.75259-004
ALH	0.16549-003	ALN	0.73620-006	ALCL3	0.12946-005
ALHO	0.13162-004	ALO	0.59849-003	AL2CL6	0.30642-011
AL2O	0.42455-003	AL2O2	0.81429-005	CCL	0.81334-010
CCLN	0.10227-007	CCL2	0.16695-005	CCL2	0.86615-012
CCL2O	0.24876-009	CCL3	0.43193-015	CCL4	0.96046-014
CH	0.42641-008	CHCL3	0.14086-014	CHNO	0.27533-006
CH2	0.13878-008	CH2CL2	0.50619-012	CH2O	0.57599-006
CH3	0.24731-007	CH3CL	0.48737-010	CN	0.74020-007
C2	0.38478-012	C2H3	0.19424-012	C2H4	0.65655-015
C2H4O	0.80261-017	C2H6	0.73955-017	C2N2	0.88697-012
C3	0.63334-016	C3H2	0.17600-015	C3H3	0.22605-014
C3H4	0.74144-018	C3H5	0.18828-017	C3O2	0.44876-014
CLHO	0.69882-005	CLNO	0.40536-007	CLNO2	0.90882-011
CLO	0.71918-005	CLO2	0.58690-010	CL2O	0.42011-010
HN	0.21879-004	HNO	0.90332-006	HNO2	0.43280-005
HNO3	0.69318-013	HO2	0.51182-004	H2N	0.98284-005
H3N	0.52621-005	H4N2	0.19570-012	N	0.15671-004
NO3	0.20825-013	N2O	0.57175-007	N2O3	0.19940-015
N2O4	0.85634-021	N2O5	0.80714-025	O3	0.19228-010
C4	0.42113-022	C4H	0.14409-018	C4H2	0.16951-012
C4H3	0.24040-021	C4H4	0.15633-022	C4N2	0.13839-021
AL*	0.	ALCL3*	0.	ALCL3*	0.
AL2O3*	0.	AL2O3*	0.15146+000	C3AL4*	0.
CL-4N*	0.	CLH4NO4*	0.	C*	0.

ENTHALPY =-0.278864+003 CAL/GM ENTROPY = 0.21808+001 CAL/GM-DEG K
DENSITY = 0.119952+000 LB/CU.FT. MASS CONDENSED/MASS GAS = 0.32471+000 H-PRIME = 0.
VEL = 0.489+004 FT/SEC MACH = 0.153+001 AREA = 0.172-002 SQFT/LB/SEC
H-GAS= 0.14029+004 BTU/LB H-KINETIC = 0.47484+004 BTU/LB

TURBULENCE THERMOCHEMISTRY INPUT

```
C11   C GC 3827.2   48.0                                                    COLS. 1-2
  8
  1 HYDROGEN     1.008     0.0322563
  6 CARBON      12.011     0.0054473
  7 NITROGEN    14.008     0.0053722
  8 OXYGEN      16.000     0.0095231
 13 ALUMINUM    26.970     0.0017600
 17 CHLORINE    35.457     0.0053752
112 SURF CARBON12.011                    1.0
144 FROZEN CO2 44.011     0.0002082
  2  1  1  8  C  C  C  0  0  0  0  0  0  OJANAF 03/61                          H2O
-577980+5 302010+5 112254+2 811397-3-260800+7 684210+2  500. 3000.1   0.H2O
-577980+5 302010+5 157278+2-191548-3-173599+8 684210+2 3000. 5000.1   0.H2O
 1112      C  C  C  0  0  C  0  0  0  0  0  OJANAF 03/61                     C*
 CCCCCC-0 144120+5 586075+1 953976-4-766621+6 121290+2  500. 3000.2 100.C*
 CCCCCC-0 144120+5 485134+1 291605-3 307202+7 121290+2 3000. 5000.2 100.C*
  1  1  1  8  C  0  C  0  0  0  0  0  0  OJANAF 03/61                        CO
-264170+5 223570+5 865040+1 117021-3-898211+6 653700+2  500. 3000.1   0.CO
-264170+5 223570+5 115496+2-424139-3-131563+8 653700+2 3000. 5000.1   0.CO
  2  1  0  0  C  C  C  0  0  0  0  0  0  OJANAF 03/61                        H2
 CCCCCC-0 212100+5 711963+1 621950-3-71269+6 484650+2  500. 3000.1   0.H2
 CCCCCC-0 212100+5 681794+1 589854-3 265106+7 484650+2 3000. 5000.1   0.H2
 1144               0  0  0  0  0  0  0  OJANAF 03/61                       CO2
-940540+5 365350+5 144559+2 210386-3-182392+7 798480+2  500. 3000.1   0.CO2
-940540+5 365350+5 156451+2-381561-4-602768+7 798480+2 3000. 5000.1   0.CO2
  2  7  0  0  0  0  0  0  0  0  0  0  0  OJANAF 03/61                        N2
 CCCCCC-0 221650+5 862699+1 116090-3-103715+7 637650+2  500. 3000.1   0.N2
 CCCCCC-0 221650+5 984175+1-116232-3-612728+7 637650+2 3000. 5000.1   0.N2
  1  1  1 17  C  C  0  0  0  0  0  0  0  OJANAF 03/61                       CLH
-219700+5 218640+5 839693+1 214828-3-125475+7 623640+2  500. 3000.1   0.CLH
-219700+5 218640+5 837177+1 193261-3-446002+6 623640+2 3000. 5000.1   0.CLH
  1  8  0  C  C  0  0  0  0  0  0  0  0  OJANAF 06/62                         O
 595590+5 135220+5 497228+1 380768-5 154749+5 500960+2  500. 3000.1   0.O
 595590+5 135220+5 657489+1-224268-3-891782+7 500960+2 3000. 5000.1   0.O
  2  8  0  C  C  C  0  0  0  0  0  0  0  OJANAF 03/61                        O2
 CCCCCC-0 234460+5 804370+1 510872-3-152718+6 679730+2  500. 3000.1   0.O2
 CCCCCC-0 234460+5 103071+2 290991-4-783079+7 679730+2 3000. 5000.1   0.O2
  1  1  3  6  C  C  0  0  0  0  0  0  0  ODUFF BAUER 6/61                    C3H
 127703+6 489620+5 194464+2 508379-3-311933+7 928820+2  500. 3000.1   0.C3H
 127703+6 489620+5 199582+2 245687-3-632514+6 928820+2 3000. 5000.1   0.C3H
  1  1  2  6  C  C  C  0  0  0  0  0  0  ODUFF BAUER 6/61                    C2H
 117395+6 349620+5 134210+2 469100-3-187509+7 781140+2  500. 3000.1   0.C2H
 117395+6 349620+5 148516+2 109402-3-503862+7 781140+2 3000. 5000.1   0.C2H
  4  1  1  6  C  C  0  0  0  0  0  0  0  OJANAF 03/61                       CH4
-178950+5 530790+5 230948+2 677896-3-755061+7 825970+2  500. 3000.1   0.CH4
-178950+5 530790+5 236053+2 374323-3-368234+7 825970+2 3000. 5000.1   0.CH4
  1  6  0  C  C  0  0  0  0  0  0  0  0  OJANAF 03/61                         C
 170886+6 135500+5 444433+1 228125-3 409830+6 492870+2  500. 3000.1   0.C
 170886+6 135500+5 412212+1 261908-3 262886+7 492870+2 3000. 5000.1   0.C
  2  1  2  6  C  C  0  0  0  0  0  0  0  OJANAF 03/61                       C2H2
 541900+5 482570+5 189960+2 769044-3-409039+7 849690+2  500. 3000.1   0.C2H2
 541900+5 482570+5 203952+2 389062-3-645297+7 849690+2 3000. 5000.1   0.C2H2
```

SPECIAL BASE SPECIES SET FOR KINETICS CALCULATIONS

GENERAL GAS PHASE SPECIES SET

```
  1  1  0  C  0  0  0  0  0  0  0  0  0  0 OJANAF 12/60                          H
 521C20+5 134230+5 480223+1 555469-4 173095+6 388620+2  500. 3000.1    0.H
 521C20+5 134230+5 308752+1 315025-3 929744+7 388620+2 3000. 5000.1    0.H
  1  1  1  8  C  0  0  0  0  0  0  0  0  0 OJANAF 12/60                         HO
 933CC0+4 214C40+5 773193+1 394386-3-973561+6 613820+2  500. 3000.1    0.HO
 933CC0+4 214C4C+5 965144+1-443528-4-686115+7 613820+2 3000. 5000.1    0.HO
  1  7  1  8  C  0  0  0  0  0  0  0  0  0 OJANAF 06/63                         NO
 2158C0+5 227CC0+5 877623+1 899031-4-789656+6 688490+2  500. 3000.1    0.NO
 2158C0+5 227CC0+5 916260+1 657885-5-212519+7 688490+2 3000. 5000.1    0.NO
  1  1  1  6  1  8  0  0  0  0  0  0  0  0 OJANAF 03/61                        CHO
-290CC0+4 323670+5 128033+2 300638-3-201721+7 789830+2  500. 3000.1    0.CHO
-290CCC+4 323670+5 103028+2 633312-3 121615+8 789830+2 3000. 5000.1    0.CHO
  1 17  0  0  C  0  0  0  0  0  0  0  0  0 OJANAF 03/61                         CL
 289220+5 140280+5 508338+1-272037-4 290013+6 516230+2  500. 3000.1    0.CL
 289220+5 140280+5 539251+1-770696-4-114573+7 516230+2 3000. 5000.1    0.CL
  2 17  0  C  0  0  0  0  0  0  0  0  0  0 OJANAF 03/61                        CL2
 CCCCC0-0 244290+5 852234+1 273227-3 287718+6 737600+2  500. 3000.1    0.CL2
 CCCCC0-0 244290+5 100329+2-141907-4-554731+7 737600+2 3000. 5000.1    0.CL2
  1  1  1  6  1  7  0  0  0  0  0  0  0  0 OJANAF 03/61                        CHN
 312CC0+5 355930+5 137023+2 552243-3-228955+7 758620+2  500. 3000.1    0.CHN
 312CC0+5 355930+5 178895+2-295052-3-183671+8 758620+2 3000. 5000.1    0.CHN
  1  7  2  8  0  0  0  0  0  0  0  0  0  0 OJANAF 06/63                        NO2
 8011C0+4 3458C0+5 137819+2 315611-4-133765+7 848890+2  500. 3000.1    0.NO2
 8011C0+4 3458CC+5 130154+2 172586-3 175340+7 848890+2 3000. 5000.1    0.NO2
  10:3 01 17                                    JANAF 06/61                      ALCL
-116200+5 244690+5 895305+1 115091-3-929251+5 750380+2  500. 3000.1    0.ALCL
-116200+5 244690+5 951089+1 835189-5-223156+7 750380+2 3000. 5000.1    0.ALCL
  1013 02 17                                    JANAF 06/61                      ALCL2
-78CCC0+5 371170+5 138896+2 586012-5-137329+6 100813+3  500. 3000.1    0.ALCL2
-78CCC0+5 371170+5 136493+2 486738-4 869684+6 100813+3 3000. 5000.1    0.ALCL2
  1001 02 08 01 13                              JANAF 12/60                      ALHO2
-1C9CC0+6 4805C0+5 191451+2 162758-3-253257+7 989760+2  500. 3000.1    0.ALHO2
-1C9CC0+6 4805CC+5 208743+2-198656-3-833764+7 989760+2 3000. 5000.1    0.ALHO2
  1 13  0  C  C  0  0  0  0  0  0  0  0  0 OJANAF 03/61                         AL
 78CCC0+5 134610+5 492905+1 113634-4 706967+5 508440+2  500. 3000.1    0.AL
 78CCC0+5 134610+5 395674+1 204094-3 361777+7 508440+2 3000. 5000.1    0.AL
  1  6  1 13  C  0  0  0  0  0  0  0  0  0 OJANAF 12/60                         ALC
 209958+6 240440+5 896909+1-757687-5-752532+5 746650+2  500. 3000.1    0.ALC
 209958+6 240440+5 961609+1-128042-3-264567+7 746650+2 3000. 5000.1    0.ALC
  1  8  1 13  1 17  C  0  C  0  0  0  0  0 OJANAF 12/60                        ALCLO
-55CCC0+5 391990+5 148879+2 423287-5-392535+6 920440+2  500. 3000.1    0.ALCLO
-55CCC0+5 391990+5 158613+2-186492-3-400349+7 920440+2 3000. 5000.1    0.ALCLO
  1  8  1  9  1 13  0  0  0  0  0  0  0  0 OJANAF 03/64                  111    ALFO
-1402C0+6 3869C0+5 148800+2 650586-5-589929+6 876980+2 1000. 3000.1    0.ALFO    1
-1402C0+6 3869C0+5 148945+2 160258-5-588334+6 876980+2 3000. 5000.1    0.ALFO    1
  1  1  1 13  C  0  0  0  0  0  0  0  0  0 OJANAF 06/63                         ALH
 62CCC0+5 233870+5 885387+1 181289-3-708658+6 638290+2  500. 3000.1    0.ALH
 620CC0+5 233870+5 951195+1 483217-4-304128+7 638290+2 3000. 5000.1    0.ALH
  1  7  1 13  C  0  0  0  0  0  0  0  0  0 OJANAF 12/60                         ALN
 1045C0+6 240670+5 892460+1 115329-3-212370+6 742970+2  500. 3000.1    0.ALN
 1045C0+6 240670+5 861677+1 172650-3 101045+7 742970+2 3000. 5000.1    0.ALN
  1 13  3 17  C  0  0  0  0  0  0  0  0  0 OJANAF 06/61                        ALCL3
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-140423+6 528160+5 199485+2-209903-4-446442+6 119584+3  500. 3000.1   0.ALCL3
-140423+6 528160+5 204484+2-109302-3-256062+7 119584+3 3000. 5000.1   0.ALCL3
  1  1  1  8  1 13  0  0  0  0  0  0  0 OJANAF 12/60                     ALHO
-3447C0+4 36734C+5 148C73+2 231376-4-155462+7 803550+2  500. 3CC0.1   0.ALHO
-3447C0+4 367340+5 143991+2 973440-4 115747+6 803550+2 30C0. 5CC0.1   0.ALHO
  1  8  1 13  C  0  0  0  C  0  0  0  0 OJANAF 03/62                     ALO
 213980+5 238C5C+5 895587+1 772498-4-329625+6 718590+2  500. 3000.1   0.ALO
 213980+5 238C5C+5 916408+1 387904-4-116511+7 718590+2 30C0. 5000.1   0.ALO
  2 13  6 17  C  0  0  0  0  0  0  0  0 OJANAF 03/64              111    AL2CL6
-3C92C0+6 116290+6 437070+2 353763-5-644812+6 211446+3 1000. 3000.1   0.AL2CL6 1
-3C92C0+6 116290+6 437101+2 159950-5-620287+6 211446+3 3000. 5000.1   0.AL2CL6 1
  1  8  2 13  C  0  0  0  C  0  0  0  0 OJANAF 09/61                     AL2O
-3144C0+5 359700+5 138891+2 485413-5-663265+6 912000+2  500. 3000.1   0.AL2O
-3144C0+5 3597C0+5 144656+2-108570-3-278920+7 912000+2 3000. 5000.1   0.AL2O
  2  8  2 13  C  0  0  0  0  0  0  0  0 OJANAF 12/61                     AL2O2
-953970+5 5C4970+5 198593+2 224091-5-134144+7 105665+3  500. 3000.1   C.AL2O2
-953970+5 5C4970+5-185468+2 738440-2 144995+9 105665+3 3000. 5CCC.1   0.AL2O2
  1  4  C  C  C  C  0  0  0  0  0  0  0 OJANAF 09/61                     BE
 78255C+5 13438C+5 464695+1 112298-3 334374+6 440210+2  500. 3000.1   0.BE
 782550+5 134380+5 105297-0 109147-2 14771+8 440210+2 3000. 5000.1   0.BE
  1  4  1 17  C  C  C  0  0  0  0  0  0 OJANAF 03/64              111    BECL
 3CCCC0+4 239830+5 893411+1 908676-4-222435+6 719C90+2 1000. 30C0.1   0.BECL   1
 3C0CC0+4 239830+5 894691+1 882523-4-267069+6 719090+2 3000. 5000.1   0.BECL   1
  1  4  2 17  C  C  C  0  0  0  0  0  0 OJANAF 09/61                     BECL2
-579119+5 3882C9+5 146996+2 608946-4-425949+6 899049+2  500. 3000.1   0.BECL2
-579119+5 3882C9+5 149007+2 485558-6-604893+6 899049+2 3000. 5000.1   0.BECL2
  1  4  1  9  C  0  0  0  0  0  0  0  0 OJANAF 03/63                     BEF
-496780+5 234680+5 888699+1 919571-4-42176+6 684020+2  500. 3CC0.1   0.BEF
-496780+5 234680+5 842934+1 174020-3 148137+7 684020+2 3000. 5000.1   0.BEF
  1  4  2  9  C  0  0  0  0  0  0  0  0 OJANAF 12/63                     BEF2
-1513C0+6 374160+5 1479C5+2 289774-4-115672+7 822830+2  500. 3000.1   0.BEF2
-1913C0+6 374160+5 138154+2 209528-3 27448l+7 822830+2 30C0. 5000.1   0.BEF2
  1  1  1  4  C  0  0  C  C  0  0  0  0 OJANAF 3/63                     BEH
 767680+5 229360+5 877224+1 184173-3-924908+6 607720+2  500. 3CC0.1   0.BEH
 767680+5 22936C+5 884739+1 160554-3-963556+6 607720+2 3000. 5CC0.1   0.BEH
  1  1  1  4  1  8  0  0  C  0  0  0  0 OJANAF 09/63                     BEHO
-25CCC0+5 321730+5 129854+2 208547-3-239494+7 78513C+2  500. 30C0.1   0.BEHO
-25CC00+5 321730+5 139C33+2-916197-5-477784+7 785130+2 300C. 5CC0.1   0.BEHO
  2  1  1  4  C  C  0  0  0  0  0  0  0 OJANAF 12/60                     BEH2
 3CCCC0+5 345780+5 145807+2 757364-4-277162+7 676530+2  500. 30C0.1   0.BEH2
 3CCCC0+5 345780+5 153556+2-872682-4-534470+7 676530+2 3000. 5CC0.1   0.BEH2
  2  1  1  4  2  8  0  0  0  0  0  0  0 OJANAF 09/63                     BEH2O2
-1585C0+6 593950+5 244524+2 313890-3-473550+7 103667+3  500. 30C0.1   0.BEH2O2
-1585CC+6 593950+5 252829+2 957844-4-632116+7 103667+3 3000. 5CCC.1   0.BEH2O2
  1  4  1  7  C  C  C  C  0  0  0  0  0 CJANAF 06/63                     BEN
 1C1599+6 236599+5 871835+1 168927-3-253217+6 692929+2  500. 3000.1   0.BEN
 101599+6 236599+5 894126+1 102713-3-471704+6 692929+2 3000. 5CCC.1   0.BEN
  1  4  1  8  C  C  C  0  0  0  0  0  0 OJANAF 09/63                     BEO
 31CCC0+5 231840+5 885450+1 909641-4-552570+6 661420+2  50C. 3000.1   0.BEO    1
 31CCC0+5 231840+5 894167+1 685229-4-73120+6 661420+2 30C0. 5000.1   0.BEO    1
  2  4  4 17  C  C  0  C  C  0  0  0  0 OJANAF 12/60                     BE2CL4
-178599+6 844529+5 316826+2 340183-4-456569+6 162027+3  5C0. 3CC0.1   C.BE2CL4
```

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-178559+6 844529+5 317876+2 141294-5-521197+6 162027+3 3000. 5000.1   0.BE2CL4
  2  4  1  8  C  C  0  C  0  0  0  0  0  OJANAF 09/63                    BE20
-15CCCC+5 375349+5 141882+2 210823-3-681583+6 829279+2  500. 3000.1   0.BE20
-15CCCC+5 375349+5 149040+2-185011-6-142668+7 829279+2 3000. 5000.1   0.BE20
  2  4  2  8  C  C  C  C  0  0  0  0  0  OJANAF 09/63                    BE202
-58CCCC+5 458360+5 197854+2 208746-4-163011+7 988560+2  500. 3000.1   0.BE202
-58CCCC+5 458360+5 192883+2 113721-3 337096+6 988560+2 3000. 5000.1   0.BE202
  3  4  3  8  C  C  0  0  0  0  0  0  0  OJANAF 09/63                    BE303
-252CCC+6 7688CC+5 316149+2 406679-4-413048+7 124702+3  500. 3000.1   0.BE303
-252CCC+6 7688CC+5 320268+2-453443-4-551555+7 124702+3 3000. 5000.1   0.BE303
  4  4  4  8  C  C  C  C  C  0  0  0  0  OJANAF 09/63                    BE404
-38CCCC+6 1C7856+6 436112+2 233046-4-439314+7 156562+3  500. 3000.1   0.BE404
-38CCCC+6 1C7856+6 439409+2-408308-4-562941+7 156562+3 3000. 5000.1   0.BE404
  5  4  5  8  C  0  C  C  0  0  0  0  0  OJANAF 09/63                    BE505
-5C5CCC+6 137169+6 553874+2 617881-4-542571+7 184299+3  500. 3000.1   0.BE505
-5C5CCC+6 137169+6 555197+2 226391-4-555927+7 184299+3 3000. 5000.1   0.BE505
  6  4  6  8  C  C  0  0  0  0  0  0  0  OJANAF 09/63                    BE606
-636CCC+6 166373+6 672405+2 798827-4-658038+7 211572+3  500. 3000.1   0.BE606
-636CCC+6 166373+6 665239+2 197656-3-331145+7 211572+3 3000. 5000.1   0.BE606
  1  5  0  C  C  C  0  0  0  0  0  0  0  OJANAF 12/60                    B
 132618+6 134240+5 506024+1-307108-4-995641+5 481210+2  500. 3000.1   0.B
 132618+6 134240+5 507458+1-121838-4-726353+6 481210+2 3000. 5000.1   0.B
  1  5  2  9  1 17  0  0  0  0  0  0  0  OJANAF 12/63                    BCLF2
-2116C0+6 503830+5 198311+2 886329-5-147403+7 106267+3  500. 3000.1   0.BCLF2
-2116C0+6 5C3830+5 195580+2 581861-4-347534+6 106267+3 3000. 5000.1   0.BCLF2
  1  5  1  9  2 17  0  0  0  0  0  0  0  OJANAF 12/63                    BCL2F
-154CC0+6 511180+5 198460+2 578157-5-110178+7 110423+3  500. 3000.1   0.BCL2F
-154CCC+6 511180+5 198057+2 126436-4-924350+6 110423+3 3000. 5000.1   0.BCL2F
  1  5  1  9  C  0  0  0  0  0  0  0  0  OJANAF 12/60                    BF
-454690+5 232890+5 887795+1 901824-4-526109+6 669360+2  500. 3000.1   0.BF
-454690+5 232890+5 816859+1 210898-3 279334+7 669360+2 3000. 5000.1   0.BF
  1  5  1  8  1  9  0  0  0  0  0  0  0  OJANAF 12/63                    BFO
-144CC0+6 374660+5 148017+2 227294-4-134052+7 843900+2  500. 3000.1   0.BFO
-144CC0+6 374660+5 157870+2-169659-3-501345+7 843900+2 3000. 5000.1   0.BFO
  1  5  2  9  C  0  C  0  0  0  0  0  0  OJANAF 12/62                    BF2
-13CC00+6 352490+5 137981+2 306556-4-979515+6 874860+2  500. 3000.1   0.BF2
-13CCC0+6 352490+5 148647+2-178860-3-507255+7 874860+2 3000. 5000.1   0.BF2
  1  1  1  5  2  9  0  0  0  0  0  0  0  OJANAF 12/65                    BF2H
-175399+6 472799+5 175176+2 676573-3-126325+7 949169+2  500. 3000.1   0.BF2H
-175399+6 472799+5 198231+2 682930-5-392997+7 949169+2 3000. 5000.1   0.BF2H
  1  5  1  8  2  9  0  0  0  0  0  0  0  OJANAF 12/65                    BF20
-249999+6 497319+5 190106+2 255063-3-106089+7 103271+3  500. 3000.1   0.BF20
-249999+6 497319+5 198673+2 528861-6-189838+7 103271+3 3000. 5000.1   0.BF20
  1  5  3  9  C  C  0  0  0  0  0  0  0  OJANAF 12/63                    BF3
-27C1C0+6 496940+5 197643+2 260131-4-174925+7 100317+3  500. 3000.1   0.BF3
-27C1C0+6 496940+5 190100+2 163117-3 133775+7 100317+3 3000. 5000.1   0.BF3
  1  1  1  5  C  0  0  0  0  0  0  0  0  OJANAF 03/63                    BH
 105630+6 226370+5 871723+1 193099-3-113880+7 593240+2  500. 3000.1   0.BH
 105630+6 226370+5 962344+1 127652-4-442568+7 593240+2 3000. 5000.1   0.BH
  1  1  1  5  1  8  C  0  C  0  0  0  0  OJANAF 12/60                    BHO
-471270+5 356C30+5 142974+2 167620-3-201136+7 764730+2  500. 3000.1   0.BHO
-471270+5 356C30+5 112392+2 644865-3 134967+8 764730+2 3000. 5000.1   0.BHO
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  1  1  1  5  2  8  0  0  0  0  0  0  0  OJANAF 06/63                          BHO2
-1341C0+6 456640+5 182280+2 425108-3-30104+7 924900+2  500. 3000.1   0.BHO2
-1341CC+6 456640+5 168746+2 521159-3 699798+7 924900+2 3000. 5CC0.1   0.BHO2
  2  1  1  5  C  C  C  0  C  0  0  0  0  OJANAF 12/60                          BH2
 66CCCC+5 327480+5 131819+2 199298-3-211346+7 728220+2  5C0. 3C00.1   0.BH2
 66CCCC+5 32748C+5 133411+2 907704-4-580069+6 728220+2 3000. 5000.1   0.BH2
  2  1  1  5  2  8  C  0  0  0  0  0  0  OJANAF 12/60                          BH2O2
-45CCCC+5 597C6C+5 246307+2 263481-3-476319+7 109074+3  5C0. 3000.1   0.BH2O2
-45CCCC+5 597C6C+5 246C15+2 206036-3-244306+7 109074+3 30C0. 5C00.1   0.BH2O2
  3  1  1  5  C  C  C  C  C  0  0  0  0  OJANAF 12/60                          BH3
 19CCCC+5 4245SC+5 179CC7+2 501613-3-495709+7 763790+2  5C0. 3CC0.1   0.BH3
 18CCCC+5 4245SC+5 186890+2 214061-3-464131+7 763790+2 3000. 50C0.1   0.BH3
  3  1  1  5  3  8  0  0  0  0  0  0  0  OJANAF 03/61                          BH3O3
-2386CC+6 860730+5 356846+2 478490-3-720419+7 131808+3  500. 3000.1   0.BH3O3
-2386CC+6 86C73C+5 377529+2-105305-4-127237+8 131808+3 30C0. 5CC0.1   0.BH3O3
  1  5  1  7  C  0  C  0  0  0  0  0  0  OJANAF 09/63                          BN
 152CC0+6 244620+5 88C110+1 108795-3-11246+6 699360+2  500. 3CC0.1   0.BN
 152CC0+6 24462C+5 88C750+1 998189-4 723668+5 699360+2 3CC0. 5000.1   0.BN
  1  5  1  8  C  0  0  C  0  0  0  0  0  OJANAF 06/62                          BO
 5744CC+4 226450+5 862197+1 136981-3-63170+6 670240+2  500. 3000.1   0.BO
 5744CC+4 226450+5 8C3486+1 210252-3 264653+7 670240+2 30CC. 5000.1   0.BO
  1  5  2  8  C  C  0  0  0  0  0  0  0  OJANAF 06/63                          BO2
-726CC0+5 3793C0+5 148552+2 119400-4-999435+6 856360+2  5C0. 30C0.1   0.BO2
-726CC0+5 3793C0+5 118268+2 637770-3 935859+7 856360+2 3000. 5000.1   0.BO2
  2  5  C  0  C  C  0  0  0  0  0  0  0  OJANAF 12/60                          B2
 1993C0+6 238C90+5 891017+1 112093-3-321955+6 678510+2  500. 30C0.1   0.B2
 1993C0+6 238C90+5 724425+1 412560-3 687918+7 678510+2 3000. 500C.1   0.B2
  1  4  2  5  4  8  C  0  0  0  0  0  0  OJANAF 12/62                          B2BE04
-3196CC+6 9C2510+5 373115+2 103876-3-543732+7 142956+3  5C0. 3000.1   0.B2BE04
-3196C0+6 9C2510+5 364687+2 244001-3-163534+7 142956+3 3000. 5000.1   0.B2BE04
  2  5  4  9  C  C  0  0  0  0  0  0  0  OJANAF 12/64                          B2F4
-34219C+6 771CC9+5 29445C+2 401125-3-162754+7 137490+3  5C0. 3000.1   0.B2F4
-34219C+6 771CC9+5 307935+2 121509-5-29627C+7 137490+3 3000. 5000.1   0.B2F4
  4  1  2  5  4  8  C  0  0  0  0  0  0  OJANAF 03/66                          B2H4O4
-3C6S99+6 125740+6 450887+2 266027-2-332605+7 179643+3  500. 3000.1   0.B2H4O4
-30699C+6 125740+6 543119+2 450391-4-15723S+8 179643+3 3000. 5000.1   0.B2H4O4
  6  1  2  5  C  C  C  0  C  0  0  0  0  OJANAF 12/64                          B2H6
 97S9S9+4 957649+5 341573+2 274368-2-380166+7 125539+3  500. 3CC0.1   0.B2H6
 979S59+4 957649+5 435286+2 258895-4-147630+8 125539+3 3000. 5000.1   0.B2H6
  2  5  2  8  C  C  0  0  0  0  0  0  0  OJANAF 03/61                          B2O2
-1116C0+6 5155C0+5 207885+2 370455-5-251331+7 983970+2  500. 3000.1   0.B2O2
-1116C0+6 5155CC+5 196641+2 203148-3 284908+7 983970+2 3000. 5000.1   0.B2O2
  2  5  3  8  C  0  0  0  0  0  0  0  0  OJANAF 03/61                          B2O3
-2101C0+6 615C70+5 257777+2-153675-4-427514+7 111710+3  500. 3000.1   0.B2O3
-2101C0+6 615C70+5 239286+2 345774-3 329402+7 111710+3 3000. 5000.1   0.B2O3
  2  1  3  5  3  8  1  9  0  0  0  0  0  OJANAF 12/65                          B3FH2O3
-381999+6 118199+6 444942+2 15C977-2-352413+7 166007+3  500. 3CC0.1   0.B3FH2O3
-381999+6 118199+6 496065+2 101166-4-904406+7 166007+3 3000. 5000.1   0.B3FH2O3
  1  1  3  5  3  8  2  9  0  0  0  0  0  OJANAF 12/65                          B3F2HO3
-474999+6 12C733+6 460250+2 107470-2-330485+7 172502+3  500. 3000.1   0.B3F2HO3
-474999+6 12C733+6 496410+2 544339-5-697826+7 172502+3 3000. 5CC0.1   0.B3F2HO3
  3  5  3  8  3  9  0  0  C  0  0  0  0  OJANAF 03/65                          B3F3O3
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-5653CC+6 123234+6 472395+2 722094-3-292334+7 179085+3  5C0. 3CCC.1   0.B3F3O3
-5653C0+6 123234+6 496561+2 357165-5-527295+7 179085+3 3000. 5C00.1   0.B3F3O3
  3  1  3  5  3  8  C  0  C  0  0  0  0  OJANAF 03/65                    B3H3O3
-291CCC+6 115496+6 427771+2 198595-2-368114+7 157365+3  5C0. 3000.1   0.B3H3O3
-291CCC+6 115496+6 495563+2 166186-4-11521C+8 157365+3 30C0. 5CCC.1   C.B3H3C3
  3  1  3  5  6  8  C  0  C  0  0  0  0  OJANAF 12/64                    B3H3O6
-542999+6 16C889+6 59469+2 222751-2-381642+7 208309+3  500. 3000.1   0.B3H3O6
-542999+6 160889+6 672365+2 437510-4-147581+8 208309+3 3000. 5CC0.1   0.B3H3O6
  6  1  3  5  3  7  C  0  C  0  0  0  0  OJANAF 03/65                    B3H6N3
-1218S9+6 15C18C+6 537397+2 387996-2-518944+7 180383+3  5C0. 3CCC.1   C.B3H6N3
-1218S9+6 15C18C+6 671331+2 581970-4-225429+8 180383+3 3000. 5CC0.1   0.B3H6N3
  1  5  1  6  C  C  0  0  C  0  0  0  0  OJANAF 06/63                    CB
 198CCC+6 233870+5 887101+1 987600-4-461666+6 689650+2  5C0. 3000.1   0.CB
 198CCC+6 233870+5 864500+1 134780-3 599853+6 689650+2 3000. 5CC0.1   0.CB
  1  6  1 17  C  C  0  0  C  0  0  0  0  OJANAF 12/60                    CCL
 132CCC+6 237850+5 890513+1 416720-4-154333+6 736510+2  50C. 3CCC.1   0.CCL
 132CCC+6 237850+5 857088+1 993826-4 129567+7 736510+2 30CC. 5CC0.1   0.CCL
  1  6  3  9  1 17  0  0  C  0  0  0  0  OJANAF 03/64          111      CCLF3
-166CC0+6 654320+5 257053+2 334186-4-172444+7 120680+3 1000. 3000.1   0.CCLF3  1
-1660C0+6 654320+5 258243+2 146187-5-193275+7 120680+3 30C0. 50C0.1   0.CCLF3  1
  1  6  1  7  1 17  C  C  C  0  0  0  0  OJANAF 12/60                    CCLN
 322CC0+5 375090+5 415997+3-109631-0-651419+9 868930+2  500. 3CCC.1   0.CCLN
 322CC0+5 375C90+5 134744+2 286947-3 348958+7 868930+2 30CC. 5000.1   0.CCLN
  1  6  1  8  1 17  0  C  C  0  0  0  0  OJANAF 12/65                    CCLO
-15CCC0+5 355119+5 131269+2 228137-3-408663+6 926619+2  500. 3CCC.1   0.CCLO
-15CCC0+5 355119+5 139003+2 148315-5-124889+7 926619+2 3000. 5C00.1   0.CCLO
  1  6  2 17  C  C  0  0  0  0  0  0  0  OJANAF 03/65                    CCL2
 75CCC0+5 363CC9+5 137335+2 526254-4-381617+6 936489+2  5C0. 30C0.1   0.CCL2
 75CCC0+5 363CC9+5 139114+2-748804-7-560298+6 936489+2 30CC. 5000.1   0.CCL2
  1  6  2  9  2 17  0  0  0  0  0  0  0  OJANAF 03/64          111      CCL2F2
-115CC0+6 662240+5 257477+2 222257-4-139026+7 125629+3 1000. 3000.1   0.CCL2F2 1
-115CC0+6 662240+5 258288+2 864195-6-154245+7 125629+3 3000. 5CC0.1   0.CCL2F2 1
  1  6  1  8  2 17  0  C  C  0  0  0  0  OJANAF 12/60                    CCL2O
-526CC0+5 5C5950+5 197348+2 333599-4-133141+7 108899+3  500. 3000.1   C.CCL2O
-526CC0+5 5C5950+5 189745+2 170558-3 180683+7 108899+3 3000. 5000.1   0.CCL2O
  1  6  3 17  C  C  0  0  C  0  0  0  0  OJANAF 03/65                    CCL3
 349999+5 5166C9+5 195967+2 821072-4-60355C+6 113242+3  5CC. 3000.1   0.CCL3
 349959+5 5166C9+5 198625+2 165563-5-823646+6 113242+3 3000. 5000.1   0.CCL3
  1  6  1  9  3 17  0  0  C  0  0  0  0  OJANAF 03/64          111      CCL3F
-68CCC0+5 669930+5 257811+2 137845-4-106628+7 128911+3 10CC. 3CCC.1   C.CCL3F  1
-68CCC0+5 669930+5 258333+2 838371-7-116610+7 128911+3 3000. 5CCC.1   0.CCL3F  1
  1  6  4 17  C  C  0  0  0  0  0  0  0  OJANAF 12/60                    CCL4
-2594C0+5 67654C+5 258277+2 144070-5-828977+6 129983+3  500. 3CC0.1   0.CCL4
-2594C0+5 676540+5 253023+2 998371-4 124339+7 129983+3 3000. 5000.1   0.CCL4
  1  6  1  9  0  C  0  0  0  0  0  0  0  OJANAF 03/61                    CF
 744CC0+5 234630+5 889829+1 942918-4-469503+6 701280+2  500. 3000.1   0.CF
 744CC0+5 234630+5 810974+1 241697-3 264745+7 701280+2 3000. 5CCC.1   0.CF
  1  6  1  7  1  9  0  0  0  0  0  0  0  OJANAF 06/61                    CFN
-3CCCC0+4 37C140+5 146756+2 528937-4-15692+7 836950+2  5C0. 3CCC.1   0.CFN
-3CCCC0+4 37C14C+5 156821+2-153382-3-505794+7 836950+2 3000. 5000.1   0.CFN
  1  6  1  8  1  9  C  C  C  0  0  0  0  OJANAF 12/65                    CFO
-4099S9+5 347970+5 13CC71+2 264190-3-618325+6 873199+2  5C0. 3CC0.1   0.CFO
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-4C9999+5 347970+5 139862+2-131517-4-194234+7 873199+2 3000. 5000.1    0.CFO
  1  6  2  9  C  0   0  C  0   0  0  0  0  OJANAF 12/63                  CF2
-3CCCCC+5 349740+5 138552+2 128704-4-118696+7 876320+2  500. 3000.1    0.CF2
-3CCCCC+5 34974C+5 142542+2-646408-4-268538+7 876320+2 3000. 5000.1    0.CF2
  1  6  1  8  2  9   0  0  C   0  0  0  0  OJANAF 12/63                  CF2O
-1525CC+6 49C560+5 196967+2 418619-4-206358+7 100607+3  500. 3000.1    0.CF2O
-1525CC+6 49C56C+5 195291+2 621854-4-110477+7 1C0607+3 3000. 5000.1    0.CF2O
  1  6  3  9  C  C   0  0  0   0  0  0  0  OJANAF 12/63                  CF3
-1165CC+6 4586CC+5 197865+2 200977-4-166384+7 1C2161+3  500. 3000.1    0.CF3
-1165CC+6 4586CC+5 196575+2 404917-4-105310+7 102161+3 3000. 5000.1    0.CF3
  1  6  4  9  C  C   0  0  C   C  0  0  0  OJANAF 12/63                  CF4
-222CCC+6 645420+5 243637+2 395728-3 723010+5 113627+3  5C0. 3000.1    0.CF4
-222CCC+6 645420+5 265430+2-135803-3-518966+7 113627+3 3000. 5000.1    0.CF4
  1  1  1  6  C  C   0  C  0   0  0  0  0  OJANAF 03/61                  CH
 142CC6+6 2213CC+5 826079+1 302211-3-100184+7 616120+2  5CC. 3000.1    0.CH
 142CC6+6 2213CC+5 707C91+1 463281-3 552860+7 616120+2 3000. 5000.1    0.CH
  1  1  1  6  3 17   C  0  0   0  0  0  0  OJANAF 12/60                  CHCL3
-25CCCC+5 634760+5 252779+2 125963-3-28782+7 121245+3  500. 3000.1    0.CHCL3
-25CCCC+5 634760+5 257850+2 237794-5-410561+7 121245+3 3000. 5000.1    0.CHCL3
  1  1  1  6  1  8   1  9  0   0  C  0  0  OJANAF 06/61                  CHFO
-5CCCCC+5 462359+5 167821+2 878833-3-128352+7 944419+2  500. 3000.1    0.CHFO
-5CCCCC+5 462359+5 198008+2 951575-5-498090+7 944419+2 3000. 5000.1    0.CHFO
  1  1  1  6  3  9   0  C  C   0  0  0  0  OJANAF 12/63                  CHF3
-1651CC+6 611C30+5 252113+2 141526-3-400405+7 109082+3  500. 3000.1    0.CHF3
-1651CC+6 611C30+5 259284+2-224709-4-603019+7 109082+3 3CCC. 5000.1    0.CHF3
  1  1  1  6  1  7   1  8  C   0  0  0  0  OJANAF 12/60                  CHNO
-279CCC+5 461930+5 179701+2 469024-3-200904+7 928990+2  500. 3000.1    0.CHNO
-279CCC+5 461930+5 21C167+2-229915-3-105568+8 928990+2 3000. 5000.1    0.CHNO
  2  1  1  6  C  C   0  C  0   0  0  0  0  OJANAF 12/62                  CH2
 95CCCC+5 325960+5 132894+2 413822-3-290273+7 684940+2  500. 3000.1    0.CH2
 95CCCC+5 32996C+5 140728+2 132150-3-239493+7 684940+2 3000. 5000.1    0.CH2
  2  1  1  6  2 17   0  0  0   0  0  0  0  OJANAF 12/60                  CH2CL2
-224CC0+5 595790+5 247355+2 249585-3-481774+7 110269+3  5C0. 3000.1    0.CH2CL2
-224CC0+5 595790+5 258799+2-161283-4-794316+7 110269+3 3000. 5000.1    0.CH2CL2
  2  1  1  6  2  9   0  0  C   0  0  0  0  OJANAF 12/63                  CH2F2
-1C72CC+6 579240+5 246913+2 260835-3-564164+7 102228+3  5C0. 3000.1    0.CH2F2
-1C72CC+6 579240+5 256947+2 195707-4-815777+7 102228+3 3000. 5000.1    0.CH2F2
  2  1  1  6  1  8   C  0  C   0  0  0  0  OJANAF 03/61                  CH2O
-277CC0+5 437910+5 184022+2 379921-3-431982+7 848880+2  500. 3000.1    0.CH2O
-277CC0+5 437910+5 189628+2 161963-3-372770+7 848880+2 3000. 5000.1    0.CH2O
  3  1  1  6  C  C   C  C  0   0  0  0  0  OJANAF 12/62                  CH3
 3194CC+5 434190+5 182763+2 401025-3-461203+7 786040+2  5C0. 3000.1    0.CH3
 3194CC+5 434190+5 204899+2-108028-3-114692+8 786040+2 3000. 5000.1    0.CH3
  3  1  1  6  1 17   C  C  0   0  0  0  0  OJANAF 12/60                  CH3CL
-2C634C+5 5603CC+5 241353+2 388635-3-654504+7 972200+2  500. 3000.1    0.CH3CL
-2C634C+5 5603C0+5 256598+2 197863-4-103065+8 972200+2 3000. 5000.1    0.CH3CL
  3  1  1  6  1  9   0  0  0   0  0  0  0  OJANAF 12/63                  CH3F
-56CCC0+5 552230+5 241434+2 386480-3-701904+7 935320+2  5C0. 3000.1    0.CH3F
-56CCC0+5 552230+5 257207+2 985709-5-110460+8 935320+2 3000. 5000.1    0.CH3F
  1  6  1  7  C  C   C  0  C   0  0  0  0  OJANAF 12/62                  CN
 1C9CC0+6 232490+5 655906+1 115326-2 479517+6 669760+2  500. 3000.1    0.CN
 1C9CCC+6 232490+5 988013+1 313855-3-649453+7 669760+2 3CCC. 50C0.1    C.CN
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  2  6  0  C  C  C  0  0  0  0  0  0  0  OJANAF 9/61                                  C2
 198999+6 246990+5 776612+1 696081-3 18564 9+6 685519+2  500. 3000.1   0.C2
 198599+6 246590+5 104162+2 566841-4-640205+7 685519+2 3000. 5000.1   0.C2
  1  4  2  6  C  C  0  C  C  0  0  0  0  OJANAF 12/63                                 C2BE
 135CCC+6 367740+5 174042+2-702548-3-572915+7 816180+2  500. 3000.1   0.C2BE
 135CCC+6 367740+5 136768+2 233788-3 253563+7 816180+2 3000. 5000.1   0.C2BE
  2  6  2  9  C  C  C  0  C  0  0  0  0  OJANAF 12/60                                 C2F2
-513CCC+5 526690+5 206993+2 383288-4-175788+7 102918+3  500. 3000.1   0.C2F2
-513CCC+5 526690+5 212155+2-681801-4-352776+7 102918+3 3000. 5000.1   0.C2F2
  2  6  4  9  C  0  0  C  0  0  0  0  0  OJANAF 06/63                                 C2F4
-1517CC+6 793120+5 316735+2 255243-4-306132+7 134856+3  500. 3000.1   0.C2F4
-1517CC+6 793120+5 305382+2 247246-3 116982+7 134856+3 3000. 5000.1   0.C2F4
  2  6  6  9  C  C  0  0  0  0  0  0  0  OJANAF 09/65                                 C2F6
-316799+6 1C8115+6 417073+2 306660-3-219022+7 165819+3  500. 3000.1   0.C2F6
-316799+6 1C8115+6 429440+2-413096-4-392508+7 165819+3 3000. 5000.1   0.C2F6
  3  1  2  6  C  C  0  0  0  0  0  0  0  OCUFF BAUER 6/61                              C2H3
 659250+5 562430+5 230065+2 691322-3-499095+7 965150+2  500. 3000.1   0.C2H3
 659250+5 562430+5 239033+2 331771-3-335425+7 965150+2 3000. 5000.1   0.C2H3
  4  1  2  6  C  C  C  0  0  0  0  0  0  OJANAF 12/60                                 C2H4
 124960+5 676830+5 294887+2 526568-3-865313+7 101790+3  500. 3000.1   0.C2H4
 124960+5 676830+5 313872+2 616238-4-131858+8 101790+3 3000. 5000.1   0.C2H4
  4  1  2  6  1  8  C  0  0  0  0  0  0  OJANAF 12/60                                 C2H4O
-1219CC+5 813210+5 353747+2 546144-3-964936+7 117211+3  5C0. 3000.1   0.C2H4O
-1219CC+5 813210+5 373112+2 690621-4-141968+8 117211+3 3000. 5000.1   0.C2H4O
  6  1  2  6  C  C  0  C  0  0  0  0  0  OCUFF BAUER 6/61                              C2H6
-2032CC+5 892710+5 484236+2-169721-2-193680+8 119447+3  500. 3000.1   0.C2H6
-2032CC+5 892710+5 393119+2 764877-3-383891+7 119447+3 3000. 5000.1   0.C2H6
  2  6  2  7  C  C  0  C  0  0  0  0  0  OJANAF 3/61                                  C2N2
 738699+5 511070+5 188740+2 559856-3-896873+6 985479+2  500. 3000.1   0.C2N2
 738699+5 511070+5 208204+2 630229-5-346865+7 985479+2 3000. 5000.1   0.C2N2
  3  6  0  C  C  0  0  0  0  0  0  0  0  OJANAF 12/60                                 C3
 189670+6 366220+5 146441+2 622536-4-168227+7 798410+2  500. 3000.1   0.C3
 189670+6 366220+5 144782+2 792232-4-646877+6 798410+2 3000. 5000.1   0.C3
  2  1  3  6  C  C  0  0  0  0  0  0  0  OCUFF BAUER 6/61                              C3H2
 106522+6 635170+5 247444+2 992918-3-437596+7 104666+3  500. 3000.1   0.C3H2
 106522+6 635170+5 266623+2 364767-3-467730+7 104666+3 3000. 5000.1   0.C3H2
  3  1  3  6  C  C  0  0  0  0  0  0  0  OCUFF BAUER 6/61                              C3H3
 764850+5 709520+5 286929+2 766031-3-548098+7 113604+3  500. 3000.1   0.C3H3
 764850+5 709520+5 291672+2 456238-3-138601+7 113604+3 3000. 5000.1   0.C3H3
  4  1  3  6  C  C  0  0  C  0  0  0  0  OCUFF BAUER 6/61                              C3H4
 442940+5 822470+5 372219+2-528861-4-101994+8 120293+3  500. 3000.1   0.C3H4A
 442940+5 822470+5 344271+2 578173-3-208515+7 120293+3 3000. 5000.1   0.C3H4A
  5  1  3  6  C  C  0  0  C  0  0  0  0  OCUFF BAUER 6/61                              C3H5
 324310+5 946210+5 397325+2 958555-3-904683+7 141759+3  500. 3000.1   0.C3H5
 324310+5 946210+5 395073+2 733720-3-949766+6 141759+3 3000. 5000.1   0.C3H5
  3  6  2  8  C  C  C  C  0  0  0  0  0  OJANAF 12/60                                 C3O2
-83CCC0+4 652120+5 263775+2 103904-3-350368+7 112723+3  5C0. 3000.1   0.C3O2
-83CCCC+4 652120+5 263543+2 882201-4-287091+7 112723+3 3000. 5000.1   0.C3O2
  1  1  1  8  1 17  C  0  0  0  0  0  0  OJANAF 12/60                                 CLHO
-22CCC0+5 329450+5 13C281+2 197747-3-200191+7 828260+2  500. 3000.1   0.CLHO
-22C0C0+5 329450+5 143860+2-989737-4-621082+7 828260+2 3000. 5000.1   0.CLHO
  1  7  1  8  1 17  C  0  C  0  0  0  0  OJANAF 12/60                                 CLNO
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1262C0+5 371C90+5 138156+2 387830-3-10183 4+7 925450+2  500. 3000.1   0.CLNO
1262CC+5 371C90+5 146390+2 226016-3-40594 9+7 925450+2 3000. 5000.1   0.CLNO
 1  7  2  8  1 17  C  C  C  0  0  0  0  OJANAF 12/60                      CLNO2
631CCC+4 49932C+5 19786 +2 190793-4-17114 5+7 105068+3  500. 3000.1   0.CLNO2
631CCC+4 49932C+5 19773 +2 214466-4-16519 1+7 105068+3 3000. 5000.1   0.CLNO2
 1  8  1 17  C  C  C  0  0  0  0  0  OJANAF 12/60                      CLO
241920+5 24C57C+5 889291+1 123702-3-17120 6+6 740940+2  500. 3000.1   0.CLO
241920+5 24C57C+5 810727+1 268314-3 29950 2+7 740940+2 3000. 5000.1   0.CLO
 2  8  1 17  C  C  C  C  C  0  0  0  0  OJANAF 12/60                      CLO2
25CCCC+5 3657BC+5 138491+2 190480-3-68975 9+6 911340+2  500. 3000.1   0.CLO2
25CCCC+5 3657BC+5 131788+2 311873-3 20660 8+7 911340+2 3000. 5000.1   0.CLO2
 1  8  2 17  C  C  0  0  0  0  0  0  0  OJANAF 12/60                      CL20
181CCC+5 3636C0+5 138650+2 123715-4-43322 9+6 937110+2  500. 3000.1   0.CL20
181CC0+5 3636C0+5 137574+2 285555-4 98290 9+5 937110+2 3000. 5000.1   0.CL20
 1  9  0  C  C  C  0  0  0  0  0  0  OJANAF 06/61                      F
1886CC+5 136030+5 489C30+1 256070-4 21541 3+6 497910+2  500. 3000.1   0.F
1886CC+5 136930+5 583971+1-157585-3-36587 6+7 497910+2 3000. 5000.1   0.F
 1  1  1  9  C  C  C  C  0  0  0  0  0  OJANAF 12/63                      FH
-648CCC+5 21C540+5 775546+1 348201-3-12246 0+7 586970+2  500. 3000.1   0.FH
-648CCC+5 21C54C+5 888581+1 799284-4-41903 8+7 586970+2 3000. 5000.1   0.FH
 1  1  1  8  1  9  0  C  0  0  0  0  0  OJANAF 12/60                      FHO
-261CC0+5 326680+5 127356+2 288514-3-18050 1+7 799420+2  500. 3000.1   0.FHO
-261CC0+5 326680+5 154100+2-262264-3-11881 4+8 799420+2 3000. 5000.1   0.FHO
 1  7  1  9  C  C  C  0  0  0  0  0  0  OJANAF 12/60                      FN
586CC0+5 234380+5 9CC098+1-168131-4-40090 8+6 683510+2  500. 3000.1   0.FN
586000+5 234380+5 822584+1 144314-3 22248 6+7 683510+2 3000. 5000.1   0.FN
 1  7  1  8  1  9  C  0  0  0  0  0  0  OJANAF 06/61                      FNO
-157CC0+5 3518C0+5 137563+2 383019-4-10555 7+7 878110+2  500. 3000.1   0.FNO
-157CCC+5 351800+5 129742+2 179442-3 21727 6+7 878110+2 3000. 5000.1   0.FNO
 1  7  2  8  1  9  0  0  0  0  0  0  0  OJANAF 12/62                      FNO2
-19CCC0+5 494740+5 197065+2 401052-4-18351 0+7 101532+3  500. 3000.1   0.FNO2
-19CCC0+5 49474C+5 189123+2 183090-3 14525 9+7 101532+3 3000. 5000.1   0.FNO2
 1  8  1  9  C  0  0  C  C  0  0  0  0  OJANAF 12/60                      FO
324CC0+5 234380+5 880849+1 432306-4-15731 5+6 701930+2  500. 3000.1   0.FO
324CC0+5 234380+5 763129+1 227095-3 58512 2+7 701930+2 3000. 5000.1   0.FO
 2  9  0  C  C  C  0  C  C  0  0  0  0  OJANAF 12/60                      F2
CCCCCC-0 244320+5 874852+1 271736-3-63434 0+5 685700+2  500. 3000.1   0.F2
CCCCC0-0 244320+5 591497+1 736861-3 13720 4+8 685700+2 3000. 5000.1   0.F2
 1  7  2  9  C  C  0  C  0  0  0  0  0  OJANAF 12/62                      F2N
85CCC0+4 35786C+5 138490+2 160322-4-67637 9+6 888700+2  500. 3000.1   0.F2N
85CCC0+4 357860+5 124793+2 272689-3 47208 5+7 888700+2 3000. 5000.1   0.F2N
 2  7  2  9  C  0  0  C  C  0  0  0  0  OJANAF 12/65                      F2N2
163999+5 5CCC19+5 191385+2 216848-3-10092 3+7 102008+3  500. 3000.1   0.F2N2
163999+5 5CC019+5 198696+2 383455-6-17444 1+7 102008+3 3000. 5000.1   0.F2N2
 1  8  2  9  C  C  C  C  C  0  0  0  0  OJANAF 03/61                      F20
76CCCC+4 3615BC+5 138318+2 250576-4-48974 4+6 888610+2  500. 3000.1   0.F20
76CCCC+4 3615BC+5 134205+2 770492-4 20537 8+7 888610+2 3000. 5000.1   0.F20
 1  7  3  9  C  C  C  0  0  C  0  0  0  OJANAF 03/64                  111 F3N
-3C4CCC+5 5C8C6C+5 198144+2 151977-4-11073 4+7 103342+3 1000. 3000.1   0.F3N    1
-3C4CC0+5 5C8C6C+5 198669+2 781936-6-11909 6+7 103342+3 3000. 5000.1   0.F3N    1
 2  7  4  9  C  C  C  C  C  0  0  C  0  OJANAF 03/64                  111 F4N2
-2CCCCC+4 8C672C+5 316906+2 272636-4-20112 1+7 136599+3 1000. 3000.1   0.F4N2   1
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-2CCCCO+4 8C6720+5 317863+2 152639-5-217755+7 136599+3 3000. 5CCC.1   0.F4N2    1
                                                                          HN
  1  1  1  7  C  C  0  0  0  0  0  0  0  0  OJANAF 12/60
 792CCC+5 217660+5 823133+1 281555-3-126896+7 609290+2  500. 3000.1   0.HN
 792CCC+5 217660+5 765457+1 359853-3 180778+7 609290+2 3000. 5000.1   0.HN
                                                                          HNO
  1  1  1  7  1  8  C  C  0  0  0  0  0  0  OJANAF 12/60
 238CCC+5 327550+5 133820+2 122061-3-232403+7 783850+2  5CC. 3CC0.1   0.HNO
 238CCC+5 327550+5 141523+2-470424-4-469135+7 783850+2 3000. 5000.1   0.HNO
                                                                          HNO2
  1  1  1  7  2  8  C  C  0  0  0  0  0  0  OJANAF 06/63
-1834C0+5 4688CC+5 190278+2 189744-3-309752+7 962310+2  500. 3CCC.1   0.HNO2
-1834C0+5 4688C0+5 210284+2-229017-3-978618+7 962310+2 3000. 5000.1   0.HNO2
                                                                          HNO3
  1  1  1  7  3  8  C  C  0  0  0  0  0  0  OJANAF 06/63
-321CC0+5 6C912C+5 253548+2 608154-4-450532+7 110851+3  500. 3000.1   0.HNO3
-321CCC+5 6C912C+5 266283+2-145785-3-10265C+8 110851+3 30C0. 5CC0.1   0.HNO3
                                                                          HO2
  1  1  2  8  C  0  0  0  0  0  0  0  0  0  OJANAF 03/64                 111
 5CCCCC+4 325340+5 127161+2 292770-3-172279+7 799790+2 1000. 3000.1   0.HO2     1
 5CCCCC+4 32534C+5 138028+2 147088-4-399551+7 799790+2 3000. 5000.1   0.HO2     1
                                                                          H2N
  2  1  1  7  C  C  0  0  0  0  0  0  0  0  OJANAF 12/65
 400999+5 3C5799+5 975862+1 114401-2-518970+6 701580+2  5CC. 3000.1   0.H2N
 400999+5 3C5799+5 13741C+2 229493-4-610024+7 701580+2 3000. 5000.1   0.H2N
                                                                          H3N
  3  1  1  7  C  0  0  0  0  0  0  0  0  0  OJANAF 09/65
-1097C0+5 41630C+5 125186+2 219670-2-978531+6 769080+2  500. 3000.1   0.H3N
-1097C0+5 41630C+5 166320+2 923148-3-361337+7 769080+2 3000. 5CC0.1   0.H3N
                                                                          H4N2
  4  1  2  7  C  C  C  0  0  0  0  0  0  0  OJANAF 12/65
 227859+5 685359+5 229856+2 241933-2-195931+7 108099+3  500. 3000.1   0.H4N2
 227859+5 685359+5 314319+2 487945-4-139705+8 108099+3 3000. 5000.1   0.H4N2
                                                                          N
  1  7  0  C  C  C  0  0  0  0  0  0  0  0  OJANAF 03/61
 112965+6 13437C+5 486944+1 383516-4 958460+5 480900+2  500. 3000.1   0.N
 112965+6 134370+5 428957+1 240844-3-417.73+6 480900+2 3000. 5000.1   0.N
                                                                          NO3
  1  7  3  8  C  C  0  0  0  0  0  0  0  0  OJANAF 12/64
 17CCC0+5 498219+5 192301+2 191161-3-112129+7 998970+2  500. 3CC0.1   0.NO3
 17CCC0+5 498219+5 198709+2 577142-7-172913+7 998970+2 3000. 5000.1   0.NO3
                                                                          N20
  2  7  1  8  C  0  0  0  0  0  0  0  0  0  OJANAF 12/60
 195CC0+5 365450+5 144686+2 120489-3-153478+7 815900+2  500. 3000.1   0.N20
 195CC0+5 365450+5 123036+2 459018-3 942382+7 815900+2 3000. 5CC0.1   0.N20
                                                                          N203
  2  7  3  8  C  C  0  0  0  0  0  0  0  0  OJANAF 12/64
 197999+5 617799+5 232121+2 477580-3-124103+7 123217+3  500. 3CC0.1   0.N203
 197999+5 617799+5 248304+2 102872-5-293892+7 123217+3 3000. 5000.1   0.N203
                                                                          N204
  2  7  4  8  C  0  0  C  0  0  0  0  0  0  OJANAF 9/64
 216999+4 785969+5 29773+2 594431-3-178833+7 134908+3  500. 3000.1   0.N204
 216999+4 785969+5 317815+2 175630-5-385969+7 134908+3 3000. 5CC0.1   0.N204
                                                                          N205
  2  7  5  8  C  0  0  0  0  0  0  0  0  0  OJANAF 12/64
 21699+4 915759+5 353051+2 147295-3-163850+7 156719+3  500. 3000.1   0.N205
 21699+4 915759+5 357365+2 624545-5-171267+7 156719+3 3000. 5000.1   0.N205
                                                                          03
  3  8  0  C  C  0  0  0  0  0  0  0  0  0  OJANAF 6/61
 341CC0+5 360230+5 135311+2 238739-3-606511+6 860919+2  500. 3000.1   0.03
 341CCC+5 360230+5 139121+2 125613-3-98065+6 860919+2 3000. 5000.1   0.03
                                                                          C4
  4  6  0  C  C  C  0  0  0  0  0  0  0  0  OJANAF 12/60
 242321+6 511230+5 205903+2 623436-4-257703+7 986760+2  500. 3000.1   0.C4
 242321+6 511230+5 210714+2-434895-4-404939+7 986760+2 3000. 5000.1   0.C4
                                                                          C4H
  1  1  4  6  C  C  C  0  0  0  0  0  0  0  ODUFF BAUER 6/61
 155196+6 64'C30+5 252172+2 574336-3-339547+7 113166+3  500. 3000.1   0.C4H
 155196+6 645C30+5 249358+2 402513-3 377676+7 113166+3 3000. 5000.1   0.C4H
```

```
  2  1  4  6  C  C  0  0  0  0  0  0  0  OCUFF BAUER 6/61                  C4H2
 111715+6 763230+5 298897+2 735927-3-430646+7 119311+3  500. 3000.1   0.C4H2
 111715+6 763230+5 301707+2 456896-3 69812+6 119311+3 3000. 5000.1   0.C4H2
  3  1  4  6  C  C  C  0  0  0  0  0  0  OCUFF BAUER 6/61                  C4H3
 1C1975+6 851450+5 343217+2 855861-3-624935+7 130072+3  500. 3000.1   0.C4H3
 1C1975+6 851450+5 345194+2 564141-3-151557+6 130072+3 3000. 5000.1   0.C4H3
  4  1  4  6  C  C  0  C  0  0  0  0  0  OCUFF BAUER 6/61                  C4H4
 737C5C+5 971240+5 398132+2 961427-3-792442+7 139440+3  5CC. 3000.1   0.C4H4A
 737C5C+5 971240+5 395899+2 720956-3 577880+6 139440+3 3000. 5000.1   0.C4H4A
  4  6  2  7  C  C  C  0  0  0  0  0  0  OJANAF 3/61                      C4N2
 1275CC+6 8C1239+5 297490+2 856052-3-15225S+7 133063+3  500. 3000.1   0.C4N2
 1275C0+6 8C1239+5 327212+2 952999-5-54165+7 133063+3 3000. 5000.1   0.C4N2
  1112      0  C  C  0  0  0  0  0  0  0  0  OJANAF 03/61                    C*
 CCCCC0-0 144120+5 586075+1 953976-4-766621+6 121290+2  500. 3000.2 100.C*
 CC0CC0-0 144120+5 485134+1 291605-3 307202+7 121290+2 3000. 5000.2 100.C*

CCC    0 01-4CCC.                                                    EDGE TABLE
CCC    C 01-35CC.                                                    EDGE TABLE
CCC    C C1-3CCC.                                                    EDGE TABLE
CCC    C 01-25CC.                                                    EDGE TABLE
CCC    C 01-2CCC.                                                    EDGE TABLE
CCC    0 01-15CC.                                                    EDGE TABLE
CCC    0 01-1CCC.                                                    EDGE TABLE
CCC    0 01- 5CC.                                                    EDGE TABLE
1CC    1 11 1CCC.
  4
  .52C E05  .82C E05 1.0
1.C       1.C                -1.0
                    1.C
  .744 E13  .192 E06 1.0
          2.C                1.0
-2.C                2.C      3.0
  .472 EC7  .936 E05 1.0
          1.C       -1.C                    1.0
                    1.C
1.C                 1.C
1.0                 1.C
                                1.0         1.0
1CC    C 01 15CC.                                                    INLET SURF
1CC    0 01 2CCC.                                                    INLET SURF
1CC    0 01 225C.                                                    INLET SURF
1CC    C 01 25CC.                                                    INLET SURF
1CC    C 01 275C.                                                    INLET SURF
1CC    C 01 3CCC.                                                    INLET SURF
1CC    C 01 325C.                                                    INLET SURF
1CC    C C1 35CC.                                                    INLET SURF
1CC    C 01 4CCC.                                                    INLET SURF
C1C    C OC 3692.1   31.4                                            COLS. 3-4
  8
  1 HYDROGEN     1.CC8     0.0322563
  6 CARBON      12.C11     C.CC54551
  7 NITROGEN    14.CC8     0.CC53722
```

SPECIAL UNLEIKED CARBON FOR SURFACE THERMOCHEMISTRY WITH KINETICS

```
  8 OXYGEN      16.000     0.0092299
 13 ALUMINUM    26.970     0.0015542
 17 CHLORINE    35.457     0.0053752
112 SURF CARBON12.011                          1.
144 FROZEN CO2  44.011     0.0002004
CCC    C C1-4CCC.                                          EDGE TABLE
CCC    C C1-35CC.                                          EDGE TABLE
CCC    C C1-3CCC.                                          EDGE TABLE
CCC    C C1-25CC.                                          EDGE TABLE
CCC    C C1-2CCC.                                          EDGE TABLE
CCC    C O1-15CC.                                          EDGE TABLE
CCC    C O1-10CC.                                          EDGE TABLE
CCC    C O1- 5CC.                                          EDGE TABLE
1CC    C 11 1000.                                          THROAT
  4
  .385 E05  .820 E05 1.0
1.0        1.0                 -1.0
                     1.0
  .551 E13  .192 E06 1.0
          2.0                  1.0
-2.0                 2.0       3.0
  .350 E07  .936 E05 1.0
          1.0        -1.0                  1.0
                     1.0
1.0                  1.0
1.0                  1.0
                               1.0         1.0
1CC    1 O1 15CC.
1CC    0 O1 2000.                                          THROAT
1CC    0 O1 2250.                                          THROAT
1CC    0 O1 2500.                                          THROAT
1CC    0 O1 2750.                                          THROAT
1CC    0 O1 3000.                                          THROAT
1CC    0 O1 3250.                                          THROAT
1CC    C O1 3500.                                          THROAT
1CC    C O1 4000.                                          THROAT
C1C    C OC 3487.9   16.0                                  COLS. 5-6
  2
  1 HYDROGEN     1.008     0.0322563
  6 CARBON      12.011     0.0054663
  7 NITROGEN    14.008     0.0053722
  8 OXYGEN      16.000     0.0088130
 13 ALUMINUM    26.970     0.0012613
 17 CHLORINE    35.457     0.0053752
112 SURF CARBON12.011                          1.
144 FROZEN CO2  44.011     0.0001892
CCC    C O1-4CCC.                                          EDGE TABLE
CCC    C C1-3500.                                          EDGE TABLE
CCC    O O1-3000.                                          EDGE TABLE
CCC    O O1-2500.                                          EDGE TABLE
CCC    O O1-2000.                                          EDGE TABLE
CCC    C O1-1500.                                          EDGE TABLE
```

```
CCC    C 01-1CCC.                                                          EDGE TABLE
CCC    C 01- 5CC.                                                          EDGE TABLE
1CC    C 11 1CCC.                                                          EXIT SURF
  4
  .482 EC5  .82C EC5 1.0
1.C        1.C               -1.0
                   1.C
  .691 E13  .152 EC6 1.C
        2.C                  1.0
-2.C               2.C       3.0
  .438 EC7  .936 EC5 1.0
        1.0        -1.0               1.0
                   1.0
1.C                1.C
1.C                1.0
                             1.0      1.0
1CC    0 01 15C0.                                                          EXIT SURF.
1CC    C 01 2CCC.                                                          EXIT SURF.
1CC    0 01 225C.                                                          EXIT SURF.
1C0    0 01 25CC.                                                          EXIT SURF.
1CC    C 01 275C.                                                          EXIT SURF.
1CC    C 01 3C0C.                                                          EXIT SURF.
1CC    C 01 325C.                                                          EXIT SURF.
1CC    C 01 35C0.                                                          EXIT SURF.
1CC    0 01 4C0C.                                                          EXIT SURF.
8CC    C 0C

                                                           CARD COUNT -       650
```

SURFACE THERMOCHEMISTRY OUTPUT

```
      AEROTHERM CHEMICAL EQUILIBRIUM JOB COLS. 1-2       0113000000

RELATIVE ELEMENTAL COMPOSITIONS, ATOMIC WTS/UNIT MASS
  AT.NO.   ELEMENT     ATOMIC WT     COMPONENT 1   COMPONENT 2  COMPONENT 3
     1     HYDROGEN     1.00800      0.0563149      0.           0.
     6     CARBON      12.01100      0.0095102      0.           0.
     7     NITROGEN    14.00800      0.0093791      0.           0.
     8     OXYGEN      16.00000      0.0166260      0.           0.
    13     ALUMINUM    26.97000      0.0030727      0.           0.
    17     CHLORINE    35.45700      0.0093843      0.           0.
   112     SURF CARBON 12.01100      0.             0.           0.0832570
   144     FROZEN CO2  44.01100      0.0003435      0.           0.

 ELEMENT   HYDROGEN    CARBON      NITROGEN     OXYGEN      ALUMINUM    CHLORINE
  SURF CARBON FROZEN CO2
 BASE ST      H2         CO           N2          H2O         ALCl        CLH
    C*        CO2
```

AEROTHERM CHEMICAL EQUILIBRIUM (ACE) SOLUTION

BOUNDARY LAYER EDGE EQUILIBRIUM SOLUTION
(COLUMN 1-2)

```
CP-FROZEN     CP-EQUIL     DLNM/DLNT    DLNM/DLNP     GAMMA
0.14558+001 0.14435+001-0.81164+000 0.41261-001 0.11703+001

PROPERTY ROUTINE OUTPUT IN LB-MASS,FT,SEC,BTU,AND DEG-R
  TEMP        VISC         COND         DBAR         PR          SC
0.68890+004 0.42163-004 0.93793-004 0.33884-003 0.32183+000 0.68678+000
  MU1         MU2         MOL.WT        WTIL        OMTTI
0.70735+000 0.19807+002 0.19147+002 0.67484+004 0.99105+000
ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . . . .
     1           6           7           8          13          17         112         144
 0.56765-001 0.11423+000 0.12138+000 0.24602+000 0.82871-001 0.33274+000 0.          0.15997-001
 0.16904+000 0.11079+000 0.12497+000 0.28076+000 0.52473+001 0.24816+000 0.          0.12335-001

TEMP = 3827.2000 DEG-K     PRES = 48.0000 ATM     MOL WT = 19.1468277
```

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
H2O	0.10535+000	C*	0.	CO	0.18190+000
H2	0.37822+000	CO2	0.69596-002	N2	0.88964-001
CLH	0.94185-001	ALCL	0.28903-001	O	0.28519-002
O2	0.35947-003	C3H	0.44331-013	C2H	0.54238-009
CH4	0.11743-007	C	0.42327-007	C2H2	0.10039-008
H	0.95844-001	HO	0.17554-0[illegible]	NO	0.14984-002
CHO	0.14938-003	CL	0.18321-001	CL2	0.18589-004
CHN	0.11150-004	NO2	0.13707-006	ALCL2	0.18802-001
ALHO2	0.24709-002	AL	0.37455-002	ALO	0.50153-011
ALCLO	0.15062-003	ALH	0.46327-003	ALN	0.36241-005
ALCL3	0.14610-003	ALHO	0.41299-004	ALO	0.14601-002
AL2CL6	0.94705-011	AL2O	0.11965-002	AL2O2	0.26648-004
CCL	0.49479-009	CCLN	0.31033-007	CCLO	0.85979-005
CCL2	0.52291-011	CCL2O	0.77306-009	CCL3	0.33663-014
CCL4	0.74536-017	CH	0.24207-007	CHCL3	0.87642-014
CHNO	0.78685-006	CH2	0.73101-008	CH2CL2	0.25888-011
CH2O	0.15771-005	CH3	0.97560-007	CH3CL	0.28717-009
CN	0.29616-006	C2	0.49783-011	C2H3	0.20021-011
C2H4	0.58513-012	C2H4O	0.13624-015	C2H6	0.12472-015
C2N2	0.66651-011	C3	0.11095-014	C3H2	0.33248-014
C3H3	0.46309-015	C3H4	0.17193-016	C3H5	0.65017-016
C3O2	0.43323-013	CLHO	0.14885-004	CLNO	0.14541-006
CLNO2	0.77073-012	CLO	0.16892-004	CLO2	0.35648-009
CL2O	0.18692-009	HN	0.57221-004	HNO	0.29312-005
HNO2	0.21520-007	HNO3	0.75534-012	HO2	0.19006-005
H2N	0.25741-004	H3N	0.12264-004	H4N2	0.21916-011
N	0.39269-004	NO3	0.25098-012	N2O	0.18861-006
N2O3	0.43220-014	N2O4	0.49638-019	N2O5	0.97819-023
O3	0.14141-009	C4	0.25060-020	C4H	0.49539-017
C4H2	0.57244-018	C4H3	0.11747-019	C4H4	0.91897-021
C4N2	0.61958-020	C*	0.		

```
ENTHALPY = 0.10581A5+004 CAL/GM     ENTROPY = 0.29520+001 CAL/GM-DEG K
DENSITY = 0.19244+000 LB/CU.FT.     MASS CONDENSED/MASS GAS = 0.          H-PRIME = 0.
VEL = 0.        FT/SEC    MACH = 0.          AREA = 0.          SQFT/LB/SEC
H-GAS=, 0.19047+004 BTU/LB   H-KINETIC = 0.        BTU/LB
```

AEROTHERM CHEMICAL EQUILIBRIUM JOB EDGE TABLE 0000000001

TYPICAL EITHALPY ALLOCATION FOR EDGE COMPUTATION & PRINTOUT (COLUMN 1-2)

CP-FROZEN	CP-EQUIL	DLNM/DLNT	DLNM/DLNP	GAMMA
0.47241+000	0.20178+001	-0.77664+000	0.41241+001	0.11378+001

PROPERTY ROUTINE OUTPUT IN LB-MASS,FT,SEC,BTU,AND DEG-R

TEMP	VISC	RGAS	DRHP	PR	SC
0.54300+003	0.52947-004	0.77769-004	0.22622-003	0.32162+000	0.68678+000

ML1	MU2	MOL.WT	WTIL	GRTTI
0.70736+000	0.19807+002	0.19147+002	0.52939+004	0.96359+001

ELEMENTAL 1 AND 2 MASS FRACTIONS BY ATOMIC NUMBER . . . .

1	6	7	8	13	17	112	144
0.56765-001	0.11423+000	0.13138+000	0.26602+000	0.82871-001	0.33274+000	0.	0.15997-001
0.16904+000	0.11039+000	0.12697+000	0.28076+000	0.52333-001	0.24816+000	0.	0.12385-001

TEMP = 3000.0000 DEG-K PRES = 48.0000 ATM MOL WT = 19.1468277

SPECIES	MOLE FR.	SPECIES	MOLE FR.	SPECIES	MOLE FR.
H2O	0.10535+000	O*	0.	CO	0.18190+000
H2	0.32822+000	CO2	0.69596-002	N2	0.88944-001
CLH	0.94185-001	ALCL	0.28903-001	O	0.28519-002
O2	0.35947-003	C3H	0.44331-013	C2H	0.54238-009
CH4	0.11743-007	C	0.42327-007	C2H2	0.10039-008
H	0.95844-001	HO	0.17554-001	NO	0.14984-002
CHO	0.16938-003	CL	0.18321-001	CL2	0.18549-004
CHN	0.11150-004	NO2	0.13707-004	ALCL2	0.18802-001
ALHO2	0.24709-002	AL	0.37455-002	ALO	0.50153-011
ALCLO	0.15062-003	ALN	0.46327-003	ALN	0.36241-005
ALCL3	0.14610-003	ALHO	0.41299-004	ALO	0.14601-002
AL2CL6	0.94705-011	AL2O	0.11965-002	AL2O2	0.26648-004
CCL	0.49479-009	CCLO	0.31033-007	CCLO	0.85979-005
CCL2	0.52291-011	CCL2O	0.77304-009	CCL3	0.33643-014
CCL4	0.74536-017	CH	0.24207-007	CHCL3	0.87642-014
CHNO	0.79685-006	CH2	0.73101-008	CH2CL2	0.25888-011
CH2O	0.15771-005	CH3	0.97560-007	CH3CL	0.28717-009
CN	0.28616-006	C2	0.45783-011	C2H3	0.20021-011
C2H4	0.58513-012	C2H4O	0.13624-015	C2H6	0.12472-015
C2H2	0.66691-011	C3	0.11095-014	C3H2	0.33248-014
C3H3	0.44309-015	C3H4	0.17193-016	C3H5	0.65017-016
C3O2	0.43323-013	CLHO	0.14885-004	CLNO	0.14561-006
CLNO2	0.77073-012	CLO	0.16892-004	CLO2	0.35648-009
CL2O	0.18692-009	HN	0.57221-004	HNO	0.29312-005
HNO2	0.21520-007	HNO3	0.75534-012	HO2	0.19006-005
H2N	0.25741-004	H3N	0.12264-004	H4N2	0.21916-011
N	0.30240-004	NO3	0.25098-012	N2O	0.18841-006
N2O3	0.43220-014	N2O4	0.40638-013	N2O5	0.97819-023
O3	0.15141-009	C4	0.25060-020	C4H	0.49539-017
C4H2	0.57244-018	C4H3	0.11767-019	C4H4	0.91897-021
C4H2	0.61958-020	C*	0.		

0.4800+002 0. 0. 0. 0. 0.30000+004 0. 0.66155+003 0.66155+003000000EDGE TABLE
4800+2 0+0 0+0 0+0 030000+4 0+0 66155+3 66155+3000000 EDGE TABLE *

ENTHALPY = 0.4615535+007 CAL/GM ENTROPY = 0.28353+001 CAL/GM-DEG K

DENSITY = 0.233036+000 LB/CU.FT. MASS CONDENSED/MASS GAS = 0. H-PRIME = 0.

VEL = 0. FT/SEC MACH = 0. AREA = 0. SQFT/LB/SEC

H-GAS=, 0.11908+004 BTU/LB H-KINETIC = 0. BTU/LB

* THIS PRINT FORMAT IN EKKK, CORRECTED IN MASTEK PROGRAM DEC

AEROTHERM CHEMICAL EQUILIBRIUM JOB 1000001011

OUTPUT OF KINETIC EQUATIONS AND KINETIC CONSTANTS (COLUMN 1-2)

*INETIC REACTION---	1	2	3	4
REACTANT COEFFICIENTS				
H2O	1.00	0.	0.	1.00
C*	1.00	2.00	1.00	0.
CC	0.	0.	-1.00	1.00
H2	-1.00	1.00	0.	0.
CO2	0.	0.	1.00	0.
N2	0.	0.	0.	0.
CLH	0.	0.	0.	0.
ALCL	0.	0.	0.	0.
PRODUCT COEFFICIENTS				
H2O	0.	-2.00	0.	0.
C*	0.	0.	0.	0.
CC	1.00	2.00	1.00	0.
H2	0.	3.00	0.	1.00
CO2	0.	0.	0.	1.00
N2	0.	0.	0.	0
CLH	0.	0.	0.	0.
ALCL	0.	0.	0.	0.
PRE-EXPONENT FACTOR	0.520+009	0.944+013	0.472+007	0.100+001
ACTIVATION ENERGY	0.820+005	0.192+004	0.936+005	0.
REACTION ORDER	0.100+001	0.100+001	0.100+001	0.100+001

TYPICAL SURFACE THERMOCHEMICAL CALCULATION (COLUMN I-2)

```
 AEROTHERM CHEMICAL EQUILIBRIUM JOB INLET SURF     1000000001

  CP-FROZEN     CP-EQUIL    PLNM/DLNT    DLNM/DLNP       GAMMA
 0.13968+001 0.15294+001-0.58468-001-0.31107+000 0.16192+001

 PROPERTY ROUTINE OUTPUT IN LB-MASS,FT,SEC,BTU,AND DEG-R
   TEMP          VISC          COND          DBAR          PR            SC
0.49500+004 0.48756-004 0.75408-004 0.19581-003 0.98513+000 0.66975+000
    MU1           MU2         MOL.WT         WTIL          GRTI
0.72510+000 0.20303+002 0.20408+002 0.31164+004 0.96461+000
ELEMENTAL - AND 7 MASS FRACTIONS BY ATOMIC NUMBER . . . .
      1             6             7             8            13            17           112           144
 0.50285-001 0.21922+000 0.11458+000 0.24593+000-0.73496+000-0.76800+000 0.18711+001 0.21600-004
 0.17100+000 0.22171+000 0.11731+000 0.24718+000 0.41449-001 0.20174+000 0.18808+009 0.17318-004

      TEMP = 2750.0000 DEG-K     PRESS = 48.0000 ATM     MOL WT = 20.4081030

   SPECIES   MOLE FR.      SPECIES   MOLE FR.      SPECIES   MOLE FR.
   H2O      0.93906-004   C*       0.             CO       0.31348+000
   H2       0.44078+000   CO2      0.10014-004    N2       0.70349-001
   CLH      0.68177-001   ALCL     0.11466-001    H        0.35247-008
   O2       0.30729-012   C3H      0.16883-003    C2H      0.28259-003
   CH4      0.78117-003   C        0.81659-007    C2H2     0.13396-001
   N        0.65230-002   HO       0.38794-004    NO       0.12937-007
   CHC      0.10374-003   CL       0.71649-003    CL2      0.67912-006
   CHN      0.29680-001   NO2      0.69111-014    ALCL2    0.42685-001
   ALHO2    0.75125-009   AL       0.71919-004    ALC      0.16318-011
   ALCLC    0.13865-007   ALH      0.24363-004    ALN      0.16223-007
   ALCL3    0.13011-002   ALHO     0.16905-008    ALO      0.16367-007
   AL2CL6   0.18212-008   AL2O     0.23353-004    AL2O2    0.35266-011
   CCL      0.15144-008   CCLN     0.12530-004    CCLO     0.14942-005
   CCL2     0.56688-010   CCL2O    0.15178-009    CCL3     0.45911-013
   CCL4     0.36393-015   CH       0.26787-004    CHCLS    0.28247-011
   CHNO     0.13283-005   CH2      0.10334-005    CH2CL2   0.49831-008
   CH2O     0.37995-005   CH3      0.41405-003    CH3CL    0.33849-005
   CN       0.12681-004   C2       0.30301-007    C2H3     0.19565-004
   C2H4     0.98136-004   C2H4O    0.21339-011    C2H6     0.14574-006
   C2N2     0.17335-004   C3       0.16681-006    C3H2     0.34721-004
   C3H3     0.31520-004   C3H4     0.47838-005    C3H5     0.49296-004
   C3C2     0.11197-009   CLHO     0.32738-009    CLNO     0.33571-012
   CLNO2    0.68005-022   CLO      0.27082-010    CLO2     0.15331-019
   CL2O     0.78177-016   HN       0.99275-006    HNO      0.26888-010
   HNO2     0.44192-016   HNO3     0.80848-025    HO2      0.15867-014
   H2N      0.42642-005   H3N      0.31359-004    H4N2     0.75752-012
   N        0.91258-007   NO       0.19164-026    N2O      0.13776-011
   N2O3     0.24181-028   N2O4     0.12380-037    N2O5     0.82324-046
   O3       0.66876-024   C4       0.30334-000    C4H      0.52506-004
   C4H2     0.61674-004   C4H3     0.26561-005    C4H4     0.94775-006
   C4N2     0.14950-006   C*       0.31792+001
 0.48000+002 0.          0.1289+000 0.5200+0050.   0.27500+004 0.          0.44589+003 0.44589+003C*    2INLET SURF
4810+2     0+72884+05200+5   027501+4    0+0 46588+3 46588+3C*    2    INLET SURF *
        E THALPY = 0.46588E4+003 CAL/GM     ENTROPY = 0.44637+001 CAL/GM-DEG K
        DENSITY = 0.27096E+000 LB/CU.FT.     MASS CONDENSED/MASS GAS = 0.          B-PRIME = 0.12888+000
```

* THIS PRINT FORMAT IN ERROR. CORRECTED IN MAIN PROGRAM DECK

APPENDIX G

FORTRAN IV LISTING OF ARCACE COMPUTER PROGRAM

MITCHELL R. WOOL

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```
CSHACE
      REAL NFIA(10) ,NFIB(10) ,FFIN(10) ,UM(10,10) ,TAU(10,10)                SHAC0050
      DIMENSION TF(150),CIJ(150,1)
      DIMENSION X(1 ),VLAM(150,1 ),CC(7960)
      COMMON KIN,KOUT,JAN,MOL,NAB,IDC,N ,KKX(5)
      COMMON FAMCA(150),FAMCB(150),RB(150,2),RC(150,2),
     1  RD(150,2),RE(150,2),RF(150,2),TU(150,2),VN(150),Y(150),WTM(150),
     2  VAL(150,10),FF(150),IFC(150),IP(150),CP(150),H(150),SB(150),
     3  TC(150),VLEX(150),E(150),LAMI(150),GAMK(  1, 1)
      COMMON A(16,16),W(3),WP,B(16),SCH,RHC,VEL,BI,KR(10),TILE(3),NFF,
     1  XC(50),XG(50)
      COMMON ZKE(10),TLC(10),DMCLC(10),WALJP(10),EB(10),ALP(10),GAMH(10)
     1 ,GAMF(10),TQ(10,3),TK(10,3),WAT(10),IR(10),IOAT(10),KAT(10),UM
     2 ,EBL(10)
      COMMON FFA,IS,ISP,P,T,SIP,HIP,EL,ENL,FLIQ,NG,IFL,ISPC,KRALP,CPF,IRE
     1,IER,AA,ITS,IN,IL,IT,MCDE,HMELT,SMELT,TMAX,TMIN,MELT,SUMN,SUML,JC,
     2HG,CPG,SVA,SVB,SVC,SVD,SUMC
      COMMON NNXC,SA1,VMACH,KRZZ,SP1,GAM,THI,MX,DMCHI,HCH,NCV,TBT,IFRZ,NOA
     1T,SR1,IXG,SV1,KKJ,IXC,NXG,SM1,NCATO,SA2,FFF,WS,RV,CMF
      COMMON VA,HOS,DUM1,DUM2,EP,IFCJC,ISP2,WTG,VMU2,WTL
      COMMON NMT,FKF(10) ,EAK(10) ,EXK(10) ,PMU(10,10) ,RMU(10,10)
      COMMON IB(11) ,FNL(10) ,PNUS(10) ,SLAM(10) ,BE(10) ,RY(10) ,
     1         IBC(10) ,JJ(10)
      COMMON SLB(16),SLA(16,16)
      EQUIVALENCE (CC(1),FAMCA(1)),(B(1),X(1)),(GAMK(1),VLAM(1))
      EQUIVALENCE(TU(151),TF(1)),(VNU(1),CIJ(1))
      EQUIVALENCE(TAU(1),A(151)),              (NFIA(1),A(1)),(NFIB(1),
     1A(51)),(FFIN(1),A(101))
    5 FORMAT(I3,F8.2,11E10.3/91X3E10.3)                                       SHAC0320
C   I/O SPECIFICATIONS ALSO IN RERAY                                          SHAC0340
      KIN=8
      KOUT=5
      JAN=13
      REWIND JAN
      ITS = 0                                                                 SHAC0330
   10 CALL ZIPIN                                                              SHAC0370
      IF (KR(2) + KR(3)) 15,15,20                                             SHAC0380
   15 IF (KRALP) 40,45,40
   20 II = C                                                                  SHAC0400
      IF (KR(2)) 30,30,25                                                     SHAC0410
   25 CALL IMELP                                                              SHAC0420
      IF (KR(3)) 40,40,30                                                     SHAC0430
   30 IF (KR(3) - 9) 35,40,40                                                 SHAC0440
   35 CALL INPLT                                                              SHAC0450
      CALL BELCH                                                              SHAC0460
      CALL INPLT                                                              SHAC0470
      REWIND JAN
   40 CALL ALPST                                                              SHAC0480
   45 IF (KR(7) - 1) 80,80,75                                                 SHAC0490
   50 IF (SVA) 60,60,55                                                       SHAC0500
   55 SVA = C.                                                                SHAC0510
      GOTO 65                                                                 SHAC0520
```

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   6C IF(KR(1)-2) 65,7C,70
   65 MCDE = 2                                                          SHAC0540
      JJC = JC                                                          SHAC0550
      CALL MAT1                                                         SHAC0560
      CALL MAT2                                                         SHAC0570
      CALL MAT3                                                         SHAC0580
      JC = JJC                                                          SHAC0590
   7C MCDE=KR(1)
      CALL RERAY(ISPC,A,0,B,0,0,IG)
      CALL PRCPS                                                        SHAC0620
   75 CALL CUTPT                                                        SHAC0630
C*****PRINCIPAL ITERATIVE LOOP                                          SHAC0640
   8C IF (ITS) 10,90,85                                                 SHAC0650
   85 IF (MCDE) 95,95,90                                                SHAC0660
   9C CALL THERM                                                        SHAC0670
      IF (IFRZ) 95,95,150                                               SHAC0680
   95 MODE = KR(1)                                                      SHAC0690
      FLIC = C.                                                         MAT10280
      CALL MAT1                                                         SHAC0700
      CALL MAT2                                                         SHAC0710
      CALL MAT3                                                         SHAC0720
      ITS = ITS + 1                                                     SHAC0730
      B1 = B(1)                                                         SHAC0740
      IF (KR(8)) 105,105,1CC                                            SHAC0750
  1CC CALL KINET                                                        SHAC0760
  1C5 MCE = 1                                                           SHAC0770
      IF (KR(7) - 1) 125,120,110                                        SHAC0780
  11C IQQ = - 2                                                         SHAC0790
      WRITE(KCLT,115)(I,I=1,IS)                                         SHAC0800
  115 FORMAT(/5CH1ITS TEMP   PRES*MWT  EQUIL ER  MASBAL ER  SCALE  7(I3,SHAC0810
     17H MASBAL)/90X3(I3,7H MASBAL))                                    SHAC0820
  12C WRITE(KCLT,5)ITS,T,AA,EL,ENL,CMF,(E(I),I=1,IS)                    SHAC0830
  125 IF (ITS) 5C,75,130                                                SHAC0840
  13C IF (ITS - 60) 14C,135,140                                         SHAC0850
  135 KR(7) = 9                                                         SHAC0860
      IQQ = - 2                                                         SHAC0870
  140 IF (ITS - 7C) 155,155,145                                         SHAC0880
  145 NCV = 1                                                           SHAC0890
      KR(7) = 1                                                         SHAC0900
  15C ITS = - 1                                                         SHAC0910
      GOTC 5C                                                           SHAC0920
  155 CALL SWAP(SLA,SLB,A,B)
      ICT = 1C                                                          SHAC0940
      DUM1=C.
      IQI = IQC                                                         SHAC0950
  16C DO 17C I=1,IS                                                     SHAC0960
      IF (IFC(I) - 1) 170,170,165                                       SHAC0970
  165 A(I + 2,I + 2) = 1.E + 10                                         SHAC0980
  17C CONTINUE                                                          SHAC0990
      IQQ = IQI                                                         SHAC1000
      CALL RERAY(IN,A(IL,IL) ,0,B(IL) ,1,0,IQC)                        SHAC1010
      ICT = ICT - 1                                                     SHAC1020
```

```
      IF (ICT) 190,175,175                                          SHAC1030
  175 IF (IQQ) 190,180,180                                          SHAC1040
  180 CALL AFMAT                                                    SHAC1050
      GOTO(180,90,145,185),NC                                       SHAC1060
  185 CALL SCALE(MOE)                                               SHAC1070
      CALL CRECT(MOE)                                               SHAC1080
      IF (CMF - 1.E - 12) 190,190,205                               SHAC1090
  190 IF (NCV) 195,200,195                                          SHAC1100
  195 CALL SWAP(A,B,SLA,SLB)
      GOTO 145                                                      SHAC1120
  200 NCV = 1                                                       SHAC1130
      GOTO 90                                                       SHAC1140
  205 IF (KR(7) - 1) 80,80,75                                       SHAC1150
      END                                                           SHAC1160

                                          CARD COUNT -      118
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      SUBROUTINEAFMAT                                                    AFMA0010
      REALNFIA(10) ,NFIB(10) ,FFIN(10) ,UM(10,10) ,TAU(10,10)            AFMA0030
      DIMENSION TF(150),CIJ(150,1)
      DIMENSION X(1 ),VLAM(150,1 ),CC(7960)
      COMMONKIN,KOUT,JAN,MCL,NAB,IDC,N ,KKX(5)
      COMMON FAMOA(150),FAMOB(150),RB(150,2),RC(150,2),
     1  RD(150,2),RE(150,2),RF(150,2),TU(150,2),VN(150),Y(150),WTM(150),
     2  VNU(150,10),FF(150),IFC(150),IP(150),CP(150),M(150),SB(150),
     3  TC(150),VLNK(150),E(150),LAMI(150),GAMK(  1, 1)
      COMMON A(16,16),W(3),WM,B(16),SCH,RHO,VEL,B1,KR(10),TILE(3),NFF,
     1  XC(50),XG(50)
      COMMON ZKE(10),TLO(10),DMCLO(10),WALJP(10),EB(10),AL*(10),GAMH(10)
     1 ,GAMF(10),TQ(10,3),TK(10,3),WAT(10),IR(10),IOAT(10),KAT(10),UM
     2 ,EBL(10)
      COMMONFFA,IS,ISP,P,T,SIP,HIP,EL,ENL,FLIQ,NQ,IFL,ISPQ,KRALP,CPF,IRE
     1,IER,AA,ITS,IN,IL,IT,MODE,HMELT,SMELT,TMAX,TMIN,MELT,SUMN,SUML,JC,
     2HG,CPG,SVA,SVB,SVC,SVD,SUMC
      COMMONNXC,SA1,VMACH,KRZZ,SP1,GAM,THI,MX,DMCHI,HCH,NCV,TBT,IFRZ,NOA
     1T,SR1,IXG,SV1,KKJ,IXC,NXG,SH1,NOATO,SA2,FFF,WS,RV,CMF
      COMMONVA,HOS,DUM1,DUM2,EP,IFCJC,ISP2,WTG,VMU2,WTL
      COMMONMT,FKF(10) ,EAK(10) ,EXK(10) ,PMU(10,10) ,RMU(10,10)
      COMMONIB(11) ,FNU(10) ,PNUS(10) ,SLAM(10) ,BE(10) ,BY(10) ,
     1        IBC(10) ,JJ(10)
      COMMON SLB(16),SLA(16,16)
      EQUIVALENCE (CC(1),FAMOA(1)),(B(1),X(1)),(GAMK(1),VLAM(1))
      EQUIVALENCE(TU(151),TF(1)),(VMU(1),CIJ(1))
      EQUIVALENCE(TAU(1),A(151)),          (NFIA(1),A(1)),(NFIB(1),
     1A(51)),(FFIN(1),A(101))
C*****IF TRYING TO PUSH THROUGH TMIN OR TMAX -- REINVERT AND DT TO ZERO AFMA0300
      IF (T - TMIN) 5,5,10                                               AFMA0310
    5 IF (X(1)) 70,20,10                                                 AFMA0320
   10 IF (T - TMAX) 20,15,15                                             AFMA0330
   15 IF (X(1)) 20,20,70                                                 AFMA0340
C*****IF NEW CONDENSED HAS NEG CORRECTION, DELETE AFTER REINVERT         AFMA0350
   20 IF (IER) 30,40,25                                                  AFMA0360
   25 IF (VN(IRE)) 30,30,40                                              AFMA0370
   30 IF (X(IER) + 1.E - 4) 35,40,40                                     AFMA0380
   35 CONTINUE
      CALL SWAP(A,B,SLA,SLB)
      A(IER,IER) = 1.E20                                                 AFMA0410
      B(IER) = - 1.E15                                                   AFMA0420
      IF (DUM1) 135,150,150                                              AFMA0430
C*****IF S.E. ERROR AND CORRECTION ON T OF CONFLICTING SIGN,REINVERT     AFMA0440
   40 IF (MODE - 1) 120,45,125                                           AFMA0450
   45 IF (X(1) + 81) 70,50,50                                            AFMA0460
C*****ON S.E. IF DELTA LN T .GT. .9 REINVERT NO DT IF EL AND ENL ARE SMAAFMA0470
   50 IF (ABS(X(1)) - 0.9) 125,125,55                                    AFMA0480
   55 IF (ENL - 0.02) 60,65,65                                           AFMA0490
   60 IF (EL - 100.) 125,65,65                                           AFMA0500
   65 MODE = 0                                                           AFMA0510
C*****REINVERT                                                          AFMA0520
   70 CALL SWAP(A,B,SLA,SLB)
```

```
C*****IF CONVERGED EXCEPT FOR T ON H OR S OPTIONS  --  NON CONVERGENT    AFMA0540
      IF (MODE - 1) 115,80,75                                            AFMA0550
   75 IF (EL + 100. * ENL - 1.E - 4) 160,160,115                         AFMA0560
C*****ON S.E. OPTION RESULTIN IN CONFLICTING ERROR/CORRECTION OR T PUSH   AFMA0570
C*****IF OTHER BALANCES RELATIVELY GOOD, SET T TO TMIN/TMAX AS PER ERROR  AFMA0580
C*****AND GO TC THERM (IF T ALREADY THERE - NONCONVERGE) ELSE DT TO ZERO  AFMA0590
   80 IF (ABS(B1) - 100. * (EL + ENL)) 115,85,85                         AFMA0600
   85 IF (B1) 90,90,100                                                  AFMA0610
   90 IF (T - TMIN) 160,160,95                                           AFMA0620
   95 T = AMAX1(TMIN,T - 1000.)                                          AFMA0630
      GOTO 155                                                           AFMA0640
  100 IF (T - TMAX) 105,160,160                                          AFMA0650
  105 T = AMIN1(TMAX,T + 1000.)                                          AFMA0660
      IF (ABS(T - TF(JC)) - .001) 110,155,155                            AFMA0670
  110 IFC(JC) = 1                                                        AFMA0680
      VN(JC) = 1.E - 3 / WTM(JC) * WTG                                   AFMA0690
      X(JC) = 0.                                                         AFMA0700
      GOTO 155                                                           AFMA0710
  115 X(1) = 0.                                                          AFMA0720
      MODE = 0                                                           AFMA0730
      TMIN = 300.                                                        AFMA0740
      TMAX = 20000.                                                      AFMA0750
      IN = IN - 1                                                        AFMA0760
      IL = 2                                                             AFMA0770
      GOTO 150                                                           AFMA0780
  120 X(1) = 0.                                                          AFMA0790
  125 IF (X(2) + 1.) 130,165,165                                         AFMA0800
  130 CALL SWAP(A,B,SLA,SLB)
  135 X(2)=WTG
      IF (NR(6)) 140,145,145                                             AFMA0830
  140 X(2) = X(2) + WTL                                                  AFMA0840
  145 X(2)=1.E25*ALOG(X(2)/AA)
      DUM1=-1.                                                           AFMA0860
      A(2,2) = 1.E25                                                     AFMA0870
  150 NQ = 1                                                             AFMA0880
      GOTO 170                                                           AFMA0890
  155 NQ = 2                                                             AFMA0900
      GOTO 170                                                           AFMA0910
  160 NQ = 3                                                             AFMA0920
      GOTO 170                                                           AFMA0930
  165 NQ = 4                                                             AFMA0940
  170 RETURN                                                             AFMA0950
      END

                                                  CARD COUNT -      95
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      SUBROUTINEZIPIN                                                    ZIPI0010
      REALNFIA(10) ,NFIB(10) ,FFIN(10) ,UM(10,10) ,TAU(10,10)            ZIPI0030
      DIMENSIONWR(3)                                                     ZIPI0040
      DIMENSION TF(150),CIJ(150,1)
      DIMENSION X(1 ),VLAM(150,1 ),CC(7960)
      COMMONKIN,KOUT,JAN,MOL,NAB,IDC,N ,KKX(5)
      COMMON FAMOA(150),FAMOB(150),RB(150,2),RC(150,2),
     1  RD(150,2),RE(150,2),RF(150,2),TU(150,2),VN(150),Y(150),WTM(150),
     2  VNU(150,10),FF(150),IFC(150),IP(150),CP(150),H(150),SB(150),
     3  TC(150),VLNK(150),E(150),LAMI(150),GAMK(  1, 1)
      COMMON A(16,16),W(3),WM,B(16),SCH,RHO,VEL,B1,KR(10),TILE(3),NFF,
     1  XC(50),XG(50)
      COMMON ZKE(10),TLO(10),DMCLO(10),WALJP(10),EB(10),ALP(10),GAMH(10)
     1 ,GAMF(10),TQ(10,3),TK(10,3),WAT(10),IR(10),IOAT(10),KAT(10),UM
     2 ,EBL(10)
      COMMONFFA,IS,ISP,P,T,SIP,HIP,EL,ENL,FLIQ,NQ,IFL,ISPQ,KRALP,CPF,IRE
     1,IER,AA,ITS,IN,IL,IT,MODE,HMELT,SMELT,TMAX,TMIN,MELT,SUMN,SUML,JC,
     2HG,CPG,SVA,SVB,SVC,SVD,SUMC
      COMMONNXC,SA1,VMACH,KRZZ,SP1,GAM,THI,MX,DMCHI,HCH,NCV,TBT,IFRZ,NOA
     1T,SR1,IXG,SV1,KKJ,IXC,NXG,SH1,NOATQ,SA2,FFF,WS,RV,CMF
      COMMONVA,HOS,DUM1,DUM2,EP,IFCJC,ISP2,WTG,VMU2,WTL
      COMMONMT,FKF(10) ,EAK(10) ,EXK(10) ,PMU(10,10) ,RMU(10,10)
      COMMONIC(11) ,ALPT(10) ,C(10) ,SORCE(8) ,RA(2) ,IM(10) ,
     1II ,KK ,J ,VINT ,YINT ,JAT(10)
      EQUIVALENCE (CC(1),FAMOA(1)),(B(1),X(1)),(GAMK(1),VLAM(1))
      EQUIVALENCE(TU(1),TF(1)),(VNU(1),CIJ(1))
      EQUIVALENCE(TAU(1),A(151)),          (NFIA(1),A(1)),(NFIB(1),
     1A(51)),(FFIN(1),A(101))
    5 FORMAT(10I1,6F10.5,2A4,A2)                                         ZIPI0290
   10 FORMAT (2I3)
   15 FORMAT (8F10.5)                                                    ZIPI0310
      NFF = 0                                                            ZIPI0320
      Z = 0.0                                                            ZIPI0330
      PR = 0.0                                                           ZIPI0340
      II=0
      IF (ITS + 1) 20,25,20                                              ZIPI0350
   20 FFA = 0.5                                                          ZIPI0360
      W(1) = 1.0                                                         ZIPI0370
      W(2)=0.                                                            ZIPI0380
      W(3)=0.                                                            ZIPI0390
      MX = - 1                                                           ZIPI0400
      NCV = 0                                                            ZIPI0410
      NOAT = 0                                                           ZIPI0420
      WM = 20.                                                           ZIPI0430
      T = 3000.                                                          ZIPI0440
      HIP = 0.                                                           ZIPI0450
      SIP = 0.                                                           ZIPI0460
      KR(4)=0
   25 ITS = 0                                                            ZIPI0480
      IDC = 1                                                            ZIPI0490
      KRALP = KR(4)
      KKJ = 0                                                            ZIPI0510
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```
     30 WS = 1.0                                                          ZIPI0520
    135 READ(KIN,5)KR,Z,PR,FFR,WR,TILE                                    ZIPI1020
        KKX(1) = KR(10)
        WRITE(KCLT,140)TILE,KR                                           ZIPI1030
        KR(8) = 0
    140 FORMAT (1H1 9X35HAEROTHERM CHEMICAL EQUILIBRIUM JOB 2A4,A2,5X10I1) ZIPI1040
        KR(5)=4-KR(1)
        KR(6)=-1
        W(3)=0.0
        KR(4)=-1
        IF (KR(1)-1) 155,150,155
    150 KR(4)=0
        W(3)=2.0
        KR(6)=0
        KR(8)=1
        KR(1)=0
        KR(5)=0
    155 IF (KR(7)) 220,220,156
    156 KR(7) = 5 * (KR(7) - 1) + 1                                      ZIPI1110
    220 MODE = KR(1)                                                     ZIPI1380
    225 IFRZ = 0                                                         ZIPI1410
        IF (MODE - 8) 275,230,275
    230 STOP                                                             ZIPI1430
    275 IF (Z) 280,430,280
    280 IF (MODE - 1) 285,285,300                                        ZIPI1570
    285 T = Z                                                            ZIPI1580
        IF (T) 290,295,295                                               ZIPI1590
    290 T = - T                                                          ZIPI1600
        IFRZ = 1                                                         ZIPI1610
    295 CONTINUE                                                         ZIPI1620
        GOTO 430                                                         ZIPI1630
    300 IF (MODE - 2) 430,415,420
    415 HIP = Z                                                          ZIPI2030
        GOTO 430                                                         ZIPI2040
    420 SIP = Z                                                          ZIPI2050
        IF (SIP + 9999.) 430,425,430                                     ZIPI2060
    425 SIP = SCH                                                        ZIPI2070
    430 IF (PR) 440, 40,435                                              ZIPI2080
    435 P = PR                                                           ZIPI2090
        AA = P * WM                                                      ZIPI2100
    440 KRALP=KR(4)-KRALP
        RETURN
        END                                                              ZIPI2120

                                                  CARD COUNT -       95
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      SUBROUTINEIMELM                                                    IMEL0010
      REALNFIA(10) ,NFIB(10) ,FFIN(10) ,UM(10,10) ,TAU(10,10)            IMEL0030
      DIMENSIONATA(10) ,ATB(10) ,ATC(10)                                 IMEL0040
      DIMENSION TF(150),CIJ(150,1)
      DIMENSION X(1 ),VLAM(150,1 ),CC(7960)
      COMMONKIN,KOUT,JAN,MOL,NAB,IDC,N ,KKX(5)
      COMMON FAMOA(150),FAMOB(150),RB(150,2),RC(150,2),
     1  RD(150,2),RE(150,2),RF(150,2),TU(150,2),VN(150),Y(150),WTM(150),
     2  VNU(150,10),FF(150),IFC(150),IP(150),CP(130),H(150),SB(150),
     3  TC(150),VLNK(150),E(150),LAMI(150),GAMK(  1, 1)
      COMMON A(16,16),W(3),WM,B(16),SCH,RHO,VEL,B1,KR(10),TILE(3),NFF,
     1  XC(50),XG(50)
      COMMON ZKE(10),TLO(10),DMCLO(10),WALJP(10),EB(10),ALP(10),GAMH(10)
     1 ,GAMF(10),TQ(10,3),TK(10,3),WAT(10),IR(10),IOAT(10),KAT(10),UM
     2 ,EBL(10)
      COMMONFFA,IS,ISP,P,T,SIP,HIP,EL,ENL,FLIQ,NQ,IFL,ISPQ,KRALP,CPF,IRE
     1,IER,AA,ITS,IN,IL,IT,MODE,HMELT,SMELT,TMAX,TMIN,MELT,SUMN,SUML,JC,
     2HG,CPG,SVA,SVB,SVC,SVD,SUMC
      COMMONXC,SA1,VMACH,KRZZ,SP1,GAM,THI,MX,DMCHI,HCH,NCV,TBT,IFRZ,NOA
     1T,SR1,IXG,SV1,KKJ,IXC,NXG,SH1,NOATQ,SA2,FFF,MS,RV,CMF
      COMMONVA,HOS,DUM1,DUM2,EP,IFCJC,ISP2,WTG,VMU2,WTL
      COMMONMT,FKF(10) ,EAK(10) ,EXK(10) ,PMU(10,10) ,RMU(10,10)
      COMMONIB(11) ,ENU(10) ,PNUS(10) ,SLAM(10) ,BE(10) ,BY(10) ,
     1        IBC( 3) ,JJ(10)
      EQUIVALENCE (CC(1),FAMOA(1)),(B(1),X(1)),(GAMK(1),VLAM(1))
      EQUIVALENCE(TU(1,1),TF(1)),(VNU(1),CIJ(1))
      EQUIVALENCE(TAU(1),A(151)),              (NFIA(1),A(1)),(NFIB(1),
     1A(51)),(FFIN(1),A(101))
      EQUIVALENCE(TQ(1),ATA(1)),(TQ(11),ATB(1)),(TQ(21),ATC(1))          IMEL0290
    5 FORMAT (I3)                                                        IMEL0300
   10 FORMAT(I3,3A4,4F10.5)                                              IMEL0310
   15 FORMAT(54HORELATIVE ELEMENTAL COMPOSITIONS, ATOMIC WTS/UNIT MASS   IMEL0320
     1/6X6HAT.NO.3X7HELEMENT4X9HATOMIC WT4X38HCOMPONENT 1  COMPONENT 2   IMEL0330
     1COMPONENT 3 /(7X13,3X3A4,F10.5,3F13.7))                            IMEL0340
   20 READ(KIN,5)IS                                                      IMEL0350
      IX = 3                                                             IMEL0360
      IF (IS - 10) 25,25,80                                              IMEL0370
   25 READ(KIN,10)(KAT(J),ATA(J),ATB(J),ATC(J),WAT(J),TK(J,1),TK(J,2),TKIMEL0380
     1(J,3),J=1,IS)                                                      IMEL0390
   30 DO 55 K=1,3                                                        IMEL0400
      VA = 0.                                                            IMEL0410
      DO 50 J=1,IS                                                       IMEL0420
      IF (KAT(J) - 99) 35,45,35                                          IMEL0430
   35 IF (TK(J,K)) 40,50,45                                              IMEL0440
   40 VA = VA - TK(J,K)                                                  IMEL0450
      TK(J,K) = - TK(J,K) / WAT(J)                                       IMEL0460
      GOTO 50                                                            IMEL0470
   45 VA = VA + TK(J,K) * WAT(J)                                         IMEL0480
   50 CONTINUE                                                           IMEL0490
      DO 55 J=1,IS                                                       IMEL0500
   55 TK(J,K) = TK(J,K) / VA                                             IMEL0510
      WRITE(KOUT,15)(KAT(J),ATA(J),ATB(J),ATC(J),WAT(J),TK(J,1),TK(J,2),IMEL0520
```

```
     1TK(J,3),J=1,IS)                                                    IMEL0530
      ISP = IS + 1                                                       IMEL0540
      IF (KR(3)) 65,65,60                                                IMEL0550
   6C IF (KR(3) - 9) 85,65,85                                            IMEL0560
   65 CONTINLE
      DO 7C L=1,3                                                        IMEL0580
      DC 7C I=1,IS                                                       IMEL0590
      TQ(I,L) = 0.                                                       IMEL0600
      DO 7C K=1,IS                                                       IMEL0610
   70 TQ(I,L) = TQ(I,L) + UM(I,K) * TK(K,L)                              IMEL0620
   75 FORMAT (////31H PROGRAM LIMITED TO 10 ELEMENTS)                    IMEL0630
   85 RETURN                                                             IMEL0660
   80 WRITE(KOUT,75)                                                     IMEL0640
      STOP                                                               IMEL0650
      END                                                                IMEL0670

                                                  CARD COUNT -      67
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      SUBROUTINEINPUT                                                    INPU0010
      REALNFIA(10) ,NFIB(10) ,FFIN(10) ,UM(10,10) ,TAU(10,10)            INPU0030
      DIMENSION TF(150),CIJ(150,1)
      DIMENSION X(1 ),VLAM(150,1 ),CC(7960)
      COMMONKIN,KOUT,JAN,MCL,NAB,IDC,N ,KKX(5)
      COMMON FAMOA(150),FAMOB(150),RB(150,2),RC(150,2),
     1  RD(150,2),RE(150,2),RF(150,2),TU(150,2),VN(150),Y(150),WTM(150),
     2  VNU(150,10),FF(150),IFC(150),IP(150),CP(150),H(150),SB(150),
     3  TC(150),VLNK(150),E(150),LAMI(150),GAMK(  1, 1)
      COMMON A(16,16),W(3),WM,B(16),SCH,RHO,VEL,B1,KR(10),TILE(3),NFF,
     1  XC(50),XG(50)
      COMMON ZKE(10),TLO(10),DMCLO(10),WALJP(10),EB(10),ALP(10),GAMH(10)
     1 ,GAMF(10),TQ(10,3),TK(10,3),WAT(10),IR(10),IOAT(10),KAT(10),UM
     2 ,EBL(10)
      COMMONFFA,IS,ISP,P,T,SIP,HIP,EL,ENL,FLIQ,NQ,IFL,ISPQ,KRALP,CPF,IRE
     1,IER,AA,ITS,IN,IL,IT,MODE,HMELT,SMELT,TMAX,TMIN,MELT,SUMN,SUML,JC,
     2HG,CPG,SVA,SVB,SVC,SVD,SUMC
      COMMONNXC,SA1,VMACH,KRZZ,SP1,GAM,THI,MX,DMCHI,HCH,NCV,TBT,IFRZ,NOA
     1T,SR1,IXG,SV1,KKJ,IXC,NXG,SH1,NOATO,SA2,FFF,WS,RV,CMF
      COMMONVA,NOS,DUM1,DUM2,EP,IECJC,ISP2,HTG,VMU2,HTL
      COMMONMT,FKF(10) ,EAK(10) ,EXK(10) ,PMU(10,10) ,RMU(10,10)
      COMMONIC(11) ,ALPT(10) ,C(10) ,SORCE(8) ,RA(2) ,IM(10) ,
     1II ,KK ,J ,YINT ,YINT ,JAT(10) ,KPHA(2)
      EQUIVALENCE (CC(1),FAMOA(1)),(B(1),X(1)),(GAMK(1),VLAM(1))
      EQUIVALENCE(TU(151),TF(1)),(VNU(1),CIJ(1))
      EQUIVALENCE(TAU(1),A(151),          (NFIA(1),A(1)),(NFIB(1),
     1A(51)),(FFIN(1),A(101))
    5 FORMAT (I3)                                                        INPU0290
   10 FORMAT (6E9.6,6XF6.0,I1)                                           INPU0300
   15 FORMAT(1X6E12.5,F10.4,I2/1X6E12.5,F10.4,I2,F7.4)                   INPU0310
   20 FORMAT(2A4,E12.4,2A4,E12.4,2A4,E12.4,2A4,E12.4)                    INPU0320
   25 FORMAT( 7(F3.0,I3),A2,9A4)
      J = ISP                                                            INPU0340
      IF (II) 30,30,35                                                   INPU0350
   30 CONTINUE
      NFF = 0                                                            INPU0370
      JC=KR(3) - (KR(3) / 2) * 2
      VINT = P * 1.E - 6                                                 INPU0390
      YINT = ALOG(VINT)                                                  INPU0400
      JAT(8) = 0                                                         INPU0410
      N = 0                                                              INPU0420
      II = ISP                                                           INPU0430
      J = 1                                                              INPU0440
      IFL = - 1                                                          INPU0450
      IDC = 1                                                            INPU0460
   35 IF (KR(3) - 5) 40,50,50                                            INPU0470
   40 READ(KIN,25)(ALPT(K),JAT(K),K=1,7),SORCE,AMOA,AMOB
      IF (KR(3) - 3) 55,45,45                                            INPU0490
   45 WRITE(  JAN) ALPT,JAT,SORCE,AMOA,AMOB
      GOTO 55                                                            INPU0510
   50 READ (  JAN) ALPT,JAT,SORCE,AMOA,AMOB
   55 IF (ALPT(1)) 60,375,60                                             INPU0530
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```
   60 IF (JAT(1)) 65,65,85                                          INPU0540
   65 INF = NFF + 1                                                 INPU0550
      K = ALPT(1)                                                   INPU0560
      NFF = K + NFF                                                 INPU0570
      IF (KR(3) - 5) 70,80,80                                       INPU0580
   70 READ(KIN,20)(NFIA(I),NFIB(I),FFIN(I),I=INF,NFF)               INPU0590
      IF (KR(3) - 3) 35,75,75                                       INPU0600
   75 WRITE(  JAN) (NFIA(I) ,NFIB(I) ,FFIN(I) ,I = INF,NFF)
      GOTO 35                                                       INPU0620
   80 READ(  JAN) (NFIA(I) ,NFIB(I) ,FFIN(I) ,I = INF,NFF)
      GOTO 35                                                       INPU0640
   85 DO 90 K=1,IS                                                  INPU0650
   90 C(K) = 0.                                                     INPU0660
      DO 110 I=1,7                                                  INPU0670
      IF (JAT(I)) 95,110,95                                         INPU0680
   95 DO 100 K=1,IS                                                 INPU0690
      IF (JAT(I) - KAT(K)) 100,105,100                              INPU0700
  100 CONTINUE                                                      INPU0710
      KK = II                                                       INPU0720
      GOTO 285                                                      INPU0730
  105 C(K) = ALPT(I)                                                INPU0740
  110 CONTINUE                                                      INPU0750
  115 WT = 0.                                                       INPU0760
      IF (JC) 125,120,125
  120 WRITE(KOUT,25)(ALPT(K),JAT(K),K=1,7),SORCE,AMOA,AMOB
  125 L = 1                                                         INPU0790
      LAMKK = 0                                                     INPU0800
      DO 140 I=1,IS                                                 INPU0810
      IF (C(I)) 130,135,130                                         INPU0820
  130 LAMKK = LAMKK + L                                             INPU0830
  135 L = L + L                                                     INPU0840
      ALPT(I) = C(I)                                                INPU0850
  140 WT = WT + C(I) * WAT(I)                                       INPU0860
      IF (J - IS) 145,145,215                                       INPU0870
  145 JM = J - 1                                                    INPU0880
      IF (JM) 175,175,150                                           INPU0890
  150 DO 170 L=1,JM                                                 INPU0900
      IML = IM(L)                                                   INPU0910
      UGH = C(IML)                                                  INPU0920
      UM(L,J) = 0.                                                  INPU0930
      IF (UGH) 155,170,155                                          INPU0940
  155 DO 160 I=1,L                                                  INPU0950
  160 UM(I,J) = UM(I,J) - UM(I,L) * UGH                             INPU0960
      DO 165 I=IML,IS                                               INPU0970
  165 C(I) = C(I) - TAU(I,L) * UGH                                  INPU0980
  170 UM(J,L) = 0.                                                  INPU0990
  175 DO 180 I=1,IS                                                 INPU1000
      IF (ABS(C(I)) - .001) 180,180,185                             INPU1010
  180 TAU(I,J) = 0.                                                 INPU1020
      GOTO 215                                                      INPU1030
  185 IM(J) = I                                                     INPU1040
      UM(J,J) = 1.                                                  INPU1050
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      DO 190 L=1,J                                                      INPU1060
  190 UM(L,J) = UM(L,J) / C(I)                                          INPU1070
      DO 195 L=I,IS                                                     INPU1080
  195 TAU(L,J) = C(L) / C(I)                                            INPU1090
  205 YC = YINT                                                         INPU1150
      DO 210 L=1,IS                                                     INPU1160
  210 CIJ(J,L) = ALPT(L)                                                INPU1170
      KK = J                                                            INPU1180
      KKK = J                                                           INPU1190
      J = J + 1                                                         INPU1200
      GOTO 285                                                          INPU1210
  215 CONTINUE
  250 IF (J - IS) 255,255,270                                           INPU1350
  255 DO 260 I=1,JM                                                     INPU1360
  260 VNU(II,I) = - UM(I,J)                                             INPU1370
      DO 265 I=J,IS                                                     INPU1380
  265 VNU(II,I) = 0.                                                    INPU1390
      GOTO 280                                                          INPU1400
  270 DO 275 L=1,IS                                                     INPU1410
      VNU(II,L) = 0.                                                    INPU1420
      DO 275 I=1,IS                                                     INPU1430
  275 VNU(II,L) = VNU(II,L) + C(I) * UM(L,I)                            INPU1440
  280 KK = II                                                           INPU1450
      KKK = II                                                          INPU1460
      II = II + 1                                                       INPU1470
      YC = 0.                                                           INPU1480
  285 IF (KR(3) - 5) 290,300,300                                        INPU1490
  290 READ(KIN,10)(RA(K),RB(KK,K),RC(KK,K),RD(KK,K),RE(KK,K),RF(KK,K),TUINPU1500
     1(KK,K),KPHA(K),K=1,2)                                             INPU1510
      IF (KR(3) - 3) 305,295,295                                        INPU1520
  295 WRITE(  JAN) (RA(K) ,RB(KK,K) ,RC(KK,K) ,RD(KK,K) ,RE(KK,K) ,RF(KK
     1,K) ,TU(KK,K) ,KPHA(K) ,K = 1,2)                                  INPU1540
      GOTO 305                                                          INPU1550
  300 READ(  JAN) (RA(K) ,RB(KK,K) ,RC(KK,K) ,RD(KK,K) ,RE(KK,K) ,RF(KK,
     1K) ,TU(KK,K) ,KPHA(K) ,K = 1,2)                                   INPU1570
  305 IF (KK - II) 310,35,310                                           INPU1580
  310 TF(KK) = 20000.                                                   INPU1590
      IF (KPHA(1) - KPHA(2)) 315,330,320                                INPU1600
  315 IF (KPHA(1) + KPHA(2) - 5) 320,335,320                            INPU1610
  320 WRITE(KOUT,325)APOA,AMOB                                          INPU1620
      STOP                                                              INPU1630
  325 FORMAT (////25H BAD PHASE NUMBERING FOR 2A4)                      INPU1640
  330 IF (KPHA(1) - 1) 345,345,340                                      INPU1650
  335 TU(KK,1) = - TU(KK,1)                                             INPU1660
  340 FF(KK) = 1.E + 10                                                 INPU1670
      IFC(KKK) = - 1                                                    INPU1680
      VN(KK) = 0.                                                       INPU1690
      Y(KK) = AMAX1(YC,0.)                                              INPU1700
      GOTO 355                                                          INPU1710
  345 FF(KK) = (WT / 20.) * * FFA                                       INPU1720
  350 IFC(KKK) = C                                                      INPU1730
      VN(KK) = VINT                                                     INPU1740
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      Y(KK) = YINT                                                          INPU1750
  355 IF (JC)  365,360,365
  360 WRITE(KOUT,15)(RA(K),RB(KK,K),RC(KK,K),RD(KK,K),RE(KK,K),RF(KK,K),INPU1770
     1TU(KK,K),KPHA(K),K=1,2),FF(KK)                                        INPU1780
                                                                            INPU1790
  365 FAMOA(KK) = AMOA                                                      INPU1800
      FAMOB(KK) = AMOB                                                      INPU1810
      LAMI(KK) = LAMKK                                                      INPU1820
      WTM(KK) = WT                                                          INPU1830
      RB(KK,1) = RB(KK,1) + RA(1)                                           INPU1840
      RB(KK,2) = RB(KK,2) + RA(2)                                           INPU1850
      N = N + 1                                                             INPU1860
      IF (KK - IS) 35,370,35
  370 CONTINUE
  375 CONTINUE
  390 RETURN                                                                INPU1920
      END                                                                   INPU1930

                                                  CARD COUNT -        172
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      SUBROUTINEBELCH                                                    BELC0010
      REALNFIA(10) ,NFIB(10) ,FFIN(10) ,UM(10,10) ,TAU(10,10)            BELC0030
      DIMENSIONFAMA(10) ,FAMB(10)                                        BELC0040
      DIMENSIONATA(10) ,ATB(10) ,ATC(10)                                 BELC0050
      DIMENSIONLIM(10,10)                                                BELC0060
      DIMENSION TF(150),CIJ(150,1)
      DIMENSION X(1 ),VLAM(150,1 ),CC(7960)
      COMMONKIN,KOUT,JAN,MOL,NAB,IDC,N ,KKX(5)
      COMMON FAMOA(150),FAMOB(150),RB(150,2),RC(150,2),
     1  RD(150,2),RE(150,2),RF(150,2),TU(150,2),VN(150),Y(150),WTM(150),
     2  VNU(150,10),FF(150),IFC(150),IP(150),CP(150),H(150),SB(150),
     3  TC(150),VLNK(150),E(150),LAMI(150),GAMK(  1, 1)
      COMMON A(16,16),W(3),WM,B(16),SCH,RHO,VEL,B1,KR(10),TILE(3),NFF,
     1  XC(501,XG(50)
      COMMON ZKE(10),TLO(10),DMCLO(10),WALJP(10),EB(10),ALP(10),GAMH(10)
     1 ,GAMF(10),TQ(10,3),TK(10,3),WAT(10),IR(10),IOAT(10),KAT(10),UM
     2 ,EBL(10)
      COMMONFFA,IS,ISP,P,T,SIP,HIP,EL,EML,FLIQ,NQ,IFL,ISPQ,KRALP,CPF,IRE
     1,IER,AA,ITS,IN,IL,IT,MODE,HMELT,SMELT,TMAX,TMIN,MELT,SUMN,SUML,JC,
     2MG,CPG,SVA,SVB,SVC,SVD,SUMC
      COMMONNXC,SA1,VMACH,KRZZ,SP1,GAM,THI,MX,DMCHI,HCH,NCV,TBT,IFRZ,NOA
     1T,SR1,IXG,SV1,KKJ,IXC,NXG,SH1,NOATO,SA2,FFF,WS,RV,CMF
      COMMONVA,MOS,DUM1,DUM2,EP,IFCJC,ISP2,WTG,VMU2,WTL
      COMMONWT,PKF(10) ,EAK(10) ,EXK(10) ,PMU(10,10) ,RMU(10,10)
      COMMONIC(11) ,ALPT(10) ,C(10) ,SORCE(8) ,RA(2) ,IN(10) ,
     1II ,KK ,J ,VINT ,YINT ,JAT(10)
      EQUIVALENCE (CC(1),FAMOA(1)),(B(1),X(1)),(GAMK(1),VLAM(1))
      EQUIVALENCE(TU(151),TF(1)),(VNU(1),CIJ(1))
      EQUIVALENCE(TAU(1,1),A(15,11),          (NFIA(1),A(1,1)),(NFIB(1),
     1A(51)),(FFIN(1),A(101))
      EQUIVALENCE(TQ(1),ATA(1)),(TQ(11),ATB(1)),(TQ(21),ATC(1))          BELC0310
      IF (N - 150) 15,15,5                                               BELC0320
    5 NEX = N - 150                                                      BELC0330
      WRITE(KOUT,10)NEX                                                  BELC0340
   10 FORMAT(////11H THERE ARE I2,15H EXCESS SPECIES)                    BELC0350
      STOP                                                               BELC0360
   15 IF (J - IS) 20,20,35                                               BELC0370
   20 JM = J - 1                                                         BELC0380
      WRITE(KOUT,25)JM,IS,(FAMOA(I),FAMOB(I),I=1,JM)                     BELC0390
      WRITE(KOUT,30)(FAMOA(I),FAMOB(I),I=ISP,N)                          BELC0400
      STOP                                                               BELC0410
   25 FORMAT(////15H ONLY FOLLOWINGI3,23H BASE SPECIES FOUND FORI3,       BELC0420
     19H ELEMENTS/(2X20A4))                                              BELC0430
   30 FORMAT(/30H OTHER SPECIES CONSIDERED WERE/(2X20A4))                 BELC0440
   35 DO 45 L=2,IS                                                       BELC0450
      JM = ISP - L                                                       BELC0460
      IMJ = IM(JM + 1)                                                   BELC0470
      IF (JM - 1) 50,40,40                                               BELC0480
   40 DO 45 K=1,JM                                                       BELC0490
      UGH = TAU(IMJ,K)                                                   BELC0500
      DO 45 I=1,IS                                                       BELC0510
   45 UM(I,K) = UM(I,K) - UGH * UM(I,JM + 1)                             BELC0520
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   50 CONTINUE                                                          BELC0530
      DO 70 I=1,IS                                                      BELC0540
   55 IMI = IM(I)                                                       BELC0550
      IF (IMI - I) 60,70,60                                             BELC0560
   60 DO 65 K=1,IS                                                      BELC0570
      V = UM(K,IMI)                                                     BELC0580
      UM(K,IMI) = UM(K,I)                                               BELC0590
   65 UM(K,I) = V                                                       BELC0600
      IM(I) = IM(IMI)                                                   BELC0610
      IM(IMI) = IMI                                                     BELC0620
      GOTO 55                                                           BELC0630
   70 CONTINUE                                                          BELC0640
C-----ELEMENT -- BASE GAS CORRESPONDENCE                                BELC0680
C     INITIALIZE ROW AND COLUMN SUMS                                    BELC0690
      IG = IS                                                           BELC0700
      DO 75 I=1,IS                                                      BELC0710
      IR(I) = - 1                                                       BELC0720
   75 IC(I) = - 1                                                       BELC0730
C     EVALUATE INITIAL SUMS                                             BELC0740
      LAMD = 1                                                          BELC0750
      DO 90 I=1,IS                                                      BELC0760
      DO 85 J=1,IS                                                      BELC0770
      LAMT = LAMI(J) / LAMD                                             BELC0780
      LIM(I,J) = LAMT - (LAMT / 2) * 2                                  BELC0790
      IF (LIM(I,J)) 80,85,80                                            BELC0800
   80 IC(J) = IC(J) + 1                                                 BELC0810
      IR(I) = IR(I) + 1                                                 BELC0820
   85 CONTINUE                                                          BELC0830
   90 LAMD = LAMD + LAMD                                                BELC0840
C     CHECK FOR ZEROS                                                   BELC0850
   95 IZ = 0                                                            BELC0860
  100 DO 185 I=1,IS                                                     BELC0870
      IF (IC(I) - IZ) 140,105,140                                       BELC0880
  105 DO 110 J=1,IS                                                     BELC0890
      IF (LIM(J,I)) 115,110,115                                         BELC0900
  110 CONTINUE                                                          BELC0910
  115 IC(I) = - J                                                       BELC0920
      IR(J) = - I                                                       BELC0930
      LIM(J,I) = 0                                                      BELC0940
      DO 135 K=1,IS                                                     BELC0950
      IF (LIM(J,K)) 120,125,120                                         BELC0960
  120 IC(K) = IC(K) - 1                                                 BELC0970
      LIM(J,K) = 0                                                      BELC0980
  125 IF (LIM(K,I)) 130,135,130                                         BELC0990
  130 LIM(K,I) = 0                                                      BELC1000
      IR(K) = IR(K) - 1                                                 BELC1010
  135 CONTINUE                                                          BELC1020
      GOTO 190                                                          BELC1030
  140 IF (IR(I) - IZ) 185,145,185                                       BELC1040
  145 DO 155 J=1,IS                                                     BELC1050
      IF (LIM(I,J)) 150,155,150                                         BELC1060
  150 IC(J) = - I                                                       BELC1070
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      IR(I) = - J                                                        BELC1080
      LIM(I,J) = 0                                                       BELC1090
      GOTO 160                                                           BELC1100
  155 CONTINUE                                                           BELC1110
  160 DO 180 K=1,IS                                                      BELC1120
      IF (LIM(K,J)) 165,170,165                                          BELC1130
  165 IR(K) = IR(K) - 1                                                  BELC1140
      LIM(K,J) = 0                                                       BELC1150
  170 IF (LIM(I,K)) 175,180,175                                          BELC1160
  175 LIM(I,K) = 0                                                       BELC1170
      IC(K) = IC(K) - 1                                                  BELC1180
  180 CONTINUE                                                           BELC1190
      GOTO 190                                                           BELC1200
  185 CONTINUE                                                           BELC1210
      IZ = IZ + 1                                                        BELC1220
      GOTO 100                                                           BELC1230
  190 IG = IG - 1                                                        BELC1240
      J = IS + 1                                                         BELC1250
      IF (IG) 195,195,95                                                 BELC1260
  195 DO 200 I=1,IS                                                      BELC1270
      K = - IR(I)                                                        BELC1280
      FAMA(I) = FAMOA(K)                                                 BELC1290
  200 FAMB(I) = FAMOB(K)                                                 BELC1300
      WRITE(KOUT,205)(ATA(I),ATB(I),ATC(I),I=1,IS)                       BELC1310
      WRITE(KOUT,210)(FAMA(I),FAMB(I),I=1,IS)                            BELC1320
  205 FORMAT(/5X9HELEMENT   18A4/(5X21A4))                               BELC1330
  210 FORMAT( 5X9HBASE SP   6(4X2A4)/5X7(4X2A4))                         BELC1340
      DO 215 L=1,3                                                       BELC1350
      DO 215 I=1,IS                                                      BELC1360
      TQ(I,L) = 0.                                                       BELC1370
      DO 215 K=1,IS                                                      BELC1380
  215 TQ(I,L) = TQ(I,L) + UR(I,K) * TK(K,L)                              BELC1390
  220 RETURN                                                             BELC1400
      END                                                                BELC1410

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      SUBROUTINEALPST                                                    ALPS0010
      REALNFIA(10) ,NFIB(10) ,FFIN(10) ,UM(10,10) ,TAU(10,10)
      DIMENSION TF(150),CIJ(150,1)
      DIMENSION X(1 ),VLAM(150,1 ),CC(7960)
      COMMONKIN,KCUT,JAN,MCL,NAB,IDC,N ,KKX(5)
      COMMON FAMOA(150),FAMCB(150),RB(150,2),RC(150,2),
     1  RD(150,2),RE(150,2),RF(150,2),TU(150,2),VN(150),Y(150),WTM(150),
     2  VNU(150,10),FF(150),IFC(150),IP(150),CP(150),H(150),SB(150),
     3  TC(150),VLNK(150),E(150),LAMI(150),GAMK(  1, 1)
      COMMON A(16,16),W(3),WM,B(16),SCH,RHO,VEL,B1,KR(10),TILE(3),NFF,
     1  XC(50),XG(50)
      COMMON ZKE(10),TLO(10),DMCLO(10),WALJP(10),EB(10),ALP(10),GAMH(10)
     1 ,GAMF(10),TQ(10,3),TK(10,3),WAT(10),IR(10),IOAT(10),KAT(10),UM
     2 ,EBL(10)
      COMMONFFA,IS,ISP,P,T,SIP,HIP,EL,ENL,FLIQ,NQ,IFL,ISPQ,KRALP,CPF,IRE
     1,IER,AA,ITS,IN,IL,IT,MODE,HMELT,SMELT,TMAX,TMIN,MELT,SUMN,SUML,JC,
     2HG,CPG,SVA,SVB,SVC,SVD,SUMC
      COMMONNXC,SA1,VMACH,KRZZ,SP1,GAM,THI,MX,DMCHI,MCH,NCV,TBT,IFRZ,NOA
     1T,SR1,IXG,SV1,KKJ,IXC,NXG,SH1,NOATO,SA2,FFF,WS,RV,CMF
      COMMONVA,HOS,DUM1,DUM2,EP,IFCJC,ISP2,WTG,VMU2,WTL
      COMMONMT,FKF(10) ,EAK(10) ,EXK(10) ,PMU(10,10) ,RMU(10,10)
      COMMONIB(11) ,FNU(10) ,PNUS(10) ,SLAM(10) ,BE(10) ,BY(10) ,
     1       IBC(10) ,JJ(10)
      EQUIVALENCE (CC(1),FAMOA(1)),(B(1),X(1)),(GAMK(1),VLAM(1))
      EQUIVALENCE(TU(151),TF(1)),(VNU(1),CIJ(1))
      EQUIVALENCE(TAU(1),A(151)),                (NFIA(1),A(1)),(NFIB(1),
     1A(51)),(FFIN(1),A(101))
    5 FORMAT(I3,/244,E12.5,2A4,E12.5,2A4,E12.5,2A4,E12.5)                ALPS0280
   10 FORMAT(51H  UPDATE OF FAIL TEMPERATURES AND DIFFUSION FACTORS/10X,ALPS0290
     17HSPECIES5X16HFAIL TEMPERATURE5X16HDIFFUSION FACTOR)               ALPS0300
   15 FORMAT(11X2A4,6XF10.3,2A2)                                         ALPS0310
   20 FORMAT(11X2A4,22XF15.5,2A2)                                        ALPS0320
   25 FORMAT(I3)                                                         ALPS0330
   30 FORMAT(8E10.4)                                                     ALPS0340
  125 WS = 1.0                                                           ALPS0840
  155 NOATO = NOAT                                                       ALPS0920
      NOAT = 0                                                           ALPS0930
      DUM1 = 0.                                                          ALPS0940
      DO 200 K=1,IS                                                      ALPS0950
      ALPH = (W(1) * TK(K,1) + W(2) * TK(K,2) + W(3) * TK(K,3)) / WS     ALPS0960
      IF (ALPH) 160,160,200                                              ALPS0970
  160 IF (KAT(K) - 99) 165,200,165                                       ALPS0980
  165 IF (KR(6)) 195,170,170                                             ALPS0990
  170 IF (TK(K,1)) 195,195,200                                           ALPS1000
  195 NOAT = NOAT + 1                                                    ALPS1070
      DUM1 = DUM1 - ALPH                                                 ALPS1080
      IOAT(NOAT) = K                                                     ALPS1090
  200 CONTINUE                                                           ALPS1100
      WS = WS * (1. + DUM1)                                              ALPS1110
      DO 205 K=1,IS                                                      ALPS1120
  205 ALP(K) = (W(1) * TQ(K,1) + W(2) * TQ(K,2) + W(3) * TQ(K,3)) / WS   ALPS1130
      TEST = 1.0                                                         ALPS1140
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      IF (KR(6)) 280,215,210                                          ALPS1150
  210 STOP2222                                                        ALPS1160
C*****SURFACE MASS BALANCE PACKAGE GOES HERE                          ALPS1170
  215 DO 270 K=1,IS                                                   ALPS1350
      GAMF(K) = 0.                                                    ALPS1360
      IF (KAT(K) - 99) 255,260,255                                    ALPS1370
  255 IF (W(1) - 0.9) 265,265,270                                     ALPS1380
  260 ALP(K) = 0.                                                     ALPS1390
      GOTO 270                                                        ALPS1400
  265 ALP(K) = ALP(K) + ZKE(K)                                        ALPS1410
  270 CONTINUE                                                        ALPS1420
  275 TEST=1.+W(2)+W(3)                                               ALPS1430
  280 DO 285 K=1,IS                                                   ALPS1440
  285 TEST = TEST - ALP(K) * WTM(K)                                   ALPS1450
      IF (ABS(TEST) - .001) 300,300,290                               ALPS1460
  290 WRITE(KOUT,295)                                                 ALPS1470
      STOP                                                            ALPS1480
  295 FORMAT(////10X25HBAD EDGE TABLE * * * STOP)                     ALPS1490
  300 IF (KR(3)) 305,305,370                                          ALPS1500
  305 IF (NOATO) 370,370,310                                          ALPS1510
C     REINITIALIZE SPECIES                                            ALPS1520
  310 PIN = P / 10.                                                   ALPS1530
      PLOG = ALOG(PIN)                                                ALPS1540
      J = 1                                                           ALPS1550
  315 DO 365 IK=1,N                                                   ALPS1560
      IF (IFC(J) + 1) 320,365,330                                     ALPS1570
  320 IFC(J) = IFC(J) + 3                                             ALPS1580
      IF (J - IS) 340,340,325                                         ALPS1590
  325 YC = 0.                                                         ALPS1600
      GOTO 345                                                        ALPS1610
  330 IF (IFC(J) - 1) 365,365,335                                     ALPS1620
  335 IFC(J) = IFC(J) - 3                                             ALPS1630
  340 YC = PLOG                                                       ALPS1640
  345 IF (IFC(J)) 355,360,350                                         ALPS1650
  350 IFC(J) = - 1                                                    ALPS1660
  355 VN(J) = 0.                                                      ALPS1670
      Y(J) = YC                                                       ALPS1680
      GOTO 365                                                        ALPS1690
  360 VN(J) = PIN                                                     ALPS1700
      Y(J) = PLOG                                                     ALPS1710
  365 J=J+1                                                           ALPS1720
  370 IF (NOAT) 425,425,375                                           ALPS1730
  375 J = 1                                                           ALPS1740
  380 DO 405 IK=1,N                                                   ALPS1750
  385 DO 395 L=1,NOAT                                                 ALPS1770
      K = IOAT(L)                                                     ALPS1780
      LAMT = LAMI(J) / 2 * * (K - 1)                                  ALPS1790
      LAMT = LAMT - (LAMT / 2) * 2                                    ALPS1800
      IF (LAMT) 390,395,390                                           ALPS1810
  390 VN(J) = 0.                                                      ALPS1820
      IFC(J) = IFC(J) - 3                                             ALPS1830
      GOTO 405                                                        ALPS1840
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395 CONTINUE                                                    ALPS1850
405 J=J+1
410 DO 415 L=1,NCAT                                             ALPS1890
    K = IOAT(L)                                                 ALPS1900
    J = - IR(K)                                                 ALPS1910
415 IFC(J) = IFC(J) + 6                                         ALPS1920
425 RETURN                                                      ALPS1940
    END                                                         ALPS1950

                                                  CARD COUNT -      112
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      SUBROUTINETHERM                                                    THER0010
      REALNFIA(10) ,NFIB(10) ,FFIN(10) ,UM(10,10) ,TAU(10,10)            THER0030
      DIMENSIONBLNK(10) ,BC(10)                                          THER0040
      DIMENSION TF(150),CIJ(150,1)
      DIMENSION X(1 ),VLAM(150,1 ),CC(7960)
      COMMONKIN,KOUT,JAN,MOL,NAB,IDC,N ,KKX(5)
      COMMON FAMOA(150),FAMCB(150),RB(150,2),RC(150,2),
     1  RD(150,2),RE(150,2),RF(150,2),TU(150,2),VN(150),Y(150),WTM(150),
     2  VNU(150,10),FF(150),IFC(150),IP(150),CP(150),H(150),SB(150),
     3  TC(150),VLNK(150),E(150),LAMI(150),GAMK(  1, 1)
      COMMON A(16,16),W(3),WM,B(16),SCH,RHO,VEL,B1,KR(10),TILE(3),NFF,
     1  XC(50),XG(50)
      COMMON ZKE(10),TLO(10),DMCLO(10),WALJP(10),EB(10),ALP(10),GAMH(10)
     1 ,GAMF(10),TQ(10,3),TK(10,3),WAT(10),IR(10),IOAT(10),KAT(10),UM
     2 ,EBL(10)
      COMMONFFA,IS,ISP,P,T,SIP,HIP,EL,ENL,FLIQ,NQ,IFL,ISPQ,KRALP,CPF,IRE
     1,IER,AA,ITS,IN,IL,IT,MODE,HMELT,SMELT,TMAX,TMIN,MELT,SUMN,SUML,JC,
     2HG,CPG,SVA,SVB,SVC,SVD,SUMC
      COMMONNXC,SA1,VMACH,KRZZ,SP1,GAM,THI,MX,DMCHI,HCH,NCV,TBT,IFRZ,NOA
     1T,SR1,IXG,SV1,KKJ,IXC,NXG,SH1,NOATO,SA2,FFF,WS,RV,CMF
      COMMONVA,HOS,DUM1,DUM2,EP,IFCJC,ISP2,WTG,VMU2,WTL
      COMMONMT,FKF(10) ,EAK(10) ,EXK(10) ,PMU(10,10) ,RMU(10,10)
      COMMONIB(11) ,FNU(10) ,PNUS(10) ,SLAM(10) ,BE(10) ,BY(10) ,
     1        IBC(10) ,JJ(10)
      EQUIVALENCE (CC(1),FAMOA(1)),(B(1),X(1)),(GAMK(1),VLAM(1))
      EQUIVALENCE(TU(151),TF(1)),(VNU(1),CIJ(1))
      EQUIVALENCE(TAU(1),A(151)),              (NFIA(1),A(1)),(NFIB(1),
     1A(51)),(FFIN(1),A(101))
    5 MODE = KR(1)                                                       THER0300
      IF (ITS) 20,10,20                                                  THER0310
   10 WTG = 0.                                                           THER0320
      WTL = 0.                                                           THER0330
      DUM2 = 0.                                                          THER0340
      SUMN = 0.                                                          THER0350
      DO 15 I=1,IS                                                       THER0360
      PNUS(I) = 0.                                                       THER0370
   15 SLAM(I) = 0.                                                       THER0380
   20 HMELT = 0.                                                         THER0390
      FLIQ = 0.                                                          THER0400
      SMELT = 0.                                                         THER0410
      MELT = 1                                                           THER0420
      TMAX = 20000.                                                      THER0430
      TMIN = 500.                                                        THER0440
      TFMAX = 500.                                                       THER0450
      VA = ALOG(T / 3000.)                                               THER0460
      VB = T - 3000.                                                     THER0470
      VC = (T + 3000.) / 2.                                              THER0480
      VD = T * 3000.                                                     THER0490
      VE = VC / (VD * VD)                                                THER0500
      RT = 1.9869 * T                                                    THER0510
      IF (NCV) 35,35,25                                                  THER0520
   25 PIN = P * 10.E - 3                                                 THER0530
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      WM = 20.                                                          THER0550
      AA = P * WM                                                       THER0560
      IF (MODE) 35,35,30                                                THER0570
   30 T = 3000.                                                         THER0580
   35 CONTINUE                                                          THER0590
      I = 1                                                             THER0600
   40 DO 215 IK=1,N                                                     THER0610
      IF (NCV) 55,55,45
   45 IF (IFC(I)) 55,50,55                                              THER0630
   50 VN(I) = VN(I) + PIN                                               THER0640
      Y(I) = ALOG(VN(I))                                                THER0650
   55 CONTINUE                                                          THER0660
      IF (IFC(I) + 1) 130,60,60                                         THER0670
   60 J = 2                                                             THER0680
      IF (IFC(I)) 65,70,95                                              THER0690
   65 IF (MODE - 1) 130,185,130                                         THER0700
   70 IF (ITS) 130,75,130                                               THER0710
   75 SUMN = SUMN + VN(I)                                               THER0720
      DUM1 = WTM(I) * VN(I)                                             THER0730
      WTG = WTG + DUM1                                                  THER0740
      DUM2 = DUM2 + DUM1 / FF(I)                                        THER0750
      IF (IK - IS) 80,80,85                                             THER0760
   80 PNUS(I) = VN(I)                                                   THER0770
      SLAM(I) = VN(I) / FF(I)                                           THER0780
      GOTO 130                                                          THER0790
   85 DO 90 K=1,IS                                                      THER0800
      DUM1 = VNU(I,K) * VN(I)                                           THER0810
      PNUS(K) = PNUS(K) + DUM1                                          THER0820
   90 SLAM(K) = SLAM(K) + DUM1 / FF(I)                                  THER0830
      GOTO 130                                                          THER0840
   95 IF (IFC(I) - 1) 100,100,130                                       THER0850
  100 IF (ITS) 125,105,125                                              THER0860
  105 IF (KR(6) - KR(8)) 120,110,110                                    THER0870
  110 IF (T - TF(I) + .001) 115,115,120                                 THER0880
  115 IFC(I) = - 1                                                      THER0890
      VN(I) = 0.                                                        THER0900
      GOTO 65                                                           THER0910
  120 WTL = WTL + VN(I) * WTM(I)                                        THER0920
  125 IF (MODE - 1) 130,180,130                                         THER0930
  180 TMIN = AMAX1(TMIN,TF(I))                                          THER1100
  185 TFMAX = AMAX1(TF(I) ,TFMAX)                                       THER1110
  130 IF (T - ABS(TU(I,1))) 135,140,140                                 THER0940
  135 J = 1                                                             THER0950
  140 CP(I) = RC(I,J) + T * RD(I,J) + RE(I,J) / (T * T)                 THER0960
      H(I) = RB(I,J) + VB * (RC(I,J) + RD(I,J) * VC + RE(I,J) / VD)     THER0970
      SB(I) = RF(I,J) + RC(I,J) * VA + VB * (RD(I,J) + RE(I,J) * VE)
  145 IF (MODE - 2) 190,150,150                                         THER0980
  150 IF (IFC(I) - 1) 190,155,190                                       THER0990
  155 IF (TU(I,1)) 160,190,190                                          THER1000
  160 IF (T + TU(I,1)) 170,165,175                                      THER1010
  165 HMELT = - H(I) - HMELT                                            THER1020
      SMELT = - SB(I) - SMELT                                           THER1030
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      MELT = I                                                          THER1040
      IF (J - 2) 190,135,190                                            THER1050
  170 TMAX = AMIN1(TMAX, - TU(I,1))                                     THER1060
      GOTO 190                                                          THER1070
  175 TMIN = AMAX1(TMIN, - TU(I,1))                                     THER1080
  190 TC(I) = - H(I) / RT                                               THER1130
      VLNK(I) = TC(I) + SB(I) / 1.9869                                  THER1140
      IF (IK - IS) 195,195,200                                          THER1150
  195 BLNK(I) = VLNK(I)                                                 THER1160
      IBC(I) = IFC(I)                                                   THER1170
      BC(I) = TC(I)                                                     THER1180
      GOTO 215                                                          THER1190
  200 DO 210 K=1,IS                                                     THER1200
      IF (IBC(K) + 1) 210,205,205                                       THER1210
  205 VLNK(I) = VLNK(I) - VNU(I,K) * BLNK(K)                            THER1220
      TC(I) = TC(I) - VNU(I,K) * BC(K)                                  THER1230
  210 CONTINUE                                                          THER1240
  215 I=I+1
      NCV = -IABS(NCV)
      IF (MODE - 1) 230,220,230                                         THER1260
  220 IF (TFMAX - T) 225,230,230                                        THER1270
  225 T = TFMAX                                                         THER1280
      GOTO 5                                                            THER1290
  230 IF (ITS) 355,235,355                                              THER1300
  235 AA = P * WR                                                       THER1310
      NCV = 0                                                           THER1320
  240 FORMAT(8F10.6)                                                    THER1330
  245 FORMAT (2I3)                                                      THER1340
  250 FORMAT(3E10.4)                                                    THER1350
      IF (WR(9))   335,335,255
  255 READ(KIN,245)MT                                                   THER1370
      DO 260 M=1,MT                                                     THER1380
      READ(KIN,250)FKF(M),EAK(M),EXK(M)                                 THER1390
      READ(KIN,240)(RNU(I,M),I=1,IS)                                    THER1400
  260 READ(KIN,240)(PNU(I,M),I=1,IS)                                    THEP1410
  265 FORMAT (//3X,7HKINETIC)
  270 FORMAT (3X,11HREACTION--,I7,9I10)
  275 FORMAT (/3X,8HREACTANT)
  280 FORMAT (5X,12HCOEFFICIENTS/)
  285 FORMAT (8X,2A4,F8.2,9F10.2)                                       THER1460
  290 FORMAT (/3X,7HPRODUCT)
  295 FORMAT (/3X,12HPRE-EXPONENT)
  300 FORMAT (5X,6HFACTOR,4X,10E10.3)
  305 FORMAT (/3X,10HACTIVATION)
  310 FORMAT (5X,6HENERGY,4X,10E10.3)
  315 FORMAT (/3X,8HREACTION)
  320 FORMAT (5X,5HORDER,5X,10E10.3)
      WRITE(KOUT,265)
      WRITE(KOUT,270)(M,M=1,MT)                                         THER1
      WRITE(KOUT,275)
      WRITE(KOUT,280)
      DO 325 I=1,IS                                                     THER1580
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  325 WRITE(KOUT,285)FAMOA(I),FAMOB(I),(RMU(I,M),M=1,MT)                    THER1
      WRITE(KOUT,290)
      WRITE(KOUT,280)
      DO 330 I=1,IS                                                        THER1620
  330 WRITE(KOUT,285)FAMOA(I),FAMOB(I),(PMU(I,M),M=1,MT)                     THER1
      WRITE(KOUT,295)
      WRITE(KOUT,300)(FKF(M),M=1,MT)
      WRITE(KOUT,305)
      WRITE(KOUT,310)(EAK(M),M=1,MT)
      WRITE(KOUT,315)
      WRITE(KOUT,320)(EXK(M),M=1,MT)
  335 SUMN = SUMN / P                                                      THER1710
      SUML = ALOG(SUMN)                                                    THER1720
      FFF = WTG / DUM2                                                     THER1730
      WTG = WTG / SUMN                                                     THER1740
      WTL = WTL / SUMN                                                     THER1750
      DO 340 I=1,IS                                                        THER1760
      PNUS(I) = PNUS(I) / SUMN + GAMF(I) * AA                              THER1770
  340 SLAM(I) = SLAM(I) / SUMN * FFF                                       THER1780
      WS=W(2)+W(3)                                                         THER1800
      SUMC = 1.0                                                           THER1810
      IF (XRALP + RR(2)) 355,355,345                                       THER1820
  345 IF (WTL / WTG - WS) 355,355,350                                      THER1830
  350 SUMC = WTL / (WTG * WS)                                              THER1840
      WTL = WTL / SUMC                                                     THER1850
  355 RETURN                                                               THER1860
      END                                                                  THER1870

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      SUBROUTINEMAT1                                                    MAT10010
      REALNFIA(10) ,NFIB(10) ,FFIN(10) ,UM(10,10) ,TAU(10,10)           MAT10030
      DIMENSION TF(150),CIJ(150,1)
      DIMENSION X(1 ),VLAM(150,1 ),CC(7960)
      COMMONKIN,KOUT,JAN,MCL,NAB,IDC,N ,XKX(5)
      COMMON FAMOA(150),FAMOB(150),RB(150,2),RC(150,2),
     1  RD(150,2),RE(150,2),RF(150,2),TU(150,2),VN(150),Y(150),WTM(150),
     2  VNU(150,10),FF(150),IFC(150),IP(150),CP(150),H(150),SB(150),
     3  TC(150),VLNK(150),E(150),LAMI(150),GAMK(  1, 1)
      COMMON A(16,16),W(3),WM,B(16),SCH,RHO,VEL,B1,KR(10),TILE(3),NFF,
     1  XC(50),XG(50)
      COMMON ZME(10),TLO(10),DMCLO(10),WALJP(10),EB(10),ALP(10),GAMH(10)
     1 ,GAMF(10),TQ(10,3),TK(10,3),WAT(10),IR(10),IOAT(10),KAT(10),UM
     2 ,EBL(10)
      COMMONFFA,IS,ISP,P,T,SIP,HIP,EL,ENL,FLIQ,NG,IFL,ISPQ,KRALP,CPF,IRE
     1,IER,AA,ITS,IN,IL,IT,MODE,HMELT,SMELT,TMAX,TMIN,MELT,SUMN,SUML,JC,
     2HG,CPG,SVA,SVB,SVC,SVD,SUMC
      COMMONXC,SA1,VMACH,KRZZ,SP1,GAM,THI,MX,DMCHI,MCH,NCV,TBT,IFRZ,MOA
     1T,SR1,IXG,SV1,KKJ,IXC,NXG,SH1,NOATO,SA2,FFF,WS,RV,CMF
      COMMONVA,MOS,DUM1,DUM2,EP,IFCJC,ISP2,WTG,VMU2,WTL
      COMMONMT,FKF(10) ,EAK(10) ,EXK(10) ,PMU(10,10) ,RMU(10,10)
      COMMONIB(11) ,FNU(10) ,PNUS(10) ,SLAM(10) ,BE(10) ,BY(10) ,
     1        IBC(10) ,JJ(10)
      EQUIVALENCE (CC(1),FAMOA(1)),(B(1),X(1)),(GAMK(1),VLAM(1))
      EQUIVALENCE(TU(151),TF(1)),(VNU(1),CIJ(1))
      EQUIVALENCE(TAU(1,1),A(151)),          (NFIA(1),A(1)),(NFIB(1),
     1A(51)),(FFIN(1),A(101))
      RV = WS - WTL / WTG                                               MAT10300
      IF (KR(7) - 1) 30,5,10                                            MAT10310
    5 IF (ITS) 30,20,30                                                 MAT10320
   10 WRITE(KOUT,15)FFF,WTL,WTG,AA,RV,ALP,PNUS,SLAM                     MAT10330
   15 FORMAT(32H FFF,WTL,WTG,AA,RV/ALP/PNUS/SLAM/1X5E12.5/(1X10E12.5))  MAT10340
      KR(7) = KR(7) - 1                                                 MAT10350
      IF (KR(7) - 1) 30,20,30                                           MAT10360
   20 WRITE(KOUT,25)(I,I=1,IS)                                          MAT10370
   25 FORMAT (50H1ITS TEMP   PRES*PNT  EQUIL ER  MASBAL ER  SCALE  7(I3,MAT10380
     17H MASBAL)/90X3(I3,7H MASBAL))                                    MAT10390
C     INITIALIZE                                                        MAT10400
   30 EL = 0.                                                           MAT10410
      CPG = 0.                                                          MAT10420
      EP = P                                                            MAT10440
      CPF = 0.                                                          MAT10450
      JC = 0                                                            MAT10460
      ISPQ = IS + 2                                                     MAT10470
      B(1) = 0.                                                         MAT10480
      B(2) = 0.                                                         MAT10490
      A(1,1) = 0.                                                       MAT10500
      A(1,2) = 0.                                                       MAT10510
      A(2,1) = 0.                                                       MAT10520
      A(2,2) = 0.                                                       MAT10530
C-----INITIALIZE CONTRIBUTION OF MOST SIGNIFICANT SPECIES IN EACH MASS BMAT10540
      DO 35 I=1,IS                                                      MAT10550
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      EB(I) = 0.                                                        MAT10560
   35 E(I) = AA * ALP(I)                                                MAT10570
      ISP2 = ISPQ                                                       MAT10580
C - - - MAIN BASE SPECIES LOOP                                          MAT10590
   40 DO 25C I=3,ISPQ                                                   MAT10600
C     ZERO MATRIX                                                       MAT10610
   45 DO 5C K=1,ISPQ                                                    MAT10620
   5C A(K,I) = 0.                                                       MAT10630
      IF (ITS) 70,55,70                                                 MAT10640
C     NORMALIZE ON PRESSURE ON FIRST PASS                               MAT10650
   55 VN(I - 2) = VN(I - 2) / SUMN                                      MAT10660
      EBL(I - 2) = 0.                                                   MAT10670
      IF (IFC(I - 2)) 70,60,65                                          MAT10680
   60 Y(I - 2) = Y(I - 2) - SUML                                        MAT10690
      GOTO 70                                                           MAT10700
   65 VN(I - 2) = VN(I - 2) / SUMC                                      MAT10710
C     INITIALIZE SOME MORE                                              MAT10720
   70 B(I) = 0.                                                         MAT10730
      A(I,1) = 0.                                                       MAT10740
      IP(I - 2) = 0.                                                    MAT10750
C     SET FLAG INDICATING SIGNIFICANCE OF SPECIES IN MASS               MAT10760
C     BALANCE(S) AND INCREMENT COUNT ON SIGNIFICANT SPECIES             MAT10770
   75 IF (VN(I - 2) - EBL(I - 2)) 85,85,80                              MAT10780
   80 IP(I - 2) = - 1                                                   MAT10790
C     TREAT BASE SPECIES CONTAINING BUT NOT REPRESENTING NON-PRESENT    MAT10810
C     ELEMENTS IN SAME MANNER AS NON-PRESENT CONDENSED SPECIES          MAT10820
   85 IF (IFC(I - 2) + 1) 290,90,90                                     MAT10830
   90 IF (IFC(I - 2)) 140,170,95                                        MAT10840
   95 A(I,I) = 1.                                                       MAT10850
      VA = VN(I - 2)                                                    MAT10860
      IF (IFC(I - 2) - 1) 100,100,240                                   MAT10870
  100 IF (EB(I - 2) - ABS(VA)) 105,110,110                              MAT10880
  105 EB(I - 2) = ABS(VA)                                               MAT10890
      IB(I - 2) = I - 2                                                 MAT10900
  110 E(I - 2) = E(I - 2) - VA                                          MAT10910
      IF (KR(6)) 115,120,120                                            MAT10920
  115 IF (MODE - 1) 240,130,240                                         MAT10940
  120 DO 125 K=1,IS                                                     MAT10950
  125 A(K + 2,I) = - WTM(I - 2) / WTG * PNUS(K)                         MAT10960
      A(I,I) = A(I,I) + 1.                                              MAT10970
  130 TMIN = AMAX1(TMIN,TF(I - 2))                                      MAT10980
      IF (T - TF(I - 2) + .001) 135,135,140                             MAT10990
  135 A(I,I) = 1.0E + 10                                                MAT11000
      E(I - 2) = - VN(I - 2) * 1.001E + 10                              MAT11010
      MODE = 0                                                          MAT11020
  140 IF (MODE - 1) 290,145,290                                         MAT11030
  145 IF (TF(I - 2) + .001 - T) 290,150,150                             MAT11040
  150 IF (JC) 165,165,155                                               MAT11050
  155 IF (Y(I - 2) - B(1)) 290,290,160                                  MAT11060
  160 A(1,JC + 2) = 0.                                                  MAT11070
  165 B(1) = Y(I - 2)                                                   MAT11080
      TMAX = TF(I - 2)
```

```
      JC = I - 2                                                        MAT11090
      IFCJC = IFC(I - 2)                                                MAT11100
      A(1,I) = - 1.                                                     MAT11110
      GOTO 290                                                          MAT11120
C-----GAS PHASE                                                         MAT11130
  170 VA = VN(I - 2)                                                    MAT11140
      CPG = CPG + VA * CP(I - 2)                                        MAT11150
      A(1,I) = VA                                                       MAT11160
      A(2,I) = VA                                                       MAT11170
      EP = EP - VA                                                      MAT11180
      IF (KAT(I - 2) - 99) 175,235,175                                  MAT11190
  175 IF (KR(6)) 235,210,180                                            MAT11200
  180 DO 185 K=1,IS                                                     MAT11210
  185 A(K + 2,I) = GAMK(I - 2,K) + GAMH(K) * H(I - 2)                   MAT11220
      A(I,I) = A(I,I) + VA * RV                                         MAT11230
  190 DUM2 = WTM(I - 2) / WTG * WTL / WTG * VA                          MAT11240
      DO 205 K=1,IS                                                     MAT11250
      IF (EB(K) - ABS(A(K + 2,I))) 195,200,200                          MAT11260
  195 EB(K) = ABS(A(K + 2,I))                                           MAT11270
      IB(K) = I - 2                                                     MAT11280
  200 E(K) = E(K) - A(K + 2,I)                                          MAT11290
  205 A(K + 2,I) = A(K + 2,I) + DUM2 * PNUS(K)                          MAT11300
      GOTO 240                                                          MAT11310
  210 DUM1 = WTM(I - 2) / WTG * VA                                      MAT11320
      DUM2 = WTL / WTG * DUM1                                           MAT11330
      IF (KR(4)) 215,215,220                                            MAT11340
  215 DUM1 = 0.                                                         MAT11350
      VA = (RV + 1.) * VA                                               MAT11360
      GOTO 225                                                          MAT11370
  220 DUM1 = DUM1 * (1. - FFF / FF(I - 2))                              MAT11380
      VA = (RV + FFF / FF(I - 2)) * VA                                  MAT11390
  225 DO 230 K=1,IS                                                     MAT11400
  230 A(K + 2,I) = DUM1 * SLAM(K) + DUM2 * PNUS(K)                      MAT11410
      A(I,I) = A(I,I) + VA                                              MAT11420
  235 EB(I - 2) = ABS(VA)                                               MAT11430
      IB(I - 2) = I - 2                                                 MAT11440
      E(I - 2) = E(I - 2) - VA                                          MAT11450
  240 IF (MODE - 2) 285,260,245                                         MAT11460
  245 IF (IFC(I - 2)) 290,255,250                                       MAT11470
  250 HOS = SB(I - 2)                                                   MAT11480
      GOTO 270                                                          MAT11490
  255 HOS = SB(I - 2) - 1.9869 * Y(I - 2) - 1.9869                      MAT11500
      GOTO 275                                                          MAT11510
  260 HOS = H(I - 2)                                                    MAT11520
  265 IF (IFC(I - 2)) 290,275,270                                       MAT11530
  270 A(1,I) = HOS                                                      MAT11540
      GOTO 280                                                          MAT11550
  275 A(1,I) = HOS * VN(I - 2)                                          MAT11560
  280 A(1,2) = A(1,2) - HOS * VN(I - 2)                                 MAT11570
  285 CPF = CPF + CP(I - 2) * VN(I - 2)                                 MAT11580
  290 CONTINUE                                                          MAT11590
      DO 295 I=1,IS                                                     MAT11600
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      BE(I) = E(I)                                                    MAT11610
      BY(I) = Y(I)                                                    MAT11620
  295 IBC(I) = IFC(I)                                                 MAT11630
      RETURN                                                          MAT11640
      END                                                             MAT11650

                                                  CARD COUNT -        161
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      SUBROUTINEMAT2                                                    MAT20010
      REALNFIA(10) ,NFIB(10) ,FFIN(10) ,UM(10,10) ,TAU(10,10)           MAT20030
      DIMENSION TF(150),CIJ(150,1)
      DIMENSION X(1 ),VLAM(150,1 ),CC(7960)
      COMMONKIN,KOUT,JAN,MOL,NAB,IDC,N ,KKX(5)
      COMMON FAMOA(150),FAMCB(150),RB(150,2),RC(150,2),
     1  RD(150,2),RE(150,2),RF(150,2),TU(150,2),VN(150),Y(150),WTM(150),
     2  VNU(150,10),FF(150),IFC(150),IP(150),CP(150),H(150),SB(150),
     3  TC(150),VLNK(150),E(150),LAMI(150),GAMK(  1, 1)
      COMMON A(16,16),W(3),WP,B(16),SCH,RHO,VEL,B1,KR(10),TILE(3),NFF,
     1  XC(50),XG(50)
      COMMON ZKE(10),TLO(10),DMCLO(10),WALJP(10),EB(10),ALP(10),GAMH(10)
     1 ,GAMF(10),TQ(10,3),TK(10,3),WAT(10),IR(10),IOAT(10),KAT(10),UM
     2 ,EBL(10)
      COMMONFFA,IS,ISP,P,T,SIP,HIP,EL,ENL,FLIQ,NQ,IFL,ISPQ,KRALP,CPF,IRE
     1,IER,AA,ITS,IN,IL,IT,MODE,HMELT,SMELT,TMAX,TMIN,MELT,SUMN,SUML,JC,
     2HG,CPG,SVA,SVB,SVC,SVD,SUMC
      COMMONNXC,SA1,VMACH,KRZZ,SP1,GAM,THI,MX,DMCHI,HCH,NCV,TBT,IFRZ,NOA
     1T,SR1,IXG,SV1,KKJ,IXC,NXG,SH1,NOATO,SA2,FFF,WS,RV,CMF
      COMMONVA,HOS,DUM1,DUM2,EP,IFCJC,ISP2,WTG,VMU2,WTL
      COMMONMT,FKF(10) ,EAK(10) ,EXK(10) ,PMU(10,10) ,RMU(10,10)
      COMMONIB(11) ,FNU(10) ,PNUS(10) ,SLAM(10) ,BE(10) ,BY(10) ,
     1        IBC(10) ,JJ(10)
      EQUIVALENCE (CC(1),FAMOA(1)),(B(1),X(1)),(GAMK(1),VLAM(1))
      EQUIVALENCE(TU(151),TF(1)),(VNU(1),CIJ(1))
      EQUIVALENCE(TAU(1),A(151)),          (NFIA(1),A(1)),(NFIB(1),
     1A(51)),(FFIN(1),A(101))
      ISPQ = IS + 2                                                     MAT20300
      ISP2 = ISPQ                                                       MAT20310
      IER = 0                                                           MAT20340
      IRE = 0                                                           MAT20350
      EER = 0.                                                          MAT20360
C - - - MAIN NON-BASE SPECIES LOOP                                      MAT20370
      IF (N - ISP) 350,5,5                                              MAT20380
    5 J = ISP                                                           MAT20390
   10 DO 345 IK=ISP,N                                                   MAT20400
      IF (IFC(J) + 1) 345,15,15                                         MAT20410
   15 IF (ITS) 35,20,35                                                 MAT20420
   20 VN(J) = VN(J) / SUMN                                              MAT20430
      IF (IFC(J)) 35,30,25                                              MAT20440
   25 VN(J) = VN(J) / SUMC                                              MAT20450
      GOTO 35                                                           MAT20460
   30 Y(J) = Y(J) - SUML                                                MAT20470
   35 E(J) = VLNK(J) - Y(J)                                             MAT20480
      DO 50 I=1,IS                                                      MAT20490
      IF (IBC(I)) 45,45,40                                              MAT20500
   40 FNU(I) = 0.                                                       MAT20510
      GOTO 50                                                           MAT20520
   45 FNU(I) = VNU(J,I)                                                 MAT20530
      E(J) = E(J) + FNU(I) * BY(I)                                      MAT20540
   50 CONTINUE                                                          MAT20550
      EAB = ABS(E(J))                                                   MAT20560
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      IF (IFC(J)) 55,215,85                                          MAT20570
C*****CONDENSED SPECIES                                              MAT20580
   55 EAB = E(J)                                                     MAT20590
      IF (KR(6) - KR(8)) 65,60,60                                    MAT20600
   60 IF (T - TF(J) + .001) 180,65,65                                MAT20610
   65 IF (E(J) - EER) 170,170,70                                     MAT20620
   70 EER = E(J)                                                     MAT20630
      IF (IER) 75,75,80                                              MAT20640
   75 ISPQ = ISPQ + 1                                                MAT20650
      IER = ISPQ                                                     MAT20660
   80 IE = IER                                                       MAT20670
      IRE = IK                                                       MAT20680
      GOTO 90                                                        MAT20690
   85 ISPQ = ISPQ + 1                                                MAT20700
      IE = ISPQ                                                      MAT20710
   90 WTR = 0.                                                       MAT20720
      IF (KR(6)) 100,95,95                                           MAT20730
   95 TMIN = AMAX1(TF(J) ,TMIN)                                      MAT20740
      WTR = WTM(J) / WTG                                             MAT20750
  100 DO 105 I=1,ISPQ                                                MAT20760
      A(I,IE) = 0.                                                   MAT20770
  105 A(IE,I) = 0.                                                   MAT20780
      DO 145 K=1,IS                                                  MAT20790
      DUM1 = VNU(J,K)                                                MAT20800
      IF (T - TF(J) + .001) 110,120,120                              MAT20810
  110 IF (KR(8)) 120,120,115                                         MAT20820
  115 DUM1 = TQ(K,3) + WTM(J)                                        MAT20830
      JC=J                                                           
  120 IF (IBC(K) - 1) 125,125,145                                    MAT20840
  125 VA = DUM1 * VN(J)                                              MAT20850
  130 A(K + 2,IE) = DUM1 - WTR * PNUS(K)                             MAT20860
  135 BE(K) = BE(K) - VA                                             MAT20870
      IF (ABS(VA) - EB(K)) 145,145,140                               MAT20880
  140 EB(K) = ABS(VA)                                                MAT20890
      IB(K) = IK                                                     MAT20900
  145 CONTINUE                                                       MAT20910
      K = IE - ISP2                                                  MAT20920
      JJ(K) = J                                                      MAT20930
      A(IE,1) = TC(J)                                                MAT20940
      B(IE) = E(J)                                                   MAT20950
      IF (T + .001 - TF(J)) 150,165,165                              MAT20960
  150 IF (MODE - 1) 155,160,155                                      MAT20970
  155 IF (KR(6) - KR(8)) 165,160,160                                 MAT20980
  160 A(IE,IE) = 1.E + 10                                            MAT20990
      B(IE) = - VN(J) * 1.001E + 10                                  MAT21000
      MODE = 0                                                       MAT21010
  165 IE (MODE - 2) 170,200,205                                      MAT21020
  170 IF (MODE - 1) 335,175,335                                      MAT21030
  175 IF (T - TF(J) - .001) 180,180,335                              MAT21040
  180 IF (JC) 190,190,185                                            MAT21050
  185 IF (E(J) - B(1)) 345,345,190                                   MAT21060
  190 B(1) = E(J)                                                    MAT21070
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      JC = IK                                                          MAT21080
      IFCJC = IFC(JC)                                                  MAT21090
      TMAX = TF(J)                                                     MAT21100
      DO 195 K=1,IS                                                    MAT21110
  195 A(1,K + 2) = - FNU(K)                                            MAT21120
      A(2,1) = TC(J)                                                   MAT21130
      GOTO 345                                                         MAT21140
  200 HOS = H(J)                                                       MAT21150
      GOTO 210                                                         MAT21160
  205 HOS = SB(J)                                                      MAT21170
  210 A(1,IE) = HOS                                                    MAT21180
      A(1,2) = A(1,2) - VN(J) * HOS                                    MAT21190
      CPF = CPF + CP(J) * VN(J)                                        MAT21200
      GOTO 335                                                         MAT21210
C*****GAS PHASE SPECIES                                                MAT21220
  215 IP(J) = 0                                                        MAT21230
      IF (VN(J)) 220,335,220                                           MAT21240
  220 IQ = 0                                                           MAT21250
      CPG = CPG + VN(J) * CP(J)                                        MAT21260
      IF (KR(6)) 245,225,230                                           MAT21270
  225 FFJ = FFF / FF(J)                                                MAT21280
  230 DUM1 = WTM(J) / WTG * VN(J)                                      MAT21290
      DUM2 = DUM1 / WTG * WTL                                          MAT21300
      IF (KR(4)) 235,235,240                                           MAT21310
  235 DUM1 = 0.                                                        MAT21320
      FFJ = 1.0                                                        MAT21330
      GOTO 245                                                         MAT21340
  240 DUM1 = DUM1 * (1. - FFJ)                                         MAT21350
  245 DO 300 I=3,ISP2                                                  MAT21360
      VA = VNU(J,I - 2) * VN(J)                                        MAT21370
      IF (KR(6)) 265,255,250                                           MAT21380
  250 VA = VA * RV + VN(J) * (VLAM(J,I - 2) + GAMH(I - 2) * H(J))      MAT21390
      BE(I - 2) = BE(I - 2) - VA                                       MAT21400
      ABSVA = ABS(VA)                                                  MAT21410
      VA = VA + PNUS(I - 2) * DUM2                                     MAT21420
      GOTO 270                                                         MAT21430
  255 IF (KAT(I - 2) - 99) 260,265,260                                 MAT21440
  260 VB = VA * FFJ                                                    MAT21450
      VA = RV * VA + VB                                                MAT21460
      BE(I - 2) = BE(I - 2) - VA                                       MAT21470
      ABSVA = ABS(VA)                                                  MAT21480
      VA = VA + SLAM(I - 2) * DUM1 + DUM2 * PNUS(I - 2)                MAT21490
      GOTO 270                                                         MAT21500
  265 BE(I - 2) = BE(I - 2) - VA                                       MAT21510
      ABSVA = ABS(VA)                                                  MAT21520
  270 IF (ABSVA - EBL(I - 2)) 280,280,275                              MAT21530
  275 IQ = 1                                                           MAT21540
      IF (ABSVA - EB(I - 2)) 290,290,285                               MAT21550
  280 IF (ABS(VA) - EBL(I - 2)) 300,300,290                            MAT21560
  285 EB(I - 2) = ABSVA                                                MAT21570
      IB(I - 2) = IK                                                   MAT21580
  290 DO 295 K=3,ISP2                                                  MAT21590
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  295 A(I,K) = A(I,K) + VA * FNU(K - 2)                                 MAT21600
      B(I) = B(I) - VA * E(J)                                           MAT21610
      A(I,1) = A(I,1) - VA * TC(J)                                      MAT21620
      A(2,I) = A(2,I) + VN(J) * FNU(I - 2)                              MAT21630
  300 CONTINUE                                                          MAT21640
      IF (IQ) 335,335,305                                               MAT21650
  305 EP = EP - VN(J)                                                   MAT21660
      IP(J) = - 1                                                       MAT21680
      B(2) = B(2) - VN(J) * E(J)                                        MAT21690
      A(2,1) = A(2,1) - VN(J) * TC(J)                                   MAT21700
      IF (MODE - 2) 330,310,315                                         MAT21710
  310 HOS = H(J) * VN(J)                                                MAT21720
      GOTO 320                                                          MAT21730
  315 HOS = VN(J) * (SB(J) - 1.9869 * Y(J) - 1.9869)                    MAT21740
  320 DO 325 I=3,ISP2                                                   MAT21750
  325 A(1,I) = HOS * FNU(I - 2) + A(1,I)                                MAT21760
      A(1,2) = A(1,2) - HOS                                             MAT21770
      A(1,1) = A(1,1) - HOS * TC(J)                                     MAT21780
      B(1) = B(1) - HOS * E(J)                                          MAT21790
  330 CPF = CPF + VN(J) * CP(J)                                         MAT21800
  335 IF (EL - EAB) 340,345,345                                         MAT21810
  340 EL = EAB                                                          MAT21820
  345 J=J+1
  350 CONTINUE                                                          MAT21840
      RETURN                                                            MAT21850
      END                                                               MAT21860

                                                  CARD COUNT -      182
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      SUBROUTINEMAT3
      REALNFIA(10) ,NFIB(10) ,FFIN(10) ,UM(10,10) ,TAU(10,10)                    MAT30010
      DIMENSIONL(10) ,AR(10)                                                     MAT30030
      DIMENSION TF(150),CIJ(150,1)                                               MAT30060
      DIMENSION X(1 ),VLAM(150,1 ),CC(7960)
      COMMONKIN,KOUT,JAN,MOL,NAB,IDC,N ,KKX(5)
      COMMON FAMOA(150),FAMOB(150),RB(150,2),RC(150,2),
     1  RD(150,2),RE(150,2),RF(150,2),TU(150,2),VN(150),Y(150),WTM(150),
     2  VNL(150,10),FF(150),IFC(150),IP(150),CP(150),H(150),SB(150),
     3  TC(150),VLNK(150),E(150),LAMI(150),GAMK(  1, 1)
      COMMON A(16,16),W(3),WM,B(16),SCH,RHO,VEL,B1,KR(10),TILE(3),NFF,
     1  XC(50),XG(50)
      COMMON ZKE(10),TLO(10),DMCLO(10),WALJP(10),EB(10),ALP(10),GAMH(10)
     1 ,GAMF(10),TQ(10,3),TK(10,3),WAT(10),IR(10),IOAT(10),KAT(10),UM
     2 ,EBL(10)
      COMMONFFA,IS,ISP,P,T,SIP,HIP,EL,ENL,FLIQ,NQ,IFL,ISPQ,KRALP,CPF,IRE
     1,IER,AA,ITS,IN,IL,IT,MODE,HMELT,SMELT,TMAX,TMIN,MELT,SUMN,SUML,JC,
     2HG,CPG,SVA,SVB,SVC,SVD,SUMC
      COMMONNXC,SA1,VMACH,KRZZ,SP1,GAM,THI,MX,DMCHI,HCH,NCV,TBT,IFRZ,NOA
     1T,SR1,IXG,SV1,KKJ,IXC,MXG,SH1,NOATO,SA2,FFF,WS,RV,CMF
      COMMONVA,HOS,DUM1,DUM2,EP,IFCJC,ISP2,WTG,VMU2,WTL
      COMMONMT,FKF(10) ,EAK(10) ,EXK(10) ,PMU(10,10) ,RMU(10,10)
      COMMONIB(111) ,FNU(10) ,PNUS(10) ,SLAM(10) ,BE(10) ,BY(10) ,
     1         IBC(10) ,JJ(10)
      EQUIVALENCE (CC(1),FAMOA(1)),(B(1),X(1)),(GAMK(1),VLAM(1))
      EQUIVALENCE(TU(151),TF(1)),(VMU(1),CIJ(1))
      EQUIVALENCE(TAU(1),A(151)),              (NFIA(1),A(1)),(NFIB(1),
     1A(51)),(FFIN(1),A(101))
      ISP3 = IS + 3
      IF (MODE - 2) 50,5,25                                                      MAT30310
    5 CPA = CPF * T                                                              MAT30320
      SHMLT = HMELT * VN(MELT)                                                   MAT30330
      EHS = AA * HIP + A(1,2)                                                    MAT30340
      IF (SVA) 15,15,10                                                          MAT30350
   10 DUM1 = SVA / AA * T * T                                                    MAT30360
      EHS = AA * SVC - DUM1 + A(1,2)                                             MAT30370
      HIP = - A(1,2) / AA                                                        MAT30380
      A(1,2) = - AA * SVC - DUM1                                                 MAT30390
      CPA = (CPF + 2. * DUM1 / T) * T                                            MAT30400
      DUM2 = SVB / AA * T                                                        MAT30410
      P = P - EP                                                                 MAT30420
      EP = - P + SVD - DUM2                                                      MAT30430
      A(2,1) = A(2,1) + DUM2                                                     MAT30440
      A(2,2) = - DUM2                                                            MAT30450
   15 IF (KR(2) - MODE) 30,20,30                                                 MAT30460
   20 A(1,2) = - AA * HIP                                                        MAT30470
      GOTO 30                                                                    MAT30480
   25 CPA = CPF                                                                  MAT30490
      SHMLT = SMELT * VN(MELT)                                                   MAT30500
      EHS = AA * SIP + A(1,2) - 1.9869 * (P - EP)                                MAT30510
      A(1,2) = - AA * SIP                                                        MAT30520
   30 B(1) = B(1) + EHS                                                          MAT30530
                                                                                 MAT30540
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      A(1,1) = A(1,1) + CPA                                              MAT30550
      IF (SHMLT) 50,50,35                                                MAT30560
   35 IF (EHS) 50,50,40                                                  MAT30570
   40 EHS = EHS - SHMLT                                                  MAT30580
      B(1) = B(1) - SHMLT                                                MAT30590
      IF (EHS) 45,50,50                                                  MAT30600
   45 FLIQ = 1. + EHS / SHMLT                                            MAT30610
      MODE = 0                                                           MAT30620
      TMIN = 500.                                                        MAT30630
      TMAX = 5000.                                                       MAT30640
   50 ENL = ABS(EP) / P                                                  MAT30650
      DO 75 I=3,ISP2                                                     MAT30660
      L(I - 2) = I - 2                                                   MAT30670
      E(I - 2) = BE(I - 2)                                               MAT30680
      EBL(I-2)=EB(I-2)*1.E-7
      A(I,2) = - AA * ALP(I - 2)                                         MAT30700
      IF (IFC(I - 2) - 1) 60,60,55                                       MAT30710
   55 NFM = NFM + 1                                                      MAT30720
      GOTO 75                                                            MAT30730
   60 IF (KR(6)) 70,70,65                                                MAT30740
   65 A(I,1) = A(I,1) + GAMH(I - 2) * T * CPG                            MAT30750
      DUM1 = GAMF(I - 2) * RV * AA                                       MAT30760
      A(I,2) = A(I,2) - DUM1                                             MAT30770
      E(I - 2) = E(I - 2) - DUM1                                         MAT30780
   70 ER = E(I - 2)                                                      MAT30790
      ABER = ABS(ER) / (EB(I - 2) + 1.E - 20)                            MAT30800
      ENL = AMAX1(ABER,ENL)                                              MAT30810
      B(I) = B(I) + ER                                                   MAT30820
   75 CONTINUE                                                           MAT30830
      IF (ISP2 - ISPQ) 80,255,255                                        MAT30840
   80 IV = 0                                                             MAT30850
      JZ = 0                                                             MAT30860
C     ADD CONDENSED NONBASE SPECIES TO ARRAY                             MAT30870
   85 DO 90 IE=ISP3,ISPQ                                                 MAT30880
      J = IE - ISP2                                                      MAT30890
      J = JJ(J)                                                          MAT30900
      DO 90 K=1,IS                                                       MAT30910
   90 A(IE,K + 2) = - VNU(J,K)                                           MAT30920
      IF (IV) 95,95,215                                                  MAT30930
C     CHECK FOR SINGULAR CONDENSED SET                                   MAT30940
   95 DO 140 IE=ISP3,ISPQ                                                MAT30950
      IV = IV + 1                                                        MAT30960
      IF (IV - 1) 120,120,100                                            MAT30970
C     REDUCE NEW ROW BY PREVIOUS ROWS                                    MAT30980
  100 DO 115 J=2,IV                                                      MAT30990
      K = L(J - 1)                                                       MAT31000
      DIV = - A(IE,K + 2)                                                MAT31010
      IF (DIV) 105,115,105                                               MAT31020
  105 A(IE,K + 2) = 0.                                                   MAT31030
      JM = J + ISP                                                       MAT31040
      DO 110 M=3,ISP2                                                    MAT31050
  110 A(IE,M) = A(IE,M) + DIV * A(JM,M)                                  MAT31060
```

```
  115 CONTINUE                                                    MAT31070
C     SEEK VALID NON-ZERO ELEMENT                                 MAT31080
  120 DO 130 J=IV,IS                                              MAT31090
      M = L(J)                                                    MAT31100
      IF (ABS(A(IE,M + 2)) - .01) 130,130,125                     MAT31110
  125 IF (IFC(M)) 135,135,130                                     MAT31120
  130 CONTINUE                                                    MAT31130
C     SINGULAR CONDENSED SET                                      MAT31140
      GOTO 145                                                    MAT31150
  135 L(J) = L(IV)                                                MAT31160
      L(IV) = M                                                   MAT31170
      DIV = A(IE,M + 2)                                           MAT31180
      A(IE,M + 2) = 1.                                            MAT31190
C     NORMALIZE NEW ROW                                           MAT31200
      DO 140 J=3,ISP2                                             MAT31210
  140 A(IE,J) = A(IE,J) / DIV                                     MAT31220
C     COMPLETES MAJOR LOOP=NON SINGULAR                           MAT31230
      GOTO 85                                                     MAT31240
C     EXTRACT COEFFICIENTS ON SINGULAR SET-NONBASE                MAT31250
  145 DO 150 J=2,IV                                               MAT31260
      K = L(J - 1)                                                MAT31270
  150 AR(J - 1) = A(IE,K + 2)                                     MAT31280
      AR(IV) = 1.                                                 MAT31290
C     EXTRACT COEFFICIENTS ON SINGULAR SET - BASE                 MAT31300
      DO 165 K=1,IS                                               MAT31310
      IF (IFC(K)) 165,165,155                                     MAT31320
  155 IF (ABS(A(IE,K + 2)) - .01) 165,165,160                     MAT31330
  160 IV = IV + 1                                                 MAT31340
      AR(IV) = - A(IE,K + 2)                                      MAT31350
      JJ(IV) = K                                                  MAT31360
  165 CONTINUE                                                    MAT31370
C     ISOLATE NEW CONDENSED CANDIDATE                             MAT31380
      DO 175 J=1,IV                                               MAT31390
      K = JJ(J)                                                   MAT31400
      IF (VN(K)) 170,170,175                                      MAT31410
  170 JZ = J                                                      MAT31420
      KZ = K                                                      MAT31430
      GOTO 185                                                    MAT31440
  175 CONTINUE                                                    MAT31450
  180 STOP                                                        MAT31460
C     WHO MUST GO TO ALLOW ENTRY OF NEW CANDIDATE                 MAT31470
  185 TEST = - 1.0E10                                             MAT31480
      JX = 0                                                      MAT31490
      DO 200 J=1,IV                                               MAT31500
      IF(ABS(AR(J))-.01) 200,200,186
  186 DUM1=AR(JZ)/AR(J)
      IF(DUM1) 190,200,200
  190 K = JJ(J)                                                   MAT31530
      DUM1 = DUM1 * VN(K)                                         MAT31540
      IF (DUM1 - TEST) 200,200,195                                MAT31550
  195 TEST = DUM1                                                 MAT31560
      JX = J                                                      MAT31570
```

```
      KX = K                                                              MAT31580
  200 CONTINUE                                                            MAT31590
      TEST = VN(KX) / AR(JX)                                              MAT31600
C      DOES NEW CANDIDATE ENTER                                           MAT31610
      IF (E(KZ) - E(KX)) 85,85,205                                        MAT31620
C     YES                                                                 MAT31630
  205 DO 210 J=1,IV                                                       MAT31640
      K = JJ(J)                                                           MAT31650
  210 VN(K) = VN(K) - TEST * AR(J)                                        MAT31660
      KR(7) = KR(7) + 1                                                   MAT31670
      VN(KX) = 0.                                                         MAT31680
      KZ = KX                                                             MAT31690
      JZ = JX                                                             MAT31700
      GOTO 85                                                             MAT31710
C     ELIMINATE TERMS CORRESPONDING TO PRESENT BASE CONDENSED             MAT31720
  215 DO 230 K=1,IS                                                       MAT31730
      IF (IFC(K)) 230,230,220                                             MAT31740
  220 DO 225 IE=ISP3,ISPQ                                                 MAT31750
  225 A(IE,K + 2) = 0.                                                    MAT31760
  230 CONTINUE                                                            MAT31770
      IF (JZ) 250,250,235                                                 MAT31780
C     FIX MATRIX TO YIELD SMALL NEG CORRECTION ON ELIMINATED SPECIES      MAT31790
  235 IF (KX - IS) 245,245,240                                            MAT31800
  240 KZ = JZ + IS                                                        MAT31810
  245 A(KZ + 2,KZ + 2) = 1.E + 15                                         MAT31820
      B(KZ + 2) = - 1.E + 10                                              MAT31830
  250 CONTINUE                                                            MAT31840
  255 B(2) = EP + B(2)                                                    MAT31850
      IF (MODE - 1) 290,270,260                                           MAT31860
  260 IF (ABS(EHS / A(1,1)) - .0001) 290,290,300                          MAT31870
  265 IF (ABS(B(1)) - 1.E - 4) 290,290,300                                MAT31880
  270 IF (IFC(JC) 275,265,285                                             MAT31890
  275 IF (JC - IRE) 280,285,280                                           MAT31900
  280 GOTO 265                                                            MAT31910
  285 MODE = 0                                                            MAT31920
      TMIN = 500.                                                         MAT31930
      TMAX = 5000.                                                        MAT31940
      GOTO 265                                                            MAT31950
  290 IF (EL - 1.E - 4) 295,295,300                                       MAT31960
  295 IF (ENL - 1.E - 5) 315,315,300                                      MAT31970
  300 IN = ISPQ                                                           MAT31980
      IL = 1                                                              MAT31990
      IF (MODE) 305,305,310                                               MAT32000
  305 IN = ISPQ - 1                                                       MAT32010
      IL = 2                                                              MAT32020
      X(1) = 0.                                                           MAT32030
  310 RETURN                                                              MAT32040
  315 ITS = - 2                                                           MAT32050
      GOTO 310                                                            MAT32060
      END                                                                 MAT32070
```

CARD COUNT - 206

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      SUBROUTINESCALE(MCE)                                                  SCAL0010
      REALNFIA(10) ,NFIB(10) ,FFIN(10) ,UM(10,10) ,TAU(10,10)               SCAL0030
      DIMENSIONCMFF(150)
      DIMENSIONDY(1) ,DYA(150,1)
      DIMENSION TF(150),CIJ(150,1)
      DIMENSION X(1 ),VLAM(150,1 ),CC(7960)
      COMMONKIN,KOUT,JAN,MOL,NAB,IDC,N ,KKX(5)
      COMMON FAMDA(150),FAMDB(150),RB(150,2),RC(150,2),
     1  RD(150,2),RE(150,2),RF(150,2),TU(150,2),VN(150),Y(150),WTM(150),
     2  VNU(150,10),FF(150),IFC(150),IP(150),CP(150),H(150),SB(150),
     3  TC(150),VLNK(150),E(150),LAMI(150),GAMK(  1, 1)
      COMMON A(16,16),W(3),WM,B(16),SCH,RHO,VEL,B1,KR(10),TILE(3),NFF,
     1  XC(50),XG(50)
      COMMON ZKE(10),TLO(10),DMCLO(10),WALJP(10),EB(10),ALP(10),GAMH(10)
     1 ,GAMF(10),TQ(10,3),TK(10,3),WAT(10),IR(10),IOAT(10),KAT(10),UM
     2 ,EBL(10)
      COMMONFFA,IS,ISP,P,T,SIP,HIP,EL,ENL,FLIQ,NQ,IFL,ISPQ,KRALP,CPF,IRE
     1,IER,AA,ITS,IN,IL,IT,MODE,HMELT,SMELT,TMAX,TMIN,MELT,SUMN,SUML,JC,
     2HG,CPG,SVA,SVB,SVC,SVD,SUMC
      COMMONNXC,SA1,VMACH,KRZZ,SP1,GAM,THI,MX,DMCHI,MCH,NCV,TBT,IFRZ,NOA
     1T,SR1,IXG,SV1,KKJ,IXC,NXG,SH1,NOATO,SA2,FFF,WS,RV,CMF
      COMMONVA,MOS,DUM1,DUM2,EP,IFCJC,ISP2,WTG,VMU2,WTL
      COMMONNT,FKF(10) ,EAK(10) ,EXK(10) ,PMU(10,10) ,RMU(10,10)
      COMMONIB(11) ,FNU(10) ,PNUS(10) ,SLAM(10) ,BE(10) ,BY(10) ,
     1        IBC(10) ,JJ(10)
      EQUIVALENCE (CC(1),FAMDA(1)),(B(1),X(1)),(GAMK(1),VLAM(1))
      EQUIVALENCE(TU(151),TF(1)),(VNU(1),CIJ(1))
      EQUIVALENCE(TAU(1),A(151)),              (NFIA(1),A(1)),(NFIB(1),
     1A(51)),(FFIN(1),A(101))
      EQUIVALENCE(A(1),DY(1),DYA(1))                                        SCAL0300
      CLIN = AMAX1(1.,W(2) + W(3)) * 0.2 * WTG                              SCAL0350
      DWTL = 0.                                                             SCAL0360
      DWTG = 0.                                                             SCAL0370
      DUMP = P * 1.E - 7                                                    SCAL0380
      BUMP = P * 1.E - 4                                                    SCAL0390
      BULP = ALOG(BUMP)                                                     SCAL0400
   15 CMF = 1.                                                              SCAL0410
   20 K = 0                                                                 SCAL0420
      DO 35 J=2,IS                                                          SCAL0430
      IF (IB(J) - IB(J - 1)) 25,30,35                                       SCAL0440
   25 JA = IB(J)                                                            SCAL0450
      IB(J) = IB(J - 1)                                                     SCAL0460
      IB(J - 1) = JA                                                        SCAL0470
      K = 1                                                                 SCAL0480
      GOTO 35                                                               SCAL0490
   30 IB(J) = 1000                                                          SCAL0500
   35 CONTINUE                                                              SCAL0510
      IF (K) 40,40,20                                                       SCAL0520
   40 IB(IS + 1) = 1000                                                     SCAL0530
      M = IB(1)                                                             SCAL0540
      M1 = 1                                                                SCAL0550
      L = IS + 2                                                            SCAL0560
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      I = C                                                              SCALC570
      LL = 1                                                             SCAL0600
   45 DO 320 IK=1,N                                                      SCAL0610
      I = I + 1                                                          SCAL0620
   65 IF (IK - IS) 70,70,85                                              SCAL069C
   70 SLAM(I) = 0.                                                       SCAL0700
      IBC(I)=IFC(I)
      PNUS(I) = 0.                                                       SCAL0710
      IF (IFC(I) - 1) 75,75,115                                          SCAL0720
   75 DYI = X(I + 2)                                                     SCAL0730
      IF (IFC(I) + 1) 315,80,80                                          SCAL0740
   80 IF (IFC(I)) 245,135,270                                            SCAL0750
   85 IF (IFC(I) + 1) 115,90,90                                          SCAL0760
   90 IF (IFC(I)) 110,95,125                                             SCAL0770
   95 VA = E(I) - TC(I) * X(1)                                           SCAL0780
      DO 105 J=1,IS                                                      SCAL0790
      IF (IBC(J)) 100,100,105                                            SCAL0800
  100 VA = VA + VNU(I,J) * X(J + 2)                                      SCAL0810
  105 CONTINUE                                                           SCAL0820
      DYI = VA                                                           SCAL0830
      GOTO 135                                                           SCAL0840
  110 IF (IK - IRE) 115,120,115                                          SCAL0850
  115 DYI = 0.                                                           SCAL0860
      GOTO 315                                                           SCAL0870
  120 IFC(I) = 1                                                         SCAL0880
      DYI = X(IER)                                                       SCAL0890
      GOTO 270                                                           SCAL0900
  125 L = L + 1                                                          SCAL0910
      IF (L - IER) 130,125,130                                           SCAL0920
  130 DYI = X(L)                                                         SCAL0930
      GOTO 270                                                           SCAL0940
  135 DWTG = DWTG + VN(I) * DYI * WTM(I)                                 SCAL0950
      IF (IP(I)) 140,235,140                                             SCAL0960
  140 IF (IK - M) 145,185,145                                            SCAL0970
  145 IF (VN(I) - BUMP) 150,180,180                                      SCAL0980
  150 IF (MOE) 235,235,155                                               SCAL0990
  155 IF (DYI) 160,315,165                                               SCAL1000
  160 IF (VN(I) / BUMP - .9999995 - CMF * DYI) 315,315,170               SCAL1010
  165 IF (BUMP / VN(I) - 1. - CMF * DYI) 175,315,315                     SCAL1020
  170 CMF = (VN(I) / BUMP - .9999995) / DYI                              SCAL1030
      GOTO 315                                                           SCAL1040
  175 CMF = (BUMP / VN(I) - 1.) / DYI                                    SCAL1050
      GOTO 315                                                           SCAL1060
  180 IF (MOE) 215,215,190                                               SCAL1070
  185 M1 = M1 + 1                                                        SCAL1080
      M = IB(M1)                                                         SCAL1090
  190 IF (DYI) 195,315,200                                               SCAL1100
  195 IF (DYI * CMF + .999) 205,315,315                                  SCAL1110
  200 IF (DYI * CMF - 9.) 315,315,210                                    SCAL1120
  205 CMF = - .999 / DYI                                                 SCAL1130
      GOTO 315                                                           SCAL1140
  210 CMF = 9. / DYI                                                     SCAL1150
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      GOTO 315                                                          SCAL1160
  215 IF (DYI * CMF - 2.303) 220,230,230                                SCAL1170
  220 IF (DYI * CMF + 6.909) 225,315,315                                SCAL1180
  225 CMF = - 6.909 / DYI                                               SCAL1190
      GOTO 315                                                          SCAL1200
  230 CMF = 2.303 / DYI                                                 SCAL1210
      GOTO 315                                                          SCAL1220
  235 IF (Y(I) - BULP + ABS(DYI) * CMF) 315,240,240                     SCAL1230
  240 CMF = - (Y(I) - BULP) / ABS(DYI)                                  SCAL1240
      GOTO 315                                                          SCAL1250
C     NON-PRESENT BASE                                                  SCAL1260
  245 IF (KR(6)) 255,250,250                                            SCAL1270
  250 IF (T - TF(I) + .001) 315,255,255                                 SCAL1280
  255 IF (Y(I) + CMF * DYI - 0.1) 315,260,260                           SCAL1290
  260 DUM1 = (.1 - Y(I)) / DYI                                          SCAL1300
      IF (DUM1 - .001) 315,315,265                                      SCAL1310
  265 CMF = DUM1                                                        SCAL1320
      GOTO 315                                                          SCAL1330
  270 DWTL = DWTL + DYI * WTM(I)                                        SCAL1340
      IF (DYI) 275,315,290                                              SCAL1350
  275 IF (VN(I)) 290,290,280                                            SCAL1360
  280 IF (VN(I) + DYI * CMF) 285,290,290                                SCAL1370
  285 CMF = - VN(I) / DYI * 1.00001                                     SCAL1380
  290 IF (KR(6)) 305,295,295                                            SCAL1390
  295 CLIP = CLIM / WTM(I)                                              SCAL1400
      IF (ABS(CMF * DYI) - CLIP) 315,315,300                            SCAL1410
  300 CMF = CLIP / ABS(DYI)                                             SCAL1420
      GOTO 315                                                          SCAL1430
  305 IF (ABS(CMF * DYI) - P) 315,315,310                               SCAL1440
  310 CMF = P / ABS(DYI)                                                SCAL1450
  315 CMFF(I) = CMF                                                     SCAL1460
  320 DY(IK) = DYI                                                      SCAL1470
      IF(KR(6)) 322,321,321
  321 RVL=AMAX1(.1,RV/2.)
      CMF = AMIN1(CMF,WTG / ABS(ABS(DWTL - DWTG / WTG * WTL) / RVL - DWTSCAL1490
     1G))                                                               SCAL1500
  322 IF(KR(7)-1) 355,355,330                                           SCAL1520
  325 FORMAT (1X2(8X2HVN9X1HY8X2HDY7X5HSCALE7X1HE4X6HIFC IP)/(1XA4,5E    SCAL1530
     110.3,I3,I2,1X,A4,5E10.3,I3,I2))                                   SCAL1540
  330 NQ = I                                                            SCAL1550
  335 WRITE(KOUT,325)(FANCA(J),VN(J),Y(J),DYA(J,LL),CMFF(J),E(J),IFC(J),SCAL1560
     1IP(J),J=1,NQ)                                                     SCAL1580
  340 WRITE(KOUT,350)(EB(I),I=1,IS)                                     SCAL1590
      WRITE(KOUT,350)(X(I),I=1,ISPQ)                                    SCAL1600
      WRITE(KOUT,345)(IB(I),I=1,IS)                                     SCAL1610
  345 FORMAT(10I5)                                                      SCAL1620
  350 FORMAT(8E12.4)                                                    SCAL1630
  355 CONTINUE                                                          SCAL1690
      IF (X(1)) 370,415,370                                             SCAL1700
  370 X1 = X(1) * CMF                                                   SCAL1710
      ABX = ABS(X(1))                                                   SCAL1720
      IF (ABS(X1) - .5) 380,380,375
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375 CMF = .5 / ABX                                                    SCAL1730
    X1 = CMF * X(1)                                                   SCAL1740
380 IF (X1) 390,415,385                                               SCAL1750
385 TM = TMAX                                                         SCAL1760
    X1 = AMIN1(.2,X1)                                                 SCAL1770
    GOTO 395                                                          SCAL1780
390 TM = TMIN                                                         SCAL1790
    X1 = AMAX1( - 0.2,X1)                                             SCAL1800
395 DTM = (TM - T) / (TM * X1)                                        SCAL1810
    IF (DTM - 1.) 400,410,410                                         SCAL1820
400 CMF = DTM * CMF                                                   SCAL1830
405 T = TM                                                            SCAL1840
    GOTO 415                                                          SCAL1850
410 T = T / (1. - X1)                                                 SCAL1860
415 AA = AA * EXP(CMF * X(2))                                         SCAL1870
    RETURN                                                            SCAL1880
    END                                                               SCAL1890

                                                  CARD COUNT -        173
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      SUBROUTINECRECT(MCE)                                                  CREC0010
      REALNFIA(10) ,NFIB(10) ,FFIN(10) ,UM(10,10) ,TAU(10,10)               CREC0030
      DIMENSIONDY(1) ,DYA(15,1)                                             CREC0060
      DIMENSION TF(150),CIJ(150,1)
      DIMENSION X(1 ),VLAM(150,1 ),CC(7960)
      COMMONKIN,KCUT,JAN,MCL,NAB,IDC,N ,KKX(5)
      COMMON FAMOA(150),FAMOB(150),RB(150,2),RC(150,2),
     1  RD(150,2),RE(150,2),RF(150,2),TU(150,2),VN(150),Y(150),WTM(150),
     2  VNU(150,10),FF(150),IFC(150),IP(150),CP(150),H(150),SB(150),
     3  TC(150),VLNK(150),E(150),LAMI(150),GAMK(  1, 1)
      COMMON A(16,16),W(3),WM,B(16),SCH,RHO,VEL,B1,KR(10),TILE(3),NFF,
     1  XC(50),XG(50)
      COMMON ZKE(10),TLO(10),DMCLO(10),WALJP(10),EB(10),ALP(10),GAMH(10)
     1 ,GAMF(10),TQ(10,3),TK(10,3),WAT(10),IR(10),IOAT(10),KAT(10),UM
     2 ,EBL(10)
      COMMONFFA,IS,ISP,P,T,SIP,HIP,EL,ENL,FLIG,NQ,IFL,ISPQ,KRALP,CPF,IRE
     1,IER,AA,ITS,IN,IL,IT,MODE,HMELT,SMELT,TMAX,TMIN,MELT,SUMN,SUML,JC,
     2HG,CPG,SVA,SVB,SVC,SVD,SUMC
      COMMONNXC,SA1,VMACH,KRZZ,SP1,GAM,THI,MX,DMCHI,HCH,NCV,TBT,IFRZ,NOA
     1T,SR1,IXG,SV1,KKJ,IXC,NXG,SHI,NOATO,SA2,FFF,WS,RV,CMF
      COMMONVA,HOS,DUM1,DUM2,EP,IFCJC,ISP2,WTG,VMU2,WTL
      COMMONMT,FKF(10) ,EAK(10) ,EXK(10) ,PMU(10,10) ,RMU(10,10)
      COMMONIB(11) ,FNU(10) ,PNUS(10) ,SLAM(10) ,BE(10) ,BY(10) ,
     1        IBC(10) ,JJ(10)
      EQUIVALENCE (CC(1),FAMOA(1)),(B(1),X(1)),(GAMK(1),VLAM(1))
      EQUIVALENCE(TU(151),TF(1)),(VNU(1),CIJ(1))
      EQUIVALENCE(TAU(1),A(151)),          (NFIA(1),A(1)),(NFIB(1),
     1A(51)),(FFIN(1),A(101))
      EQUIVALENCE(A(1),DY(1),DYA(1))                                        CREC0290
      M1 = 1                                                                CREC0300
      M = IB(1)                                                             CREC0310
      WTL = 0.                                                              CREC0320
      WTG = 0.                                                              CREC0330
      DUM2 = 0.                                                             CREC0340
      I = 1                                                                 CREC0350
      DO 115 IK=1,N                                                         CREC0360
    5 DYI = CMF * DY(IK)                                                    CREC0370
      IF (DYI) 10,115,10                                                    CREC0380
   10 IF (IFC(I)) 75,15,100                                                 CREC0390
   15 IF (IP(I)) 20,50,20                                                   CREC0400
   20 IF (M - IK) 25,30,25                                                  CREC0410
   25 IF (MCE) 50,50,25                                                     CREC0420
   30 M1 = M1 + 1                                                           CREC0430
      M = IB(M1)                                                            CREC0440
   35 VN(I) = VN(I) * (1. + DYI)                                            CREC0450
      IF (VN(I)) 40,40,45                                                   CREC0460
   40 Y(I) = - 100.                                                         CREC0470
      GOTO 115                                                              CREC0480
   45 Y(I) = ALOG(VN(I))                                                    CREC0490
      GOTO 55                                                               CREC0500
   50 Y(I) = Y(I) + DYI                                                     CREC0510
      VN(I) = EXP(Y(I))                                                     CREC0520
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   55 VA = WTM(I) * VN(I)                                    CREC0530
      WTG = WTG + VA                                         CREC0540
      DUM2 = DUM2 + VA / FF(I)                               CREC0550
      IF (IK - IS) 60,60,65                                  CREC0560
   60 PNUS(I) = VN(I)                                        CREC0570
      SLAM(I) = VN(I) / FF(I)                                CREC0580
      GOTO 115                                               CREC0590
   65 DO 70 K=1,IS                                           CREC0600
      VA = VNU(I,K) * VN(I)                                  CREC0610
      PNUS(K) = PNUS(K) + VA                                 CREC0620
   70 SLAM(K) = SLAM(K) + VA / FF(I)                         CREC0630
      GOTO 115                                               CREC0640
C     NON-PRESENT BASE CORRECTIONS AND TESTS                 CREC0650
   75 Y(I) = Y(I) + DYI                                      CREC0660
      IF (Y(I)) 115,80,80                                    CREC0670
   80 IF (IFC(I) + 1) 115,85,85                              CREC0680
   85 IF (KR(6)) 95,90,90                                    CREC0690
   90 IF (T - TF(I) + .001) 115,95,95                        CREC0700
   95 Y(I) = 0.                                              CREC0710
      IFC(I) = + 1                                           CREC0720
      GOTO 115                                               CREC0730
  100 VN(I) = VN(I) + DYI                                    CREC0740
      IF (VN(I)) 110,110,105                                 CREC0750
  105 WTL = WTL + VN(I) * WTM(I)                             CREC0760
      GOTO 115                                               CREC0770
  110 VN(I) = 0.                                             CREC0780
      IFC(I) = - 1                                           CREC0790
  115 I=I+1
      EFF = WTG / DUM2                                       CREC0810
      DO 120 I=1,IS                                          CREC0820
      PNUS(I) = PNUS(I) + AA * GAMF(I)                       CREC0830
  120 SLAM(I) = SLAM(I) * FFF                                CREC0840
      RETURN                                                 CREC0850
      END                                                    CREC0860

                                        CARD COUNT -         86
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      SUBROUTINEOUTPT                                                    OUTP0010
      REALNFIA(10) ,NFIB(10) ,FFIN(10) ,UM(10,10) ,TAU(10,10)            OUTP0030
      DIMENSION TF(150),CIJ(150,1) ,IO(25)
      DIMENSION X(1 ),VLAM(150,1 ),CC(7960)
      COMMONKIN,KOUT,JAN,MOL,NAB,IDC,N ,KKX(5)
      COMMON FAMOA(150),FAMOB(150),RB(150,2),RC(150,2),
     1  RD(150,2),RE(150,2),RF(150,2),TU(150,2),VN(150),Y(150),WTM(150),
     2  VNU(150,10),FF(150),IFC(150),IP(150),CP(150),H(150),SB(150),
     3  TC(150),VLNK(150),E(150),LAMI(150),GAMK(  1,  1)
      COMMON A(16,16),W(3),WM,B(16),SB1,RHO,VEL,B1,KR(10),TILE(3),NFF,
     1  XC(50),XG(50)
      COMMON ZKE(10),TLC(10),DMCLO(10),WALJP(10),EB(10),ALP(10),GAMH(10)
     1 ,GAMF(10),TQ(10,3),TK(10,3),WAT(10),IR(10),IOAT(10),KAT(10),UM
     2 ,EBL(10)
      COMMONFFA,IS,ISP,P,T,SIP,HIP,EL,ENL,FLIQ,NQ,IFL,ISPQ,KRALP,CPF,IRE
     1,IER,AA,ITS,IN,IL,IT,MODE,HMELT,SMELT,TMAX,TMIN,MELT,SUMN,SUML,JC,
     2HG,CPG,SVA,SVB,SVC,SVD,SUMC
      COMMONNXC,SA1,VMACH,KRZZ,SP1,GAM,THI,MX,DMCHI,HCH,NCV,TBT,IFRZ,NOA
     1T,SR1,IXG,SV1,KKJ,IXC,NXG,SH1,NOATO,SA2,FFF,WS,RV,CNF
      COMMONVA,HOS,DUM1,DUM2,EP,IFCJC,ISP2,WTG,VMU2,WTL
      COMMONMT,FKF(10) ,EAK(10) ,EXK(10) ,PMU(10,10) ,RMU(10,10)
      COMMONIB(11) ,FNU(10) ,PNUS(10) ,SLAM(10) ,BE(10) ,BY(10) ,
     1       IBC(10) ,JJ(10)
      EQUIVALENCE (CC(1),FAMOA(1)),(B(1),X(1)),(GAMK(1),VLAM(1))
      EQUIVALENCE(TU(151),TF(1)),(VNU(1),CIJ(1))
      EQUIVALENCE(TAU(1),A(151)),              (NFIA(1),A(1)),(NFIB(1),
     1A(51)),(FFIN(1),A(101))
    5 FORMAT(/9X6HTEMP =F10.4,17H DEG-K      PRES =F8.4,17H ATM      MOL WOUTP0280
     1T =E11.7)                                                          OUTP0290
   10 FORMAT( /87H  SPECIES  MOL.FRAC.   D-LN-KP/D-LN-T  LOG-PP        LOOUTP0300
     1G-KP      FLAG    ERROR            CP  /(1X2A4,4E13.5,I5,2E13.5))  OUTP0310
   15 FORMAT(10X10HENTHALPY =E14.7,20H CAL/GM    ENTROPY =E12.5,13H CAL/OUTP0320
     1GM-DEG K/10X 9HDENSITY =E13.6,10H LB/CU.FT.
     15X25HMASS CONDENSED/MASS GAS =E12.5,11H  B-PRIME =,E12.5)          OUTP0340
   20 FORMAT(//)                                                         OUTP0350
   25 FORMAT(5X 5HVEL =E10.3,16H FT/SEC    MACH =E10.3,  9H   AREA =E10.3OUTP0360
     1,12H SQFT/LB/SEC,/9H  H-GAS=,E12.5,21H BTU/LB    H-KINETIC =E12.5,
     27H BTU/LB)
   30 FORMAT(10X17HFRACTION LIQUID =F8.5)                                OUTP0380
      TAN(Q) = SIN(Q) / COS(Q)                                           OUTP0390
      HEPS = 0.01                                                        OUTP0400
C     FIND VKIN AS FIRST NONZERO FKF(M)
      IF(MT) 702,702,699
  699 DO 704 M=1,MT
      IF(FKF(M)) 701,704,701
  704 CONTINUE
  701 VKIN=FKF(M)
      GO TO 703
  702 VKIN=0.0
  703 CONTINUE
   35 WM = AA / P                                                        OUTP0410
      WRITE(KOLT,5)T,P,WM                                                OUTP0420
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```
      SHIP = HIP                                                        OUTP0450
      SSIP = SIP                                                        OUTP0460
      HG = C.                                                           OUTP0470
      HL = C.                                                           OUTP0480
      HIP = 0.                                                          OUTP0490
      WTLS=WTL
      SIP = 0.                                                          OUTP0500
      PMU2 = 0.                                                         OUTP0510
      HTIL = 0.                                                         OUTP0520
      BPRM=W(3)
   60 NINT = - 1                                                        OUTP0630
   65 IKMM=N
   70 DO 100 J=1,IKMM                                                   OUTP0650
      HTIL = HTIL + VN(J) / FF(J) * H(J)                                OUTP0660
      PMU2 = PMU2 + VN(J) / FF(J) * WTM(J)                              OUTP0670
      VA = VN(J) * H(J)                                                 OUTP0680
      IF (IFC(J)) 80,75,80                                              OUTP0690
   75 HG = HG + VA                                                      OUTP0700
      GOTO 95                                                           OUTP0710
   80 HL = HL + VA                                                      OUTP0720
      IF (KR(8)) 95,95,85                                               OUTP0730
   85 IF (TF(J) - .001 - T) 95,95,90                                    OUTP0740
   90 BPRM = BPRM - VN(J) * WTM(J) / WTG                                OUTP0750
      HL = HL - VA                                                      OUTP0760
      WTLS=WTLS-VN(J) * WTM(J)
   95 SIP = SIP + VN(J) * (SB(J) - 1.9869 * Y(J))                       OUTP0780
  100 CONTINUE                                                          OUTP0790
      IF (ITS) 105,135,135                                              OUTP0800
  105 DO 110 I=1,IKMM                                                   OUTP0810
  110 VN(I) = VN(I) / P                                                 OUTP0820
      IF (NCV) 115,115,120                                              OUTP0830
  115 WRITE(KOUT,270)(FAMOA(I),FAMOB(I),VN(I),I=1,IKMM)                 OUTP0840
      GOTO 125                                                          OUTP0850
  120 WRITE(KOUT,10)(FAMOA(I),FAMOB(I),VN(I),TC(I),Y(I),VLNK(I),IFC(I),EOUTP0860
     1(I),CP(I),I=1,IKMM)                                               OUTP0870
  125 DO 130 I=1,IKMM                                                   OUTP0880
  130 VN(I) = VN(I) * P                                                 OUTP0890
  135 CONTINUE
      HTIL = HTIL / PMU2                                                OUTP0950
      WTR = WTLS/WTG
      HIP = HG + HL                                                     OUTP0970
      HIP = (HIP + VN(MELT) * FLIQ * HMELT) / AA                        OUTP0980
      SIP = (SIP + VN(MELT) * FLIQ * SMELT) / AA                        OUTP0990
      KR1 = KR(1) - IFRZ + KR(8)                                        OUTP1000
  150 HTIL = HG / AA                                                    OUTP1030
      FAF = 0.                                                          OUTP1040
      IF (KR(4)) 160,155,155
  155 HIP = (HG + (HL - WTR * HG) / WS) / AA                            OUTP1050
  160 IF (KR(10)) 165,180,165                                           OUTP1060
  165 IF (NCV + ITS) 166,180,180                                        OUTP1070
  166 IF(KKX(1)) 180,180,168
  168  CONTINUE
```

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C*****THE SQUEE CALLS AND FORMAT 167 YIELD A COMPRESSED OUTPUT TO BE
C*****READ AS (E6.4,E8.5,2E6.4,F4.2,E7.5,E6.4,2E8.5,.....)
      CALL SQUEE (P,IO(1),4)
      CALL SQUEE (W(2),IO(4),4)
      CALL SQUEE (BPRM,IO(7),5)
      CALL SQUEE (VKIN,IO(10),4)
      IO(13) = FAF*100.
      CALL SQUEE (T,IO(14),5)
      CALL SQUEE (WTR,IO(17),4)
      CALL SQUEE (HTIL,IO(20),5)
      CALL SQUEE (HIP,IO(23),5)
      KR1=KR1+1
      WRITE (KOUT,169)  P,W(2),BPRM,VKIN,FAF,
     1                  T,WTR,HTIL,HIP,FAMOA(JC), FAMOB(JC),KR1,TILE
      WRITE(KOUT,1675) IO,FAMOA(JC),FAMOB(JC),KR1,TILE
      PUNCH 167,  IO,FAMOA(JC), FAMOB(JC), KR1,TILE
      KR1=KR1-1
  167 FORMAT (I4,A1,I1,I4,A1,I1,I6,A1,I1,I4,A1,I1,
     1        I4,I5,A1,I1,I4,A1,I1,I6,A1,I1,I6,A1,I1,A4,A2,I1,4X,2A4,A2)
 1675 FORMAT(1X,I4,A1,I1,I4,A1,I1,I6,A1,I1,I4,A1,I1,I4,I5,A1,I1,
     1   I4,A1,I1,I6,A1,I1,I6,A1,I1,A4,A2,I1,4X,2A4,A2)
  169 FORMAT(1X,E11.4,E12.5,2E11.4,F4.2,E12.5,E11.4,2E12.5,A4,A2,I1,
     1   2A4,A2)
  180 RHO = P / T * WM / 1.3146                                          OUTP1100
      WRITE(KOUT,15)HIP,SIP,RHO,WTR,BPRM                                 OUTP1110
      IF (FLIQ) 185,190,185                                              OUTP1120
  185 WRITE(KOUT,30)FLIQ                                                 OUTP1130
  190 IF (ITS) 245,260,260
  245 IF (KR(5) - 1) 260,255,250                                         OUTP1420
  250 HCH = HIP                                                          OUTP1430
      SCH = SIP                                                          OUTP1440
  255 VELSQ = (HCH - HIP) * 2.                                           OUTP1450
      VMACH = SQRT(VELSQ / GAM * WM / (1.9869 * T))                      OUTP1460
      VEL = SQRT(VELSQ * 45054.)                                         OUTP1470
      AREA = 1. / (VEL * RHO)                                            OUTP1480
      HG=HG/WTG*1.8
      HKIN=(HCH-HIP)*1.8
      WRITE(KOUT,25)VEL,VMACH,AREA,HG,HKIN                               OUTP1490
  260 CONTINUE                                                           OUTP1500
  265 FORMAT(22H   SURFACE SPECIES IS 2A4)                               OUTP1510
  270 FORMAT(/3(5X7HSPECIES3X8HMOLE FR.2X)/(5X2A4,E12.5,5X2A4,E12.5,5X2AOUTP1520
     14,E12.5))                                                          OUTP1530
      IF (MODE - 1) 280,275,280                                          OUTP1540
  275 WRITE(KOUT,265)FAMOA(JC),FAMOB(JC)                                 OUTP1550
  280 WRITE(KOUT,20)                                                     OUTP1560
      IF (ITS) 285,315,315                                               OUTP1570
  285 RETURN
  315 HIP = SHIP                                                         OUTP1700
      SIP = SSIP                                                         OUTP1710
      RETURN                                                             OUTP1720
      END                                                                OUTP1730

                                                  CARD COUNT -      155
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      SUBROUTINEPROPS                                                    PROP0010
      REALNFIA(10) ,NFIB(10) ,FFIN(10) ,UM(10,10) ,TAU(10,10)            PROP0030
      DIMENSIONTT(1) ,RHO(1) ,CPBAR(1) ,SC(1) ,PR(1) ,VK(10)             PROP0040
      DIMENSIONZK(10)                                                    PROP0050
      DIMENSIONZI(10)                                                    PROP0060
      DIMENSION VI(10)
      DIMENSIONCAPC(1)                                                   PROP0070
      DIMENSION TF(150),CIJ(150,1)
      DIMENSION X(1 ),VLAM(150,1 ),CC(7960)
      COMMONKIN,KOUT,JAN,MOL,NAB,IDC,N ,KKX(5)
      COMMON FAMOA(150),FAMOB(150),RB(150,2),RC(150,2),
     1  RD(150,2),RE(150,2),RF(150,2),TU(150,2),VN(150),Y(150),WTM(150),
     2  VNU(150,10),FF(150),IFC(150),IP(150),CP(150),H(150),SB(150),
     3  TC(150),VLNK(150),E(150),LAMI(150),GAMK(  1, 1)
      COMMON A(16,16),W(3),WM,B(16),SCH,RHO,VEL,B1,KR(10),TILE(3),NFF,
     1  XC(50),XG(50)
      COMMON ZKE(10),TLC(10),DMCLO(10),WALJP(10),EB(10),ALP(10),GAMH(10)
     1 ,GAMF(10),TQ(10,3),TK(10,3),WAT(10),IR(10),IOAT(10),KAT(10),UM
     2 ,EBL(10)
      COMMONFFA,IS,ISP,P,T,SIP,HIP,EL,ENL,FLIQ,NQ,IFL,ISPQ,KRALP,CPF,IRE
     1,IER,AA,ITS,IN,IL,IT,MODE,HMELT,SMELT,TMAX,TMIN,MELT,SUMN,SUML,JC,
     2HG,CPG,SVA,SVB,SVC,SVD,SUMC
      COMMONNXC,SA1,VMACH,KRZZ,SP1,GAM,THI,MX,DMCHI,HCH,NCV,TBT,IFRZ,NOA
     1T,SR1,IXG,SV1,KKJ,IXC,NXG,SH1,NOATO,SA2,FFF,WS,RV,CMF
      COMMONVA,HOS,DUM1,DUM2,EP,IFCJC,ISP2,WTG,VMU2,WTL
      COMMONMT,FKF(10) ,EAK(10) ,EXK(10) ,PMU(10,10) ,RMU(10,10)
      COMMONIB(11) ,FNU(10) ,PNUS(10) ,SLAM(10) ,BE(10) ,BY(10) ,
     1        IBC(10) ,JJ(10)
      EQUIVALENCE (CC(1),FAMOA(1)),(B(1),X(1)),(GAMK(1),VLAM(1))
      EQUIVALENCE(TU(151),TF(1)),(VNU(1),CIJ(1))
      EQUIVALENCE(TAU(1),A(151)),              (NFIA(1),A(1)),(NFIB(1),
     1A(51)),(FFIN(1),A(101))
    5 FORMAT(/10X60H CP-FROZEN     CP-EQUIL    DLNM/DLNT    DLNM/DLNP      GPROP0320
     1AMMA          /10X5E12.5)                                            PROP0330
   10 FORMAT(1H1115X45HAEROTHERM CHEMICAL EQUILIBRIUM (ACE) SOLUTION//)    PROP0340
   15 FORMAT (4H1---50H-----FOLLOWING OUTPUT NON-CONVERGENT-------------PROP0350
     1-//)                                                                 PROP0360
      IF (NCV) 25,25,20                                                  PROP0370
   20 WRITE(KOUT,15)                                                     PROP0380
      GOTO 35                                                            PROP0390
   25 IF (KR(10) / 2 + KR(7) + KR(2) + KR(3)) 35,35,30                   PROP0400
   30 WRITE(KOUT,10)                                                     PROP0410
   35 CPF = CPF / AA                                                     PROP0420
      ALF = A(2,1) / A(1,1)                                              PROP0430
      CSP = 1. / (A(1,1) * AA)                                           PROP0440
      IF (MODE - 3) 40,45,40                                             PROP0450
   40 CSP = CSP / T                                                      PROP0460
   45 BETA = P * (A(2,2) - A(1,2) / A(1,1) * A(2,1)) - 1.                PROP0470
      GAM = 1. - ALF                                                     PROP0480
      GAM = 1. / (1. + BETA - 1.9869 / AA * GAM / CSP * GAM * P)         PROP0490
      WRITE(KOUT,5)CPF,CSP,ALF,BETA,GAM                                  PROP0500
      ITS = - 1                                                          PROP0510
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```
      CAPC(1) = 1.                                                    PROP0520
      II = 1                                                          PROP0530
      WM = AA / P                                                     PROP0540
      ISM = IS - 1                                                    PROP0550
      TT(II) = T * 1.8                                                PROP0560
      RHO(II) = AA / (1.3146 * T)                                     PROP0570
      CPBAR(II) = CPF                                                 PROP0580
      AISTR = 1.13                                                    PROP0590
C     FORM NECESSARY SUMMATIONS                                       PROP0600
      PMU2 = 0.                                                       PROP0610
      CPTIL = 0.                                                      PROP0620
      HTIL = 0.                                                       PROP0630
      PMU1 = 0.                                                       PROP0640
      TMU3 = 0.                                                       PROP0650
      I = 1                                                           PROP0660
   50 DO 60 IK=1,N                                                    PROP0670
      IF (IFC(I)) 60,55,60                                            PROP0680
   55 PMU1 = PMU1 + VN(I) * FF(I)                                     PROP0690
   60 I=I+1
      VMU1 = PMU1 / P                                                 PROP0710
      DO 66 K=1,ISM
      VK(K)=VN(K)
      IF(WTM(K)-1.) 66,65,65
   65 ZK(K) = VN(K) / FF(K)                                           PROP0730
   66 CONTINUE
      AMU5 = 0.                                                       PROP0740
      PMU6 = 0.                                                       PROP0750
      WD2 = 1.385                                                     PROP0760
      WD7 = WD2 / PMU1                                                PROP0770
      WD2 = 1.2 * AISTR / (PMU1 * WM)                                 PROP0780
      WD4 = 0.284 * WD2                                               PROP0790
      WD5 = .32 * AISTR / (PMU1 * WM)                                 PROP0800
      WD8 = WD4 / PMU1                                                PROP0810
      I = 1                                                           PROP0820
      DO 90 IK=1,N                                                    PROP0830
      IF (WTM(I) - 1.) 90,70,70                                       PROP0840
   70 VA = VN(I) / FF(I)                                              PROP0850
      VB = VA * WTM(I)                                                PROP0860
      VC = VN(I) * FF(I)                                              PROP0870
      IF (IK - IS) 85,85,75                                           PROP0880
   75 DO 80 K=1,ISM                                                   PROP0890
      VK(K)=VK(K)+VN(I)*VNU(I,K)
   80 ZK(K) = ZK(K) + VA * VNU(I,K)                                   PROP0900
   85 PMU2 = PMU2 + VB                                                PROP0910
      TMU3 = TMU3 + VA                                                PROP0920
      CPTIL = VA * CP(I) + CPTIL                                      PROP0930
      HTIL = HTIL + VA * H(I)                                         PROP0940
      AMU5 = AMU5 + VB / (WDZ + VC * (WTM(I) * WD2 - WD7))            PROP0950
      PMU6 = PMU6 + VA / (WD4 + (WD5 * WTM(I) - WD8) * VC)            PROP0960
   90 I=I+1
      VMU5 = AMU5 / AA                                                PROP0980
      VMU6 = (PMU6 + CPTIL / 1.9869 - 2.5 * TMU3) / P                 PROP0990
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      VMU2 = PPU2 / P                                                    PROP1000
      VMU3 = TPU3 / PMU2                                                 PROP1010
      ZKS = 1.0                                                          PROP1020
      VKS=1.0
      DO 95 K=1,ISM                                                      PROP1030
      VK(K)=VK(K)/AA*WTM(K)
      ZK(K) = ZK(K) / PMU2 * WTM(K)                                      PROP1050
      VKS=VKS-VK(K)
   95 ZKS = ZKS - ZK(K)                                                  PROP1060
      DO 100 I=1,IS                                                      PROP1070
      ZI(I) = ZKS * CIJ(IS,I) / WTM(IS) * WAT(I)                         PROP1080
      VI(I)=VKS*CIJ(IS,I)/WTM(IS)*WAT(I)
      DO 100 K=1,ISM                                                     PROP1090
      VI(I) = VI(I) + CIJ(K,I) * VK(K) / WTM(K) * WAT(I)
  100 ZI(I) = ZI(I) + CIJ(K,I) * ZK(K) / WTM(K) * WAT(I)                 PROP1100
      CPTIL = CPTIL / PMU2                                               PROP1110
      HTIL = HTIL / PMU2 * 1.8                                           PROP1120
      OMEGA = 1.07 / (T / 106.7) ** 0.159                                PROP1130
      DBAR = 4.16E - 8 * T / P * SQRT(T) / OMEGA                         PROP1140
      VMU = RHO(II) * DBAR * VMU5 / VMU1                                 PROP1150
  105 CONTINUE                                                           PROP1160
      TCOND = RHO(II) * DBAR / WM * VMU6 / VMU1 * 1.9869                 PROP1170
      SC(II) = VMU5 / VMU2 * WM                                          PROP1180
      PR(II) = CPF / VMU6 * VMU5 / 1.9869 * WM                           PROP1190
      VMU12 = VMU1 * VMU2                                                PROP1200
      WRITE(KOUT,110)T1,VMU,TCOND,DBAR,PR,SC,VMU1,VMU2,WM,HTIL,CPTIL
  110 FORMAT(/58H  PROPERTY ROUTINE OUTPUT IN LB-MASS,FT,SEC,BTU,AND DEGPROP1230
     1-R     /67H     TEMP          VISC          COND          DBAR          PR PROP1240
     1          SC/6E12.5/57H      MU1           MU2        MOL.WT        HTILPROP1250
     1         CPTIL/5E12.5)
  115 FORMAT(1X10E12.5)                                                  PROP1270
  120 FORMAT (58H ELEMENTAL K AND Z MASS FRACTIONS BY ATOMIC NUMBER . .
     1. ./1X10(4XI3,5X))
      WRITE(KOUT,120)(KAT(J),J=1,IS)                                     PROP1300
      WRITE(KOUT,115)(VI(J),J=1,IS)
      WRITE(KOUT,115)(ZI(J),J=1,IS)                                      PROP1310
      RETURN                                                             PROP1320
      END                                                                PROP1330

                                                  CARD COUNT -       142
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      SUBROUTINE RERAY(N,C,NN,D,NNN,LS,IS)
C     DIRECT INVERSION PROCEDURE  --  C IS REPLACED BY C**-1
      DIMENSION D(16,1),SD(16),C(16,1),L(16),S(16),LL(16),LLL(16),LS(1)
      N1=N+1
      KOUT=5
      NP=N+NN
      DO 11 I=1,NP
      LLL(I)=I
      IF(LS(1)) 113,113,112
  112 L(I)=LS(I)
      GO TO 11
  113 L(I)=I
   11 CONTINUE
      IX=-1
      IF(IS+2) 111,109,111
  106 FORMAT(11H  L(I),I=1,I3,5X (30I3))
  107 FORMAT(15H  ((C(I,J),J=1,I3,12H),(D(J),J=1,I3, 6H),I=1,I3,15H)  BE
     1FORE RERAY)
  108 FORMAT(2X  11E10.3/(12X  10E10.3))
  109 WRITE(KOUT,107) NP,NNN,N
      WRITE(KOUT,106)NP,(L(I),I=1,NP)
      IX=0
      DO 110 I=1,N
  110 WRITE(KOUT,108)(C(I,J),J=1,NP),(D(I,J),J=1,NNN)
  111 IS=-1
C     TRIANGULATE MATRIX
      DO 15 I=1,N
      DO 160 M=1,NP
  160 S(M)=ABS(C(I,M))
      IF(IS) 18,16,16
   18 IS=0
      SD(1)=1.
      GO TO 12
C     REDUCE ROW I BY PRECEEDING ROWS
   16 DO 17 J=2,I
      K=L(J-1)
      DIV=-C(I,K)
      IF(DIV) 161,17,161
  161 C(I,K)=0.
      DO162 M=1,NP
      DIVC=DIV*C(J-1,M)
      S(M)=AMAX1(S(M),ABS(DIVC))
  162 C(I,M)=C(I,M)+DIVC
      IF(NNN) 17,17,163
  163 DO 164 M=1,NNN
  164 D(I,M)=D(I,M)+DIV*D(J-1,M)
   17 CONTINUE
C     SEEK MAXIMUM PIVOT
   12 DIV=0.
      DO 13 JJ=I,N
      M=L(JJ)
      IF(ABS (C(I,M))-DIV)13,13,121
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```
  121 DIV=ABS (C(I,M))
      K=M
      J=JJ
   13 CONTINUE
      SD(I)=DIV/S(K)
      L(J)=L(I)
      L(I)=K
      IF(SD(I)-1.E-8) 131,131,14
C     SINGULAR MATRIX RETURN
  131 IS=-1
      WRITE(KOUT,151) (II,L(II),SD(II),II=1,I)
      RETURN
   14 DIV=C(I,K)
      C(I,K)=1.0
      K=LLL(J)
      LLL(J)=LLL(I)
      LLL(I)=K
      LL(K)=I
C     NORMALIZE ROW
      IF(NNN) 143,143,141
  141 DO 142 J=1,NNN
  142 D(I,J)=D(I,J)/DIV
  143 DO 15 J=1,NP
   15 C(I,J)=C(I,J)/DIV
      IF(IX) 152,150,152
  151 FORMAT(24H PIVOT ROW/COL/RES.RATIO 5(I4,1H/I3,1H/E9.2,1H,))
  150 WRITE(KOUT,151) (I,L(I),SD(I),I=1,NP)
C     DIAGONALIZE MATRIX
  152 NM=N-1
      DO 20 I=1,NM
      K=L(I+1)
      DO 20 J=1,I
      DIV=-C(J,K)
      IF(DIV)19,20,19
   19 C(J,K)=0.
      IF(NNN) 191,191,192
  192 DO 193 M=1,NNN
  193 D(J,M)=D(J,M)+DIV*D(I+1,M)
  191 DO 201 M=1,NP
  201 C(J,M)=C(J,M)+DIV*C(I+1,M)
   20 CONTINUE
C     INTERCHANGE COLUMNS
      DO 30 II=1,NP
      I=II
   21 J=L(I)
      L(I)=I
      IF(J-I)22,30,22
   22 IF(IS)25,23,25
   23 DO 24 M=1,N
      S(M)=C(M,I)
   24 C(M,I)=C(M,J)
      IS=I
```

```
      I=J
      GO TO 21
   25 IF(IS-J)26,28,26
   26 DO 27 M=1,N
   27 C(M,I)=C(M,J)
      I=J
      GO TO 21
   28 DO 29 M=1,N
   29 C(M,I)=S(M)
      IS=0
   30 CONTINUE
C     INTERCHANGE ROWS
      DO 40 II=1,N
      I=II
   31 J=LL(I)
      LL(I)=I
      IF(J-I)32,40,32
   32 IF(IS)35,33,35
   33 DO 34 M=1,NP
      S(M)=C(I,M)
   34 C(I,M)=C(J,M)
      IF(NNN) 343,343,341
  341 DO 342 M=1,NNN
      SD(M)=D(I,M)
  342 D(I,M)=D(J,M)
  343 IS=I
      I=J
      GO TO 31
   35 IF(IS-J)36,38,36
   36 DO 37 M=1,NP
   37 C(I,M)=C(J,M)
      IF(NNN) 373,373,371
  371 DO 372 M=1,NNN
  372 D(I,M)=D(J,M)
  373 I=J
      GO TO 31
   38 DO 39 M=1,NP
   39 C(I,M)=S(M)
      IF(NNN) 393,393,391
  391 DO 392 M=1,NNN
  392 D(I,M)=SD(M)
  393 IS=0
   40 CONTINUE
      IF(IX) 411,409,411
  407 FORMAT(15H  ((C(I,J),J=1,I3,12H),(D(J),J=1,I3, 6H),I=1,I3,15H)  AF
     1TER RERAY  )
  409 WRITE(KOUT,407) NP,NNN,N
      DO 410 I=1,N
  410 WRITE(KOUT,108)(C(I,J),J=1,NP),(D(I,J),J=1,NNN)
  411 RETURN
      END
```

CARD COUNT - 155

```
      SUBROUTINEKINET                                                    KINE0010
      REALNFIA(10) ,NFIB(10) ,FFIN(10) ,UM(10,10) ,TAU(10,10)            KINE0030
      DIMENSIONPRMU(10,10)
      DIMENSION TF(150),CIJ(150,1)
      DIMENSION X(1 ),VLAM(150,1 ),CC(7960)
      COMMONKIN,KOUT,JAN,MOL,NAB,IDC,N ,KKX(5)
      COMMON FAMOA(150),FAMOB(150),RB(150,2),RC(150,2),
     1  RD(150,2),RE(150,2),RF(150,2),TU(150,2),VN(150),Y(150),WTM(150),
     2  VNU(150,10),FF(150),IFC(150),IP(150),CP(150),H(150),SB(150),
     3  TC(150),VLNK(150),E(150),LAMI(150),GAMK(  1, 1)
      COMMON A(16,16),W(3),WM,B(16),SCH,RHO,VEL,B1,KR(10),TILE(3),NFF,
     1  XC(50),XG(50)
      COMMON ZKE(10),TLO(10),DMCLO(10),WALJP(10),EB(10),WLP(10),GAMH(10)
     1 ,GAMF(10),TQ(10,3),TK(10,3),WAT(10),IR(10),IOAT(10),KAT(10),UM
     2 ,EBL(10)
      COMMONFFA,IS,ISP,P,T,SIP,HIP,EL,ENL,FLIQ,NQ,IFL,ISPQ,KRALP,CPF,IRE
     1,IER,AA,ITS,IN,IL,IT,MODE,HMELT,SMELT,TMAX,TMIN,MELT,SUMN,SUML,JC,
     2HG,CPG,SVA,SVB,SVC,SVD,SUMC
      COMMONNXC,SA1,VMACH,KRZZ,SP1,GAM,THI,MX,DMCHI,HCH,NCV,TBT,IFRZ,NOA
     1T,SR1,IXG,SV1,KKJ,IXC,NXG,SH1,NOATQ,SA2,FFF,WS,RV,CMF
      COMMONVA,HOS,DUM1,DUM2,EP,IFCJC,ISP2,WTG,VMU2,WTL
      COMMONMT,FKF(10) ,EAK(10) ,EXK(10) ,PMU(10,10) ,RMU(10,10)
      COMMONIB(11) ,DKPT(10) ,PKP(10) ,PKR(10) ,PMR(10) ,RAI(10) ,
     1VKP(10) ,LL(10) ,MA(10)
      EQUIVALENCE (CC(1),FAMOA(1)),(B(1),X(1)),(GAMK(1),VLAM(1))
      EQUIVALENCE(TU(1511,TF(1)),(VNU(1),CIJ(1))
      EQUIVALENCE(TAU(1),A(151)),          (NFIA(1),A(1)),(NFIB(1),
     1A(51)),(FFIN(1),A(101))
    5 FORMAT(13I3)                                                       KINE0320
   10 RT = 1.9869 * T                                                    KINE0330
      DO 40 M=1,MT                                                       KINE0340
      SUMD = 0.                                                          KINE0350
      SUMK = 0.                                                          KINE0360
      SUMR = 0.                                                          KINE0370
      SUMP = 0.                                                          KINE0380
      DO 15 I=1,IS                                                       KINE0390
      PRMU(I,M) = PMU(I,M) - RMU(I,M)                                    KINE0400
      SUMK = SUMK + PRMU(I,M) * VLNK(I)                                  KINE0410
      SUMR = SUMR + RMU(I,M) * Y(I)                                      KINE0420
      SUMP = SUMP + PMU(I,M) * Y(I)                                      KINE0430
   15 SUMD = SUMD + PRMU(I,2) * H(I)                                     KINE0440
C     EQUILIBRIUM CONSTANTS FOR KINETIC REACTIONS IN TERMS OF BASE SPECIKINE0450
C          LOG KP-S                                                     KINE0460
C     DERIVATIVES OF LOGS OF ABOVE KP-S WITH RESPECT TO LOG T           KINE0480
      DKPT(M) = SUMD / RT                                                KINE0490
C     RIGHT HAND SIDE (OR REVERSE PART) OF DRIVING POTENTIAL             KINE0500
      PKP(M) = EXP(SUMP - SUMK)                                          KINE0510
C     LEFT HAND SIDE (OR FORWARD PART) OF DRIVING POTENTIAL              KINE0520
      PKR(M) = EXP(SUMR)                                                 KINE0530
      VK1 = PKR(M) - PKP(M)                                              KINE0540
      IF (VK1) 25,20,25                                                  KINE0550
   20 VK1 = 1.E - 9 * PKR(M)                                             KINE0560
```

```
   25 CONTINUE
      VK2 = AA * FKF(M) * (ABS(VK1)) * * (EXK(M) - 1.) * EXP( - EAK(M) /KINE0580
     1RT)                                                                KINE0590
      VK3 = VK2                                                          KINE0600
      IF (EXK(M) - 1.) 35,30,30                                          KINE0610
   30 VK3 = VK2 * EXK(M)                                                 KINE0620
C     PM TIMES FORWARD RATE OF REACION I  (PM=AA)                        KINE0630
   35 PMR(M) = VK2 * VK1                                                 KINE0640
      PKP(M) = PKP(M) * VK3                                              KINE0650
      PKR(M) = PKR(M) * VK3                                              KINE0660
      RAT(M)=AMAX1(PKP(M),PKR(M))
      IF(KR(7)-1) 40,40,36
   36 IF(M-1) 37,37,39
   37 WRITE(KOUT,38)
   38 FORMAT(2X1HM7X3HLKP6X8HDLKP/DLT6X4HPMRR8X4HPMRP9X3HPMR9X3HRAT)
   39 WRITE(KOUT,41) M,SUMK,DKPT(M),PKR(M),PKP(M),PMR(M),RAT(M)
   40 MA(M) = M                                                          KINE0680
   41 FORMAT(I3,2X,6E12.5)
   45 FORMAT(1X26HA(I,J),B(I),I=1,8,J=1,8 IN)                            KINE0690
   50 FORMAT(1X12E10.3)                                                  KINE0700
   55 FORMAT(1X27HA(I,J),B(I),I=1,8,J=1,8 OUT)                           KINE0710
      IF (KR(7) - 1) 80,80,65                                            KINE0730
   65 CONTINUE
      WRITE(KOUT,50)PRMU                                                 KINE0810
      WRITE(KOUT,215)                                                    KINE0820
      WRITE(KOUT,50)(FR(I),I=1,IS)                                       KINE0830
   70 WRITE(KOUT,45)                                                     KINE0840
      DO 75 I=1,ISP2                                                     KINE0850
   75 WRITE(KOUT,50)(A(I,J),J=1,ISP2),B(I)                               KINE0860
   80 CONTINUE                                                           KINE0870
C******ORDER REACTIONS                                                  KINE0880
   85 IF (MT - 1) 105,105,90                                             KINE0890
   90 K = 0                                                              KINE0900
      DO 100 M=2,MT                                                      KINE0910
      IF (RAT(M) - RAT(M - 1)) 100,100,95                                KINE0920
   95 K = MA(M)                                                          KINE0930
      MA(M) = MA(M - 1)                                                  KINE0940
      MA(M - 1) = K                                                      KINE0950
      DUM1 = RAT(M)                                                      KINE0960
      RAT(M) = RAT(M - 1)                                                KINE0970
      RAT(M - 1) = DUM1                                                  KINE0980
  100 CONTINUE                                                           KINE0990
      IF (K) 105,105,85                                                  KINE1000
C******START SECOND MAJOR LOOP ON REACTIONS                             KINE1010
  105 DO 200 MM=1,MT
      M = MA(MM)
C******IS IT A CONTROLLING REACTION                                     KINE1030
      LL(MM) = 0                                                         KINE1040
      DO 125 L=1,IS                                                      KINE1050
      IF (PRMU(L,M)) 110,125,110                                         KINE1060
  110 DO 115 K=1,MM                                                      KINE1070
      IF (L - LL(K)) 115,125,115                                         KINE1080
                                                                         KINE1090
```

```
  115 CONTINUE                                                          KINE1100
      IF (RAT(MM) - EB(L)) 125,125,120                                  KINE1110
C* * * YES,IT IS FOR MASS BALANCE L                                     KINE1120
  120 LL(MM) = L                                                        KINE1130
      GOTO 130                                                          KINE1140
  125 CONTINUE                                                          KINE1150
C* * *NO, IT IS NOT, ADD INTO ALL MASS BALANCES                         KINE1160
      I1 = 1                                                            KINE1170
      I2 = IS                                                           KINE1180
      GOTO 170                                                          KINE1190
C******REARRANGE ACCORDING TO CONTROLLING REACTION                      KINE1200
  130 DUM1 = PRMU(L,M)                                                  KINE1210
      PRMU(L,M) = 0.                                                    KINE1220
      DO 165 I=1,IS                                                     KINE1230
      IF (PRMU(I,M)) 135,165,135                                        KINE1240
  135 DUM2 = PRMU(I,M) / DUM1                                           KINE1250
      MP = MM + 1                                                       KINE1260
      IF (MT - MP) 155,140,140                                          KINE1270
  140 DO 150 K=MP,MT                                                    KINE1280
      MI = MA(K)                                                        KINE1290
      PRMU(I,MI) = PRMU(I,MI) - DUM2 * PRMU(L,MI)                       KINE1300
      IF (ABS(PRMU(I,MI)) - .001) 145,150,150                           KINE1310
  145 PRMU(I,MI) = 0.                                                   KINE1320
  150 CONTINUE                                                          KINE1330
  155 DO 160 K=1,ISPQ                                                   KINE1340
  160 A(I + 2,K) = A(I + 2,K) - DUM2 * A(L + 2,K)                       KINE1350
      B(I + 2) = B(I + 2) - DUM2 * B(L + 2)                             KINE1360
      E(I)=E(I)-DUM2*E(L)
      DUM2 = ABS(DUM2)                                                  KINE1370
      EB(I) = AMAX1(EB(I) ,DUM2 * EB(L))                                KINE1380
  165 CONTINUE                                                          KINE1390
      PRMU(L,M) = DUM1                                                  KINE1400
C*****ADD CONTROLLING REACTION INTO ITS MASS BALANCE                    KINE1410
      I1 = L                                                            KINE1420
      I2 = L                                                            KINE1430
  170 DO 175 J=1,IS                                                     KINE1440
      SUMD = RMU(J,M) * PKR(M) - PMU(J,M) * PKP(M)                      KINE1450
      DO 175 I=I1,I2                                                    KINE1460
  175 A(I + 2,J + 2) = A(I + 2,J + 2) - SUMD * PRMU(I,M)                KINE1470
      SUMD = - PKP(M) * DKPT(M) - EAK(M) / RT * PMR(M)                  KINE1480
      DO 180 I=I1,I2                                                    KINE1490
      DUM1 = PMR(M) * PRMU(I,M)                                         KINE1500
      A(I+2,2)=A(I+2,2)-DUM1
      A(I + 2,1) = A(I + 2,1) + SUMD * PRMU(I,M)                        KINE1510
      E(I)=E(I)+DUM1
      B(I + 2) = B(I + 2) + DUM1                                        KINE1520
  180 EB(I) = AMAX1(EB(I) ,ABS(PRMU(I,M) * RAT(MM)))                    KINE1530
      IF (KR(7) - 1) 200,200,185                                        KINE1540
  185 WRITE(KOUT,215)                                                   KINE1550
      WRITE(KOUT,50)(EB(I),I=1,IS)                                      KINE1560
  190 WRITE(KOUT,55)                                                    KINE1570
      DO 195 I=1,ISP2                                                   KINE1580
```

```
      WRITE(KOLT,50)(A(1,J),J=1,ISP2),B(I)                              KINE1590
  195 CONTINUE                                                          KINE1600
      WRITE(KOLT,5)M,I1,I2,L,LL,MM,MA                                   KINE1610
      WRITE(KOLT,50)PRMU                                                KINE1620
  200 CONTINUE                                                          KINE1630
      DO 206 MM=1,MT
      L=LL(MM)
      IF(L) 201,206,201
  201 M=MA(MM)
      AR=1.
      EXEL=(PKR(M)+1.E-36)/(PKP(M)+1.E-36)
      IF(ABS(EXEL-1.)-.1) 204,204,202
  202 ELK=ALOG(EXEL)
      AR=EXEL/(EXEL-1.)-1./ELK
  204 DO 205 J=1,IS
  205 A(L+2,J+2)=A(L+2,J+2)+E(L)*(PMU(J,M)*(1.-AR)+AR*RMU(J,M))
      A(L+2,1)=A(L+2,1)-E(L)*DKPT(M)*(1.-AR)
  206 CONTINUE
      ENL = 0.                                                          KINE1650
      DO 210 I=3,ISP2                                                   KINE1660
  210 ENL = AMAX1(ABS(E(I-2)) / EB(I-2) ,ENL)
  215 FORMAT(1X12HEB(M),M=1,MT)                                         KINE1680
      IF(ENL-1.E-5) 216,216,225
  216 IF(EL-1.E-4) 220,225,225
  220 ITS = - 1                                                         KINE1700
  225 RETURN                                                            KINE1710
      END                                                               KINE1720

                                                CARD COUNT =      183
```

```
      SUBROUTINE SQUEE  (A,I,IDEE)
      DIMENSION I(1)
      DATA LUS,INUS/1H+,1H-/
      I(1)=C
      I(3)=C
      B=ABS(A)*1.000001
      IF(ABS(A)-1.E-10) 7,7,1
    1 IF(B-1.C) 3,2,2
    2 B=B/1C.
      I(3) = I(3)+1
      GO TO 1
    3 IF(B-0.1) 4,5,5
    4 B=B*10.
      I(3) = I(3)-1
      GO TO 3
    5 I(1) = A*10.** (IDEE-I(3))*1.000001
      IF(I(3)) 6,7,7
    6 I(2) = INUS
      GO TO 8
    7 I(2) = LUS
    8 I(3) = IABS(I(3))
      RETURN
      END
```

CARD COUNT - 23

```
      SUBROUTINE SWAP(A,B,SLA,SLB)
      DIMENSION A(16,1),B(1),SLA(16,1),SLB(1)
      DO 5 I=1,16
      B(I)=SLB(I)
      DO 5 J=1,16
    5 A(I,J)=SLA(I,J)
      RETURN
      END
```

CARD COUNT - 8

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13. ABSTRACT

The report describes and gives user's instructions for a computer program (ASTHMA) for predicting the in-depth temperature history and the surface recession (ablation) history of a two-dimensional, axi-symmetric, non-charring material. The in-depth solution procedure is of the conventional explicit finite-difference type. It will account for anisotropic heat conduction in the main material and allows several back-up materials. The heated surface boundary condition can have any one of three forms at each surface location at each instant:

1. Very general film-coefficient-based simultaneous heat and mass transfer type, including any number of equilibrium reactions for an environment and any ablating material, and four specific kinetically controlled reactions for carbon surfaces.
2. Simplified radiation energy balance type, no ablation ("cooldown" option).
3. Specified temperature and surface recession rate.

The program was designed specifically for rocket nozzle use but has sufficient generality that it can be employed for many axi-symmetric shapes.

A User's Manual Brief Description is also presented for a computer program (ARCACE) for calculating surface thermochemical response of materials, including kinetically controlled surface reactions. This program provides for surface thermochemical boundary condition information input to the ASTHMA program. The program was designed specifically for graphitic material and solid propellant combustion products environment but can be employed for many materials and chemical systems.

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