AD-782 023

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AeroChem Research Laboratories, Incorporated

Prepared for:

Air Force Cambridge Research Laboratories

January 1974

AFCRL-TR- 74-0074 AeroChem TP-308

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by

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January 1974

Contract No. F19628-73-0045
Project No. 5635
Task No. 563504
Work Unit No. 56350401

Final Report for Period 1 October 1972 - 30 November 1973

Contract Monitor: Sheldon B. Herskovitz, Microwave Physics Laboratory

Prepared for

AIR FORCE CAMBRIDGE RESEARCH LABORATORIES
Air Force Systems Command
United States Air Force
Bedford, Massachusetts 01730

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

AD-782 023

REPORT DOCUMENTATION PAGE

READ INSTRUCTIONS BEFORE COMPLETING FORM

1. REPORT NUMBER: AFCRL-TR-74-0074	2. GOVT ACCESSION NO
3. RECIPIENT'S CATALOG NUMBER	
4. TITLE (and Subtitle): A COMPUTER CODE TO PREDICT THE EFFECTS OF ELECTROPHILIC LIQUID INJECTION ON RE-ENTRY PLASMA SHEATH PROPERTIES	5. TYPE OF REPORT & PERIOD COVERED: Final, 1 October 1972 to 30 November 1973
	6. PERFORMING ORG. REPORT NUMBER: AeroChem TP-308
7. AUTHOR(s): Harold S. Pergament, Chung-jen Kau	8. CONTRACT OR GRANT NUMBER(s): F19628-73-C-0045
9. PERFORMING ORGANIZATION NAME AND ADDRESS: AeroChem Research Laboratories, Inc., P.O. Box 12, Princeton, New Jersey 08540	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS: 61102F, 5635, 563504, 56350401
11. CONTROLLING OFFICE NAME AND ADDRESS: Air Force Cambridge Research Laboratories (LZ), L.G. Hanscom Field, Bedford, Massachusetts 01730	12. REPORT DATE: January 1974
	13. NUMBER OF PAGES: 143
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)	15. SECURITY CLASS (of this report): Unclassified
	15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

A - Approved for public release; distribution unlimited.

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

18. SUPPLEMENTARY NOTES

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

Re-entry Plasma Sheaths, Electrophilic Liquid Injection, Liquid Jet Breakup, Electron/Ion Recombination, Electron Attachment/Detachment, Computer Codes, Shock Layer Properties

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

A detailed description of a computer code to predict the influence of electrophilic liquid injection on re-entry plasma sheath properties is presented. The code requires input data on the liquid injection system parameters (i.e. electrophilic liquid properties, injection velocity, number of orifices, etc.) and the plasma sheath (shock layer) properties for no material addition, and predicts altered shock layer flow properties and species concentrations. Of primary interest is the ability of the

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code to predict reductions in shock layer electron concentrations, which determine the effectiveness of the injectant in alleviating re-entry blackout.

The physical processes incorporated into the model include: flash vaporization of the liquid jet, penetration and breakup of the jet, droplet acceleration and vaporization, diffusion of the spray/vapor cloud into the shock layer, vapor decomposition, heterogeneous and homogeneous charged species recombination and homogeneous electron attachment/detachment kinetics. The influence of the electrophilic liquid and vapor is assumed to be limited to the volume contained within a droplet-vapor-air (DVA) tube, which extends in a streamwise direction from the location of liquid jet breakup to the end of the body. Flow properties and species concentrations are assumed to be constant over the tube cross section, so that only the streamwise influence of the droplets and vapor on integrated electron and ion concentrations is predicted.

This report includes the equations utilized to describe the model and serves as a Program User's Manual, incorporating instructions for preparing input data, sample input and output and Fortran listings for two versions of the code (specialized and generalized chemistry versions).

ACKNOWLEDGMENTS

The authors gratefully acknowledge the efforts of J.T. Kelly in helping to formulate the model and for critically reviewing the computer code and J.S. Weber for the programming assistance needed to develop a working code.

We also thank the personnel at the AFCRL Microwave Physics Laboratory, particularly S.B. Herskovitz, J.F. Lennon and D.T. Hayes for their helpful suggestions, encouragement and support during the course of this work.

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I. INTRODUCTION

It has been established that the injection of electrophilic liquids into re-entry plasma sheaths can significantly reduce electron and positive ion concentrations[1,2] and alleviate re-entry blackout for signal frequencies ranging from VHF to X-band.[1,2] Prior to the present study, however, a systematic computational technique to predict the alteration of plasma sheath properties as a result of liquid injection (and to subsequently interpret flight data[1,2]) from given injection system parameters was not available. In this report we discuss an analysis and computer code which can be used to predict altered re-entry plasma sheath fluid mechanic, chemical and electrical properties when flow field (shock layer) properties for no material injection are given as input data. The computer code is a considerable advance over the one developed by Pergament, et al,[3] which has been used to analyze electrostatic probe and signal recovery data taken during the RAM C-III flight.[2]

The fundamental assumption in the present model is that the influence of the injected liquid (and the electrophilic vapor) is limited to the volume contained within a droplet-vapor-air (DVA) tube which extends in a streamwise direction from the location of liquid jet breakup to the end of the body (see Fig. 1). The boundaries of the tube normal to and circumferentially around the body are defined by the expansion and spread of the electrophilic vapor. Flow properties and species concentrations are assumed to be constant over the tube cross section. Therefore only the streamwise influence of the injected liquid on integrated electron and ion concentrations within the plasma sheath can be predicted. This appears to be a reasonable first approach considering the overall complexity of this problem and the number of physical processes which must be incorporated into a realistic model.

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[1] Hayes, D.T., Herskovitz, S.B., Lennon, J.R., and Poirier, J.L., " Preliminary Report on the Trailblazer II Chemical Alleviation Flight of 28 July 1972,'' AFCRL-72-0640, 25 October 1972; see also, " Inflight Electrostatic Probe Measurements of the Effect of Chemical Injection on the Properties of the Re-Entry Flow Field," AIAA Paper 73-692, AIAA 6th Fluid and Plasma Dynamics Conference, Palm Springs, 16-18 July 1973.

[2] Schroeder, L.C. and Akey, N.D., " Material Injection Alleviation during the RAM C-III Flight," J. Spacecraft Rock. 10, 170 (1973).

[3] Pergament, H.S., Mikatarian, R.R., and Kurzius, S.C., " Fluid Mechanic and Chemical Kinetic Effects of Water and Freon E-3 Injection into Re-Entry Plasma Sheaths," Final Report, AeroChem TP-291, NASA CR-132309, October 1973.

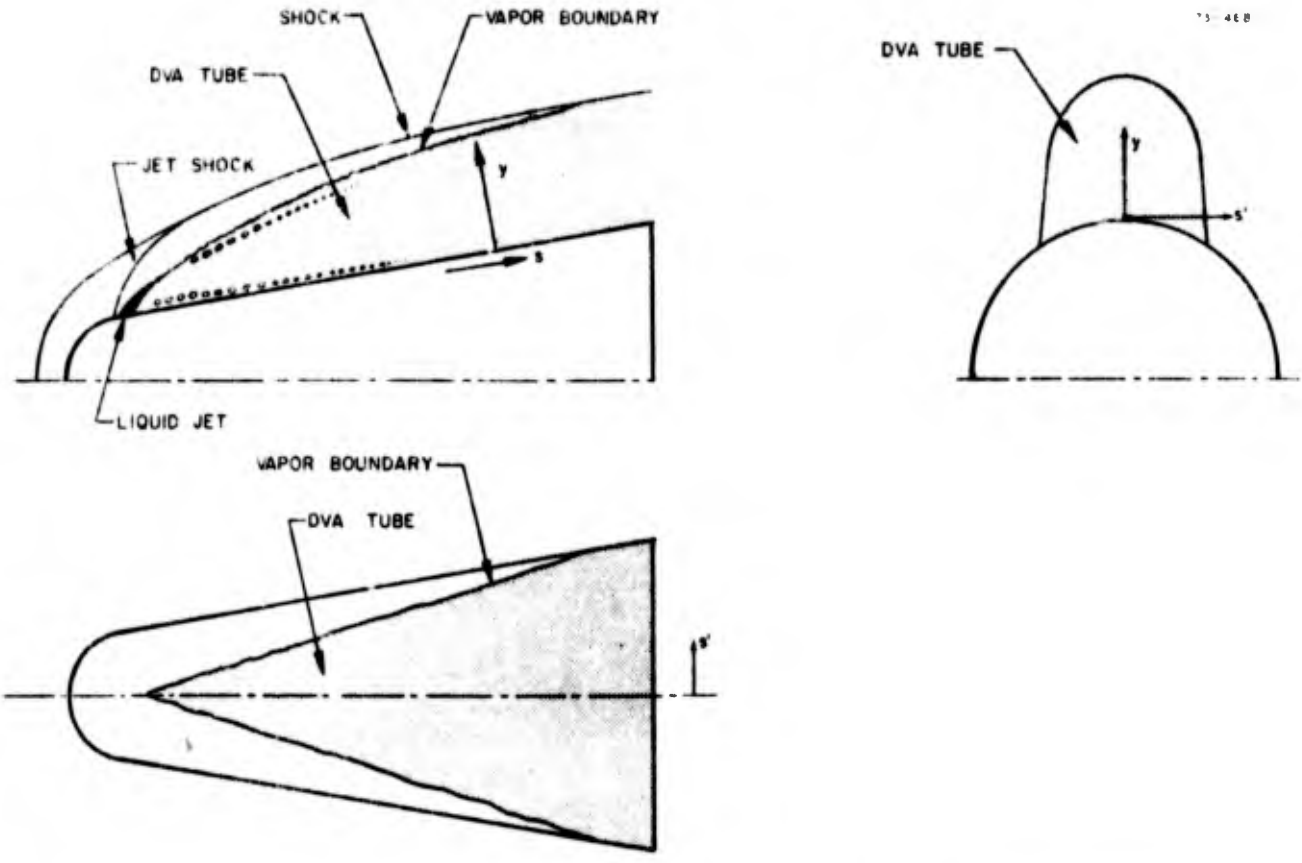

Figure 1. Schematic of liquid injection into a re-entry plasma sheath

The processes included in the model are: flash vaporization, penetration and breakup of the liquid jet, droplet acceleration and vaporization, diffusion of the spray/vapor cloud into the external (shock layer) flow field, decomposition of the vapor, heterogeneous and homogeneous charged species recombination kinetics and homogeneous electron attachment/detachment kinetics.

This report is a detailed description of the analysis, including all equations utilized in the computer code. The code is written in such a manner that it should be relatively easy to replace existing pieces of the model (e.g. droplet vaporization, vapor diffusion, etc.) with more sophisticated treatments, when these become available. There are two basic versions of the code (versions C and D), which are almost identical except for the chemistry routine. Version C incorporates a specialized chemistry routine which considers specific heterogeneous and homogeneous electron/ion recombination reactions and electron attachment/detachment reactions and does not allow for vapor decomposition. Version D incorporates a generalized chemistry routine in which up to 50 different species involved in 100 different reactions can be employed. (Unfortunately, version D has not yet been completely debugged.)

This report also serves as a Program User's Manual, incorporating instructions for preparing input data, sample input data, sample output and Fortran listings for versions C and D.

II. MATHEMATICAL MODEL

A. Phenomenological Description

A schematic of liquid injection into a re-entry plasma sheath is shown in Fig. 1. For blunt re-entry bodies, shock layer Mach numbers immediately downstream of the sphere-cone junction (the location of injection orifices for both Trailblazer[1] and RAM C-III[2] flight test vehicles) are, typically, about 2 to 3. Thus the presence of the liquid jet induces a strong shock which is nearly normal at the surface and rapidly decays to a weak shock before it finally coalesces into the air shock surrounding the body. The liquid jet is therefore exposed to air pressures and temperatures which are greater than the undisturbed shock layer values at the injection orifice. If the temperature of the injected liquid is greater than its boiling point at the post-shock pressure a fraction of the liquid will " flash" into vapor (flash vaporization) in order to reach pressure equilibrium with the surroundings. The remaining liquid is deformed and turned downstream by the air flow while simultaneously disintegrating into droplets; the droplets are accelerated and vaporized by the momentum and heat transferred from the high velocity, high temperature shock layer.

Mixing between the droplet/vapor spray and shock layer air influences the plasma sheath chemistry by: (i) reducing the shock layer temperature (which reduces ionization rates), (ii) enhancing the rate of electron/ion recombination over the dominant homogeneous recombination reaction, $NO^+ + e^- \rightarrow N + O$ via heterogeneous recombination, and (iii) attaching electrons. It is anticipated that the efficiency of electrophilic vapor attachment will exceed that of heterogeneous electron/ion recombination in reducing electron concentrations.[3]

The top of Fig. 1 shows the normal penetration of vapor and droplets into the shock layer, while the bottom of Fig. 1 shows the circumferential (lateral) spread of the vapor and droplets around the body. Flight tests[1,2] have shown that the extent of the lateral spread of the vapor off the injection axis can be substantial.

B. Model Formulation

In principle, the accurate prediction of plasma sheath properties during liquid injection cycles requires a three-dimensional analysis. However the effort to model the complex interactions between the liquid jet, droplets, vapor and shock layer air in three dimensions was beyond the scope of the present study;* therefore a one-dimensional approach was taken. The present model

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* In addition, the uncertainties in some of the input data, e.g. droplet sizes, entrainment rates, rate coefficients, etc., are sufficiently large that a three-dimensional analysis is not warranted at this time. However after a number of calculations have been performed with the present computer code to interpret flight data[1,2] and obtain a feeling for the relative importance of all the input parameters on altered plasma sheath properties, it may be desirable to extend the present model to three dimensions.

should give an adequate description of the significant physical/chemical processes without unnecessarily complicating the analysis.

Referring to Fig. 2, the normal shock air passing through a cross sectional area determined by the liquid jet penetration and the spray lateral spread distance is assumed to mix perfectly with the " flashed" vapor. This mixture, together with the droplets, enters the DVA tube at the point of liquid jet breakup, establishing the initial gas and droplet conditions for the DVA tube calculations. Droplet vaporization and droplet/vapor/air chemical reactions, occurring within the DVA tube, are assumed to be functions only of streamwise distance, parallel to the re-entry body. Shock layer air is continually ingested into the DVA tube (Fig. 2) and instantaneously mixed with the air/vapor mixture flowing within the tube. The neutral species entering the tube are assumed to be frozen at their shock layer values at the point of entry, whereas the charged species (e.g. NO^+, e^-) will, of course, be depleted via the recombination and attachment reactions taking place within the tube.

The pressure along the tube must be specified as input data. The initial pressure is that behind the normal (jet) shock, and the streamwise distribution is assumed to exponentially decay* to the shock layer pressure for no material injection.

Expressions for momentum, energy and mass (vaporization) transfer rates between the droplets and the vapor/air mixture, together with a suitable chemical reaction mechanism are incorporated into the DVA tube governing equations. During vaporization the droplets are assumed to remain at their (initial) boiling point temperature. The problem is completely formulated once the pressure distribution, initial conditions at the point of liquid jet breakup and the shock layer properties for no material injection are known; the gas and droplet conservation equations are then integrated along the DVA tube in the streamwise direction.

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* The " relaxation" length is an input parameter to the computer code. Preliminary calculations show that the streamwise property distributions are relatively insensitive to this parameter if a reasonable value is chosen (say, 1/2 the body length).

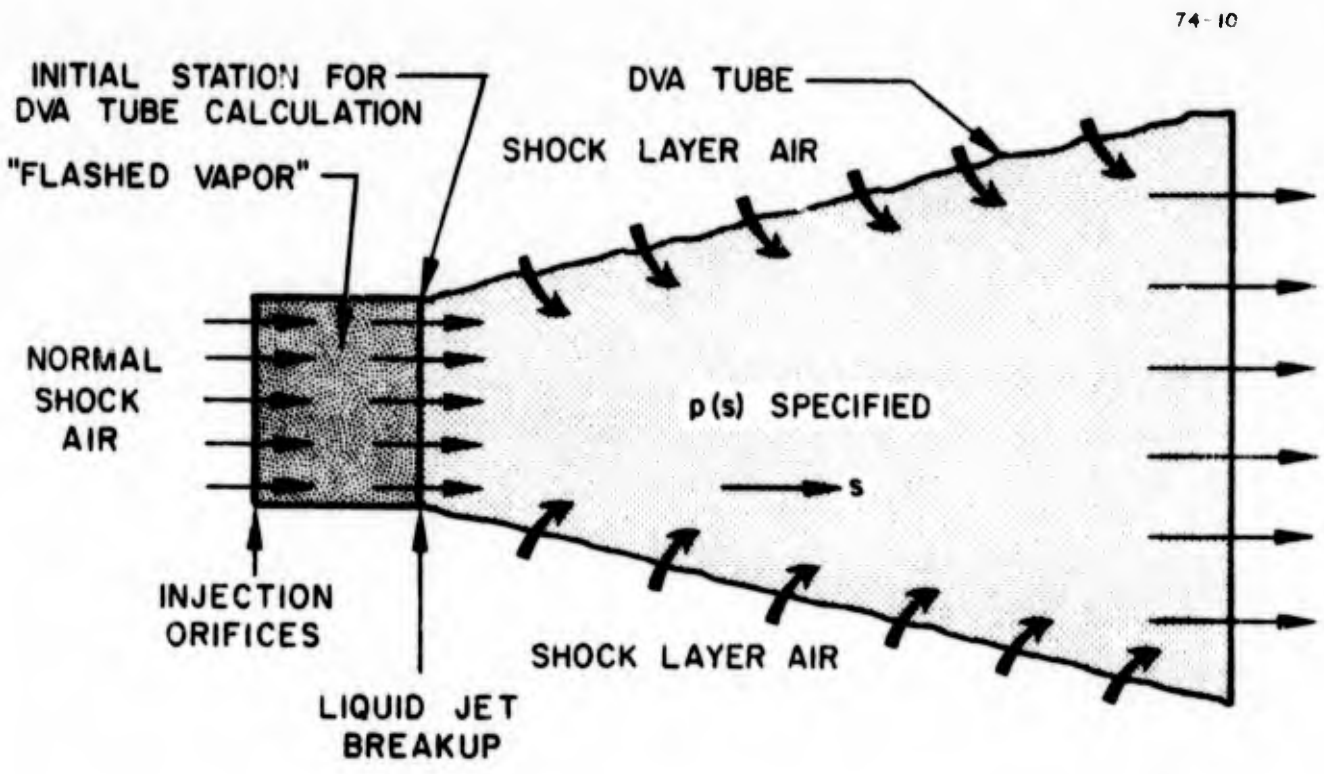

Figure 2. Schematic of Droplet-Vapor-Air (DVA) tube model.

III. SHOCK LAYER PROPERTIES

Several programs have been used[4-7] to calculate the shock layer properties for no material injection for different re-entry test vehicles. For example, the method of Lew[4] has been applied to the Trailblazer flight tests; the fully viscous shock layer theory of Kang, et al[5] has been used to make RAM C-III

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[4] Lew, H.G., "A Study of Electron Density Distribution in Viscous Flows," AFCRL-72-0718, November 1972

[5] Kang, S.W., Jones, W.L., and Dunn, M.G., "Theoretical and Measured Electron-Density Distributions at High Altitudes," AIAA J. 11, 141 (1973).

[6] Schexnayder, C.J., Jr., Huber, P.W., and Evans, J.S., "Calculations of Electron Concentration for a Blunt Body at Orbital Speeds and Comparison with Experimental Data," NASA TN D-6294, 1971.

[7] Kiel, R.E., Bergenn, R.F., Jr., Kessler, T.J., and Kaplan, A.E., "Boundary Layer Plasma of a Re-entry Vehicle: A Comparison of Prediction Models and Flight Measurements," AIAA J. 11, 1235 (1973).

flight calculations,* as has the inviscid flow/boundary layer analysis of Schexnayder, et al.[6] Kiel, et al[7] have combined several programs to interpret electrostatic probe flight data taken in the Re-entry Measurements Program-Phase B.

The shock layer properties required as input data are, pressure, temperature, velocity and the following species concentrations: NO^+, e^-, O, N, O_2, N_2, NO. These properties must be specified (input cards 10 and 11) as a function of distance normal to the body for a selected number of streamwise locations measured from the liquid injection station. Average property values are determined by the program at each input value of s as follows:

$$\bar{p}_e(s) = \frac{1}{y_{max}} \int_0^{y_{max}} \bar{p}_e(s,y)\, dy \tag{1}$$

with similar definitions for $\bar{T}_e(s)$, $\bar{u}_e(s)$ and $\bar{F}_{e_i}(s)$. The molecular weight of the entrained air is then determined from

$$\bar{w}_a(s) = \left[\sum_i \bar{F}_{e_i} \right]^{-1} \tag{2}$$

The entrained air density is then computed from the equation of state,

$$\bar{\rho}_e(s) = \frac{\bar{p}_e(s)\ \bar{W}_a(s)}{R\ \bar{T}_e(s)} \tag{3}$$

and the stagnation enthalpy is computed from,

$$h_{s_e}(s) = \bar{h}_e(s) + \bar{u}_e^2/2 \tag{4}$$

where† $$\bar{h}_e(s) = \bar{h}_e[\,\bar{T}_e(s)\,] \tag{5}$$

A linear interpolation scheme is used to obtain shock layer properties at values of s other than the input points.

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* Recently, Miner and Lewis[8] have also reported shock layer calculations for the RAM C-III vehicle.

† The enthalpy-temperature relation used in the program is described in Section VIII.

[8] Miner, E.W. and Lewis, C.H., "Hypersonic Chemically Reacting Viscous Shock Layers over Sphere-Cones and Cylinder-Wedges," AIAA Paper 74-172, AIAA 12th Aerospace Sciences Meeting, Washington DC, 30 January-1 February 1974.

The actual pressure distribution along the DVA tube is different than $\bar{p}_e$ due to the displacement of the shock layer air by the liquid jet and electrophilic vapor. At the injection station the pressure increases to the value immediately downstream of the normal shock and is assumed to remain constant until the point of liquid jet breakup (i.e. the start of the DVA tube calculations). Downstream of this point the pressure is assumed to decay to the undisturbed shock layer value, according to,

$$\bar{p} = \bar{p}_e + \bar{\rho}_e \bar{u}_e^2 \left(1 - \frac{\rho_x}{\rho_y}\right) e^{-(s - s_{bk})/L_s} \qquad (6)$$

where L_s is a relaxation length within which the dynamic pressure decreases to 1/e of its local normal shock value. L_s is input to the code and should be taken to be some fraction of the body length.

IV. JET SHOCK, FLASH VAPORIZATION AND LIQUID JET BREAKUP

In this section analyses are described for determining (i) conditions downstream of the liquid jet shock, (ii) the amount of liquid that "flashes" into vapor, (iii) the position of the liquid jet at breakup and (iv) the initial droplet properties. The general procedure is to compute properties downstream of the jet (normal) shock using, first, the integrated average properties in the shock layer at the injection station (see Section III) as the pre-shock properties. The computed post-shock properties are then used to compute flash vaporization and liquid jet breakup. After the distance normal to the body at which breakup occurs (y_{bk}) is determined, <u>all</u> calculations are repeated using as input data to the normal shock calculations integrated average property values up to y_{bk} instead of y_{max}. This single iteration* accounts for the fact that the jet shock is normal only in a region relatively near the body and that y_{max} is approximately equal to the total shock layer thickness.

A. <u>Jet Shock</u>

The properties immediately downstream of the jet shock are computed via solution of the conservation equations through a normal shock. These equations are:

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* This iteration is performed by the program even if all the liquid flashes into vapor. In that case the y_{bk} is used only to establish a reasonable value for the initial entrainment area (see Eq. (35)).

$$p_y = p_x + \rho_x u_x^2 \left(1 - \frac{\rho_x}{\rho_y}\right) \tag{7}$$

$$h_y = h_x + (u_x^2/2)\left(1 - \frac{\rho_x^2}{\rho_y^2}\right) \tag{8}$$

$$u_y = u_x \frac{\rho_x}{\rho_y} \tag{9}$$

$$T_y = T(h_y) \tag{10}$$

The method of solution is to assume ρ_x/ρ_y and solve for p_y and h_y from Eqs. (7) and (8). The enthalpy-temperature polynomial is then inverted (via the procedure described in Section VIII.B) to determine T_y, and ρ_y is computed from the equation of state

$$\rho_y = \frac{W_y p_y}{R\, T_y} \tag{11}$$

A solution is obtained when the computed value of ρ_x/ρ_y equals the assumed value of ρ_x/ρ_y.

B. Flash Vaporization

Assuming that the vapor pressure of the superheated liquid jet is in equilibrium with the surrounding pressure, p_y, the fraction of liquid that "flashes" into vapor can be computed from,

$$f = \frac{C_{p,\ell}(T_{\ell,o} - T_{bp})}{\Delta H_v} \tag{12}$$

If the temperature of the liquid jet is lower than T_{bp} there is no flash vaporization. For large temperature differences f can be computed from Eq. (12) to be greater than unity; in that case the program will set f = 1.*

The boiling point of the electrophilic liquid is usually known at 1 atm. The program uses this value as input data and computes T_{bp} at the local pressure, p_y, from the following expression,[9]

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* The program will also set f = 1 if f is greater than some input number (FFVI, Card 2, Cols. 51-60).

[9] Weast, R.C., ed., Handbook of Chemistry and Physics, 52nd edition (Chemical Rubber Co., Cleveland, 1971), p. D-144.

$$T_{bp} = \left(\frac{1}{T_{bp}(1)} - \frac{R}{\Delta H_v} \ln p_y \right)^{-1} \tag{13}$$

where ΔH_v is assumed to be a constant equal to its value at 1 atm, and $T_{bp}(1)$ is the boiling point at 1 atm.

C. Liquid Jet Breakup

The program allows for the occurrence of either aerodynamic breakup or vapor pressure breakup, depending on whether the Weber number exceeds or is less than the critical Weber number. The value for the critical Weber number is input to the program; from the literature,[10] a reasonable value appears to be $We_{cr} = 6.2$. The Weber number is defined as,

$$We = \rho_y u_y^2 \, d_{eq} / 2\sigma_\ell \tag{14}$$

where d_{eq} is the diameter of an equivalent single orifice having the same total mass flow as all the in-line (with the flow direction) orifices (i.e. $d_{eq} = \sqrt{N}\, d_o$).* It is necessary to introduce the concept of an equivalent single orifice since both the Air Force (Trailblazer)[1] and NASA (RAM C-III)[2] flight test vehicles used multiple orifices for increasing the penetration of the jet into the shock layer.

1. Aerodynamic Breakup ($We > We_{cr}$)

Aerodynamic breakup of the liquid jet is assumed to occur via the jet stripping mechanism discussed in Ref. 3. From that analysis we obtain the following expression for the jet breakup time,

$$t_{bk} = 0.536 \left(\frac{\rho_\ell}{\rho_y} \right)^{2/3} \left(\frac{\mu_y}{\mu_\ell} \right)^{1/3} \frac{d_{eq}}{2u_y} \sqrt{\frac{Re_y}{1 + \frac{2We}{Re_y}}} \tag{15}$$

In Eq. (15) the air viscosity is computed from Sutherland's law,[11]

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[10] Lane, W.R., " Shatter of Drops in Streams of Air," I and EC 43, 1312 (1951).

* The justification for the use of this equivalent orifice diameter is given in Ref. 3.

[11] Sutherland, W., " The Viscosity of Gases and Molecular Force," London, Edinburgh and Dublin Phil. Mag. J. Sci.--5th Series 36, 507 (1895).

$$\mu = \mu_{ref} \left(\frac{T}{T_{ref}} \right)^{3/2} \left[\frac{T_{ref} + 110}{T + 110} \right] \tag{16}$$

or

$$\mu = 1.21 \times 10^{-8} \frac{T^{3/2}}{T + 110} \text{ g/cm-sec} \tag{16a}$$

where T is in °K. The Reynolds number, Re_y is defined as,

$$Re_y = \frac{\rho_y u_y d_{eq}}{2 \mu_y} \tag{17}$$

From a force balance on the jet the location of jet breakup (s_{bk}, y_{bk}) is[3]

$$s_{bk} = \frac{C_D \rho_y}{\pi d_{eq} \rho_\ell} (u_y - V_\ell \sin\Theta)^2 t_{bk}^2 + V_\ell \sin\Theta \, t_{bk} \tag{18}$$

$$y_{bk} = V_\ell \cos\Theta \, t_{bk} \tag{19}$$

The streamwise jet velocity component at breakup is,

$$u_{bk} = \frac{2 C_D}{\pi d_{eq}} \frac{\rho_y}{\rho_\ell} (u_y - V_\ell \sin\Theta)^2 t_{bk} + V_\ell \sin\Theta \tag{20}$$

The vertical jet velocity component is assumed to be constant, i.e.

$$V_{bk} = V_\ell \cos\Theta \tag{21}$$

The drag coefficient C_D is taken to be that for a cylinder in hypersonic cross flow ($C_D = 1.2$).

A modified form of the Volynsky correlation[12] is used to estimate the mass-averaged droplet diameter, i.e.

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[12] Kurzius, S.C. and Raab, F.H., "Measurement of Droplet Sizes in Liquid Jets Atomized in Low-Density Supersonic Streams," AeroChem TP-152, NASA CR-1242, March 1967.

$$\frac{d_{30}}{d_{eq}} = 48\, W_L^{-3/8} (Re_y/M_y)^{-1/4} \tag{22}$$

where M_y is the air Mach number downstream of the normal shock, defined as

$$M_y = u_y/(\gamma_y R T_y)^{1/2} \tag{23}$$

and W_L is defined as $2(\rho_\ell/\rho)We$. The specific heat ratio is computed from,

$$\gamma = (1 - \frac{R}{W_y C_{p_y}})^{-1} \tag{24}$$

where W_y and C_{p_y} are evaluated assuming the composition of the air remains frozen through the jet shock at its input value at the injection location ($s = 0$).

The mean droplet size, d_{32}, is then obtained from the expression given by Gooderum and Bushnell,[13]

$$d_{32} = 1.38\, d_{30} \tag{25}$$

The droplet diameter computed from Eq. (25) is the initial droplet diameter for the DVA tube calculations.

2. Vapor Pressure Breakup ($We < We_{cr}$)

For Weber numbers less than the critical Weber number breakup occurs via "boiling" of the liquid jet after emerging from the nozzle. It has been observed[14] that breakup is initiated at some characteristic temperature of the jet, designated the "shatter temperature". Gooderum and Bushnell[14] have correlated this temperature with orifice diameter for water jets and have obtained the following relation,

$$\frac{T_{sh} - T_{bp}}{T_{sh}} = \xi \tag{26}$$

where $\xi \approx 0.1$ for orifice diameters from 0.01 in. to 0.04 in. Droplet

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[13] Gooderum, P. and Bushnell, D.M., "Atomization, Drop Size and Penetration for Cross-Stream Water Injection During High Altitude Re-entry with Application to the Ram C-I Flight," NASA TN D-6747, July 1972.

[14] Bushnell, D.M. and Gooderum, P.B., "Atomization of Superheated Water Jets at Low Ambient Pressures," J. Spacecraft Rock. 5, 231 (1968).

diameters are calculated from additional results of Gooderum and Bushnell[15] who correlated water droplet sizes with jet injection temperature and orifice diameter. A curve fit of the data given in Ref. 15 results in the following expression

$$\frac{d_{32}}{d_o} = A_k \exp(- B_k T) \quad , \tag{26a}$$

where $A_k = 612$ and $B_k = 0.0244$ and T is in °K. The extrapolation to electrophilic liquid jets must obviously be made with caution.

a. $T_{\ell,o} < T_{sh}$ - For liquid injection temperatures less than the shatter temperature the breakup time can be calculated from the time to heat the jet from $T_{\ell,o}$ to T_{sh}, i.e..

$$t_{bk} = \frac{C_{p,\ell} (T_{sh} - T_{\ell,o}) \rho_\ell d_{eq}}{4 q''} \tag{27}$$

The heat transfer to the jet is computed from the expression for free molecular heat transfer rate given in Section VI.B. The position and velocity of the jet at breakup are then obtained from Eqs. (18) - (21).

b. $T_{\ell,o} > T_{sh}$ - In this case the jet will 'flash' immediately into vapor, reaching the boiling point at the post-shock pressure. The jet breakup time is then computed assuming the jet is heated from T_{bp} to T_{sh}.

The present version of the program automatically goes into the vapor pressure breakup routine if $We < We_{cr}$, <u>after</u> calculating liquid jet breakup parameters from the aerodynamic breakup analysis and completing the DVA tube calculations. This is done because the <u>precise</u> value of We_{cr} is not well known and, if We is only marginally less than We_{cr}, it appears worthwhile to calculate DVA tube properties for both jet breakup modes and compare the predicted distributions of charged species concentrations for the two cases.

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[15] Gooderum, P.B. and Bushnell, D.M., "Measurement of Mean Drop Sizes for Sprays from Superheated Waterjets," J. Spacecraft Rock. 6, 201 (1969).

V. INITIAL CONDITIONS FOR DVA TUBE CALCULATIONS

The initial conditions for DVA tube calculations are determined via an analysis that assumes perfect mixing between 'flashed' vapor and the shock layer air passing through a semi-elliptical cross sectional area, defined by the maximum jet penetration,* y_{bk}, and the lateral spread of the spray at the point of jet breakup, s'_{bk}.

A. Lateral Spread at Breakup

The lateral spread of the spray has been estimated via interpretation of data obtained for water sprays by Horn and Reichenbach,[16] who showed that the lateral spread distance scaled by the orifice diameter (at $s = 150\ d'_{eq}$) depends approximately on the inverse square root of the free stream Mach number. In order to interpret the data of Ref. 16 in terms of the lateral spread of electrophilic liquid sprays, a simple dimensional analysis of the lateral motion of a droplet was formulated (see Appendix A). The results of this analysis indicate that,

$$\frac{s'}{d'_{eq}} = K' \frac{d'_{eq}}{r_p} \tag{28}$$

Using Eq. (28) to interpret the data[16] shows that the proportionality constant is approximately unity. The equivalent diameter, d'_{eq}, to be used in Eq. (28) is one having a mass flow equal to the total mass flow from all the side-by-side orifices,† i.e.

$$d'_{eq} = \sqrt{N'}\, d_o \tag{29}$$

In Ref. 16 it was found that at a downstream distance (from the orifice) of about $70\ d'_{eq}$ the lateral spread distance approached its asymptotic value. In order to calculate the lateral spread downstream of this point we

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* If all the liquid flashes into vapor ($f = 1$) y_{bk} will still be computed via the methods described in Section IV.C. However, in this case y_{bk} will be a fictitious value, used only to determine an approximate initial cross sectional area for the DVA tube calculations.

[16] Horn, K.P. and Reichenbach, R.E., " Further Experiments on Spreading of Liquids Injected into a Supersonic Flow," AIAA J. 7, 358 (1969).

† Note that this equivalent diameter is different from d_{eq}, used to compute penetration distances and liquid jet breakup.

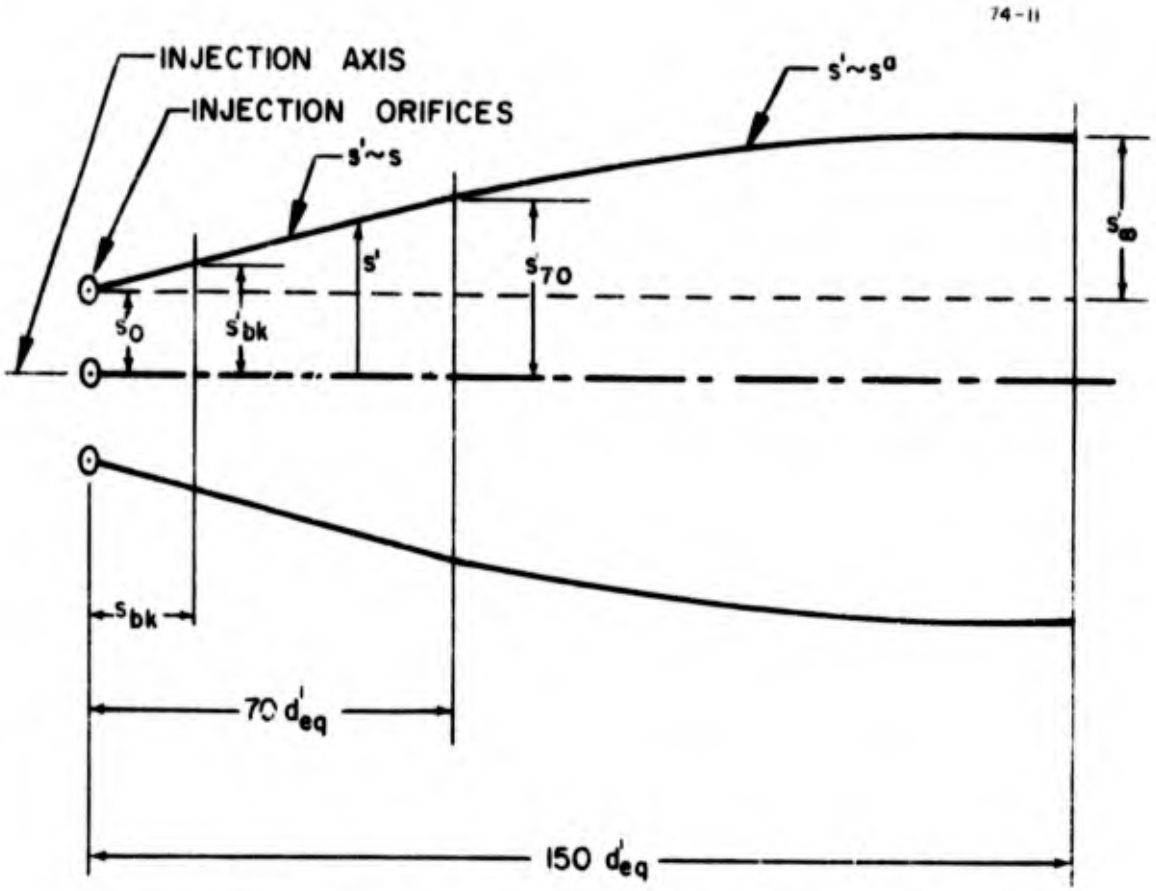

Figure 3. Significant dimensions for lateral spread calculations.

assume that the growth of the spray is similar to that for the wake growth[17] behind circular cylinders and spheres. Thus for $s > 70\ d'_{eq}$ (see Fig. 3),

$$s' = s'_o + C\, s^a \tag{30}$$

We assume that the lateral growth of the spray is linear from the orifice to $70\ d'_{eq}$. Thus, for $s' < 70\ d'_{eq}$

$$s' = s'_o + \frac{s'_{70} - s'_o}{70\ d'_{eq}} \tag{31}$$

The constant C in Eq. (30) is evaluated in terms of a at $s = 150\ d'_{eq}$, the position at which the data of Ref. 16 were taken and where the correlation expressed by Eq. (28) applies. Thus,

$$C = s'_\infty/(150\ d'_{eq})^a \tag{32}$$

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[17] Herrman, J., Slattery, R.E., and Clay, W.G., "Measured Properties of the Wakes of Hypersonic Cones," AIAA Paper No. 68-687, 1968.

where

$$s'_\infty = d'^{2}_{eq}/r_{p_o} \tag{33}$$

Then, we get for $s' > 70\ d'_{eq}$

$$s' = s'_o + s'_\infty \left(\frac{s}{150\ d'_{eq}}\right)^a \tag{30a}$$

Now s'_{70} is evaluated from Eq. (30a),

$$s'_{70} = s'_o + s'_\infty \left(\frac{70}{150}\right)^a \tag{34}$$

and, finally, we get for $s' < 70\ d'_{eq}$

$$s' = s'_o + s'_\infty \left(\frac{70}{150}\right)^a \left(\frac{s}{70\ d'_{eq}}\right) \tag{31a}$$

Usually the streamwise position of jet breakup will be less than $70\ d'_{eq}$. Thus, substituting s_{bk} in Eq. (31a) will give the lateral spread distance at breakup, s'_{bk}. The entrainment area from which the mass flow of shock layer air is computed is then given by

$$A^*_{bk} = \frac{\pi}{2}\, y_{bk}\, s'_{bk} \tag{35}$$

for the assumed semi-elliptical cross section.

B. Shock Layer Air/Flashed Vapor Mixing

Assuming perfect mixing between the shock layer air and flashed vapor, the conservation equations are solved across a control volume bounded by the jet shock and the droplet/vapor/air mixture at the streamwise location of jet breakup. The mass flow of vapor is computed from

$$\dot{m}_v = f\, \dot{m}_i \tag{36}$$

and the mass flow of air is determined by

$$\dot{m}_a = \bar{\rho}_x \bar{u}_x A^*_{bk} \tag{37}$$

The conservation equations are:

Continuity

$$\dot{m}_a + \dot{m}_v = \rho_o u_o A_o \tag{38}$$

Momentum (assuming $p = p_y$ throughout the control volume)

$$\dot{m}_a u_y + \dot{m}_v u_\ell = \rho_o u_o^2 A_o \tag{39}$$

Energy

$$\dot{m}_a H_{s_a} + \dot{m}_v H_{s_v} = (\dot{m}_a + \dot{m}_v) H_{s_o} \tag{40}$$

$$H_{s_v} = C_{p_\ell} T_{bp} + \Delta H_v + V_\ell^2/2 \tag{41}$$

The momentum and energy equations are first solved to get u_o and H_{s_o}, respectively; the static temperature is then computed by inverting the enthalpy-temperature relation. The equation of state is then used to compute ρ_o, noting that the molecular weight of the mixture now includes the molecular weight of the vapor. Finally the initial DVA tube area is obtained from the continuity equation, Eq. (38). This area is larger than the entrainment area, A^*_{bk}, because it must accommodate the vapor, which pushes the streamlines outward.

VI. DVA TUBE ANALYSIS

The DVA tube calculations are initiated at the point of liquid jet breakup using the droplet and air/vapor properties computed in Sections IV and V, respectively. One-dimensional droplet and gas conservation equations are solved along the tube with a pressure distribution specified by Eq. (6). Shock layer air is entrained continuously, the entrainment rate being a function of the entrainment area which is computed via the wake growth law given by Eqs. (30a) and (31a). The shock layer air is assumed to mix perfectly and instantaneously with the air/vapor mixture within the tube while undergoing no change in composition.

A. Governing Equations

1. Vapor/Air Mixture

The conservation equations applied in the DVA tube analysis are:

$$du = \frac{1}{\rho u A}\left[(u_p - u)\dot{\Phi}_v A ds + (\bar{\rho}_e \bar{u}_e^2 - \bar{\rho}_e \bar{u}_e u) dA^* - A\, dp - dF_p\right] \tag{42}$$

$$dH_s = \frac{1}{\rho u A}\left[(H_{p_s} - H_s)\dot{\varphi}_v\, Ads + (\bar{\rho}_e \bar{u}_e H_{s_e} - \bar{\rho}_e \bar{u}_e H_s)\, dA^* - \rho_e u_p A\, dH_{p_s}\right] \quad (43)$$

$$dY_i = \frac{1}{\rho u A}\left[W_i \dot{w}_i\, Ads + (\bar{\rho}_e \bar{u}_e \bar{Y}_{e,i} - \bar{\rho}_e \bar{u}_e Y_i)\, dA^* - Y_i \dot{\varphi}_v\, Ads\right] \quad (44)$$

$$dY_v = \frac{1}{\rho u A}\left[(1 - Y_v)\dot{\varphi}_v\, Ads - Y_v \bar{\rho}_e \bar{u}_e\, dA^*\right] \quad (45)$$

(Eq. (45) is only used for version C, in which the vapor is assumed to undergo no decomposition. For version D all species mass fractions are computed from Eq. (44)).

$$dh = \left[(H_s + dH_s) - \frac{(u + du)^2}{2}\right] - h \quad (46)$$

Then, $T = T(h)$ by inverting the enthalpy-temperature polynomial, and

$$d\rho = \frac{p + dp}{R(T + dT)}\left[\sum_j \frac{Y_j + dY_j}{W_j}\right]^{-1} - \rho \quad (47)$$

where the summation over all j species in Eq. (47) includes the vapor. Finally the change in area is computed from,

$$dA = \frac{1}{\rho u}\left[\dot{\varphi}_v\, Ads + \bar{\rho}_e \bar{u}_e\, dA^* - Au\, d\rho - A\rho\, du\right] \quad (48)$$

The droplet properties in the above equations, u_p, dFp, H_{p_s} and dH_{p_s} are determined via the droplet conservation equations; the vaporization rate $\dot{\varphi}_v$ is computed from the heat transfer rate to the droplet and the chemical production terms, $\dot{w}_i (= \sum_j \dot{w}^{(j)})$ are computed from the specified chemical reaction mechanism and rate coefficients.

2. Droplets

We assume that (i) the droplet temperature remains constant at its boiling point and, therefore, the energy equation does not have to be solved and (ii) the normal droplet velocity component remains constant at the normal liquid injection velocity, $V_\ell \cos\Theta$. The following equations are employed:

$$dF_p = \frac{9}{2} \frac{\rho_p}{\rho_\ell} \frac{f_p \mu}{r_p^2} (u - u_p) \, Ads \tag{49}$$

$$du_p = \frac{dF_p}{\rho_p u_p A} \tag{50}$$

$$\rho_p = \frac{\dot{m}_i - \rho Y_v uA}{u_p A} \tag{51}$$

$$H_{p_s} = C_{p_\ell} T_{bp} + u_p^2/2 \tag{52}$$

$$dH_{p_s} = C_{p_\ell} T_{bp} + \frac{(u_p + d u_p)^2}{2} - H_{p_s} \tag{53}$$

The term f_p in Eq. (49) is defined as the ratio of the actual droplet drag coefficient to the drag coefficient from Stokes law. In Eqs. (52) and (53) T_{bp} is the droplet boiling point temperature evaluated from Eq. (13) at the pressure behind the (normal) jet shock.

The change in droplet radius is determined from

$$dr_p = \frac{\dot{d}}{2 u_p} ds \tag{54}$$

where $\dot{d}$ is determined from the free molecular heat transfer rate (see next section).

B. Droplet Vaporization

Free molecular heat transfer to the droplet is assumed, which gives the rate of change of droplet diameter as,[3]

$$\dot{d} = - \frac{\alpha_D (T_s - T_{bp})\, p(u - u_p)}{\rho_\ell \Delta H_v T} \left[1 + \frac{\alpha_T}{\alpha_D} \left(\frac{v}{(u - u_p)} \right) \frac{T - T_{bp}}{T_s - T_{bp}} \right] \quad (55)$$

where T_s is the relative stagnation temperature between the droplets and gas determined from the relative stagnation enthalpy,

$$H_{s_r} = h + u_r^2/2 \quad (56)$$

and the enthalpy-temperature polynomial. The thermal mean velocity in Eq. (55) is computed from,

$$\dot{\varphi}_v = (3p/\rho)^{1/2} \quad (57)$$

The vaporization rate (typically, in units of g/cm^3-sec) is then expressed as,

$$\dot{\varphi}_v = 4\pi\, r_p^2\, \frac{\dot{d}}{2}\, n\, \rho_\ell \quad (58)$$

where n is the droplet number density, defined as,

$$n = \rho_p / (4/3)\, \pi\, r_p^3\, \rho_\ell \quad (59)$$

Combining Eqs. (58) and (59) gives,

$$\dot{\varphi}_v = \frac{3}{2}\, \frac{\rho_p}{r_p}\, \dot{d} \quad (60)$$

C. Droplet Drag Coefficient

The expression for the drag coefficient used in the program was taken from the work of Crowe,[18] who correlated data on small diameter spheres in flow regimes from free molecular to continuum in terms of a normalized drag coefficient, defined as,

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[18] Crowe, C.T., "On the Momentum and Heat Transfer Equations for Two-Phase Plumes," JANNAF 6th Plume Technology Meeting, CPIA Publ. No. 209 (Applied Physics Lab., Johns Hopkins Univ., Silver Spring, 1971), p. 101.

$$\bar{C}_D = (C_D - C_{D_I})/(C_{D_{FM}} - C_{D_I}) \tag{61}$$

where C_{D_I} is the incompressible high Reynolds number drag coefficient (taken to be 0.) and $C_{D_{FM}}$ is the free molecular drag coefficient. $\bar{C}_D$ is expressed as a function of Knudson number and particle Reynolds number,

$$\bar{C}_D = G(Kn) \quad D(Kn, Re_p) \tag{62}$$

where,

$$G(Kn) = \frac{Kn^{0.3} \exp(1.2\ Kn^{0.5})}{1 + Kn^{0.3} \exp(1.2\ Kn^{0.5})} \tag{63}$$

and

$$D(Kn, Re_p) = 1 - \exp\left[- \frac{Re_p}{8} Kn^{0.7}\ e^{Kn} \left(C_{D_o} - 0.48 \right) \right] \tag{64}$$

$$Kn = 1.26\ \sqrt{\gamma}\ \frac{M_p}{Re_p} \tag{65}$$

$$M_p = \frac{u - u_p}{a} \tag{66}$$

$$Re_p = \frac{\rho\ r_p\ (u - u_p)}{\mu} \tag{67}$$

C_{D_o} is obtained from Stokes drag law, (note that Re_p is defined in terms of r_p), i.e.

$$C_{D_o} = 12/Re_p \tag{68}$$

$C_{D_{FM}}$ is obtained from,

$$C_{D_{FM}} = \frac{\exp(-S_1^2/2)}{\sqrt{\pi}\ S_1^3} (1 + 2S_1^2) + \frac{4(S_1^4 - S_1^2) - 1}{2S_1^4} \operatorname{erf}(S_1) + \frac{2}{3} \frac{\sqrt{\pi}}{S_2} \tag{69}$$

where

$$S_1 = \sqrt{\gamma/2}\ M_p \tag{70}$$

and

$$S_2 = S_1 \sqrt{T/T_{bp}} \tag{71}$$

Finally, C_D is evaluated from Eq. (61) and $f_p = C_D/C_{D_o}$ is used in Eq. (49).

D. Normal Penetration and Entrainment Area

The penetration of the spray into the shock layer normal to the body as a function of streamwise distance, s, is computed by adding the penetration due to mixing with shock layer air to the local droplet penetration. The contribution due to mixing, y_{mix}, is assumed to be the same as the lateral spread distances $(s' - s'_o)$ computed via Eq. (30a) or (31a). The droplet penetration is computed from,

$$y_{pen} = V_\ell \cos\Theta \int \frac{ds}{u_p} \tag{72}$$

Thus the total penetration is $y_{tot} = y_{mix} + y_{pen}$, and the entrainment area is computed from

$$A^* = \frac{\pi}{2}\ s' y_{tot} \tag{73}$$

VII. CHEMICAL REACTION MECHANISMS

A. Specialized Chemistry Version (Version C)

This version of the code incorporates the following one-way reactions and rate coefficients.

	Reaction	Rate Coefficient Form
(1)	$NO^+ + e^- \rightarrow N + O$	$C_1\ T^{-N_1}$
(2)	$NO^+ + F^- \rightarrow NO + F$	$C_2\ T^{-N_2}$
(3)	$NO^+ + (e^- + S) \rightarrow N + O + (S)$	k_3
(4)	$NO^+ + (F^- + S) \rightarrow N + O + (S)$	k_4
(5)	$Q + e^- \rightarrow F^- + \text{Products}$	$C_5\ T^{-N_5}$
(6)	$F^- + M \rightarrow F + e^- + M$	$C_6 \exp(-B_6/RT)$
(7)	$F^- + O \rightarrow OF + e^-$	$C_7 \exp(-B_7/RT)$
(8)	$N + O \rightarrow NO^+ + e^-$	$C_8\ T^{N_8}\ (-B_8/RT)$

The following points should be noted: (i) Reaction (8) is the reverse of Reaction (1); (ii) Reactions (3) and (4) are heterogeneous recombination reactions which occur at the surface of the droplets; expressions for k_3 and k_4 are given below*; (iii) Q represents the electrophilic vapor which is assumed not to be decomposed; (iv) The rate coefficients are incorporated into the program in the form shown, with the coefficients, temperature exponents and activation energies being input data (cards 8 and 9); (v) The justification for the use of this mechanism, the form of the rate coefficients and the specific values recommended in Section XI are given by Pergament, et al.[3]

Expressions for the production rates for each of the above reactions are:

Homogeneous

$$\dot{w}^{(1)} = k_1\ \rho^2 F_{NO^+} F_{e^-} \tag{74}$$

$$\dot{w}^{(2)} = k_2\ \rho^2 F_{NO^+} F_{F^-} \tag{75}$$

$$\dot{w}^{(5)} = k_5\ \rho^2 F_Q F_{e^-} \tag{76}$$

$$\dot{w}^{(6)} = k_6\ (\rho^2/W)\ F_{F^-} \tag{77}$$

$$\dot{w}^{(7)} = k_7\ \rho^2 F_{F^-} F_O \tag{78}$$

$$\dot{w}^{(8)} = k_8\ \rho^2 F_N F_O \tag{79}$$

---

* A discussion of the derivation of these equations is given in Ref. 3.

Heterogeneous

$$\dot{w}^{(3)} = k_3 \rho F_{NO^+} \tag{80}$$

$$\dot{w}^{(4)} = k_4 \rho F_{NO^+} \tag{81}$$

where

$$k_3 = f_3 k_s \left[\frac{\rho v_{e^-} F_{e^-}}{\rho v_{e^-} F_{e^-} + (v_{F^-} + u - u_d)\rho F_{F^-}} \right] \tag{82}$$

$$k_4 = f_4 k_s \left[\frac{(v_{F^-} + u - u_d)\rho F_{F^-}}{\rho v_{e^-} F_{e^-} + (v_{F^-} + u - u_d)\rho F_{F^-}} \right] \tag{83}$$

$$k_s = \frac{3}{4} \frac{(1 + \eta)\dot{m}_i (r_p/r_{p_o})^3}{r_p \rho_\ell u_d} \left(v_{NO^+} + u - u_d \right) \tag{84}$$

The factors f_3 and f_4 (card 8) are coefficients by which the rates of the heterogeneous recombination reactions can be arbitrarily varied. η must be evaluated from the following transcendental equation,

$$\exp(-\eta) = \frac{(v_+ + u - u_d)\rho F_{NO^+} (1 + \eta)}{\rho v_{e^-} F_{e^-} + (v_{F^-} + u - u_d)\rho F_{F^-}} \tag{85}$$

Expressions for the thermal velocities are:

$$v_{NO^+} = 1.88 \times 10^5 (T/5000)^{1/2} \text{ cm/sec} \tag{86}$$

$$v_{e^-} = 4.40 \times 10^7 (T/5000)^{1/2} \text{ cm/sec} \tag{87}$$

$$v_{F^-} = 2.36 \times 10^5 (T/5000)^{1/2} \text{ cm/sec} \tag{88}$$

where T is in °K.

B. Generalized Chemistry Version (Version D)

Reaction types are given for one direction only; both forward and backward reactions and rate coefficients must therefore be specified. The generalized form of the one-way reaction (card 9) is A + B + C + D → E + F + G + H. Individual reaction types (card 9, cols. 41 and 42) are specified below.

Reaction Type	Reaction
(1)	A + B → E + F
(2)	A + B + M → E + M
(3)	A + B → E + F + G
(4)	A + B → E
(5)	A + M → E + F + M
(6)	A + B + C + M → E + M
(7)	A + M → E + F + G + M
(8)	A + B + C → E + F
(9)	A + B + C + D → E + F
(10)	A + B → E + F + G + H
(11)	A → Products

Examples: For reaction type (2) on card 9, C ≡ M and F ≡ M. For reaction type (5) on card 9, B ≡ M and G ≡ M.

Rate coefficient types (card 9, cols. 43-44) are specified below; data must be given in cm-molecule-sec units.

Rate Coefficient Type	Rate Coefficent, k
(1)	A (constant)
(2)	$A\ T^{-1}$
(3)	$A\ T^{-2}$
(4)	$A\ T^{-1/2}$
(5)	$A \exp(B/RT)$
(6)	$A\ T^{-1} \exp(B/RT)$
(7)	$A\ T^{-3/2}$
(8)*	$A\ T^{N} \exp(B/T)$
(9)*	$A\ T^{N} [(K/T) + 1] \exp(B/T)$
(10)*	$\delta\ A\ T^{N} \exp(B/T)$

* Note that for these reactions the exponential term is expressed as exp(B/T) rather than exp(B/RT) as in rate coefficient types (5) and (6).

Expressions for the production rates for each of the reaction types are given below:

$$\dot{w}^{(1)} = k_f \rho^2 F_A F_B \tag{89}$$

$$\dot{w}^{(2)} = \frac{k_f \rho^3 F_A F_B}{W} \tag{90}$$

$$\dot{w}^{(3)} = k_f \rho^2 F_A F_B \tag{91}$$

$$\dot{w}^{(4)} = k_f \rho^2 F_A F_B \tag{92}$$

$$\dot{w}^{(5)} = \frac{k_f \rho^2 F_A}{W} \tag{93}$$

$$\dot{w}^{(6)} = k_f \rho^4 F_A F_B F_C / W \tag{94}$$

$$\dot{w}^{(7)} = k_f \rho^2 F_A / W \tag{95}$$

$$\dot{w}^{(8)} = k_f \rho^3 F_A F_B F_C \tag{96}$$

$$\dot{w}^{(9)} = k_f \rho^4 F_A F_B F_C F_D \tag{97}$$

$$\dot{w}^{(10)} = k_f \rho^2 F_A F_B \tag{98}$$

$$\dot{w}^{(11)*} = \delta k_f \rho^2 F_A F_H \tag{99}$$

---

* F_H in this reaction refers to the moles/g of hydrogen atoms that might be introduced into the flow due to an ablating heat shield.

Note that reaction-type (11) only specifies one reactant (with arbitrary products) and yet $\dot{w}^{(11)}$ has the form of a 2-body reaction. This special reaction-type is introduced because of the manner in which the rate coefficients were specified[3] for the decomposition reactions involving the electrophilic vapor and hydrogen atoms, i.e.

$$Q + H \rightarrow HF + \text{Products}$$

where

$$(k)_Q = 4 \times 10^{-11} \exp(-4000/RT)$$

$$(k)_H = 9.2 \times 10^{-10} \exp(-4000/RT)$$

$$(k)_{HF} = 9.2 \times 10^{-10} \exp(-4000/RT)$$

$(k)_Q$ is the rate coefficient for depletion of Q by H; $(k)_H$ is the rate coefficient for the depletion of H by Q and $(k)_{HF}$ is the rate coefficient for the production of HF from Q. In this program these reactions would be handled by specifying the reaction Q + H → HF as reaction-type (4) with rate coefficient type (5), having $A = 4 \times 10^{-11}$; B = -4000. In the normal method of program operation this would give identical depletion rates for Q and H, (equal to the production rate of HF), via Eq. (92) above. But because of the manner of specifying the rate coefficients for this reaction, the above values of A and B only give the correct depletion rate for Q. Now we must invoke reaction type (11) and rate coefficient type (10) in the following way:

$Q \rightarrow H$ $\quad \delta = -(9.2 - 0.4)10^{-10}$ for depletion rate of H*

$\quad A = 1$

$\quad N = 0$

$\quad B = -2000$

$Q \rightarrow HF$ $\quad \delta = (9.2 - 0.4)10^{-10}$ for production rate of HF

$\quad A = 1$

$\quad N = 0$

$\quad B = -2000$

---

* δ is negative because in the reaction of interest H is actually on the left hand side.

VIII. THERMODYNAMIC DATA

A. Program Input

The thermodynamic data have been incorporated directly into the specialized chemistry version of the program (version C) via a set of block data. The specific heat of each species is expressed in the following form,

$$C_{p_i} = L_{1_i} + L_{2_i}\Theta + L_{3_i}\Theta^2 + L_{4_i}\Theta^3 + L_{5_i}\Theta^{-2} \quad \text{cal/mole-°K} \tag{100}$$

where Θ = T(°K)/1000. The enthalpy is then expressed as,

$$h_i = \int_o^T C_{p_i}\, dT + L_{6_i} \tag{101}$$

where $L_{6_i} = H^o_{f_i} - \int_o^{298} C_{p_i}\, dT$; H^o_f being the heat of formation at 298°K. Thus the block data are L_{1_i} through L_{6_i} and the molecular weight of each species, W_i. The values of the coefficients used in version C were obtained by curve fits of the JANNAF data.[19]

For the generalized chemistry version (version D) the above data have to be input (card type 8), up to a maximum of 50 species, in the manner discussed in Section XI.B.

It should be noted that thermodynamic data are used in the program only to determine the enthalpy and temperature of the mixture. They are not used to determine equilibrium constants (via the Gibbs free energy) from which backward reaction rate coefficients could be evaluated (since only one-way reactions are employed in the kinetics scheme). Thus for species with small concentrations, and for which thermodynamic data are not available, it is recommended that only some reasonable value of L_1 (i.e., constant specific heat) be input and the remaining coefficients be set equal to zero. This should result in a negligible error in the enthalpy of the system.

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[19] JANNAF Thermochemical Tables (Dow Chemical Co., Midland, continuously updated).

B. Inversion of T from h(T)

As noted above the mixture enthalpy is expressed as $h = f(\Theta)$. The following numerical procedure is used to find a given value of h. Let

$$G = f(\Theta) - h \tag{102}$$

$$G_{n+1} = G_n + \left(\frac{\partial G}{\partial \Theta}\right)_n \Delta\Theta_n \tag{103}$$

where n is the number of the iteration step. Setting $G_{n+1} = 0$ gives

$$\Delta\Theta_n = -G_n/(\partial G/\partial\Theta)_n \tag{104}$$

Since $\Delta\Theta_n = \Theta_{n+1} - \Theta_n$, we get

$$\Theta_{n+1} = \Theta_n - G_n/(\partial G/\partial\Theta)_n \tag{105}$$

The above recursion formula is used to solve for Θ from $h(\Theta)$. The iteration stops when $G_n \leq \varepsilon h$, where ε is a very small number.

IX. NUMERICAL TECHNIQUES

The ordinary differential equations given in Section VI (with the exception of the species continuity equation) are solved via a simple explicit marching procedure in which a nominal integration step size, Δs, is specified as input data. During the first 10 integration steps, however, the step size is reduced at least a factor of 10 less than the input value, and will be reduced still further if the vaporization rate is very large. This has been found to be necessary to obtain a smooth start to the calculations. After the first 10 steps the step size is allowed to increase up to 5 times the input value, but will still be controlled by the vaporization rate if φ_v is large.

The species mass fractions, Y_i are evaluated via an <u>implicit</u> integration technique; i.e. these variables are evaluated from information at the forward step (n + 1) as well as at the present step (n). This is accomplished by linearizing the production terms in the individual species continuity equations, Eq. (44). The sum of all species continuity equations then results in a matrix equation in which known coefficients (elements of the matrix) multiply the unknown species concentrations (which form a vector). This product is equal to a known vector on the right hand side of the equation. The linearizations involving species F_i and F_j (for a two-body reaction) or F_i, F_j and F_k (for a three-body reaction) at station n + 1 (all variables are known at station n), are given by

$$(F_iF_j)_{n+1} = (F_iF_j)_n + F_{jn}\left[(F_i)_{n+1} - (F_i)_n\right] + F_{in}\left[(F_j)_{n+1} - (F_j)_n\right]$$

$$= -\underline{\underline{(F_iF_j)_n}} + \underline{(F_j)_n}\,(F_i)_{n+1} + \underline{(F_i)_n}\,(F_j)_{n+1}$$

$$(F_iF_jF_k)_{n+1} = -\underline{\underline{2(F_iF_jF_k)_n}} + \underline{(F_jF_k)_n}\,(F_i)_{n+1} + \underline{(F_iF_k)_n}\,(F_j)_{n+1}$$

$$+ \underline{(F_iF_j)_n}\,(F_k)_{n+1}$$

The terms underscored by a single line contribute to the elements of the coefficient matrix, while the terms underscored by a double line contribute to the known column matrix on the right hand side of the matrix equation for the linearized system. Thus the matrix equation takes the form (for N species),

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & & a_{1N} \\ a_{21} & & & & \\ & & & & \\ a_{N1} & & & & a_{NN} \end{bmatrix} \begin{bmatrix} F_1 \\ F_2 \\ \\ F_N \end{bmatrix} = \begin{bmatrix} Q_1 \\ Q_2 \\ \\ Q_N \end{bmatrix}$$

It should be noted that the size of the matrix is determined by the number of species in the chemical system.

This implicit technique is used for both versions C and D. For the version D integration procedure, however, if any species mass fraction is predicted to be negative the step size will be halved until a positive value is obtained.* The recommended value of the initial step size (card 6) of 0.01 cm was determined from several trial calculations and should produce a stable solution. However, if the solution appears to be unstable this value should be reduced.

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* It is a straightforward matter to add this step size control to version C and to incorporate a step size control on the other dependent variables (u, H_s, etc.).

X. PROGRAM OPERATION

The program was originally written in Fortran IV for the IBM 360-91 and converted to the CDC 6600. It can readily be converted to other machines with a sufficient core storage (Version C occupies a core of 40.6 K and version D occupies a core of 54.4 K on the CDC 6600). There are no special routines which must be provided by the system, other than the usual functions.

XI. PROGRAM INPUT DATA

If two complete (identical) data sets are used the program will make complete DVA tube calculations for both aerodynamic and vapor pressure breakup if $We < We_{cr}$. If only one data set is used the program will consider only aerodynamic breakup in establishing initial conditions for the DVA tube calculations (even if $We < We_{cr}$).

A. Version C - Specialized Chemistry

Card No.	Columns	Description	Format
1	1-80	Run identification	8 A 10
2	1-10	Factor which multiplies entrainment area, A* (usually 1.0)	E 10.3
	11-20	Factor which multiplies DVA tube static pressure, p (usually 1.0)	E 10.3
	21-30	Factor which multiplies vaporization rate, $\dot{\phi}_v$ (usually 1.0)	E 10.3
	31-40	Factor which multiplies particle drag coefficient, C_D (usually 1.0)	E 10.3
	41-50	Pressure relaxation length, L_s (cm), see Eq. (6)	E 10.3
	51-60	FFVI, fraction of liquid that has flashed into vapor (f) is set equal to 1.0 if $f \geq$ FFVI	E 10.3
3	1-10	Molecular weight of liquid injectant	E 10.3
	11-20	Specific heat of liquid (assumed constant) (cal/g-°K)	E 10.3
	21-30	Injectant boiling point at one atm (°K)	E 10.3

Card No.	Columns	Description	Format
3	31-40	Injectant heat of vaporization (cal/g)	E 10.3
	41-50	Density of liquid (g/cm^3)	E 10.3
	51-60	Injectant mass flux (g/sec)	E 10.3
	61-70	Velocity of liquid jet (cm/sec)	E 10.3
	71-80	Jet injection angle (deg), measured from normal to surface	E 10.3
4	1-10	Temperature of liquid jet (°K)	E 10.3
	11-20	Surface tension of liquid jet (dyne/cm)	E 10.3
	21-30	Viscosity of liquid jet (poise)	E 10.3
	31-40	Diameter of single orifice (cm)	E 10.3
	41-50	A_k | Coefficients in expression for d_{32} for	E 10.3
	51-60	B_k | vapor pressure breakup (see Eq. 26a)	E 10.3
5	1- 5	Number of input data points per streamline (NPS)	I5
	6-10	Number of streamlines + 1 (NSL)	I5
	11-15	Number of in-line orifices	I5
	16-20	Debugging output index, If 0: No debug output 1: All debug output printed	I5
	21-25	Number of side-by-side orifices	I5
6	1-10	Value of s at injection site (must be 0)	E 10.3
	11-20	Initial integration step size DS (cm) (recommended value, 0.01 cm)	E 10.3
	21-30	Maximum integration distance (cm)	E 10.3
	31-40	Number of integration steps between print output (DSP), in multiples of DS; e.g. to print at every 10 steps, set DSP = 10 DS	E 10.3
7	1-10	Directed thermal accommodation coefficient, α_D (recommended value, 0.3)	E 10.3
	11-20	Random thermal accommodation coefficient, α_T (recommended value, 0.2)	E 10.3
	21-30	s'_o, maximum lateral spacing of orifices (cm)	E 10.3
	31-40	a, lateral spread parameter, (recommended value, 0.333)	E 10.3
	41-50	Critical Weber number (recommended value, 6.2)	E 10.3

Card No.	Columns	Description	Format

Cards 8 and 9 contain input data on the rate coefficients for the reactions in the specialized chemistry version (see Section VII.A). Values used in previous calculations[3] are given in parentheses (cm-molecule-sec units).

8	1-10	C_1 (1×10^{-2})	E 10.3
	11-20	C_2 (1×10^{-3})	E 10.3
	21-30	C_5 (3×10^{-1})	E 10.3
	31-40	C_6 (3×10^{-10})	E 10.3
	41-50	C_7 (1×10^{-10})	E 10.3
	51-60	C_8 (2.3×10^{-18})	E 10.3
	61-70	f_3 (usually 1.0)	E 10.3
	71-80	f_4 (usually 1.0)	E 10.3
9	1-10	N_1 (1.5)	E 10.3
	11-20	N_2 (1.5)	E 10.3
	21-30	N_5 (2.0)	E 10.3
	31-40	N_8 (1.5)	E 10.3
	41-50	B_6 (8.0×10^4)	E 10.3
	51-60	B_7 (3.0×10^4)	E 10.3
	61-70	B_8 (6.4×10^4)	E 10.3

The following cards specify the free stream (shock layer) properties. Card-type 10 gives the streamwise location of each data set; these cards are noted, 10.1, 10.2...10.NPS. Card-type 11 gives the streamline location normal to the body and the property values. These cards are noted, 11.1.1.1, 11.1.1.2..11.1.(NSL-1)*.2 ...11.NPS.(NSL-1).2.

10.1	1-10	Streamwise location of first data set (cm), must be at injection site, s ≡ 0	E 10.3
11.1.1.1	1-10	Normal distance from body of first streamline (cm)	E 10.3
	11-20	Pressure (dyne/cm^2)	E 10.3
	21-30	Temperature (°K)	E 10.3
	31-40	Velocity (cm/sec)	E 10.3

* Note that on Card 5, Cols. 6-10, NSL is the number of streamlines + 1.

Card No.	Columns	Description	Format
11.1.1.1	41-50*	F_{NO^+} (mole/g)	E 10.3
	51-60	F_{e^-}	E 10.3
	61-70	F_O	E 10.3
	71-80	F_{F^-} (usually 0)	E 10.3
11.1.1.2	1-10	F_N (mole/g)	E10.3
	11-20	F_{O_2}	E 10.3
	21-30	F_{N_2}	E 10.3
	31-40	F_{NO}	E 10.3
11.1.2.1	1-10	Normal distance from body of second streamline (cm)	E 10.3
	11-20	Pressure (atm)	E 10.3
	⋮		
	71-80	F_{F^-} (usually 0)	E 10.3
11.1.2.2	1-10	F_N (mole/g)	E 10.3
⋮	⋮		
	31-40	F_{NO}	E 10.3
⋮			
11.1.(NSL-1).2.			
	⋮		
	31-40	F_{NO}	E 10.3
10.2	1-10	Streamwise location of second data set (cm)	E 10.3

* Note that $F_i = Y_i/W_i = X_i/W$, where Y_i = mass fraction; X_i = mole fraction; W_i = molecular weight of ith species and W = mixture molecular weight.

Card No.	Columns	Description	Format
11.2.1.1	1-10	Normal distance from body of first streamline	E 10.3
•	•		
•			
•	•		
•			
11.2.(NSL-1).2	31-40	F_{NO}	E 10.3
•			
•			
•			
•			
10.NPS	1-10	Streamwise location of last (NPS) data set	E 10.3
•			
•			
•			
•			
•			
11.NPS.(NSL-1).2	31-40	F_{NO} for last data set (NPS) at last streamline (NSL-1) location	E 10.3

1 REPEAT ABOVE DATA SET

2

3

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B. Version D - Generalized Chemistry

Card No.	Columns	Description	Format
1	1-80	Run identification	8 A 10
2	1-10	Factor which multiplies entrainment area, A* (usually 1.0)	E 10.3
	11-20	Factor which multiplies DVA tube static pressure, p (usually 1.0)	E 10.3
	21-30	Factor which multiplies vaporization rate, $\dot{\phi}_v$ (usually 1.0)	E 10.3
	31-40	Factor which multiplies drag coefficient, C_D (usually 1.0)	E 10.3
	41-50	f_3, factor which multiplies k_s in Eq. (82) (usually 1.0)	E 10.3
	51-60	f_4, factor which multiplies k_s in Eq. (83) (usually 1.0)	E 10.3
	61-70	Pressure relaxation length, L_s (cm), see Eq. (6)	E 10.3
	71-80	FFVI, fraction of liquid that has flashed into vapor (f) is set equal to 1.0 if $f \geq$ FFVI	E 10.3
3	1-10	Molecular weight of liquid injectant	E 10.3
	11-20	Specific heat of liquid (assumed constant) (cal/g-°K)	E 10.3
	21-30	Injectant boiling point at one atm (°K)	E 10.3
	31-40	Injectant heat of vaporization (cal/g)	E 10.3
	41-50	Density of liquid (g/cm^3)	E 10.3
	51-60	Injectant mass flux (g/sec)	E 10.3
	61-70	Velocity of liquid jet (cm/sec)	E 10.3
	71-80	Jet injection angle (deg), measured from normal to surface	E 10.3
4	1-10	Temperature of liquid jet (°K)	E 10.3
	11-20	Surface tension of liquid jet (dyne/cm)	E 10.3
	21-30	Viscosity of liquid jet (poise)	E 10.3
	31-40	Diameter of single orifice (cm)	E 10.3
	41-50	A_k Coefficients in expression for d_{32}	E 10.3
	51-60	B_k for vapor pressure breakup (see Eq. 26a)	E 10.3

Card No.	Columns	Description	Format
5	1- 5	Number of input data points per streamline (NPS)	I5
	6-10	Number of streamlines + 1 (NSL)	I5
	11-15	Number of in-line orifices	I5
	16-20	Debugging output index, If 0: No debug output 1: All debug output printed	I5
	21-25	Number of homogeneous reactions (IKINE)	I5
	26-30	Number of species (NS1)	I5
	31-35	Number of side-by-side orifices	I5
6	1-10	Value of s at injection site (must be 0)	E 10.3
	11-20	Initial integration step size (DS), (cm) (recommended value, 0.01 cm)	I5
	21-30	Maximum integration distance (cm)	E 10.3
	31-40	Number of integration steps between print output	E 10.3
7	1-10	Directed thermal accommodation coefficient, α_D (recommended value, 0.3)	E 10.3
	11-20	Random thermal accommodation coefficient, α_T (recommended value, 0.2)	E 10.3
	21-30	s'_o maximum lateral spread of orifices (cm)	E 10.3
	31-40	a, lateral spread parameter (recommended value, 0.333)	E 10.3
	41-50	Critical Weber number (recommended value, 6.2)	E 10.3

The following cards (card-type 8) contain the specific heat data for each species. Data must be included for each species. The first 8 species must be in the following order: NO^+, e^-, O, F^-, N, O_2, N_2, NO. The remaining species can be in any order. Specific heats are expressed in the following form:

$$C_p = L_{1_i} + L_{2_i}\Theta + L_{3_i}\Theta^2 + L_{4_i}\Theta^3 + L_{5_i}\Theta^{-2} \quad \text{cal/mole-°K where } \Theta = T(°K)/1000$$

Card No.	Columns	Description	Format

The enthalpy of each species is then expressed as

$$h_i = \int_o^T C_{p_i}\, dT + L_{6_i}$$

where $L_{6_i} = \Delta H^o_{f_i} - \int_o^{298} C_{p_i}\, dT$

$\Delta H^o_{f_i}$ = heat of formation at 298°K

8.1	1-10	First species (NO^+) name identification	A4
	11-20	Molecular weight	E 10.3
	21-30	L_1	E 10.3
	31-40	L_2	E 10.3
	41-50	L_3	E 10.3
	51-60	L_4	E 10.3
	61-70	L_5	E 10.3
	71-80	L_6	E 10.3
8.2	1-10	Second species (e^-) name identification	A4
•	•		
•	•		
•	•		
•	•		
•	71-80	L_6 for second species (e^-)	E 10.3
•	•		
•	•		
•	•		
8.NS1	71-80	L_6 for NS1 species	E 10. 3

Card-type 9 specifies the reaction mechanism and rate coefficients (see Section VII.B). No particular order is required.

9.1	1- 4	Species A (Reaction 1)	A4
	5	+ sign	
	6- 9	Species B	A4
	10	+ sign	
	11-14	Species C	A4
	15	+ sign	
	16-19	Species D	A4

Card No.	Columns	Description	Format
9.1	20	= sign	
	21-24	Species E	A4
	25	+ sign	
	26-29	Species F	A4
	30	+ sign	
	31-34	Species G	A4
	35	+ sign	
	36-39	Species H	A4
	40	Blank	
	41-42	Reaction type (1-11)	I2
	43-44	Rate coefficient type (1-10)	I2
	45-53	A (Pre-exponential factor, cm-molecule-sec units)	E 9.2
	54-58	N (Temperature exponent)	F 5.2
	59-66	B (Activation energy, cal/mole)	E 8.1
	67-73	K (Reaction type 9 only)	E 7.1
	74-80	δ (Reaction type 10 only)	E 7.1
9.2	1- 4	Species A (Reaction 2)	A4
•			
•			
•			
9.IKINE	1- 4	Species A (Reaction IKINE)	A4
10.1	1-10	Streamwise location of first data set (cm), must be at injection site, s = 0	E 10.3
11.1.1.1	1-10	Normal distance from body of first streamline (cm)	E 10.3
	11-20	Pressure (dyne/cm^2)	E 10.3
	21-30	Temperature (°K)	E 10.3
	31-40	Velocity (cm/sec)	E 10.3
	41-50*	F_{NO} (mole/g)	E 10.3
	51-60	F_e-	E 10.3
	61-70	F_O	E 10.3
	71-80	F_F- (usually 0)	E 10.3

* Note that $F_i = Y_i/W_i = X_i/W_i$, where Y_i = mass fraction; X_i = mole fraction; W_i = molecular weight of ith species and W = mixture molecular weight.

Card No.	Columns	Description	Format
11.1.1.2	1-10	F_N (mole/g)	E 10.3
	11-20	F_{O_2}	E 10.3
	21-30	F_{N_2}	E 10.3
	31-40	F_{NO}	E 10.3
11.1.2.1	1-10	Normal distance from body of second streamline (cm)	E 10.3
	11-20	Pressure (atm)	E 10.3
	•		
	•		
	•		
	•		
	71-80	F_{F^-} (usually 0)	E 10.3
11.1.2.2	1-10	F_N (mole/g)	E 10.3
•	•		
•	•		
•	31-40	F_{NO}	E 10.3
•			
•			
11.1.(NSL-1).2	•		
	•		
	31-40	F_{NO}	E 10.3
10.2	1-10	Streamwise location of second data set (cm)	E 10.3
11.2.1.1	1-10	Normal distance from body of first streamline	E 10.3
•	•		
11.2.(NSL-1).2	31-40	F_{NO}	E 10.3
•			
•			
•			
10.NPS	1-10	Streamwise location of last (NPS) data set	E 10.3
•			
•			
•			
•			
•			
11.NPS.(NSL-1).2			
	31-40	F_{NO} for last data set (NPS) at last streamline (NSL-1) location	E 10.3
12	1-10	Initial mass fraction of H atoms (This card must be included even if the value is zero)	E 10.3

Card No.	Columns	Description	Format
1		REPEAT ABOVE DATA SET	
2			
3			
•			
•			
•			
•			
•			
•			
•			
•			
12			

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NOMENCLATURE

A	DVA tube area; also constant in rate coefficient expression for generalized chemistry version of code (version D)
A*	entrainment area
A_o	initial area for DVA tube calculations
a	exponent in expression for lateral spread, Eq. (30); also speed of sound
B	activation energies for rate coefficient types (5) and (6); activation energy/2 for rate coefficient types (8), (9), (10) (version D)
B_6, B_7, B_8	activation energies in rate coefficient expressions
C	constant, defined by Eq. (32)
C_1, C_2 ...C_8	constants in rate coefficient expressions
C_D	drag coefficient
$\overline{C}_D$	normalized drag coefficient, defined by Eq. (61)
C_{D_I}	incompressible, high Reynolds number drag coefficient
$C_{D_{FM}}$	free molecular drag coefficient
C_{D_o}	drag coefficient from Stokes law, $C_{D_o} = 12/Re_p$
C_p	specific heat
$C_{p,\ell}$	specific heat of liquid
$\dot{d}$	rate of change of droplet diameter
d_{eq}	equivalent orifice diameter based on number of in-line orifices
d'_{eq}	equivalent orifice diameter based on number of side-by-side orifices
d_o	orifice diameter
d_{30}	mass-averaged droplet diameter
d_{32}	mean droplet diameter
erf	error function
F_i	mass fraction/molecular weight (moles/g) of ith species; $F_i = Y_i/W_i$
f	fraction of liquid that flashes into vapor
f_3, f_4	factors which multiply k_s in Eqs. (82) and (83) respectively
dF_p	defined by Eq. (49)
f_p	defined as C_D/C_{D_o}
H_f°	heat of formation at 298°K

H_s	stagnation enthalpy
H_{s_o}	initial stagnation enthalpy for DVA tube calculations
ΔH_v	heat of vaporization of liquid injectant
h	static enthalpy
K	constant in rate coefficient type (9) (version D)
Kn	Knudson number
k	rate coefficient
k_s	proportional to heterogeneous rate coefficients, k_3 and k_4; defined by Eq. (84)
L_1, L_2, ...L_6	coefficients in enthalpy-temperature polynomial, Eq. (101)
L_s	pressure relaxation length, see Eq. (6)
M	Mach number
M_p	droplet Mach number, defined by Eq. (66)
$\dot{m}_a$	mass flow of shock layer air passing through A^*_{bk}
$\dot{m}_i$	mass flow of liquid injectant
$\dot{m}_v$	mass flow of 'flashed' vapor
N'	number of side-by-side orifices
N	number of in-line orifices; also temperature exponent in rate coefficient expression for generalized version D
N_1, N_2 N_5	temperature exponents in rate coefficient expression
n	droplet number density
p	DVA tube static pressure, defined by Eq. (6)
q''	heat transfer rate
R	universal gas constant
Re	Reynolds number, defined by Eq. (17)
Re_p	droplet Reynolds number, defined by Eq. (67)
r_p	droplet radius
r_{p_o}	droplet radius at liquid jet breakup; initial value for DVA tube calculations
s	streamwise distance (along the DVA tube)
s'	lateral spread distance, measured from injection axis to DVA tube boundary
s'_∞	lateral spread distance at $s = 150\ d'_{eq}$
s'_o	initial lateral spread distance

$s'_{7,o}$	lateral spread distance at $s = 70\ d'_{eq}$
T	static temperature
$T_{\ell,o}$	temperature of injected liquid
T_s	stagnation temperature
T_{sh}	shatter temperature, see Eq. (26)
t_{bk}	time for liquid jet to break up
u	velocity in s direction
u_o	initial velocity for DVA tube calculations
u_d	total droplet velocity, $u_d = [u_p^2 + (V_\ell \cos\theta)^2]^{1/2}$
u_r	velocity relative to droplet, $u_r = [(u - u_p)^2 + (V_\ell \cos\theta)^2]^{1/2}$
u_ℓ	streamwise component of injection velocity
V_ℓ	liquid jet injection velocity
v	thermal velocity of neutrals
v_{e^-}	thermal velocity of electrons
v_{F^-}	thermal velocity of negative (F^-) ions
v_{NO^+}	thermal velocity of positive (NO^+) ions
W	mixture molecular weight
$\bar{W}_a$	average molecular weight of shock layer species; defined by Eq. (2)
W_L	liquid jet Weber number, defined as $W_L = 2We(\rho_\ell/\rho)$
We	Weber number, defined by Eq. (14)
We_{cr}	critical Weber number for aerodynamic breakup
W_i	molecular weight of ith species
$\dot{w}_i$	chemical production rate of ith species
$\dot{w}^{(j)}$	chemical production rate from jth reaction
Y_i	mass fraction of ith species
Y_v	mass fraction of vapor
y	distance normal to body
y_{max}	maximum distance normal to body at which shock layer input data are given
y_{mix}	expansion distance of DVA tube in both normal and lateral directions due to mixing
y_{pen}	droplet penetration distance normal to surface
y_{tot}	normal distance of DVA tube boundary from surface

Greek

α_D	directed thermal accommodation coefficient
α_T	random thermal accommodation coefficient
γ	specific heat ratio
η	defined by Eq. (85)
Θ	liquid jet injection angle (measured from normal to body); also T(°K)/1000 in Eq. (100)
μ	viscosity
ρ	density
ρ_o	initial density for DVA tube calculations
σ	surface tension
$\dot{\varphi}_v$	vaporization rate

Subscripts

bk	value at point of liquid jet breakup
bp	boiling point
e	shock layer
i	ith species
j	jth reaction
ℓ	liquid
p	droplet
r	relative to droplets
ref	reference value
x	upstream of normal (jet) shock
y	downstream of normal (jet) shock

Superscripts

$\overline{\quad}$	average value of shock layer property, defined, e.g. by Eq. (11)

APPENDIX A

LATERAL SPREAD OF SPRAY

In order to derive an approximate expression for the lateral spread of the spray we employ the following simplified dimensional analysis. The force acting on a droplet due to a pressure gradient in the s' direction is,

$$F = \frac{4}{3}\pi r_p^3 \frac{dp}{ds'} \tag{A-1}$$

From normal momentum and dimensional considerations, the pressure gradient across the droplet formed from the jet fragment can be expressed as,

$$\frac{dp}{ds'} \propto \frac{\rho u^2}{r_p} \tag{A-2}$$

The equation of lateral motion of the droplet is,

$$m_\ell \frac{\Delta w}{\Delta t} = F \tag{A-3}$$

where w is the droplet velocity in the s' direction and $\Delta t \propto L/u_\ell$ where L is a characteristic break-up length. Combining Eqs. (A-1), (A-2) and (A-3) gives the following expression for w,

$$w \propto \frac{L}{r_p} \frac{\rho u^2}{\rho_\ell u_\ell} \tag{A-4}$$

Taking $L \sim y_{pen}$, we get

$$w \propto \left(\frac{y_{pen}}{d_o}\right)^2 \left(\frac{d_o}{r_p}\right) \frac{\rho u^2}{\rho_\ell u_\ell} \tag{A-4a}$$

The lateral distance the particle will move is,

$$s' = w\Delta t \tag{A-5}$$

Combining Eqs. (A-4) and (A-5) gives

$$s' \propto \left(\frac{y_{pen}}{d_o}\right) \frac{\rho u^2}{\rho_\ell u_\ell^2} \frac{d_o}{r_p} \cdot d_o \tag{A-6}$$

From the results of Weaver[20] we get $y_{pen}/d_o \propto [\rho_\ell u_\ell^2/\rho u^2]$. Thus it is reasonable to express s' as

$$s'/d_o = C\, d_o/r_p \tag{A-7}$$

By interpretation of available experimental data on the lateral spread of liquid sprays,[16,21] the proportionality constant (C) in Eq. (A-7) was found to be approximately unity.

APPENDIX B

SAMPLE INPUT DATA

1. Version C
2. Version D

AeroChem

COMPUTER CODE TO PREDICT THE EFFECTS OF
ELECTROPHILIC LIQUID INJECTION INTO RE-ENTRY PLASMA SHEATHS

version C

```
*******J108 RAM C-III 200KFT FREON E-3 (CASE 6-TLO=360) 12/13/73C
   1.0        1.0        1.0        1.0        50.0       0.8
  618.       0.243      428.       14.5        1.723     152.      2.40E+3      39.0
  380.       284.0      2.2E-2     0.051      612.0      0.0244
10    7    3    0    3
   0.0        0.01       100.0      2.0
   0.3        0.2        0.112      0.333      6.2
 1.0E-2     1.0E-3     3.0E-1     3.E-10     1.E-10     2.3E-18      1.0          1.0
   1.5        1.5        2.0        1.5        8.0E4      3.0E4       6.4E4
```

Note: All cards for 10 and 11 can be found under Version D input 10.1 thru 11.10

Duplicate above data set to reproduce sample output (Appendix C)

AeroChem

FORTRAN Coding Form

COMPUTER CODE TO PREDICT THE EFFECTS OF
ELECTROPHILIC LIQUID INJECTION INTO RE-ENTRY PLASMA SHEATHS

1 7

version D

1	********J108 RAM C-III 200KFT FREON E-3 (CASE 6-TL0=360) 12/13/73C									
2	1.0	1.0	1.0	1.0	1.0	1.0	50.0	0.8		
3	618.	0.243	428.	14.5	1.723	152.0	2.40E+3	39.00		
4	380.	284.0	2.2E-2	0.051	612.0	0.0244				
5	10 7	3 0	6 9	3						
6	0.0	0.01	100.0	200.0						
7	0.3	0.2	0.112	0.333	6.2					
8	NO+	30.0	6.260E+0	1.927E+0	-4.576E-1	3.634E-2	9.764E-3	2.347E+2		
	E-	5.487E-4	4.968E+0	-3.076E-4	7.913E-5	-6.637E-6	-1.709E-5	-1.481E+0		
	O	16.0	5.062E+0	-1.174E-1	3.941E-2	-2.053E-3	1.813E-2	5.812E+1		
	F-	18.99	4.968E+0	-7.323E-5	2.247E-5	-2.775E-6	-1.045E-5	-6.368E+1		
	N	14.0	5.046E+0	-8.613E-2	8.062E-3	6.133E-3	-5.908E-3	1.114E+2		
	O2	32.0	7.241E+0	1.239E+0	-1.844E-1	1.050E-2	-5.960E-2	-2.421E+0		
	N2	28.0	6.264E+0	1.932E+0	-4.615E-1	3.708E-2	9.185E-3	-1.924E+0		
	NO	30.0	6.752E+0	1.700E+0	-4.176E-1	3.412E-2	-1.677E-2	1.942E+1		
	Q	618.0	2.152E+2	0.0	0.0	0.0	0.0	0.0		
9	NO+ +E-	=N +O			1 7	1.1E-2	-1.5			
	NO+ +F-	=NF +O			1 7	1.0E-3	-1.5			
	Q +E-	=F- +Q			1 7	3.0E-1	-2.0			
	F- +M	=F +E- +M			5 5	3.E-10	-8.0E+4			
	F- +O	=OF +E-			1 5	1.E-10	-3.0E+4			
	N +O	=NO+ +E-			1 8	2.3E-18	1.5	-3.2E+4		
10.1	0.0									
11.1.1	0.11	7.80E-3	1610.	1.00E5	3.920E-8	3.920E-8	1.45E-2	0.0		

11.1.1.1	3.00E-2	4.80E-8	1.23E-2	4.40E-7				
11.1.2.1	0.69	8.25E-3	3410.	3.95E+5	2.922E-6	2.922E-6	1.45E-2	0.0
	2.40E-2	2.70E-8	1.53E-2	8.90E-6				
	1.04	8.25E-3	3840.	4.51E+5	5.264E-6	5.264E-6	1.45E-2	0.0
	2.03E-2	2.90E-7	1.72E-2	4.70E-5				
	1.47	8.25E-3	4500.	5.01E+5	7.927E-6	7.927E-6	1.45E-2	0.0
	1.55E-2	2.20E-6	1.95E-2	1.90E-4				
	3.12	7.80E-3	5320.	5.80E+5	1.084E-5	1.084E-5	1.29E-2	0.0
	5.40E-3	9.90E-5	2.38E-2	1.90E-3				
	4.86	1.23E-2	5825.	6.38E+5	7.958E-7	7.958E-7	6.40E-3	0.0
	2.30E-4	3.60E-3	2.66E-2	1.30E-3				
10.2	6.48							
11.2.1.1	0.15	6.37E-3	1700.	1.00E5	4.526E-8	4.526E-8	1.45E-2	0.0
	3.00E-2	4.80E-8	1.23E-2	4.4E-7				
	0.83	6.60E-3	3300.	4.01E5	1.980E-6	1.980E-6	1.45E-2	0.0
	2.40E-2	2.70E-8	1.53E-2	8.9E-6				
	1.21	6.60E-3	3720.	4.61E5	3.659E-6	3.659E-6	1.45E-2	0.0
	2.03E-2	2.90E-7	1.72E-2	4.7E-5				
	1.68	6.60E-3	4215.	5.11E5	5.214E-6	5.214E-6	1.45E-2	0.0
	1.55E-2	2.20E-6	1.95E-2	1.9E-4				
	3.39	6.18E-3	5025.	5.90E5	7.659E-6	7.659E-6	1.32E-2	0.0
	5.40E-3	9.90E-5	2.38E-2	1.9E-3				
	5.42	7.85E-3	5225.	6.50E5	4.782E-7	4.782E-7	6.60E-3	0.0
	2.30E-4	3.60E-3	2.66E-2	1.3E-3				

10.3		11.54								
11.3.1.1		0.16	5.73E-3		1775.	1.00E5	4.971E-8	4.971E-8	1.45E-2	0.0
	3.00E-2		4.8E-8	1.23E-2		4.4E-7				
		0.93	5.83E-3		3265.	4.03E5	1.915E-6	1.915E-6	1.45E-2	0.0
	2.40E-2		2.7E-8	1.53E-2		8.9E-6				
		1.33	5.83E-3		3690.	4.66E5	3.378E-6	3.378E-6	1.45E-2	0.0
	2.03E-2		2.9E-7	1.72E-2		4.7E-5				
		1.80	5.83E-3		4075.	5.16E5	4.757E-6	4.757E-6	1.45E-2	0.0
	1.55E-2		2.2E-6	1.95E-2		1.9E-4				
		3.45	5.59E-3		4900.	5.93E5	6.840E-6	6.840E-6	1.33E-2	0.0
	5.40E-3		9.9E-5	2.38E-2		1.9E-3				
		5.65	6.62E-3		4925.	6.54E5	4.479E-7	4.479E-7	6.65E-3	0.0
	2.30E-4		3.6E-3	2.66E-2		1.3E-3				
10.4		21.67								
11.4.1.1		0.19	4.80E-3		1900.	1.00E5	5.714E-8	5.714E-8	1.45E-2	0.0
	3.00E-2		4.8E-8	1.23E-2		4.4E-7				
		1.11	4.80E-3		3200.	4.07E5	1.729E-6	1.729E-6	1.45E-2	0.0
	2.40E-2		2.7E-8	1.53E-2		8.9E-6				
		1.52	4.80E-3		3635.	4.70E5	2.876E-6	2.876E-6	1.45E-2	0.0
	2.03E-2		2.9E-7	1.72E-2		4.7E-5				
		2.02	4.80E-3		3875.	5.23E5	4.009E-6	4.009E-6	1.45E-2	0.0
	1.55E-2		2.2E-6	1.95E-2		1.9E-4				
		3.56	4.78E-3		4700.	6.00E5	5.814E-6	5.814E-6	1.35E-2	0.0
	5.40E-3		9.9E-5	2.38E-2		1.9E-3				

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	5.99	5.30E-3	4600.	6.60E5	3.982E-7	3.982E-7	6.73E-3	0.0
	2.30E-4	3.6E-3	2.66E-2	1.3E-3				
10.5	31.79							
11.5.1	0.21	4.16E-3	2025.	9.90E4	6.320E-8	6.320E-8	1.45E-2	0.0
	3.00E-2	4.8E-8	1.23E-2	4.4E-7				
	1.25	4.08E-3	3160.	4.02E5	1.572E-6	1.572E-6	1.45E-2	0.0
	2.40E-2	2.7E-8	1.53E-2	8.9E-6				
	1.67	4.08E-3	3585.	4.70E5	2.516E-6	2.516E-6	1.45E-2	0.0
	2.03E-2	2.9E-7	1.72E-2	4.7E-5				
	2.18	4.08E-3	3740.	5.25E5	3.463E-6	3.463E-6	1.45E-2	0.0
	1.55E-2	2.2E-6	1.95E-2	1.9E-4				
	3.68	4.16E-3	4565.	6.05E5	4.957E-6	4.957E-6	1.37E-2	0.0
	5.40E-3	9.9E-5	2.38E-2	1.9E-3				
	6.25	4.48E-3	4400.	6.65E5	3.637E-7	3.637E-7	6.80E-3	0.0
	2.30E-4	3.6E-3	2.66E-2	1.3E-3				
10.6	41.92							
11.6.1	0.24	3.70E-3	2130.	9.70E4	6.663E-8	6.663E-8	1.45E-2	0.0
	3.00E-2	4.8E-8	1.23E-2	4.4E-7				
	1.36	3.55E-3	3030.	4.03E5	1.461E-6	1.461E-6	1.45E-2	0.0
	2.40E-2	2.7E-8	1.53E-2	8.9E-6				
	1.80	3.55E-3	3540.	4.65E5	2.228E-6	2.228E-6	1.45E-2	0.0
	2.03E-2	2.9E-7	1.72E-2	4.7E-5				
	2.33	3.55E-3	3650.	5.22E5	3.093E-6	3.093E-6	1.45E-2	0.0
	1.55E-2	2.2E-6	1.95E-2	1.9E-4				

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	3.80	3.70E-3	4460.	6.085	4.241E-6	4.241E-6	1.38E-2	0.0
	5.40E-3	9.9E-5	2.38E-2	1.9E-3				
	6.45	3.90E-3	4255.	6.685	3.689E-7	3.689E-7	6.80E-3	0.0
	2.30E-4	3.6E-3	2.66E-2	1.3E-3				
10.7	52.04							
11.7.1.1	0.26	3.35E-3	2225.	9.35E4	6.696E-8	6.696E-8	1.45E-2	0.0
	3.00E-2	4.8E-8	1.23E-2	4.4E-7				
	1.44	3.22E-3	3115.	3.975	1.201E-6	1.201E-6	1.45E-2	0.0
	2.40E-2	2.7E-8	1.53E-2	8.9E-6				
	1.90	3.22E-3	3495.	4.555	1.776E-6	1.776E-6	1.45E-2	0.0
	2.03E-2	2.9E-7	1.72E-2	4.7E-5				
	2.44	3.22E-3	3585.	5.185	2.732E-6	2.732E-6	1.45E-2	0.0
	1.55E-2	2.2E-6	1.95E-2	1.3E-4				
	3.91	3.36E-3	4375.	6.115	3.700E-6	3.700E-6	1.39E-2	0.0
	5.40E-3	9.9E-5	2.38E-2	1.9E-3				
	6.62	3.50E-3	4150.	6.715	3.706E-7	3.706E-7	6.80E-3	0.0
	2.30E-4	3.6E-3	2.66E-2	1.3E-3				
10.8	72.29							
11.8.1.1	0.31	2.88E-3	2385.	8.705	6.046E-8	6.046E-8	1.45E-2	0.0
	3.00E-2	4.8E-8	1.23E-2	4.4E-7				
	1.54	2.77E-3	3110.	3.785	1.219E-6	1.219E-6	1.45E-2	0.0
	2.40E-2	2.7E-8	1.53E-2	8.9E-6				
	2.02	2.77E-3	3415.	4.285	1.784E-6	1.784E-6	1.45E-2	0.0
	2.03E-2	2.9E-7	1.72E-2	4.7E-5				

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	2.60	2.77E-3	3540.	4.98E5	2.278E-6	2.278E-6	1.45E-2	0.0
	1.55E-2	2.2E-6	1.95E-2	1.9E-4				
	4.19	2.95E-3	4270.	6.15E5	3.109E-6	3.109E-6	1.41E-2	0.0
	5.40E-3	9.9E-5	2.38E-2	1.9E-3				
	6.87	3.02E-3	4025.	6.74E5	3.923E-7	3.923E-7	6.80E-3	0.0
	2.30E-4	3.6E-3	2.66E-2	1.3E-3				
10.9	87.48							
11.9.1.1	0.33	2.70E-3	2335.	8.50E4	5.083E-8	5.083E-8	1.45E-2	0.0
	3.00E-2	4.8E-8	1.23E-2	4.4E-7				
	1.58	2.59E-3	3125.	3.59E5	1.079E-6	1.079E-6	1.45E-2	0.0
	2.40E-2	2.7E-8	1.53E-2	8.9E-6				
	2.10	2.59E-3	3370.	4.19E5	1.541E-6	1.541E-6	1.45E-2	0.0
	2.03E-2	2.9E-7	1.72E-2	4.7E-5				
	2.68	2.59E-3	3555.	4.87E5	1.874E-6	1.874E-6	1.45E-2	0.0
	1.55E-2	2.2E-6	1.95E-2	1.9E-4				
	4.33	2.80E-3	4225.	6.17E5	2.586E-6	2.586E-6	1.41E-2	0.0
	5.40E-3	9.9E-5	2.38E-2	1.9E-3				
	6.99	2.82E-3	3975.	6.75E5	3.861E-7	3.861E-7	6.80E-3	0.0
	2.30E-4	3.6E-3	2.66E-2	1.3E-3				
10.10	100.0							
11.10.1.1	0.34	2.60E-3	2265.	8.50E4	4.185E-8	4.185E-8	1.45E-2	0.0
	3.00E-2	4.8E-8	1.23E-2	4.4E-7				
	1.62	2.55E-3	3130.	3.39E5	9.697E-7	9.697E-7	1.45E-2	0.0
	2.40E-2	2.7E-8	1.53E-2	8.9E-6				

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```
      2.15      2.55E-3        3330.      4.05E5    1.374E-6    1.374E-6    1.45E-2      0.0
2.03E-2         2.9E-7    1.72E-2         4.7E-5
      2.75      2.55E-3        3590.      4.82E5    1.591E-6    1.591E-6    1.45E-2      0.0
1.55E-2         2.2E-6    1.95E-2         1.9E-4
      4.48      2.73E-3        4200.      6.19E5    2.178E-6    2.178E-6    1.42E-2      0.0
5.40E-3         9.9E-5    2.38E-2         1.9E-3
      7.08      2.73E-3        3950.      6.77E5    3.889E-7    3.889E-7    6.80E-3      0.0
2.30E-4         3.6E-3    2.66E-2         1.3E-3
12    0.0
```

Duplicate above data set for vaper pressure breakup calculations ($We < We_{cr}$)

APPENDIX C

SAMPLE OUTPUT,* Version C†

(see pages E-2 - E-14)

---

* Sample output is not given for Version D since it was not completely debugged at the time this report was prepared.

† These results were obtained with π inadvertently omitted from the denominator in Eqs. (18) and (20). When this correction is made in the code, values of s_{bk} and u_{bk} will be correspondingly reduced.

APPENDIX D

SAMPLE OUTPUT-EXPLANATIONS

VERSION C

Line 1 Input data on Card 1

Line 2 Input data on Card 2

Lines 3-15 Input data on Cards 3 and 4

Line 17 Input data on Card 5

Line 19 Input data on Card 6

Line 20 Input data on Card 7

Lines 22-23 Input data on Cards 8 and 9

Lines 25-36 Starts listing input for first value of S (Card-types 10 and 11)

- J = streamline number (first streamline is designated J = 2)
- Y = normal distance from body (cm)
- PE = pressure (dyne/cm^2)
- TE = temperature (°K)
- UE = velocity (cm/sec)
- FE(I) = F_i (moles/g of ith species)--in order NO^+, e^-, O, F^-, N, O_2, N_2, NO

Line 38 AV = integrated average properties ($\bar{G}$) from the body (Y = 0) to the position of the last streamline ($Y = Y_{max}$);

$$\bar{G}(S) = \frac{1}{Y_{max}} \int_0^{Y_{max}} G(s,y)\, dy$$

First column gives input value of S (Card-type 10) at which average properties are computed.

Line 41

- I = Input data set number
- WA = mixture molecular weight
- HE = static enthalpy, cal/g
- HSE = stagnation enthalpy, cal/g
- REUE = $\bar{\rho}_e \bar{u}_e$ (g/cm^2-sec)
- REUE2 = $\bar{\rho}_e \bar{u}_e^2$ (g/cm-sec^2)

REUEHSE = $\bar{\rho}_e \bar{u}_e h_{s,e}$ (cal/cm^2-sec)

RUF1E = $\bar{\rho}_e \bar{u}_e \bar{F}_{NO^+}$ (moles/cm^2-sec)

RUF2E = $\bar{\rho}_e \bar{u}_e \bar{F}_{e^-}$ (moles/cm^2-sec)

RUF3E = $\bar{\rho}_e \bar{u}_e \bar{F}_O$ (moles/cm^2-sec)

Line 42 RUF4E = $\bar{\rho}_e \bar{u}_e \bar{F}_{F^-}$ (moles/cm^2-sec)

RUF5E = $\bar{\rho}_e \bar{u}_e \bar{F}_N$ (moles/cm^2-sec)

RUF6E = $\bar{\rho}_e \bar{u}_e \bar{F}_{O_2}$ (moles/cm^2-sec)

RUF7E = $\bar{\rho}_e \bar{u}_e \bar{F}_{N_2}$ (moles/cm^2-sec)

RUF8E = $\bar{\rho}_e \bar{u}_e \bar{F}_{NO}$ (moles/cm^2-sec)

Line 46 and following Input for second value of S

⋮

through tenth value of S (I = 10)

*CONDITIONS IN FRONT OF SHOCK (integrated average values from Y = 0 to Y = Y_{max} at the injection site, S = 0)

PX = pressure (dyne/cm^2)

UX = velocity

HSX = stagnation enthalpy, cal/g

RHOX = density, g/cm^3

TX = static temperature, °K

WAX = mixture molecular weight

MASS FRACTIONS F(I) = mass fractions (= $W_i F_i$) of species in following order NO^+, e^-, O, F^-, N, O_2, N_2, Q (vapor)

*CONDITIONS BEHIND SHOCK

PY = pressure (dyne/cm^2)

UY = velocity (cm/sec)

HY = static enthalpy (cal/g)

RHOY = density (g/cm^3)

TY = static temperature (°K)

TBPY = boiling point temperature at PY

*JET BREAK-UP INFORMATION

WE	=	Weber number
REJ	=	Jet Reynold's Number†
TBK	=	Jet breakup time (sec)
UBK	=	Jet velocity in s direction at breakup (cm/sec)
XBK	=	S breakup distance (cm)
YBK	=	Distance normal to body at breakup (cm)
WEL	=	Liquid jet Weber number†
D30	=	Droplet diameter based on mass (cm)†
D32	=	Mean droplet diameter (cm)
DMAX	=	Maximum droplet diameter (cm)†

MODIFIED FREE STREAM CONDITIONS IN SHOCK FRONT BY SINGLE ITERATION
(integrated average values--from Y = 0 to Y = YBK (above)--upstream of shock at the injection site, S = 0

Repeat of Lines 38 to 44, with new integrated average values

*CONDITIONS IN FRONT OF SHOCK

Repeat of above with new integrated average values

*CONDITIONS BEHIND SHOCK

Repeat of above with new values

*JET BREAKUP INFORMATION§

Repeat of above with new values

INITIAL FLOW RATE (G/SEC)

XMV	=	Mass flow of " flashed" vapor (g/sec)
XML	=	Mass flow of liquid (g/sec)
XMA	=	Mass flow of entrained air (g/sec)
XMM	=	Mass flow of entrained air plus vapor (g/sec)
AE	=	Initial entrainment area (cm^2)

---

† Set = 0 in first calculation of Jet Breakup Information if $We < We_{cr}$.

§ Always assumes aerodynamic breakup in calculations for first data set.

**CONDITIONS O. THE INITIAL MIXTURE AT S =

(The following are initial conditions for the DVA tube calculations at the position of jet breakup (XBK))

U	=	Velocity (cm/sec)
HSV	=	Stagnation enthalpy of vapor (cal/g)
HSR	=	Relative stagnation enthalpy of droplets (cal/g)
H	=	Static enthalpy (cal/gm)
TSR	=	Relative stagnation temperature of droplets (°K)
RHO	=	Density (g/cm^3)
A	=	DVA tube area (cm^2)

MASS FRACTIONS OF SPECIES ($Y_i = F_i W_i$) (given in the usual order)

P	=	Pressure ($dyne/cm^2$)
WM	=	Mixture molecular weight
RHO	=	Density (g/cm^3)
HS	=	Stagnation enthalpy (cal/g)
FV	=	Mass fraction of vapor (mass flow of vapor/mass flow of air + vapor)
UP	=	Droplet velocity in S direction (cm/sec)
VP	=	Droplet velocity in Y direction (cm/sec)
TP	=	Droplet (boiling point) temperature (°K)
RP	=	Droplet radius (cm)
SE	=	Lateral spread distance (cm)
YE	=	Penetration distance (cm)

INITIAL THERMODYNAMIC INFORMATION

GAMA	=	Specific heat ratio
CP	=	Specific heat
SS	=	Speed of sound (cm/sec)
MA	=	Gas Mach number
MP	=	Droplet Mach number
REP	=	Droplet Reynold's number

The results of the DVA tube calculations follow

RUN IDENTIFICATION

*S(cm) = Distance from injection site

All symbols same as above, with the addition of:

RHOP = Particle cloud density (g/cm^3)

ELECTRON DENSITY = (cm^{-3})

The following line gives the values of F_i (moles/g) for each species in the same order as the mass fractions.

CHANGES OF MASS FRACTION OVER DS =

The following line gives the changes of mass fraction (derivatives) over the present integration step, in the usual order--ending with the mass fraction of Q (vapor).

The following quantities, starting with DP are evaluated at the previous value of S

DP = Pressure derivative ($dynes/cm^2$)

DRHO = Density derivative (gm/cm^3)

DU = Velocity derivative (cm/sec)

DHS = Stagnation enthalpy derivative (cal/g)

DFV = Vapor mass fraction derivative

PHADS = (PHIV)(A)(DS)(g/cm^3-sec)

DA = DVA tube area derivative (cm^2)

DAE = Entrainment area derivative (cm^2)

DUP = Droplet velocity derivative (cm/sec)

DRP = Droplet radius derivative (cm)

QP = Free molecular heating rate ($erg/sec-cm^2$)

PHIV = Vaporization rate (g/cm^3-sec)

DFP = DUP/(RHOP)(UP)(A)

DQ = Total heat transfer over DS (ergs)

PRODUCTION RATES FOR EACH REACTION (MOL/SEC-CM3)

The following line gives the molar production rates of Reactions 1-8 (see Section VII.A) in order.

PRODUCTION RATES FOR EACH SPECIE

The following line gives the molar production rates (mole/sec-cm^3) for NO^+, e^-, O, F^-, and N, in order.

LOCAL THERMODYNAMIC INFORMATION

The first line following gives the same data as noted above at the local value of S, with the addition of, # P/sec = total number of droplets/sec within the DVA tube.

The second line following gives the following information in order: DS, ETA, SE, YE, VP, XX,a,XX, XX, XX, where

DS	=	Present integration step size (cm)
ETA	=	Used for heterogeneous rate coefficients (see Section VII.A)
SE	=	Lateral spread (cm)
YE	=	Penetration depth (cm)
VP	=	Droplet velocity normal to body (cm/sec)
a	=	Exponent in expression for lateral spread, Eq. 30
XX	=	Not used in present version of program

After printout at maximum integration distance (Card 6, cols. 21-30) program will print, AERODYNAMIC BREAK-UP IS IMPOSSIBLE, WE = (if We < We_{cr}). Then, if a second data set is included, all calculations will be repeated using the vapor pressure breakup equations to establish initial conditions for the DVA tube calculations.

APPENDIX E

FORTRAN LISTINGS*

(AND SAMPLE OUTPUT)

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* These listings do not contain π in the denominator in Eqs. (18) and (20). Corrections should be made to the code in subroutine BREAK; expressions for UBK (version C), lines 108 and 139 and XBK (version C), lines 112 and 142; UBK (version D), lines 111 and 143 and XBK (version D), lines 115 and 146.

```
******** JI 8 RAM C-III  2..KFT FREON-E-3 (BASE 6-TLD=3-6)**** 12/13/73 0
.100E+01  .100E+01  .100E+01  .100E+01  .500E+02  .500E+00
        --- PROPERTIES OF THE INJECTED LIQUID ------
                MOLECULAR WT.=     518.00
                SPECIFIC HEAT(CAL/G-K)= 2.43 E- 1
                BOILING PT. (K)= 4.280E+02
                HEAT OF VAPORIZATION(CAL/G)= 1.450E+01
                DENSITY (G/CM3)= 1.723E+00
                MASS FLUX(G/SEC)= 1.520E+02
                JET VELOCITY(CM/SEC)= 2.400E+03
                JET ANGLE(RAD.)= 6.807E-01
                TEMPERATURE(K)= 3.900E+02
                SURFACE TENSION(DYNE/CM)= 2.840E+02
                VISCOSITY(GM/CM-SEC)= 2.200E-02
                ORIFICE DIAMETER(CM)= 5.100E-02
                LIQUID DROP COEFFICIENTS
                     AK= 6.120E+ 2
                     BK= 2.440E-02

NPS=   10   NSL=    7   NDS=    3   IBUG=   -0   NSO=    3

INITIAL S=  0.000    S INCREMENT= 1.000E-02   FINAL S= 1.000E+02   PRINT INCREMENT= 2.000E+00
 .300E+00  .200E+00  .111E+00  .333E+00  .620E+01

  C1= 1.100E-02  C2= 1.300E-03  C5= 3.000E-01  C6= 3.000E-10  C7= 1.000E-10  C8= 2.30 E-16  FF3= 1.00E+ 0  FF4= 1.00 E+0
 N1= 1.500E+00  N2= 1.100E+00  N.= 2.000E+00  N9= 1. 0.E+00  B6= 8.000E+01  B7= 3.000E+04  B8= 5.400E+04

 J     Y          PE         TE         JE     FE(I) (MOLE/GM)=
 2     .11  7.901E+03  1.511E+03  1.000E+05  3.920E-08  3.920E-08  1.450E-02  .0          3.000E-02  4.800E-08  1.230E-02  4.400E-07

 3     .39  6.367E+03  3. 10E+03  3.950E+05  2.922E-06  2.922E-06  1.450E-02  0.          2.400E-02  2.700E-08  1.530E-02  8.900E-06

 4    1.04  8.357E+03  3.340E+03  4.510E+05  5.264E-06  5.264E-06  1.450E-02  0.          2.030E-02  2.900E-07  1.720E-02  4.700E-05

 5    1.47  8.357E+03  4.500E+03  5.010E+05  7.927E-06  7.92 E-06  1.450E-02  0.          1.900E-02  2.200E-06  1.950E-02  1.900E-04

 6    3.12  7.901E+03  5.320E+03  5.800E+05  1.084E-05  1.084E-05  1.290E-02  0.          5.400E-03  9.900E-05  2.380E-02  1.400E-03

 7    4.06  1.246E+04  5.425E+03  5.360E+05  7.958E- 7  7.958E- 7  6.400E-03  .          2.300E-04  3.600E-03  2.550E-02  1.300E-03

AV=   3.00  9.661E+03  5.010E+03  5.048E+05  5.372E-06  5.372E-06  1.101E-02  0.          5.257E-03  1.317E-03  2.259E-02  1.127E-03

    I       WA          ME          HSE          REUE        REUE2        REUEHSE       RUF1E        RUF2E        RUF3E
        RUF4E       RUF5E       RUF6E       RUF7E       RUF8E
    1   2.257E+01   3.084E+03   6.128E+03   2.643E-01   1.334E+05   1.620E+03   1.420E-05   1.420E-05   2.910E-03
        .0          2.183E-03   3.482E-04   5.968E-03   2.973E-04

 J     Y          PE         TE         JE     FE(I) (MOLE/GM)=
 2     .19  6.. 3E+03  1. 0.E+03  1.000E+05  4.526E-08  4.526E-08  1.450E-02  0.          3.000E-02  4.800E-08  1.230E-02  4.400E-07

 3     .63  6.686E+03  3.300E+03  4.01.E+05  1.9 3E-06  1.980E-06  1.450E-02  0.          2.400E-02  2.700E-08  1.530E-02  8.4.. E-06

 4    1.21  6.686E+03  3.720E+03  ..01.E+05  3.6.3E-06  3.6 4E-06  1.4. 0E-02  0.          2.030E-02  2.900E-07  1.720E-02  4.700E-05

 5    1.68  6.346E+03  4.215E+03  5.11.E+05  5.214E-06  5.214E-06  1.450E-02  .0          1.950E-02  2.200E-06  1.95.E-02  1.900E-04

 6    3.39  6.260E+03  5. 25E+ 3  5.0. E+05  7.659E- 6  7.659E- 6  1.320E-02  .          5.400E-03  9.900E-05  2.380E-02  1.400E-03

 7    5.42  7.952E+03  5.225E+03  6.500E+05  4.782E-07  4.782E-07  6.600E-03  .0          2.300E-04  3.600E-03  2.550E-02  1.300E-03

AV=   5.48  7..19E+03  4.630E+03  5.111E+05  3.530E-06  3.530E-06  1.1.6E-02  .0          5.342E-03  1.371E- 3  2.248E- 2  1.1.. E- 3
```

I	WA	HE	HSE	REUE	REUE2	REUEHSE	RUF1E	RUF2E	RUF3E
	RUF4E	RUF5E	RUF6E	RUF7E	RUF8E				
2	2.255E+01	2.971E+03	6.091E+03	2.102E-01	1.774E+ 5	1.280E+ 3	7.419E-07	7.419E- 7	2.324E-03
	•	1.753E-03	2.886E-04	1.72 E-03	2.311E-04				

J	Y	PE	TE	UE	FE(I) (MOLE/GM)=					
2	.16	5.804E+03	1.775E+03	1.003E+05	4.971E-08	4.971E-08	1.450E-02	3.	3.000E-02	4.300E-06	1.23 E- 2	4.40 E-07
3	.93	5.906E+03	3.250E+03	1.030E+05	1.91 E-06	1.91 E-06	1.450E-02	3.	2.400E-02	2.700E-08	1.530E-02	8.900E-06
4	1.33	5.906E+03	3.650E+03	4.660E+05	3.378E-06	3.378E-06	1.450E-02	3.	2.030E-02	2.900E-07	1.720E-02	4.700E-05
5	1. .	5.906E+03	4. 75E+03	5.160E+05	4.757E-06	4.757E- 6	1.450E-02	3.	1.550E-02	2.200E-06	1.9 0E-02	1.900E-04
6	3.45	5.663E+03	4.900E+03	5.930E+05	6.840E-06	6.840E-06	1.330E-02	3.	5.400E-03	9.900E-05	2.380E-02	1.300E-03
7	5.65	6.706E+03	4.925E+03	6.540E+05	4.479E-07	4.479E- 7	6.650E-03	.	2.3 0E- 4	3.60 E-03	2.66 E-02	1.30 E-03
AV=	11. 4	6.1 4E+03	4. 4 E+03	5.12 E+05	3.047E-06	3.047E-06	1.101E-02	3.	9.452E-03	1.421E-03	2.242E-02	1.074E-03

I	WA	HE	HSE	REUE	REUE2	REUEHSE	RUF1E	RUF2E	RUF3E
	RUF4E	RUF5E	RUF6E	RUF7E	RUF8E				
3	2.253E+01	2.913E+03	6.051E+03	1.918E-01	9.822E+04	1.161E+03	5.845E-07	5.845E-07	2.113E-03
	..	1.621E-03	2.725E-04	1.301E-03	2.063E-04				

J	Y	PE	TE	UE	FE(I) (MOLE/GM)=					
2	.19	4.862E+03	1.300E+03	1.000E+05	5.714E-08	5.714E-08	1.450E-02	3.	3.000E-02	4.900E-08	1.230E-02	4.400E-07
3	1.11	4.862E+03	3.200E+03	4.070E+05	1.729E-06	1.729E-06	1.450E-02	3.	2.400E-02	2.700E-08	1.530E-02	8.900E-06
4	1.52	4.862E+03	3.535E+03	4.700E+05	2.675E-06	2.675E-06	1.450E-02	3.	2.030E-02	2.900E-07	1.720E-02	4.700E-05
5	2.12	4.862E+03	3.975E+03	5.230E+05	4.009E-06	4.009E-06	1.450E-02	3.	1.550E-02	2.230E-06	1.950E-02	1.900E-04
6	3.56	4.842E+03	4.710E+03	6.000E+05	5.814E-06	5.814E-06	1.350E-02	.	5.400E-03	9.900E-05	2.380E-02	1.300E-03
	5.03	5.363E+03	4.360E+03	6.600E+05	3.982E-07	3.982E-07	6.730E-03	3.	2.300E-04	3.600E-05	2.660E-02	1.300E-03
AV=	21.67	5.063E+03	4.198E+03	5.119E+05	2.435E-06	2.435E-06	1.100E-02	3.	8.732E-03	1.474E-03	2.227E-02	1. 28E-03

I	WA	HE	HSE	REUE	REUE2	REUEHSE	RUF1E	RUF2E	RUF3E
	RUF4E	RUF5E	RUF6E	RUF7E	RUF8E				
4	2.247E+01	2.873E+03	6.000E+03	1.663E-01	8.540E+04	1.001E+03	4.163E-07	4.163E-07	1.835E-03
	•	1.457E-03	2.459E-04	3.716E-03	1.71 E-04				

J	Y	PE	TE	UE	FE(I) (MOLE/GM)=					
2	.21	4.214E+03	2.025E+03	9.900E+04	5.320E-08	5.320E-08	1.450E-02	3.	3.000E-02	4.800E-08	1.23 E-02	4.40 E-07
3	1.25	4.133E+03	3.180E+03	4.080E+05	1.572E-06	1.572E-06	1.450E-02	3.	2.400E-02	2.700E-08	1.530E-02	8.900E-06
4	1.67	4.133E+03	3.585E+03	4.700E+05	2.515E-06	2.515E-06	1.450E-02	3.	2.030E-02	2.900E-07	1.720E-02	4.700E-05
5	2.18	4.133E+03	3.740E+03	5.250E+05	3.463E- 6	3.463E- 6	1.450E- 2	3.	1.550E-02	2.200E-06	1.900E-02	1.900E-04
6	3.68	4.214E+03	4.365E+03	6.050E+05	4.957E-06	4.957E-06	1.370E-02	3.	5.400E-03	9.900E-05	2.380E-02	1.300E-03
7	5.25	4.538E+03	4.430E+03	6.650E+05	3.637E-07	3.637E-07	6.800E-03	.	2.3 0E- 4	3.60 E-03	2.66 E-02	1.30 E-03
AV=	31. 9	4.322E+03	4.0 0E+03	5.10 E+05	2.036E-06	2.036E-06	1.104E-02	3.	8.940E-03	1.491E-03	2.215E-02	1.002E-03

I	WA	HE	HSE	REUE	REUE2	REUEHSE	RUF1E	RUF2E	RUF3E

	RUF4E	RUF5E	RUF6E	RUF7E	RUF8E				
	2.[illegible]E+01	2.84[illegible]E+03	9.96[illegible]E+03	[illegible]E-01	7.509E+04	6.765E+02	2.994E-07	[illegible]E-07	1.624E-03
	•	[illegible]E-03	2.192E-04	[illegible]E-03	1.473E-04				

J	Y	PE	TE	UE	FE(I) (MOLE/GM)=						
2	[illegible]	[illegible]E+03	2.[illegible]E+03	[illegible]E+04	6.663E-08	6.663E-08	1.45[illegible]E-02	0.	3.000E-02	4.800E-08	1.23[illegible]E-02	4.460E-07
3	1.36	[illegible]E+03	[illegible]E+03	[illegible]E+05	1.461E-06	1.461E-06	1.45[illegible]E-02	0.	2.400E-02	2.700E-08	1.532E-02	8.900E-06
4	[illegible]	[illegible]E+03	[illegible]E+03	[illegible]E+05	2.228E-06	2.228E-06	1.450E-02	0.	2.030E-02	2.900E-07	1.720E-02	4.700E-05
5	[illegible]	[illegible]E+03	[illegible]E+03	[illegible]E+05	3.093E-06	3.093E-06	1.450E-02	0.	1.550E-02	2.200E-06	1.950E-02	1.400E-04
6	[illegible]	[illegible]E+03	[illegible]E+03	[illegible]E+05	4.241E-06	4.241E-06	1.380E-02	0.	5.400E-03	9.900E-05	2.380E-02	1.900E-03
[illegible]	[illegible]	[illegible]E+03	[illegible]E+03	[illegible]E+05	3.689E-07	3.689E-07	6.800E-03	0.	2.300E-04	3.600E-03	2.650E-02	1.300E-03
AV=	41.[illegible]	[illegible]E+03	[illegible]E+03	[illegible]E+05	1.764E-06	1.764E-06	1.108E-02	0.	9.134E-03	1.488E-03	2.2[illegible]E-02	9.786E-04

I	WA	HE	HSE	REUE	REUE2	REUE4SE	RUF1E	RUF2E	RUF3E
	RUF4E	RUF5E	RUF6E	RUF7E	RUF8E				
6	2.234E+01	2.832E+03	5.833E+03	1.319E-01	6.653E+04	7.751E+02	2.321E-07	2.321E-07	1.457E-03
	•	[illegible]E-03	1.997E-04	2.899E-03	1.28[illegible]E-04				

J	Y	PE	TE	UE	FE(I) (MOLE/GM)=						
2	.26	3.344E+03	2.226E+03	9.35[illegible]E+04	6.696E-08	6.696E-08	1.450E-02	0.	3.000E-02	4.800E-08	1.23[illegible]E-02	4.4[illegible]E-07
3	1.[illegible]	3.2[illegible]E+03	3.11[illegible]E+03	3.9[illegible]E+05	1.201E-06	1.201E-06	1.4[illegible]E-02	0.	2.400E-02	2.700E-08	1.532E-02	8.900E-06
4	1.[illegible]	3.2[illegible]E+03	3.[illegible]E+03	[illegible]E+05	1.776E-06	1.776E-06	1.450E-02	0.	2.030E-02	2.900E-07	1.720E-02	4.700E-05
5	2.44	3.26[illegible]E+03	3.3[illegible]E+03	5.18[illegible]E+05	2.732E-06	2.732E-06	1.450E-02	0.	1.550E-02	2.200E-06	1.9[illegible]E-02	1.400E-04
6	3.91	3.4[illegible]E+03	4.375E+03	6.11[illegible]E+05	3.700E-06	3.700E-06	1.390E-02	0.	5.400E-03	9.900E-05	2.38[illegible]E-02	1.400E-03
7	5.02	3.5[illegible]E+03	4.15[illegible]E+03	6.71[illegible]E+05	3.706E-07	3.706E-07	6.8[illegible]E-03	0.	2.3[illegible]E-04	3.6[illegible]E-03	2.66[illegible]E-02	1.3[illegible]E-03
AV=	52.[illegible]	3.[illegible]E+03	3.[illegible]E+03	[illegible]E+05	1.522E-06	1.522E-06	1.111E-02	0.	9.338E-03	1.482E-03	2.137E-02	9.655E-04

I	WA	HE	HSE	REUE	REUE2	REUE4SE	RUF1E	RUF2E	RUF3E
	RUF4E	RUF5E	RUF6E	RUF7E	RUF8E				
[illegible]	2.229E+01	2.831E+03	5.848E+03	1.196E-01	6.649E+04	6.992E+02	1.820E-07	1.820E-07	1.329E-03
	•	1.116E-03	1.772E-04	2.[illegible]26E-03	1.154E-04				

J	Y	PE	TE	UE	FE(I) (MOLE/GM)=						
2	.31	2.31[illegible]E+03	2.3[illegible]E+03	5.70[illegible]E+04	6.046E-08	6.046E-08	1.45[illegible]E-02	0.	3.000E-02	4.800E-08	1.23[illegible]E-02	4.460E-07
3	1.34	2.3[illegible]E+03	3.1[illegible]E+03	3.78[illegible]E+05	1.219E-06	1.219E-06	1.450E-02	0.	2.400E-02	2.700E-08	1.532E-02	8.900E-06
4	2.[illegible]2	2.3[illegible]E+03	3.[illegible]E+03	4.28[illegible]E+05	1.78[illegible]E-06	1.[illegible]E-06	1.45[illegible]E-02	0.	2.030E-02	2.900E-07	1.720E-02	4.700E-05
5	2.[illegible]8	2.[illegible]E+03	3.[illegible]E+03	4.98[illegible]E+05	2.279E-06	2.279E-06	1.450E-02	0.	1.550E-02	2.200E-06	1.950E-02	1.400E-04
6	4.19	2.4[illegible]E+03	4.27[illegible]E+03	6.15[illegible]E+05	3.1[illegible]E-06	3.1[illegible]E-06	1.41[illegible]E-02	0.	5.4[illegible]E-03	9.900E-05	2.38[illegible]E-02	1.[illegible]E-03
	5.[illegible]7	3.[illegible]59E+03	4.[illegible]E+03	6.74[illegible]E+05	3.923E-07	3.923E-07	6.800E-03	0.	2.300E-04	3.600E-03	2.65[illegible]E-02	1.300E-03
AV=	72.29	2.3[illegible]E+03	3.[illegible]E+03	4.911E+05	1.397E-06	1.397E-06	1.123E-02	0.	9.621E-03	1.413E-03	2.131E-02	9.582E-04

I	WA	HE	HSE	REUE	REUE2	REUE4SE	RUF1E	RUF2E	RUF3E
	RUF4E	RUF5E	RUF6E	RUF7E	RUF8E				
6	2.216E+01	2.84[illegible]E+03	5.726E+03	1.023E-01	6.651E+04	5.888E+02	1.436E-07	1.436E-07	1.161E-03
	•	[illegible]E-03	1.493E-04	2.243E-03	9.8[illegible]E-05				

J	Y	PE	TE	UE	FE(I) (MOLE/GM)=						
2	.33	2.735E+03	2.336E+03	8.503E+04	5.083E-06	5.083E-06	1.450E-02	..	3.001E-02	4.4..E-..	1.23 E- 2	4.4 E-.7
3	1. 6	2.02 E+03	3.12 E+03	3. .0E+0.	1.079E-06	1.079E-06	1.4.0E-02	..	2.400E-02	2.70.E-08	1.53.E-02	8.90.E-06
4	2.10	2.624E+03	3.37.E+03	4.19.E+05	1.541E-06	1.541E-06	1.450E-02	..	2.03.E-02	2.90.E-07	1.72.E-02	4.70.E-05
5	2.68	2.624E+03	3.355E+03	4.87 E+05	1.874E-06	1.874E-06	1.450E-02	..	1.95.E-02	2.20.E-06	1.9..E-02	1.90.E-04
6	4.33	2.836E+03	4.225E+03	6.17.E+05	2.566E-06	2.566E-06	1.410E-02	..	5.40.E-03	9.90.E-05	2.38.E-02	1.40.E-03
7	6. 9	2.857E+03	3.475E+03	6.75.E+05	3.861E-07	3.861E- 7	6.80.E-.3	..	2.3..E-04	3.6..E-.3	2.66 E-.2	1.3 .E-.3
4V= 6 . 8		2.7..E+03	3. 2.E+03	4.844E+05	1.211E-06	1.211E-06	1.136E-02	..	9.769E-03	1.380E-03	2.174E-02	9.945E-04

I	WA	HE	HSE	REUE	REUE2	REUEHSE	RUF1E	RUF2E	RUF3E
	RUF4E	RUF5E	RUF6E	RUF7E	RUF8E				
9	2.212E+01	2.85 E+03	5.658E+03	9.57.E-02	4.639E+04	5.419E+02	1.160E-07	1.160E-07	1.088E-03
	..	9.357.-04	1.322E-04	2.682E-03	9.142E-05				

J	Y	PE	TE	UE	FE(I) (MOLE/GM)=						
2	.34	2.03.E+03	2.3 .E+03	8. .3E+04	4.165E-06	4.165E-06	1.450E-02	..	3.00.E-02	4.80.E-08	1.23.E-02	4.40.E-07
3	1.02	2.583E+03	3.13.E+03	3.39.E+05	9.697E-07	9.697E-07	1.450E-02	..	2.40.E-02	2.70.E-08	1.53.E-02	8.90.E-06
4	2.15	2.583E+03	3.33.E+03	4.15.E+05	1.374E-06	1.3..E-06	1.450E-02	..	2.03.E-02	2.90.E-07	1.72.E-02	4.70.E-05
5	2.75	2.583E+03	3.55.E+03	4.82.E+05	1.591E-06	1.591E-06	1.450E-02	..	1.95.E-02	2.20.E-06	1.95.E-02	1.90.E-04
6	4.48	2.765E+03	4.2..E+03	6.19 E+05	2.178E-.6	2.178E-.6	1.42.E-.2	.	5.4. E-.3	9.9. E-05	2.38.E-02	1.90.E-.3
	..8	2.765E+03	3.95.E+03	6.77.E+05	3.889E-07	3.889E-07	6.80.E-03	..	2.30.E-04	3.60.E-03	2.66.E-02	1.30.E-03
4V=1....		2.687E+03	3.7.2E+03	4.783E+05	1.073E-06	1.07.E-.6	1.148E-02	..	9.913E-03	1.332E-03	2.165E-.2	9.529E-.4

I	WA	HE	HSE	REUE	REUE2	REUEHSE	RUF1E	RUF2E	RUF3E
	RUF4E	RUF5E	RUF6E	RUF7E	RUF8E				
10	2.236E+01	2.873E+03	5.605E+03	9.239E-02	4.419E+04	5.179E+02	9.966E-.8	9.966E-.8	1.061E- 3
	.	9.158E-.4	1.23.E-.4	2.6..E-03	6.86.E-.				

CONDITIONS IN FRONT OF SHOCK
PX= 9.661E+03 UX= 5.048E+05 HSX= 6.128E+03 RHOX= 5.237E-07 TX= 5.013E+03 WAX= 2.257E+01
MASS FRACTIONS F(I)= ..612E-.4 2.948E-.3 1.762E- 1 .. 1.155E-.1 4.215E-.2 6.321E-01 3.381E-02 ..

CONDITIONS BEHIND SHOCK
PY= 1.182E+05 UY= 9.462E+04 HY= 6.022E+03 RHOY= 2.811E-.6 TY= 1.141E+04 TBPY= 3.555E+02

JET BREAK-UP INFORMATION
WE= 3.865E+00 REJ= 0. TBK= 1.027E-03 UBK= 1.90.E+03 XBK= 1.751E+01 YBK= 1.915E+00
WEL= 0. D3.= 0. D32= 2.935E-03 DMAX= 0.

--------- MODIFIED FREE STREAM CONDITIONS IN SHOCK FRONT BY SINGLE ITERATION -----

J	PE	TE	UE	FE(I) (MOLE/GM)=						
4V= ...0	8.37.E+03	3.467E+03	4.598E+05	5.762E-06	5.762E- 6	1.450E-.2	.	1.947E-.2	3.362E-.7	1.762E-.2	5.4 1E-.5

I	WA	HE	HSE	REUE	REUE2	REUEHSE	RUF1E	RUF2E	RUF3E
	RUF4E	RUF5E	RUF6E	RUF7E	RUF8E				
1	1.436E+01	4.23.E+03	6.76.E+.3	2.259E-.1	1..39E+.5	1.527E+.3	1.3.2E-.5	1.3.2E- 6	3.27.E-.3
	.	.398E-03	7. 93E-.8	3.981E-03	1.22.E-.				

CONDITIONS IN FRONT OF SHOCK
PX= 5.274E+03 UX= 4.593E+05 HSX= 6.760E+03 RHOX= 4.912E-07 TX= 3.967E+03 MAX= 1.935E+ 1
MASS FRACTIONS OF SPECIES
NO+= 3.719E-07 E-= 1.759E-11 O= 1.291E-03 F-= 0. N= 1.517E-03 O2= 5.935E-08 N2= 2.746E- 3 NO= 9. 17E- 6 FV= 9.944E-01

CONDITIONS BEHIND SHOCK
PY= 3.776E+04 UY= 1.08+E+05 HY= 6.62 E+ 3 RHOY= .084E- 6 TY= 9.611E+03 TBPY= 3.474E+02

JET BREAK-UP INFORMATION
WE= 1.107E+00 REJ= 8.417E+02 TBK= 1.107E-03 UBK= 1.926E+03 XBK= 1.901E+01 YBK= 2.064E+00
WEL= 3.295E+00 D3.= 5.34.E-03 D32= 7.475E-03 DMAX= 1.739E- 2

INITIAL FLOW RATE(G/SEC)
XMV= 1.315E+01 XML= 6.855E+01 XMA= 4.653E-01 XMM= 8.361E+01 AE= 2.063E+00

------ CONDITIONS OF THE INTIAL MIXTURE AT S= 1.+.10
U= 2.5.6E+03 HSV= 9.893E+01 HSR= 1.361E+02 H= 1.359E+02 TSR= 3.432E+02 T= 3.431E+02 RHO= 1.630E-03 A= 2.345E+01
MASS FRACTIONS OF SPECIES
NO+= 3.619E-07 E-= 1.759E-11 O= 1.291E-03 F-= 0. N= 1.517E-03 O2= 5.935E-08 N2= 2.746E- 3 NO= 9. 17E- 6 FV= 9.944E-01

P= 8.315E+04 WM= 5.273E+02 RHO= 1.630E-03 HS= 1.366E+02 FV= 9.944E-01 UP= 1.926E+03 VP= 1.863E+03
TP= 3.474E+02 RP= 3.737E-03 SE= 6.354E-01 YE= 2.064E+00

INITIAL THERMODYNAMIC INFORMATION
GAMA= 1.011 CP(CAL/G)= 3.480E-01 SS= 7.395E+03 MA= 3.392E-01 MAP= 2.842E-01 REP= 7.013E+01

******** J108 RAM C-III 200KFT FREON-E-3 (CASE 6-TLO=360)**** 12/13/73 0

S(CM)= 1.920
T(K)= 343.16 P(DYNE/CM2)= 8.815E+04 RHO(GM/ML)= 1.629E-03 U(CM/SEC)= 2.511E+03 HS(CAL/GM)= 1.361E+02 FV= 9.944E-01 WM= 5.272E+02
A= 2.44E+01 UP= 1.926E+03 TP= 3.474E+02 RP= 3.737E-03 RHOP= 1.746E-03 AE= 2.062E+00 TSR= 3.432E+02 H= 1.36 E+2

MASS FRACTIONS OF SPECIES
NO+= 8.845E-07 E-= 2.999E-17 O= 1.292E-03 F-= 5.599E-07 N= 1.517E-03 O2= 1.283E-07 N2= 2.743E-3 NO= 9.78E-08
---- ELECTRON DENSITY= 3.144E+13
.321E-7 .321E-7 .8u7E- 4 0. .1.8E-.3 .187E-.8 .981E-04 .301E-05

CHANGES OF MASS FRACTION OVER DS= 1.000E-03
-7.738E-03 -1.759E-11 1.258E-06 5.599E-07 5.000E-07 6.907E-08 2.986E-06 5.849E-08 -5.513E-06
DP= -.139E+01 DRHO= -.823E-06 DU= .300E+01 DHS= .364E-01 DFV= -.562E-.5 PHADS= -.471E-.4
DA=-1.049E-.2 DAE= 2.433E-.3 DUP= 3.875E-03 DRP= 8. 29E-10 QP=-4.103E-02 PHIV=-2.304E-03
DFP= 5.111E-01 DQ=-3.549E-10

PRODUCTION RATES FOR EACH REACTION (MOL/SEC-CM3)
2.545E-.3 .. 1.827E-.6 0. 2.103E+02 0. 0. 0.

PRODUCTION RATES FOR EACH SPECIE
-2.547E-03 -2.103E+02 2.847E-.3 2.103E+02 2.847E-03

LOCAL THERMODYNAMIC INFORMATION
GAMA=D 1.011 CP(CAL/G)= 3.480E-01 SS= 7.396E+03 MA= 3.391E-01 MAP= 2.542E-01 REP= 7.013E+01 #P/SEC= 1.827E+18
.1.0E-02 .356E+01 .636E+00 .207E+01 .157E+04 .192E+13 .333E+00 .177E+22 .157E+01 .640-218

S(CM)= 4.0133
T(K)= 334.04 P(DYNE/CM2)= 8.525E+04 RHO(GM/ML)= 7.965E-04 U(CM/SEC)= 9.712E+03 HS(CAL/GM)= 2.253E+02 FV= 9.803E-01 WM= 3.915E+02
A= 1.123E+01 UP= 2.071E+03 TP= 3.474E+02 RP= 3.705E-03 RHOP= 2.692E-03 AE= 7.726E+00 TSR= 5.157E+.2 H= 2.241E+.2

MASS FRACTIONS OF SPECIES
NO+= 5.047E-08 E-= 2.255E-19 O= 4.205E-03 F-= 5.094E-08 N= 4.346E-03 O2= 2.352E-04 N2= 1.058E-02 NO= 2.358E-04
---- ELECTRON DENSITY= 1.959E+05
.268E-.8 .4 9E-15 .262E- 3 .268E- 8 .315E- 3 .888E-05 .377E-03 .783E-03

CHANGES OF MASS FRACTION OVER DS= 5.053E-03
2.176E-10 1.374E-21 6.025E-06 1.377E-10 7.131E-06 1.106E-06 2.344E-05 8.567E-07 -4.057E-05
DP= -.688E+01 DRHO= -.139E-05 DU= .205E+02 DHS= .252E+03 DFV= -.435E-04 PHADS= .133E-.1
DA=-2.342E-03 DAE= 1.751E-.2 DUP= 7.358E-01 DRP=-1.841E-07 QP= 1.885E+03 PHIV= 1.757E-01
DFP= 4.936E+01 DQ= 3.539E-07

PRODUCTION RATES FOR EACH REACTION (MOL/SEC-CM3)
4. 77E-13 2.427E- 7 1. 35E-12 3.969E-08 2.938E-07 0. 0. 0.

PRODUCTION RATES FOR EACH SPECIE
-2.824E-07 -2.938E-07 2.824E-07 1.144E-06 1.442E-12

LOCAL THERMODYNAMIC INFORMATION
GAMA=D 1.015 CP(CAL/G)= 3.471E-01 SS= 1.042E+04 MA= 9.299E-01 MAP= 7.519E-01 REP= 1.041E+02 #P/SEC= 1.827E+18
.3.5E-02 .1.8E+00 .121E+01 .405E+01 .187E+04 .192E+13 .333E+00 .177E+22 .157E+01 .660-218

S(CM)= 4.8131
T(K)= 332.52 P(DYNE/CM2)= 8.415E+04 RHO(GM/ML)= 8.086E-04 U(CM/SEC)= 1.310E+04 HS(CAL/GM)= 2.664E+02 FV= 9.736E-01 WM= 3.912E+02
A= 1.120E+01 UP= 2.218E+03 TP= 3.474E+02 RP= 3.666E-03 RHOP= 2.621E-03 AE= 1.074E+01 TSR= 5.364E+.2 H= 2.644E+.2

MASS FRACTIONS OF SPECIES
NO+= 1.190E-07 E-= 5.504E-19 O= 5.502E-03 F-= 7.535E-08 N= 5.446E-03 O2= 4.394E-04 N2= 1.452E-.2 NO= 3.927E-04
---- ELECTRON DENSITY= 3.663E+05

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-3.1[illegible]E-1[illegible]   [illegible]5E-1[illegible]   3.126E-10   8.687E-11   3.420E-15

  LOCAL   THERMODYNAMIC INFORMATION
GAMA=D 1.042   CP(CAL/G)= 3.430E-01  SS= 3.[illegible]53E+04  MA= 2.752E+[illegible]   MAP= 1.799E+0[illegible]   REP= 2.149E+0[illegible]   #P/SEC= 1.82[illegible]E+[illegible]
    .5[illegible]0E-01     .8[illegible]5E-0[illegible]     .438E+01     .192E+02     .187E+04     .192E+13     .333E+00     .177E+22     .187E+01     .[illegible]-21[illegible]

S(CM)=  99.9648
T(K)= 1545.63 P(DYNE/CM2)= 7.449E+03 RHO(GM/ML)= 8.251E-06 U(CM/SEC)= [illegible]E+04 HS(CAL/G4)= 6.254E+02 FV= 8.759E-01 WM= 1.4[illegible]3E+02
A= 2.3[illegible]6E+02  UP= 2.948[illegible]E+04  TP= 3.474E+02  RP= 1.998E-03  RHOP= 1.549E-08  AE= 1.340E+02  TSR= 1.552E+03  H= 7.3[illegible]E+ 2

MASS FRACTIONS OF SPECIES
NO+= 5.176E-07 E-= 2.885E-17 O= 2.257E-02 F-= 3.909E-07 N= 1.692E-02 O2= 5.[illegible]E-03 N2= 7.582E-02 NO= 3.526E-03
 ----   ELECTRON DENSITY= 2.610E+05
    .[illegible] 6E-07     .526E-13     .141E-02     .2[illegible]6E- 7     .121E- 2     .164E-03     .271E-02     .118E-03

CHANGES OF MASS FRACTION OVER DS= 5.[illegible]0E-02
     1.506E-10   1.596E-20   3.730E-06   9.530E-11   2.823E-06   8.656E-07   1.226E-05   5.600E-07  -2.026E-05
DP= -.598E+01  DRHO= -.531E-08  DU=  .172E+02  DHS=  .110E+00  DFV= -.2[illegible]E-0[illegible]  PHADS=  .211E- 2
DA= 1.[illegible]3E-01  DAE= [illegible].3[illegible]E-02  DUP=  .[illegible]2E+00  DRP=-1.336E-07  QP= 1.967E+00  PHIV= 1.830E-04
DFP= 7.432E+01  DQ= 5.191E-08

PRODUCTION RATES FOR EACH REACTION (MOL/SEC-CM3)
   8.[illegible]42E-15   2.663E-1   3.307E-15   9.872E-12   3.6[illegible]2E-10   8.6[illegible]2E-18   5.818E-12   8.598E-1[illegible]

PRODUCTION RATES FOR EACH SPECIE
  -2.962E-13  -3.774E-1[illegible]   2.894E-10   8.119E-11   2.650E-15

  LOCAL   THERMODYNAMIC INFORMATION
GAMA=D 1.042   CP(CAL/G)= 3.429E-01  SS= 3.068E+04  MA= 2.764E+00  MAP= 1.3[illegible]E+0[illegible]  REP= 2.058E+03  #P/SEC= 1.827E+[illegible]
    .5[illegible]E-01     .81[illegible]E-     .441E+ 1     .194E+ 2     .187E+ 4     .192E+13     .333E+00     .177E+22     .1[illegible]E+01     .[illegible]-21[illegible]

 --- AERODYNAMIC BREAK-UP IS IMPOSSIBLE, WE= 3.807E+00
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******** J108 RAM C-III  200KFT FREON-E-3 (CASE 6-TLO=360)**** 12/13/73
.100E+01  .100E+01  .100E+01  .100E+01  .500E+02  .800E+00
        --- PROPERTIES OF THE INJECTED LIQUID ------
                MOLECULAR WT.=     518.00
                SPECIFIC HEAT(CAL/G-K)= 2.430E-01
                BOILING PT. (K)= 4.280E+02
                HEAT OF VAPORIZATION(CAL/G)= 1.450E+ 1
                DENSITY (G/CM3)= 1.723E+00
                MASS FLUX(G/SEC)= 1.520E+02
                JET VELOCITY(CM/SEC)= 2.400E+03
                JET ANGLE(RAD.)= 6.807E-01
                TEMPERATURE(K)= 4.000E+02
                SURFACE TENSION(DYNE/CM)= 2.840E+02
                VISCOSITY(GM/CM-SEC)= 2.200E-02
                ORIFICE DIAMETER(CM)= 5.100E-02
                LIQUID DROP COEFFICIENTS
                     AK= 6.120E+02
                     BK= 2.440E-02

NPS=   11   NSL=    7   NDS=    3   IBUG=    -   NSO=    3

INITIAL S=  0.000     S INCREMENT= 1.000E-02   FINAL S= 1.000E+02   PRINT INCREMENT= 2.000E+00
.300E+00  .200E+00  .111E+00  .333E+00  .620E+01

   C1= 1.100E-02  C2= 1.300E-03  C5= 3.000E-01  C6= 3.000E-10  C7= 1.000E-10  C8= 2.300E-10  FF3= 1.000E+00  FF4= 1.000E+00
  N1= 1.500E+00  N2= 1.500E+00  N5= 2.000E+00  N8= 1.500E+00  B6= 8.000E+04  B7= 3.000E+04  B8= 5.400E+04

 J     Y          PE          TE          UE      FE(I) (MOLE/GM)=
 2    .11  7.901E+03  1.510E+03  1.000E+05  3.920E-08  3.920E-08  1.450E-02  1.          3.000E-02  4.800E-08  1.230E-02  4.400E-07
 3    .69  8.357E+03  3.410E+03  3.950E+05  2.922E-06  2.922E-06  1.450E-02  1.          2.400E-02  2.700E-08  1.530E-02  8.300E-06
 4   1.14  8.357E+03  3.810E+03  4.510E+05  5.264E-06  5.264E-06  1.450E-02  1.          2.030E-02  2.300E-07  1.720E-02  4.700E-05
 5   1.47  8.357E+03  4.500E+03  5.010E+05  7.927E-06  7.927E-06  1.450E-02  1.          1.550E-02  2.200E-06  1.950E-02  1.900E-04
 6   3.12  7.901E+03  5.320E+03  5.800E+05  1.084E-05  1.084E-05  1.290E-02  1.          5.400E-03  9.900E-06  2.380E-02  1.900E-03
 7   4.86  1.246E+04  5.825E+03  6.380E+05  7.958E-07  7.958E-07  6.440E-03  1.          2.300E-04  3.600E-03  2.560E-02  1.300E-03
AV=  3.00  9.651E+03  5.010E+03  5.046E+05  5.372E-06  5.372E-06  1.101E-02  1.          8.257E-03  1.317E-03  2.259E-02  1.127E-03

    I       WA          HE          HSE         REUE        REUE2       REUEHSE       RUF1E       RUF2E       RUF3E
            RUF4E       RUF5E       RUF6E       RUF7E       RUF8E
    1   2.257E+01   3.084E+03   6.128E+ 3   2.643E-01   1.334E+ 5   1.622E+03   1.424E-06   1.42.E- 6   2.910E-03
        .           2.183E-03   3.482E-04   5.968E-03   2.973E-

 J     Y          PE          TE          UE      FE(I) (MOLE/GM)=
 2    .15  6.453E+03  1.700E+03  1.000E+05  4.526E-08  4.526E-08  1.450E-02  1.          3.000E-02  4.8.0E-08  1.23 E- 2  4.4. E-07
 3    .63  8.586E+03  3.300E+03  4.010E+05  1.980E-06  1.980E-06  1.450E-02  1.          2.400E-02  2.700E-06  1.530E-02  8.300E-06
 4   1.21  8.686E+03  3.720E+03  4.610E+05  3.659E-06  3.659E-06  1.450E-02  1.          2.030E-02  2.300E-07  1.72 E- 2  4.7 E-05
 5   1.68  8.686E+03  4.210E+03  5.110E+05  5.214E-06  5.214E-06  1.440E-02  1.          1.550E-02  2.200E-06  1.950E-02  1.900E-04
 6   3.59  6.260E+03  5.025E+03  5.900E+05  7.659E-06  7.659E-06  1.320E-02  1.          5.400E-03  9.900E-06  2.380E-02  1.900E-03
 7   5.42  7.952E+03  5.225E+03  6.500E+05  4.782E- 7  4.782E-07  6.000E-03  1.          2.300E-04  3.600E-03  2.550E-02  1.300E-03
AV=  5.48  7.819E+03  4.630E+03  5.111E+05  3.530E-06  3.530E-06  1.106E-02  1.          8.342E-03  1.371E-03  2.244E-02  1.100E-03
```

I	WA	WE	WSE	REUE	REUE2	REUEWSI	RUF1E	RUF2E	RUF3E
	RUF4E	RUF5E	RUF6E	RUF7E	RUF8E				
2	2.295E+01	2.971E+03	6.091E+03	2.102E-01	1.074E+05	1.280E+13	7.419E-07	7.419E-07	2.324E-03
	..	1.753E-03	2.881E-04	4.724E-03	2.311E-04				

J	Y	PE	TE	UE	FE(I) (MOLE/GM)=					
2	.16	5.804E+03	1.775E+03	1.000E+05	4.971E-08	4.971E-08	1.450E-02	..	3.000E-02	4.830E-06	1.230E-02	4.400E-07
3	.53	5.906E+03	3.265E+03	4.030E+05	1.915E-06	1.915E-06	1.450E-02	..	2.400E-02	2.700E-06	1.530E-02	8.900E-06
4	1.33	5.906E+03	3.330E+03	4.660E+05	3.378E-06	3.378E-06	1.450E-02	..	2.030E-02	2.900E-07	1.720E-02	4.700E-05
5	1.80	5.906E+03	4.075E+03	5.160E+05	4.757E-06	4.757E-06	1.450E-02	..	1.550E-02	2.200E-06	1.950E-02	1.900E-04
6	3.45	5.863E+03	4.400E+03	5.930E+05	8.840E-06	8.840E-06	1.330E-02	..	5.400E-03	9.900E-05	2.380E-02	1.900E-03
7	5.05	6.706E+03	4.925E+03	6.540E+05	4.479E-07	4.479E-07	6.650E-03	..	2.300E-04	3.600E-03	2.650E-02	1.300E-03
4V=	11.54	6.144E+03	4.444E+03	5.121E+05	3.047E-06	3.047E-06	1.101E-02	..	8.452E-03	1.421E-03	2.262E-02	1.074E-03

I	WA	WE	WSE	REUE	REUE2	REUEWSI	RUF1E	RUF2E	RUF3E
	RUF4E	RUF5E	RUF6E	RUF7E	RUF8E				
3	2.253E+01	2.913E+03	6.011E+03	1.918E-01	9.822E+04	1.161E+13	5.845E-07	5.845E-07	2.113E-03
	..	1.621E-03	2.725E-04	4.301E-03	2.060E-04				

J	Y	PE	TE	UE	FE(I) (MOLE/GM)=					
2	.19	4.862E+03	1.810E+03	1.000E+05	5.714E-08	5.714E-08	1.450E-02	..	3.000E-02	4.800E-06	1.230E-02	4.400E-07
3	1.11	4.862E+03	3.200E+03	4.070E+05	1.729E-06	1.729E-06	1.450E-02	..	2.400E-02	2.700E-06	1.530E-02	8.900E-06
4	1.62	4.862E+03	3.535E+03	4.700E+05	2.876E-06	2.876E-06	1.450E-02	..	2.030E-02	2.900E-07	1.720E-02	4.700E-05
5	2.02	4.862E+03	3.975E+03	5.230E+05	4.009E-06	4.009E-06	1.450E-02	..	1.550E-02	2.200E-06	1.950E-02	1.900E-04
6	3.56	4.842E+03	4.710E+03	6.000E+05	8.814E-06	8.814E-06	1.350E-02	..	5.400E-03	9.900E-05	2.380E-02	1.900E-03
7	5.49	5.369E+03	4.900E+03	6.600E+05	3.982E-07	3.982E-07	6.730E-03	..	2.300E-04	3.600E-03	2.650E-02	1.300E-03
4V=	21.47	5.063E+03	4.198E+03	5.119E+05	2.435E-06	2.435E-06	1.100E-02	..	8.732E-03	1.474E-03	2.227E-02	1.028E-03

I	WA	WE	WSE	REUE	REUE2	REUEWSI	RUF1E	RUF2E	RUF3E
	RUF4E	RUF5E	RUF6E	RUF7E	RUF8E				
4	2.247E+01	2.870E+03	6.000E+03	1.668E-01	8.540E+04	1.001E+13	4.063E-07	4.063E-07	1.835E-03
	..	1.457E-03	2.459E-04	3.716E-03	1.715E-04				

J	Y	PE	TE	UE	FE(I) (MOLE/GM)=					
2	.21	4.214E+03	2.020E+03	3.900E+04	5.320E-08	5.320E-08	1.450E-02	..	3.000E-02	4.800E-06	1.230E-02	4.400E-07
3	1.29	4.133E+03	3.160E+03	4.080E+05	1.572E-06	1.572E-06	1.450E-02	..	2.400E-02	2.700E-06	1.530E-02	8.900E-06
4	1.87	4.133E+03	3.485E+03	4.700E+05	2.616E-06	2.616E-06	1.450E-02	..	2.030E-02	2.900E-07	1.720E-02	4.700E-05
5	2.18	4.133E+03	3.740E+03	5.250E+05	3.463E-06	3.463E-06	1.450E-02	..	1.550E-02	2.200E-06	1.950E-02	1.900E-04
6	3.68	4.214E+03	4.565E+03	6.150E+05	4.957E-06	4.957E-06	1.370E-02	..	5.400E-03	9.900E-05	2.380E-02	1.900E-03
7	5.29	4.538E+03	4.400E+03	6.650E+05	3.637E-07	3.637E-07	6.800E-03	..	2.300E-04	3.600E-03	2.650E-02	1.300E-03
4V=	31.79	4.322E+03	4.145E+03	5.167E+05	2.036E-06	2.036E-06	1.134E-02	..	8.940E-03	1.491E-03	2.216E-02	1.002E-03

I	WA	WE	WSE	REUE	REUE2	REUEWSI	RUF1E	RUF2E	RUF3E

	RUF4E	RUF5E	RUF6E	RUF7E	RUF8E				
5	2.240E+ 1	2.840E+ 3	5.960E+03	1.471E- 1	7.529E+04	8.750E+02	2.994E-07	2.994E-07	1.424E-03
	..	1.317E-03	2.192E-04	3.253E-03	1.473E-04				

J	Y	PE	TE	UE	FE(I) (MOLE/GM)=						
2	.24	3.748E+03	2.130E+03	9.700E+04	6.663E-08	6.663E-08	1.450E-02	..	3.000E-02	4.800E-08	1.230E-02	4.400E-07
3	1.36	3.596E+03	3.030E+03	4.030E+05	1.461E-06	1.461E-06	1.450E-02	..	2.400E-02	2.700E-08	1.530E-02	8.400E-06
4	1.80	3.596E+03	3.540E+03	4.650E+05	2.228E-06	2.228E-06	1.450E-02	..	2.030E-02	2.300E-07	1.720E-02	4.700E-05
5	2.03	3.596E+03	3.700E+03	4.220E+05	3.093E-06	3.093E-06	1.450E-02	..	1.950E-02	2.200E-06	1.950E-02	1.900E-04
6	3.00	3.748E+03	4.460E+03	6.080E+05	4.241E-06	4.241E-06	1.380E-02	..	5.400E-03	9.900E-05	2.380E-02	1.900E-03
7	5.45	3.951E+03	4.255E+03	6.680E+05	3.689E-07	3.689E-07	6.800E-03	..	2.300E-04	3.600E-03	2.660E-02	1.300E-03
AV=	41.92	3.782E+03	3.911E+03	5.063E+05	1.764E-06	1.764E-06	1.108E-02	..	9.184E-03	1.488E-03	2.204E-02	9.786E-04

I	WA	HE	HSE	REUE	REUE2	REUE4SE	RUF1E	RUF2E	RUF3E
	RUF4E	RUF5E	RUF6E	RUF7E	RUF8E				
6	2.234E+01	2.832E+03	5.893E+03	1.315E-01	6.659E+04	7.751E+02	2.321E-07	2.321E-07	1.457E-03
	..	1.208E-03	1.957E-04	2.899E-03	1.287E-04				

J	Y	PE	TE	UE	FE(I) (MOLE/GM)=						
2	.26	3.394E+03	2.225E+03	9.350E+04	5.696E-08	5.696E-08	1.450E-02	..	3.000E-02	4.800E-08	1.230E-02	4.400E-07
3	1.44	3.262E+03	3.115E+03	3.970E+05	1.201E-06	1.201E-06	1.450E-02	..	2.400E-02	2.700E-08	1.530E-02	8.900E-06
	1.90	3.262E+03	3.690E+03	4.630E+05	1.776E-06	1.776E-06	1.450E-02	..	2.030E-02	2.900E-07	1.720E-02	4.700E-05
5	2.44	3.262E+03	3.585E+03	5.180E+05	2.732E-06	2.732E-06	1.450E-02	..	1.950E-02	2.200E-06	1.950E-02	1.900E-04
6	3.91	3.404E+03	4.390E+03	6.110E+05	3.700E-06	3.700E-06	1.390E-02	..	5.400E-03	9.900E-05	2.380E-02	1.900E-03
7	5.02	3.545E+03	4.150E+03	6.710E+05	3.700E-07	3.700E-07	6.800E-03	..	2.300E-04	3.600E-03	2.660E-02	1.300E-03
AV=	52.04	3.415E+03	3.648E+03	5.026E+05	1.522E-06	1.522E-06	1.111E-02	..	9.338E-03	1.482E-03	2.197E-02	9.157E-04

I	WA	HE	HSE	REUE	REUE2	REUE4SE	RUF1E	RUF2E	RUF3E
	RUF4E	RUF5E	RUF6E	RUF7E	RUF8E				
7	2.229E+01	2.831E+03	5.848E+03	1.195E-01	6.609E+04	6.992E+02	1.820E-07	1.820E-07	1.329E-03
	..	1.116E-03	1.772E-04	2.626E-03	1.154E-04				

J	Y	PE	TE	UE	FE(I) (MOLE/GM)=						
2	.31	2.917E+03	2.365E+03	8.700E+04	5.046E-08	6.046E-08	1.450E-02	..	3.000E-02	4.800E-08	1.230E-02	4.400E-07
3	1.54	2.806E+03	3.110E+03	3.780E+05	1.219E-06	1.219E-06	1.450E-02	..	2.400E-02	2.700E-08	1.530E-02	8.400E-06
4	2.02	2.806E+03	3.715E+03	4.280E+05	1.784E-06	1.784E-06	1.450E-02	..	2.030E-02	2.300E-07	1.720E-02	4.700E-05
	2.30	2.806E+03	3.600E+03	4.980E+05	2.278E-06	2.278E-06	1.450E-02	..	1.950E-02	2.200E-06	1.950E-02	1.900E-04
6	4.19	2.988E+03	4.270E+03	6.150E+05	3.109E-06	3.109E-06	1.410E-02	..	5.400E-03	9.900E-05	2.380E-02	1.900E-03
7	5.07	3.169E+03	4.020E+03	6.740E+05	3.923E-07	3.923E-07	6.800E-03	..	2.300E-04	3.600E-03	2.660E-02	1.300E-03
AV=	72.29	2.952E+03	3.760E+03	4.911E+05	1.397E-06	1.397E-06	1.129E-02	..	9.621E-03	1.413E-03	2.181E-02	9.582E-04

I	WA	HE	HSE	REUE	REUE2	REUE4SE	RUF1E	RUF2E	RUF3E
	RUF4E	RUF5E	RUF6E	RUF7E	RUF8E				
8	2.218E+01	2.845E+03	5.726E+03	1.023E-01	5.650E+04	5.888E+02	1.436E-07	1.436E-07	1.161E-03
	..	9.694E-04	1.453E-04	2.243E-03	9.854E-05				

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J    Y      PE          TE          UE          FE(I) (MOLE/GM)=
2    .33  [illegible]  2.335E+03  [illegible]  [illegible]  5.063E-[illegible]  1.450E-02  ..        [illegible]  [illegible]  [illegible]  [illegible]
3   1.56  [illegible]  3.125E+03  3.59[illegible]E+[illegible]  [illegible]  1.079E-06  1.450E-02  ..        [illegible]  [illegible]  [illegible]  [illegible]
4   2.10  2.524E+[illegible]  3.370E+03  4.190E+0[illegible]  1.541E-06  1.541E-06  1.450E-02  ..        2.[illegible]3[illegible]E-02  [illegible]  1.722E-02  4.700E-0[illegible]
5   2.66  2.624E+0[illegible]  3.555E+03  4.670E+05  1.674E-06  1.674E- 6  1.450E-02  .        1.55[illegible]E- 2  [illegible]  1.95[illegible]E-02  1.96[illegible]E-0[illegible]
[illegible]    .33  2.536E+03  4.225E+03  6.170E+05  2.586E-06  2.586E-06  1.410E-02  0.        [illegible]  [illegible]  2.38[illegible]E-02  1.[illegible]E-03
7   6.39  2.637E+03  3.975E+03  6.750E+05  3.861E-07  3.861E-07  6.800E-03  0.        2.3[illegible]E-04  3.5[illegible]E-03  2.66[illegible]E-02  1.3[illegible]E-03
AV= 67.48  2.768E+03  3.[illegible]25E+03  4.64[illegible]E+0[illegible]  1.211E-06  1.211E-06  1.136E-02  0.        3.769E-03  1.38[illegible]E-03  2.174E-02  3.545E-04

 I      WA          HE          HSE         REUE        REUE2       REUEHSE     RUF1E       RUF2E       RUF3E
      RUF4E       RUF5E       RUF6E       RUF7E       RUF8E
 9   2.212E+01   2.8[illegible]E+03   5.5[illegible]E+03   9.578E-02   4.639E+04   5.419E+02   1.160E-07   1.160E-07   1.068E-03
     ..          9.357E-04   1.322E-04   2.062E-03   9.142E-05

J    Y      PE          TE          UE          FE(I) (MOLE/GM)=
2   [illegible]  2.534E+0[illegible]  2.265E+03  [illegible]  4.18[illegible]E-08  4.18[illegible]E-08  1.450E-02  0.        3.00[illegible]E-02  [illegible]  1.230E-02  4.400E-07
3   1.[illegible]2  2.583E+03  3.130E+03  3.390E+05  9.697E-07  9.697E-07  1.450E-02  0.        2.400E-02  2.7[illegible]E-08  1.533E-02  8.[illegible]00E-06
4   2.15  2.583E+03  3.33[illegible]E+03  4.[illegible]5[illegible]E+05  1.374E-06  1.374E-06  1.45[illegible]E-02  .        2.[illegible]3[illegible]E-02  3.900E-07  1.720E-02  4.[illegible]00E-0[illegible]
5   2.75  2.583E+03  3.390E+03  4.820E+05  1.591E-06  1.591E-06  1.450E-02  0.        1.550E-02  2.200E-06  1.950E-02  1.[illegible]E-04
6   4.48  2.765E+03  4.200E+03  6.190E+05  2.176E-06  2.176E-06  1.420E-02  .        5.4[illegible]E- 3  9.9[illegible]E-05  2.38[illegible]E-02  1.9[illegible]E-03
[illegible]  [illegible]  2.[illegible]5E+03  3.[illegible]E+03  [illegible]E+0[illegible]  3.889E-07  3.889E-07  6.800E-03  0.        2.300E-04  3.600E-03  2.550E-02  1.750E-03
AV=10[illegible]  2.697E+03  3.765E+03  4.783E+05  1.079E-06  1.079E-06  1.148E-02  0.        9.913E-03  1.332E-03  2.165E-02  9.524E-04

 I      WA          HE          HSE         REUE        REUE2       REUEHSE     RUF1E       RUF2E       RUF3E
      RUF4E       RUF5E       RUF6E       RUF7E       RUF8E
10   2.2[illegible]6E+01   2.873E+03   5.605E+03   9.239E-02   4.419E+04   5.179E+12   9.966E- 8   9.966E- 8   1.[illegible]61E- 3
     .           9.158E- 4   1.231E- 4   2.[illegible]1E-03   8.804E-0[illegible]

CONDITIONS IN FRONT OF SHOCK
PX= 3.661E+03  UX= 5.04[illegible]E+05  HSX= 6.128E+03  RHOX= 5.237E-07  TX= 5.010E+03  WAX= 2.257E+01
MASS FRACTIONS F(I)=  [illegible]612E-04  2.348E- 9  1.762E- 1  0.          1.155E- 1  4.215E-02  6.321E-01  3.361E-02  ..

CONDITIONS BEHIND SHOCK
PY= 1.182E+05  UY= 9.40[illegible]E+04  HY= 6.122E+03  RHOY= 2.811E-06  TY= 1.141E+04  TBPY= 3.555E+02

JET BREAK-UP INFORMATION
WE= 3.665E+0[illegible]  REJ= 8.417E+00  TBK= 2.692E-03  UBK= 2.532E+03  XBK= 5.442E+0[illegible]  YBK= 4.650E+00
WEL= [illegible]       D3L= 0.          D32= 5.332E-03  DMAX= 0.

---------  MODIFIED FREE STREAM CONDITIONS IN SHOCK FRONT BY SINGLE ITERATION -----

 J          PE          TE          UE       FE(I) (MOLE/GM)=
AV= [illegible]  3.661E+03  5.010E+03  5.043E+05  5.395E-06  5.395E- 6  1.1[illegible]6E-02  .        9.292E- 3  1.[illegible]E-0[illegible]  2.267E- 2  [illegible]

 I      WA          HE          HSE         REUE        REUE2       REUEHSE     RUF1E       RUF2E       RUF3E
      RUF4E       RUF5E       RUF6E       RUF7E       RUF8E
 1   2.24[illegible]E+01   3.393E+ 3   6.141E+ 3   2.632E- 1   1.329E+05   [illegible]   1.442E-05   1.442E-05   3.91[illegible]E-03
     ..          2.183E-03   3.482E-04   [illegible]E-03   2.979E-0[illegible]
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 CONDITIONS IN FRONT OF SHOCK
PX= 9.661E+03  UX= 5.043E+05  HSX= 6.141E+03  RHOX= 5.215E-07  TX= 5.010E+.3  WAX= 2.245E+ 1
MASS FRACTIONS F(I)=   1.619E-04   2.96.E- 9   1.769E-01   0.          1.1.1E-01   4.233E-02   5.3.8E-.1   3.395E-.2   0.

 CONDITIONS BEHIND SHOCK
PY= 1.178E+05  UY= 9.411E+04  HY= 6..95E+.3  RHOY= 2.797E-.6  TY= 1.14.E+.4  TRPY= 3.554E+ 2

 JET BREAK-UP INFORMATION
WE= 3.853E+00  REJ= 8.417E+00  TBK= 2.693E-03  UBK= 2.529E+03  XBK= 5.43.E+.1  YBK= 4.85.E+.4
WEL= ..          D3 = ..          D32= 5.332E-.3  DMAX= ..

INITIAL FLOW RATE(G/SEC)
XMV= 2.920E-01  XML= 1.517E+02  XMA= 4.441E+00  XMM= 4.733E+00  AE= 1.687E+01

------  CONDITIONS OF THE INTIAL MIXTURE AT S=      . 391
U= 1.364E+05  HSV= 1.069E+.2  HSK= 5.759E+03  H= 5.469E+03  TSH= 1.119E+04  T= 1.075E+04  RHO= 2.625E-.5  A= 1.134E+01
MASS FRACTIONS OF SPECIES
WO+= 1.519E-04  E-= 2.778E-.9  J= 1.66.E-.1  F-= ..          N= 1..69E- 1  O2= 3.372E-.2  N2= 5.956E-.1  WO= 3.186E-.2  FV= 6.17.E-.2

P= 9.815E+04   WM= 2.394E+01   RHO= 2.625E-06   HS= 5.756E+03   FV= 6.17.E-02   UP= 2.529E+03  VP= 1.365E+.3
TP= 3.554E+02   RP= 2.656E-03   SE= 2.210E+00   YE= 4.86.E+.0

  INITIAL THERMODYNAMIC INFORMATION
GAMA= 1.150   CP(CAL/G)= 6.365E-01  SS= 2.074E+05  MA= 7.636E-01  MAP= 7.51.E-01  REP= 8.781E-01
```

```
******** J1L3 RAM C-III  200KFT FREON-E-3 (CASE 6-TLO=360)**** 12/13/73 C


 S(CM)=   5.4336
T(K)=1739.16 P(DYNE/CM2)= 9.815E+04 RHO(GM/ML)= 2.033E-06 U(CM/SEC)= 1.591E+05 HS(CAL/GM)= 5.756E+03 FV= 6.369E-02 WM= 2.345E+01
 A= 1.146E+01  UP= 2.529E+03  TP= 3.554E+02  RP= 2.666E-03  RHOP= 5.269E-03  AE= 1.687E+01  TSR= 1.119E+04  H= 5.458E+03

 MASS FRACTIONS OF SPECIES
NO+= 1.916E-04 E-= 2.773E-09 O= 1.656E-01 F-= 7.001E-09 N= 1.687E-01 O2= 3.953E-02 N2= 5.944E-01 NO= 3.179E-02
  ----   ELECTRON DENSITY= 8.024E+12
    .3 6E-3    .5 6E-.3    .1.4E-.1   3.          .778E-.2    .124E-02    .213E-01    .10.E-02

 CHANGES OF MASS FRACTION OVER DS= 2.822E-05
    -2.720E-07  -5.192E-12  -3.507E-04   7.001E-09  -2.301E-04  -8.366E-05  -1.258E-03  -6.730E-05   1.982E-03
DP= -.153E+00  DRHO=  .368E-08  DU= -.331E+03  DHS= -.120E+02  DFV=  .198E-02  PHADS=  .1..E- 1
DA= 1.29 E-02  DAE= 1.951E-04  DUP= 1.551E-01  DRP=- .858E-06  QP= 1.312E+02  PHIV= 3.113E+01
DFP= 2.353E+.1  DQ= 1.616E-09

 PRODUCTION RATES FOR EACH REACTION (MOL/SEC-CM3)
   1. 49E-.6   ..          1.789E-.3   3.          3.4.2E-.8   3.          3.          +.230E-.1

 PRODUCTION RATES FOR EACH SPECIE
   2.396E-05   1.852E-.3  -2.396E-05   5.442E-.6  -2.396E-05

  LOCAL   THERMODYNAMIC INFORMATION
GAMA=3 1.153   CP(CAL/G)= 6.345E-01  SS= 2.371E+05  MA= 7.647E-01  MAP= 7.514E-01  REP= 8.761E-01  #P/SEC= 1.1.3E+19
    .2.2E-04    .35.E+.     .221E+.1    .486E+ 1    .187E+ 4    .192E+13    .333E+.3    .177E+22    .1 7E+.1    .380-218


 S(CM)=   5.4436
T(K)= 3579.12 P(DYNE/CM2)= 9.812E+04 RHO(GM/ML)= 4.6.2E-.6 U(CM/SEC)= 1.118E+ 5 HS(CAL/GM)= 4..8.E+ 3 FV= 3.4.4E- 1 WM= 3.345E+01
 A= 1.31.E+01  UP= 2..53E+.3  TP= 3..54E+02  RP= 2.654E-03  RHOP= 4.461E-03  AE= 1.691E+01  TSR= 3.931E+03  H= 3.931E+03

 MASS FRACTIONS OF SPECIES
NO+= 1.114E-04 E-= 1.741E-.9 O= 1.167E-01 F-= 1..25E-.5 N= 7.657E-.2 O2= 2.732E-02 N2= 4.187E-.1 NO= 2.239E-.2
  ----   ELECTRON DENSITY= 8.825E+12
    .372E-05    .319E-.3    .730E-02    .534E-.6    .548E-02    .874E-03    .150E-01    .748E-03

 CHANGES OF MASS FRACTION OVER DS= 3.37.E-05
    -1.571E- 7  -6.185E-12  -1.732E-04   1.146E-07  -1.136E-.4  -4.143E-.5  -6.213E-.4  -3.324E-.6   3.7.6E-.4
DP= -.21 E+.0  DRHO=  .118E-07  DU= -.163E+.3  DHS= -.593E+.1  DFV=  .979E-03  PHADS=  .100E-01
DA= 3.113E-03  DAE= 2.175E-04  DUP= 1.845E-01  DRP=-5.909E-.6  QP= 9.530E+.1  PHIV= 1.923E+01
DFP= 2.762E+.1  DQ= 2.246E-09

 PRODUCTION RATES FOR EACH REACTION (MOL/SEC-CM3)
   2..76E-.5   3.163E-.4   1.597E-.5   1.941E-.5   9.025E-05   5.592E-07   8.526E-07   2.185E-.5

 PRODUCTION RATES FOR EACH SPECIE
   3.748E- 6  -8.5.4E-.3  -+.601E-.6   8.873E-.3  -3.799E-.5

  LOCAL   THERMODYNAMIC INFORMATION
GAMA=3 1.169   CP(CAL/G)= 4.102E-01  SS= 1.579E+05  MA= 7.331E-01  MAP= 5.331E-01  REP= 1.204E+.0  #P/SEC= 1.1 3E+ 9
    .397E-.4    .345E+      .221E+.1    .485E+01    .187E+04    .192E+13    .333E+.3    .177E+22    .1 7E+.1    .380-218


 S(CM)=   5.4543
T(K)= 3.81.94 P(DYNE/CM2)= 9.807E+04 RHO(GM/ML)= 7.3.5E-.6 U(CM/SEC)= 8.681E+ 4 HS(CAL/GM)= 3.173E+ 3 FV= 4.913E- 1 WM= 4.261E+01
 A= 1.3 9E+.1  UP= 2.6.2E+.3  TP= 3..54E+02  RP= 2.642E-03  RHOP= 4.118E-03  AE= 1.696E+01  TSR= 7.126E+03  H= 3.193E+03

 MASS FRACTIONS OF SPECIES
NO+= 3.917E-05 E-= 3.8.1E-10 O= 9.016E- 2 F-= 4..76E-.5 N= 5.917E-.2 O2= 2.153E-02 N2= 3.235E- 1 NO= 1.73.E-02
  ----   ELECTRON DENSITY= 3.369E+12
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```
*DECK,MAIN
      PROGRAM J108(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE,)
C     ----- THIS DECK FOR CDC USE -----
C     ----- 12/18/73 -----
C*****************************************************************
C
C     ONE DIMENSIONAL REACTING DROPLET-VAPOR-AIR TUBE ANALYSIS
C          A SELF-INITIALIED REACTING DVA TUBE  (6/8/73)
C
C******* MODIFIED TUBE PRESSURE (8/30/73)
C********* ITERATED SHOCK FRONT CONDITIONS (9/13/73)
C*****************************************************************
       COMMON CPA(40),CPV(40),WA(40),RHOF(40),PSIV(40),HSE(40),UE(40),
      1 S(40),T(40),PTB(40)
      2 ,RUE(40),RU2E(40),RUHSE(40),Y(40),RUF5E(20)
      3 ,SD,DS,SMAX,RHO,FV,U,T,HS,ATO   ,P,RP,CSP,CTE,RR1,RR2,AV,C,AI,YE
      4 ,WM,SE,AE,RPO,TP,RHOP,EP,DEP,CAE,DTS,TS,DRP,DRHOP,DSE,DYE,DT,DHS
      5 ,DU,DUP,DFV,DRHO,UP,DA,ADS,ARHOP,UM,SI,SXO,BETA
      6 ,RUAI,RUEI,RUF1EI,RUF2EI,RUF3EI,RUF4EI,RUF5EI,PHATS
       COMMON RUF4E(20),D32(20),WDOT(8),RKI(8),WDOTN(5),UL(20),RUF1E(20),
      1 RUF2E(20),RUF3E(20),FQI, FE(8,20),PE(20),TE(20)
      2,       F(9),DF(9),D32I,D32II,XMLI,XMOU,EFA,ALD,ALT,DE,VLI,THETA
      3 ,F1,F2,F3,F4,F5,PI,AI1,BB,XNF5,CF5,UF,VP,GAMA,C1,C2,C3,C4,C5,C6,
      4 C7,C8 ,GP,A,RP ,XMA,XMAP,SS,UR,DUR,HSR,DHSR,XMLO
      5 ,RUF6E(20),RUF7E(20),RUF8E(20)
      6 ,RUF6EI,RUF7EI,RUF8EI,F6,F7,F8 ,F9 ,FFPE,FFTE,FFAE
      7 ,FFF,FFEV ,CF1,CF2,CF5,CF6,CF7,XNF1,XNF2,XNF5,B6,B7,FF3,FF4,XNPT
      8,XBK,YBK,TBK,PEBK,RU2BK,RHOXY,SOP,NSO,NWOR,DEOP,S150
       COMMON STB(30),TTB(30),RHOTB(30),UTB(30),FTB(8,30)
       COMMON /HEAT/ XL(6,9),WI(9)
       COMMON/LIQUID/ CPL,TBP,DHV,RHOL,WV,TCPC,SIG,TLO,UML,DO,HECR,
      1 FFVI,AK,BK,WE,ITBK,FFV,TAPY
       COMMON/INTEG/NPS,NPT,IDD(20),NSL,IOPT,KU,NS,NS1,IBUG,ID
       COMMON /SHOCK/ YO(20),PTBO(20),UTBO(20),TTBO(20),F1TBO(20),
      1               F2TBO(20),F3TBO(20),F4TBO(20),F5TBO(20),F6TBO(20),
      2               F7TBO(20),F8TBO(20)
       REWIND +
 1000  CONTINUE
       READ (5,100) (IDD(I),I=1,20)
       IF( EOF(5) )  90, 3
    3  CONTINUE
       WRITE(6,99)
       WRITE(6,100) (IDD(I),I=1,20)
       READ (5,102) FFAE,FFPE,FFEV,FFF,PRXL
       WRITE(6,102) FFAE,FFPE,FFEV,FFF,PRXL
C*****   CONSTANTS
       PI=3.14159
       SQIPI= SQRT(PI)
       AV=6.02E23
       RR=82.05
       RR1= 1.987
       RR2= 8.313E7
       CTE= 4.186E7
       AIO=1.013E6
       DO 6 I=1,9
```

```
      DF(I)=0.0
      IOK=0
      XOK=0.0
    6 CONTINUE
      DFV=0.0
      DFQ=0.0
      DU=0.0
      DP=0.0
      DRHO=0.0
      DT=0.0
      DHS=0.0
      DIS=0.0
      DRHOP=0.0
      DUP=0.0
      DRP=0.0
      DEP=0.0
      DA=0.0
      DSE=0.0
      DVE=0.0
      DAE=0.0
      DO 27 I=1,8
      WDOT(I)=0.0
   27 CONTINUE
      ETA=1.0
C***   RR IN CM3-ATM/G-MOLE-K
      CALL PUTIN
      YPEN=YE
      SEQ=SE
      EP= CPL*TP
      HPS= EP+.5*UP*UP/(2.0*GTE)
      DS1=DS
      DSMAX=5.0*DS
      DSMIN=DS/10.0
      WRITE(6,39)
      WRITE(6,100) (IDD(I),I=1,20)
      IPS=DSP/DS
      IS=-1
    1 CONTINUE
      DS=DS1
      AXX1=((U-UP)**2+VP**2)
      UR = SQRT(AXX1)
      HSR=HS-(.5*(U-UR*UR )/(2.0*GTE)
      TI=TS
      CALL TIN(HSR,TS ,TI,P,WS1,CPSR)
      RHOP=0.0
      XNP=0.0
      IF (RP..T.1.0E-9) GO TO 40
      RHOP= (XMLI*RHO*P*(WS1)*U*A)/(UP*A)
      XNP= 3.0*RHOP*UP*A/(4.0*PI*RP*RP*RP*RHOL)
      XX1=RHO*CHV*0.5
      XX2=ALO*UR*(TS-TP)
      V= SQRT(3.0*P/RHO)
C****** V IS MEAN THERMAL VELOCITY OF MIXTURE BY KINETIC THEORY
      XX3=1.0+ALI*V*(T-TP)/XX2
      DP=0.5*XX2*P*XX3/T/GTE *PPEV
```

```
      DDOT=-QP/XX1
      PHIV=-1.5*RHOP*DDOT/RP
      IF (PHIV.GT. 1.0E-6)  DS=DS1/(PHIV*A)
      IF ((IS.LT.16).AND.(DS.GT.DSMIN)) DS=DSMIN
      IF (DS.GT.DSMAX) DS=DSMAX
   40 CONTINUE
      SI=SI+DS
      IF((SI.GT. S(NPS)).OR.(SI.LT.S(1))) GO TO 999
      DO 21 ID=2,NPS
      IF (SI.GE.S(ID-1) .AND. SI.LT.S(ID)) GO TO 22
   21 CONTINUE
      WRITE(6,200)ID,S(ID),SI
      STOP
  200 FORMAT (1H ,*     OUT OF RANGE     ID=*,I5, *  S=*,2F9.3/)
   22 CONTINUE
      CALL LIPLN(SI,RUE ,S,RUEI ,ID)
      CALL LIPLN(SI,RUPE,S,RUPEI,ID)
      CALL LIPLN(SI,RUMSE,S,RUMSEI,ID)
      CALL LIPLN(SI,RUF1E,S,RUF1EI,ID)
      CALL LIPLN(SI,RUF2E,S,RUF2EI,ID)
      CALL LIPLN(SI,RUF3E,S,RUF3EI,ID)
      CALL LIPLN(SI,RUF4E,S,RUF4EI,ID)
      CALL LIPLN(SI,RUF5E,S,RUF5EI,ID)
      CALL LIPLN(SI,RUF6E,S,RUF6EI,ID)
      CALL LIPLN(SI,RUF7E,S,RUF7EI,ID)
      CALL LIPLN(SI,RUF8E,S,RUF8EI,ID)
      CALL LIPLN(SI,PTS,S,PEI ,ID)
      XXXX=(SI-XPK)/PRXL
      IF(XXXX.GT.40.0) XXXX=40.0
      P1= PEI +RUPEI*(1.0-PHUX)* EXP(-XXXX)
      P1=P1*FFPE
      IF (IBUG .NE. 0) WRITE(6,101) RUEI,RUPEI,RUMSEI,RUF1EI,RUF2EI,
     1 RUF3EI,RUF4EI,RUF5EI,RUF6EI,RUF7EI,RUF8EI,P1
      DP=P1-P
      ADS=A*DS
      SP = SE
      SE = SOP + S150*((SI/(150.*DEQP))**AI)
      IF(SI.LE.(70.*DEQP))  SE=SOP+S150*((70./150.)**AI)*SI/(70.*DEQP)
      YPEN=YPEN+VP/UP*DS
      YE = YPEN+(SE-SP)
      SE = FFBE*SE
      DAE= 0.5*PI*SE*YE +AE
      IF(IBUG.NE.0) WRITE(6,103) AE,SE,YE,YPEN,C,AI,SI,DAE
      SQGAM= SQRT(GAMA)
      XMAP=XMA* UR/U
C**********     VISCOSITY FOR AIR IN (G/CM-SEC) BY SUTHERLAND LAW
      UM=1.71E-5*(T**1.5)/(T+110)
      REP=RHO* UR*RP/UM
      PHADS=0.0
      DFP=0.0
      DRP=0.0
      DQ=0.0
      IF(RP.LT. 1.0E-9 ) GO TO 7
C        CALCULATE DRAG COEFFICIENT
      CDD=24./REP
```

```
                CDI=0.44
                CDB=1.0
                CD=CDI
                RMR=XMA**2/REP
  170           XKM=1.25 * SQRT(RMR
                IF (XKN .GT. 2.00) GO TO 4
                IF (XKN .LT. 1.E-5) GO TO 5
                XX1=XKN**0.5
                XX2= EXP(1.2* X**0.5)
  175           GKN=XX1*XX2/(1.0+XX1*XX2)
                XX3=XKN**0.7
                XX4= EXP(XKN)
                DRE=1.0- EXP(-XX3*XX4*(CDO-.48)*REP/5.)
                CDB=GKN*DRE
  180         4 CONTINUE
                S1= SQRT(0.5*GAM4)*XMAP
                S2=S1*S1
                S3=S2*S1
                S4=S3*S1
  185           S32=S2*2.5
                SQ=S1* SQRT(T/TP)
                CDFM=  EXP(-S32)*((4.+2.0*S2)/SQTPI/S3
               1      +(4.0*(S4+S2)-1.3)/2.0/S4* ERF(S1)
               2    +0.657*SQTPI/SQ
  190           CD=CDB*(CDFM-CDI)+CDI
               5 FP=CD/2.*RHO*FFF
                 DFP=4.5*RHOP*FP*U4 *(U-UP)*ADS/RHOL/PF/P2
                 DRP=0.5*DCDT*DS/UP
                 DQ=3.0*RHOF*DP*ADS*DS/(P3*RHOL*UP)
  195            IF (IBUG.NE.0) WRITE(6,101) XKN,GKN,DRE,CDFM,CD,FF,S1,S2
                 PHADS=PHIV*ADS
               7 CONTINUE
                 RU8=RHO**4
                 RU4I=1.0/RU4
  200            RU4P=RHOP**4
                 DUP=0.0
                 IF (FFV.EQ.1.0) GO TO 50
                 DUP = DFP / RU4P
              50 IF (IBUG.NE.0)
                1WRITE(6,101) RU4I,UP,U,PHADS,RU2EI,RUFI,DAE,A,UP,DFP
                 DU=RU4I*((UP-U)*PHADS+(RU2EI-RUEI*U)*DAE-A*DP-DFP+(PEI-PI)*DAE)
                 DHPS= EP*(UP+0.5*A*(UP+DUP)*(2.0*DTE) -HPS
                 DHS=RU4I*((HPS-HS)*PHADS+(RUHSEI-RUEI*HS)*DAE-RU4P*DHPS)
                 DF(NS1)= RU4I*((1.0-F(NS1))*PHADS-F(NS1)*RUEI*DAE)
  210            CALL DHSIF
                 CALCULATING DFI
                 HS=HS+DHS
                 HSHS=(U*U)*(U*U)/(2.0*GTE)
                 DO 30 I=1,NS1
  215           30 F(I)=F(I)+DF(I)
                 TI=T
                 IF (IBUG.NE.0)
                1WRITE(6,101) DP,DU,DHS,DF(NS1),DETA,DUP,HS,H,DS
                 CALL  TEMP(H,T,TI,F,NS1,DF)
  220            WM=0.0
```

```
          DO 29 I=1,NS1
          WM=WM+F(I)/WI(I)
       29 CONTINUE
          WM=1.0/WM
C          CALCULATE LOCAL SPECIFIC HEAT
          GAMA=CP/(CP-RR1/WM)
C            LOCAL SPEED OF SOUND
          SS=  SQRT(GAMA*RR2*T/WM)
C           LOCAL MACH NUMBER
          XMA=U/SS
          DRHO=P1*WM/RR2/T-RHO
C         DA=(PHADS+RUEI*DAE-A*U*DRHO-A*RHO*DU)/(RHO*U)
          DA=(PHADS+RUEI*DAE+RUA)/((RHO+DRHO)*(U+DU)) -A
          AE=AE+DAE
          RP=RP+DRP
          IF (RP.LT.0.0) RP=0.0
          UP=UP+DUP
          U=U+DU
          HPS=HPS+DHPS
          RHO=RHO+DRHO
          A=A+DA
          P=P1
          IS=IS+1
          IF ((SI+DS) .GT. SMAX ) GO TO 9
          IF(((IS/IPS)*IPS).NE. IS) GO TO 2
        9 CONTINUE
          EDEN= RHO*AV*F2
C   CALCULATING PRODUCTION RATES
          WDOT(1)= ARHO2*RKI(1)*F1*F2
          WDOT(2)= ARHO2*RKI(2)*F1*F4
          WDOT(3)= RHO*RKI(3)*F1
          WDOT(4)= RHO*RKI(4)*F1
          WDOT(5)=ARHO2*RKI(5)*FOI*F2
          WDOT(6)= ARHO2*RKI(6)*F4/WM
          WDOT(7)= ARHO2*RKI(7)*F3*F4
          WDOT(8)= ARHO2*RKI(8)*F3*F5
          WDOTN(1)=-(WDOT(1)+WDOT(2)+WDOT(3)+WDOT(4))+WDOT(8)
          WDOTN(2)=-(WDOT(1)+WDOT(3)+WDOT(5)-WDOT(6)-WDOT(7))+WDOT(8)
          WDOTN(3)= WDOT(1)+WDOT(2)+WDOT(3)+WDOT(4)-WDOT(7)-WDOT(8)
          WDOTN(4)=-(WDOT(2)+WDOT(4)-WDOT(5)+WDOT(6)+WDOT(7))
          WDOTN(5)= WDOT(1)+WDOT(3)-WDOT(8)
          WRITE(6,103) SI,T,P,RHO,U,HS,F(NS1),WM
          WRITE (6,110) A,UP,TP,RP,RHOP,AE,TS,H
          WRITE(6,105) (F(I),I=1,5),EDEN
          WRITE(4,400)  SI, T, P, U, F(1), F(2), EDEN
      400 FORMAT(2F11.4,1P,5E10.3)
          WRITE(6,101) F1,F2,F3,F4,F5,F6,F7,F8
          WRITE(6,108) DS,(DF(I),I=1,NS1)
          WRITE(6,104)         UP,DRHO,DU,DHS,DF(NS1),PHADS
          WRITE(6,111) DA,DAE,DUP     ,DRP,DP,PHIV,DFF,DQ
          WRITE(6,106) (WDOT(I),I=1,8)
          WRITE(6,107) (WDOTN(I),I=1,5)
          WRITE(6,118) GAMA,CP,SS,XMA ,XMAP,REP,XNP
          WRITE(6,101) DS,ETA,SE,FC,VP,G,PI,SXD ,ALFA
         1,BETA1
```

```
            IF ((SI+DS) .GT. SMAX ) GO TO 999
          2 CONTINUE
            GO TO 1
           91 WRITE(6,105)
260        999 CONTINUE
            GO TO 1000
           99 FORMAT(1H1)
          100 FORMAT(2I4)
          101 FORMAT (2X,10E10.3)
285       102 FORMAT (8E10.3)
          103 FORMAT(///*  S(CM)=*,F8.4/1X,*T(K)=*,F8.2,1X,*P(DYNE/CM2)=*,1PE10.3
            1,1X,*RHO(GM/ML)=*,E10.3,1X,*U(CM/SEC)=*,E10.3,1X,*MS(CAL/GM)=*,E10
            2.3,1X,*F=*,E10.3,1X,*M=*,E10.3)
          104 FORMAT(                    2X,*DP=*,E10.3,2X,*DRHO=*,E10.3,2X,*DU=*,
290         1E10.3,2X,*DMS=*,E10.3,2X,*DPV=*,E10.3,2X,*PHADS=*,E10.3)
          105 FORMAT(2X,*MASS FRACTIONS OF SPECIES*/1X,*NO=*,1PE10.3,1X,*E-=*
            1,E10.3,1X,*O=*,E10.3,1X,*F-=*,E10.3,1X,*N=*,E10.3,1X,*O2=*,E10.3,1
            2X,*NO=*,E10.3,1X,*NO=*,E10.3/*  ----  ELECTRON DENSITY=*,E10.3)
          106 FORMAT(2X,*PRODUCTION RATES FOR EACH REACTION (MOL/SEC-CM3)*/2X,1P
295         11E12.3)
          107 FORMAT(/2X,*PRODUCTION RATES FOR EACH SPECIE*,/2X,1P8E12.3)
          108 FORMAT(/*  CHANGES OF MASS FRACTION OVER DS=*,1PE10.3/4X,1P10E12.3
            1)
          109 FORMAT(1X ,*------ REACHING THE LOCAL SONIC SPEED -------*)
          110 FORMAT (2X,*A=*,E10.3,2X,*UP=*,E10.3,2X,*TP=*,E10.3,2X,*RO=*,
            *  E10.3,2X,*RHOF=*,E10.3,2X,*SE=*,E10.3,2X,*TSK=*,E10.3,2X,*M=*,
            3E10.3/)
          111 FORMAT(2X,*DA=*,1PE10.3,2X,*DAE=*,E10.3 ,2X,*DUP=*
            1, E10.3,2X,*DRP=*,E10.3,2X,*DP=*,E10.3,2X,*PHIV=*,E10.3/ 2X,*DFP=*
            2,E10.3,2X,*DV=*,E10.3/)
          112 FORMAT(/2X, *  LOCAL   THERMODYNAMIC INFORMATION */ 2X,*GAMA=*
            1 F8.3,2X,* CP(CAL/G)=*,1PE10.3,2X,*SS=*,E10.3,2X,*MA=*,E10.3,2X,
            1*MAP=*,E10.3,2X,*RLP=*,E10.3,2X,*RP/SEC=*,E10.3)
           90 REWIND 4
          310 STOP
              END
```

07 3

```
*DECK,PUTIN
      SUBROUTINE PUTIN
      DIMENSION DD(6),Y8(20)
      COMMON CPA(40),CPV(40),WA(40),RHOE(40),PSIV(40),HSE(40),UE(40),
     1 S(40),T3(40),PT3(40)
     2 ,RUE(40),RU2E(40),RUHSE(40),Y(40),RUF5E(20)
     3 ,SO,DS,SMAX,RHO,FV,U,T,HS,ATO   ,P,PP,CSP,CTE,RR1,RR2,AV,C,AI,YE
     4 ,WM,SE,AE,RPO,TP,RHOP,EP,DEP,CAE,DTS,TS,DRP,DRHOP,DSE,DYE,DT,DHS
     5 ,DU,DUP,DFV,DRHO,DP,DA,ADS,ARHO2,UM,SI,SXO,BETA
     6 ,RUAI,RUEI,RUF1EI,RUF2EI,RUF3EI,RUF4EI,RUF5EI,PHADS
      COMMON RUF4E(20),D32(20),WDOT(8),RKI(8),WDCTN(5),UL(20),RUF1E(20),
     1 RUF2E(20),RUF3E(20),FOI, FE(8,20),PE(20),TE(20)
     2,       F(9),DF(9),D32I,D32II,XMLI,XMDO,ETA,ALO,ALT,DE,VLI,THETA
     3 ,F1,F2,F3,F4,F5,PI,AI1,38,XNF8,CF8,UF,VP,GAMA,C1,C2,C3,C4,C5,C6,
     4 C7,C8 ,CP,A,RP ,XMA,XMAP,SS,UF,DUR,HSR,DHSR,XML0
     5 ,RUF6E(20),RUF7E(20),RUF8E(20)
     6 ,RUF6EI,RUF7EI,RUF8EI,F6,F7,F8 ,F9 ,FFPC,FFIE,FFAE
     7 ,FFF,FFCV ,CF1,CF2,CF5,CF6,CF7,XNF1,XNF2,XNF5,36,B7,FF3,FF4,XNPT
     8,XBK,YBK,TBK,RBK,RU2BK,RHOXY,SOP,NSO,NWCR,DEQP,T150
      COMMON ST3(30),TT3(30),RHOT3(30),UT3(30),FT3(8,30)
      COMMON /HEAT/ XL(6,9),WI(9)
      COMMON/LIQUID/ CPL,TBP,DHV,RHOL,WV,TBPO,SIG,TLO,UML,DO,WECR,
     1 FFVI,AK,BK,WE,ITBK,FFV,TBPY
      COMMON/INTEG/NPS,NPT,IDD(20),NSL,IOPT,KO,NS,NS1,IBUG,IB
      COMMON /SHOCK/ Y0(20),PT30(20),UTP0(20),TT30(20),F1T30(20),
     1              F2T30(20),F3T30(20),F4T30(20),F5T30(20),F6T30(20),
     2              F7T30(20),F8T30(20)
      READ(5,100) WV,CPL,TBPO,DHV,RHOL,XMLI,VLI,THETA
     1 ,TLO,SIG,UML,DO
      THETA=THETA*PI/180.
      VP=VLI* COS(THETA)
      WRITE(6,116)WV,CPL,TBPO,DHV,RHOL,XMLI,VLI,THETA
     1 ,TLO,SIG,UML,DO
      READ(5,101) NPS,NSL,NOS,IBUG,NSO,NWCR
      WRITE(6,107) NPS,NSL,NOS,IBUG,NSO,NWCR
      NS=8
      NS1=NS+1
      WI(NS1)=WV
      READ(5,110) SO,DS,SMAX,DSP
      WRITE(6,108) SO,DS,SMAX,DSP
      READ (5,100) ALO,ALT,SOP,AI,WECR
      WRITE(6,100) ALO,ALT,SOP,AI,WECR
      AI1=AI- 1.0
      XNOS=NOS
      DE= SQRT(XNOS) *DO
      XNSO = NSO
      DEQP = SQRT(XNSO) * DO
      READ (5,100) CF1,CF2,CF5,CF6,CF7,CF8,FF3,FF4
      WRITE(6,109) CF1,CF2,CF5,CF6,CF7,CF8,FF3,FF4
      READ (5,100) XNF1,XNF2,XNF5,XNF6,B6,B7,B8
      WRITE(6,113) XNF1,XNF2,XNF5,XNF6,B6,B7,B8
C ------> F(I) INPUT AS MOLE/GM OF MIXTURE <------
C       ASSUME ALL POSITIVE IONS ARE NO+ I.E. XNRT=1.0
      XNRT=1.0
C        CALCULATE MOLECULAR WEIGHT OF THE INITIAL MIXTURE
```

```
      DO 5 I=1,NFS
      READ(5,100) S(I)
C         COMPUTE AVERAGED FLUX OF ENTRAINMENT
      TTA(I)=0.0
      PTB(I)=0.0
      UTB(I)=0.0
      DO 11 II=1,NS
      FTB(II,I)=0.0
   11 CONTINUE
      Y(1)=0.0
      YD(1)=0.0
      UE(1)=0.0
      WRITE(6,105)
      DO 1 J=2,NSL
      READ(5,100)  Y(J),PE(J),TE(J),UE(J),(FE(II,J),II=1,NS)
C********  FE(I) ARE IN MOLES/GM-OF-MIXTURE
      PE(J)= 1.0136E6*PE(J)
C****** PE(J) INPUT AS ATM AND CONVERTED TO DYNE/CM2
      WRITE(6,106) J,Y(J),PE(J),TE(J),UE(J)
     1, (FE(II,J),II=1,NS)
    1 CONTINUE
C*********** ASSUMPTION
C     Y3(I)=YE+VE/UP*S(I)+ C*S(I)**AI
      DO 3 J=2,NSL
C     IF (Y(J).GT. Y3(I)) GO TO 4
      J1=J
      DY= Y(J)-Y(J-1)
      DY5= 0.5*DY
      PTB(I)=PTB(I)+DY*PE(J)
      TTB(I)=TTB(I)+DY*TE(J)
      UTB(I)= UTB(I)+DY5*(UE(J)+UE(J-1))
      DO 10 II=1,NS
      FTB(II,I)= FTB(II,I)+DY*FE(II,J)
   10 CONTINUE
      IF (I.GT.1) GO TO 3
      YD(J)=Y(J)
      PTBD(J)= PTB(I)/Y(J)
      TTBD(J)= TTB(I)/Y(J)
      UTBD(J)= UTB(I)/Y(J)
      F1TBD(J)= FTB(1,I)/Y(J)
      F2TBD(J)= FTB(2,I)/Y(J)
      F3TBD(J)= FTB(3,I)/Y(J)
      F4TBD(J)= FTB(4,I)/Y(J)
      F5TBD(J)= FTB(5,I)/Y(J)
      F6TBD(J)= FTB(6,I)/Y(J)
      F7TBD(J)= FTB(7,I)/Y(J)
      F8TBD(J)= FTB(8,I)/Y(J)
    3 CONTINUE
    4 UTB(I)= UTB(I)/Y(J1)
      PTB(I)=PTB(I)/Y(J1)
      TTB(I)=TTB(I)/Y(J1)
      SUM=0.0
      DO 12 II=1, NS
      FTB(II,I)= FTB(II,I)/Y(J1)
      SUM=SUM+FTB(II,I)*WI(II)
```

```
                12 CONTINUE
                   DO 14 II=1,NS
                   FTB(II,I)=FTB(II,I)/SUM
                14 CONTINUE
115          C****** NORMALIZED IN MOLE/GM OF MIXTURE
                   WA(I)=0.0
                   DO 30 II=1,NS
                   WA(I)=WA(I)+FTB(II,I)
                30 CONTINUE
120                WA(I)= 1.0/WA(I)
                   RHOTB(I) = PTB(I)*WA(I)/(RR2*TTB(I))
                   DO 31 JJ=1,6
                   DD(JJ)=0.0
                   DO 32 II=1,NS
125                DD(JJ)= DD(JJ)+ XL(JJ,II)*FTB(II,I)
                32 CONTINUE
                31 CONTINUE
                   T10=TTB(I)/ 1000.0
                   HE=1000.*(-DD(5)/T10+DD(6)+T10*(DD(1)+T10*(DD(2)/2.0+T10*(DD(3)/3.
130               1 +T10*DD(4)/4.0)))
                   HSE(I)=HE+1.5*UTB(I)*UTB(I)/CTE
                   XXX1=RHOTB(I)*UTB(I)
                   RUE(I)=XXX1
                   RU2E(I)=XXX1*UTB(I)
135                RUHSE(I)=XXX1*HSE(I)
                   RUF1E(I)=XXX1*FTB(1,I)
                   RUF2E(I)=XXX1*FTB(2,I)
                   RUF3E(I)=XXX1*FTB(3,I)
                   RUF4E(I)=XXX1*FTB(4,I)
140                RUF5E(I)=XXX1*FTB(5,I)
                   RUF6E(I)=XXX1*FTB(6,I)
                   RUF7E(I)=XXX1*FTB(7,I)
                   RUF8E(I)=XXX1*FTB(8,I)
                   WRITE(6,126)   S(I),PTB(I),TTB(I),UTB(I), (FTB(II,I),II=1,NS)
145                WRITE(6,102)
                   WRITE(6,103) I,WA(I),HE,HSE(I),   RUE(I),RU2E(I),
                  1 RUHSE(I),RUF1E(I),RUF2E(I),RUF3E(I),RUF4E(I),RUF5E(I)
                  2,RUF6E(I), RUF7E(I),RUF8E(I)
                 5 CONTINUE
150                CALL BREAK
                   GAMA=CP/(CP-RR1/WM)
             C      CALCULATE INITIAL SPEED OF SOUND
                   SS=  SQRT(GAMA*RR2*T/WM)
             C        CALCULATE INITIAL MACH NUMBER
155                XMA=U/SS
                   AXX1=((U-UP)**2+VP**2)
                   UR = SQRT(AXX1)
                   UM=1.21E-5*(T**1.5)/(T+110)
                   REP=RHO* UR*RP/UM
160                XMAP=XMA* UR/U
                   WRITE(6,116)P,WM,RHO,HS,F(NS1),UP,VP      ,TP,RP,SE,YE
                   WRITE(6,116) GAMA,CP,SS,XMA ,XMAP,REP                    .
                999 CONTINUE
                100 FORMAT(8E10.3)
165             101 FORMAT(1015)
```

```
102 FORMAT(/ 5X, *I*, 6X,*WA*,11X, *HE*,10X,*HSE*,
   1 9X,*REJE*, 7X,*REVE2*,7X,*REUEHSE*,7X,*RUF1E*,7X,*RUF2E*,7X,*RUF3
   2E*/9X,*RUF4E*,7X,*RUF5E*,7X,*RUF6E*,7X,*RUF7E*,7X,*RUF8E*)
103 FORMAT(1H ,I5,1P9E12.3/5X,8E12.3)
104 FORMAT( // 3X,*T(K)*,7X,*CP1*, 7X,*CPV*)
105 FORMAT(/ 2X,*J*, 4X,*Y*,16X,*PF*,6X,*TE*,9X,*UE*
   1,4X,*FE(I) (MOLE/GM)=*)
106 FORMAT(1X,I3,1X,F6.2,2(1P11E11.3/))
107 FORMAT(1H ,*NPS=*,I5,3X,*NSL=*,I5,3X,*NOS=*,I5,3X,*IBUG=*,I5,3X,
   1      *NSO=*,I5,3X,*BREAKUP PARAMETER=*,I3/)
108 FORMAT(1H ,*INITIAL S=*,F7.3,3X,* S INCREMENT=*,1PE10.3,3X,*FINAL
   1S=*,E10.3,3X ,
   4 *PRINT INCREMENT=*,E10.3)
109 FORMAT(/ 2X,* C1=*,1PE10.3,2X,*C2=*,E10.3,2X,*C5=*,E10.3,2X,*C6=*,
   1E10.3,2X,*C7=*,E10.3,2X,*C8=*,E10.3,2X,*FF3=*,E10.3,2X,*FF4=*,E10.
   23)
110 FORMAT(1H ,* N1=*,1PE10.3,2X,*N2=*,E10.3,2X,*N5=*,E10.3,2X,*N6=*,
   1E10.3,2X,*N6=*,E10.3,2X,*N7=*,E10.3,2X,*N8=*,E10.3)
111 FORMAT(1H ,* NNO+/N+=*,1PE10.3,2X,*FNO+=*,E10.3,2X,*FE-=*,E10.3,2
   1X,*FO=*,E10.3,2X,*FF-=*, E10.3,2X,*FN=*,E10.3,2X,*FO2=*,E10.3/
   2 3X,*FN2=*,E10.3,2X,*FNO=*,E10.3)
112 FORMAT(1H ,* --------- KINETIC CALCULATION ONLY   --------/)
115 FORMAT(3X,*   --- PROPERTIES OF THE INJECTED LIQUID ------- */
   1 20X,*MOLECULAR WT.=*,F10.2/20X,*SPECIFIC HEAT(CAL/G-K)=*,1PE10.3/
   2 20X,*BOILING PT. (K)=*,E10.3/20X,*HEAT OF VAPORIZATION(CAL/G)=*,E
   310.3  /20X,*DENSITY (G/CM3)=*,E10.3/20X,*MASS FLUX(G/SEC)=*,E10.3,
   4 /20X,*JET VELOCITY(CM/SEC)=*,E10.3/20X,*JET ANGLE(RAD.)=*,E10.3/
   5 20X,*TEMPERATURE(K)=*,E10.3/20X,*SURFACE TENSION(DYNE/CM)=*,E10.3
   6 /20X,*VISCOSITY(GM/CM-SEC)=*,E10.3  / 20X,*ORIFICE DIAMETER(CM)=*
   7 ,E10.3/)
116 FORMAT (/2X,  *[illegible]*,1PE10.3
   1,3X,*HM=*,E10.3,3X,*RHO=*,E10.3,3X,*HS=*,E10.3,3X,*[illegible]=*,E10.3,3X,
   2 *UP=*,E10.3,2X,*VP=*,E10.3/ 2X,                                *TP=*
   3,E10.3,3X,*RP=*,E10.3,3X,*[illegible]=*,E10.3,3X,*YE=*,E10.3)
118 FORMAT(/ 2X, *  INITIAL THERMODYNAMIC INFORMATION */ 2X,*GAMMA=*,
   1 F6.3,2X,* CP(CAL/G)=*,1PE10.3,2X,*SS=*,E10.3,2X,*MA=*,E10.3,2X,
   1*MAP=*,E10.3,2X,*[illegible]=*,E10.3)
119 FORMAT (/2X,*---- TE CALCULATION DOES NOT CONVERGE IN IT=*,I5/)
120 FORMAT(1X,*AV=*,F6.2,2(1P11E11.3/))
      RETURN
      END
```

```
*DECK,RATEF
      SUBROUTINE RATEF
      COMMON CPA(40),CPV(40),WA(40),RHOF(40),PSIV(40),HSE(40),UE(40),
     1 S(40),TB(40),PTH(40)
     2 ,RUE(40),RU2E(40),RUHSE(40),Y(40),RUFEE(20)
     3 ,SO,DS,SMAX,RHO,FV,U,T,HS,ATB   ,P,RR,GSP,CTE,RR1,RR2,WV,C,AI,VE
     4 ,WM,SE,AE,RPO,TP,RHOP,EP,DTP,DAE,DTS,TS,DHP,DRHOP,DSE,DYE,DT,DHS
     5 ,DU,DUP,DFV,DRHO,DP,DA,ADS,ARHO2,UM,SI,SXO,BETA
     6 ,RUAI,RUEI,RUF1EI,RUF2EI,RUF3EI,RUF4EI,RUF5EI,PHADS
      COMMON RUF4E(20),U32(20),WDDI(5),RKI(5),WDOTN(5),UL(20),RUF1E(20),
     1 RUF2E(20),RUF3E(20),FOI, FE(5,20),PE(20),TE(20)
     2,       F(9),DF(4),U32I,U32II,XMLI,XMDU,ETA,ALU,ALT,UE,VLI,THETA
     3 ,F1,F2,F3,F4,F5,PI,AI1,R8,XNF8,CF8,UP,VP,GAMA,C1,C2,C3,C4,C5,C6,
     4 C7,C8 ,DP,A,RP ,XMA,XMAP,SS,UR,DUR,HSR,DHSR,XMLO
     5 ,RUF6E(20),RUF7E(20),RUF8E(20)
     6 ,RUF6EI,RUF7EI,RUF8EI,F6,F7,F8 ,F9 ,FFPE,FFIE,FFAF
     7 ,FFF,FFIV ,CF1,CF2,CF5,CF6,CF7,XNF1,XNF2,XNF5,B6,B7,FF3,FF4,XNRT
     8,XBK,YBK,TBK,PBK,RUBBK,RHOKY,SOP,NSO,NWDR,DEOP,S15O
      COMMON STB(30),TTB(30),RHOTB(30),UTB(30),FTB(8,30)
      COMMON /HEAT/ XL(6,9),WI(9)
      COMMON/LIQUID/ CPL,TFP,DHV,RHOL,WV,TBPC,SIG,TLO,JML,DO,WCCR,
     1 FFVI,AK,BK,WE,ITBK,FFV,TPPY
      COMMON/INTEG/NPP,NFT,IDD(20),NSL,IOPT,KO,NS,NS1,IBUG,ID
      RTI=RR1*T
      RHO2=RHO*RHO
      ARHO2= AJ*RHO2
      RHOU=RHO*U
      RKI(1)= CF1*(T **(-XNF1)) *XNRT
      RKI(2)= CF2*(T **(-XNF2))
      RKI(5)= CF5*(T **(-XNF5))
      RKI(3)=0.0
      RKI(4)=0.0
      RKI(6)=0.0
      RKI(7)=0.0
      RKI(8)=0.0
      IF (T.LT.600.) GO TO 2
      RKI(6)=CF6* EXP(-B6/RTI)
      RKI(7)=CF7* EXP(-B7/RTI)
      RKI(8)=CF8*(T**XNF8)* EXP(-B8/RTI)
    2 CONTINUE
      C3=0.0
      C4=0.0
      IF ((F1.LE.0.0).OR.( F2.LE.0.0)) GO TO 25
      IF(RP    .LT. 1.0E-9) GO TO 25
      ULI=  SQRT(UP*UP+VP*VP)
      XMDU=0.5*XMLO*RR*RP/(ULI*A*RPO**3)
      TI50= T /5000.
      VPLUS= 1.88E5* SQRT(TI50)
      VEMIUS= 4.4E7* SQRT(TI50)
      VMIUS= 2.36E5* SQRT(TI50)
      DNM= (VEMIUS*RHO *F2    + (VMIUS+U -ULI)*RHO *F4   )
      CC= (VPLUS+U -ULI)*RHO *F1  /DNM
      CALL ETAST(ETA,CC,SI)
      RKS    = 1.5*(1.0+ETA)*XMDU *(VPLUS+U -ULI)/ RHOL
      RKI(5)=FF3*RKS    *VEMIUS*RHO *F2  /DNM
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```
      RKI(4)=FF4*R[illegible]   *(VMIUS+U -[illegible])*RHO *F4   /DNM
      C3=RHO*RKI(3)
      C4=RHO*RKI(4)
   25 C1= ARHO2*RKI([illegible])
      C2= ARHO2*RKI([illegible])
      C5= ARHO2*RKI([illegible])
      C6= ARHO2*RKI([illegible])/4[illegible]
      C7= ARHO2*RKI([illegible])
      C8=ARHO2*RKI([illegible])
      RETURN
      END
```

```
*DECK,ETAGT
      SUBROUTINE ETAGT(ETA,CC,SI)
      IF ((CC.LT.1.0) .AND. (CC.GT.0.3)) GO TO 4
    5 CONTINUE
      WRITE(6,100) CC,SI
      STOP
  100 FORMAT(14 ,*------  CC=*, 5E10.3)
    4 CONTINUE
      EPS1=0.01
      DETA=0.5*ETA
      ETA=1.0E-5-DETA
      DEL1=1.0
    1 CONTINUE
      ETA= ETA  +DETA
      XLHS= EXP(-ETA)
      XRHS= CC*(1.0+ETA)
      DEL= XLHS-XRHS
      EPS= ABS(XLHS*EPS1)
      IF( ABS(DEL).LE.EPS) GO TO 3
      IF ((DEL*DEL1).GE.0.0) GO TO 2
      ETA= ETA-DETA
      DETA= 0.5*DETA
      GO TO 1
    2 DEL1= DEL
      GO TO 1
    3 CONTINUE
      RETURN
      END
```

```
*DECK,CHEMF
      SUBROUTINE CHEMF
      DIMENSION B(4,4), DX(4)
      COMMON CPA(40),CPV(40),WA(40),FMOE(40),PSIV(40),HSE(40),UE(40),
     1 S(40),FT3(40),PT3(40)
     2 ,RUE(40),RUPE(40),RUHSE(40),Y(40),RUFSE(20)
     3 ,SO,DS,SMAX,RHO,FV,U,T,HS,ATO   ,P,RR,CSP,CTE,PRI,PRE,AV,C,AI,YE
     4 ,WM,SE,AE,RPO,TP,RHOP,EP,DEP,CAE,DTS,TS,DRP,DRHOP,DSE,DYE,DT,DHS
     5 ,DU,DUP,CFV,DRHO,DP,DA,ADS,ARHO2,UM,SI,SAO,BETA
     6 ,RUAI,RUEI,RUF1FI,RUF2EI,RUF3EI,RUF4EI,RUF5EI,RHAFS
      COMMON RUF4E(20),D32(20),WDOT(5),RKI(5),WDCIN(5),UL(20),RUF1E(20),
     1 RUF2E(20),RUF3E(20),FOI, FE(8,20),PE(20),TE(20)
     2,       F(9),DF(9),D32I,D32II,XMLI,XMOU,ETA,ALO,ALT,DE,VLI,THETA
     3 ,F1,F2,F3,F4,F5,PI,AI1,38,XNFS,DFS,UP,VP,GAMA,C1,C2,C3,C4,C5,C6,
     4 C7,C8 ,CP,A,RP ,XMA,XMAP,SS,UR,DUR,HSR,DHSR,XML0
     5 ,RUF6E(20),RUF7E(20),RUF8E(20)
     6 ,RUF6EI,RUF7EI,RUF8EI,F6,F7,F8 ,F9 ,FFPE,FFTE,FFAE
     7 ,FFF,FFEV ,DF1,DF2,DF5,DF6,DF7,XNF1,XNF2,XNF5,55,E7,FF3,FF4,XNPT
     8,YPK,VBK,TBK,PERK,RUBBK,RHOKY,SOF,NSO,NWOR,DEGF,S150
      COMMON STB(30),TTB(30),RHOTB(30),HTB(30),FTB(5,30)
      COMMON /HEAT/ WL(5,9),WI(9)
      COMMON/LIQUID/ CPL,TBP,DHV,RHOL,WV,TBPC,SIG,TLO,IML,DO,WECR,
     1 FFVI,AK,BK,WE,ITBK,FFV,TEPY
      COMMON/INTEG/WPS,WPT,IOD(20),NSE,IOPT,N0,NS,NS1,IAUG,ID
C        SPECIE MOLE FRACTION IN MOLE/GM-OF-MIXTURE
      F1=F(1)/WI(1)
      F2=F(2)/WI(2)
      F3=F(3)/WI(3)
      F4=F(4)/WI(4)
      F5=F(5)/WI(5)
      F6=F(6)/WI(6)
      F7=F(7)/WI(7)
      F8=F(8)/WI(8)
      FOI=F(NS1)/WI(NS1)
      CALL RATEF
      ADSM=ADS*RUAI
      DX(1)=-(C1*F1*F2+C2*F1*F4+(C3+C4)*F1-C8*F3*F5)
      B(1,1)=-(C1*F2+C2*(F1+F4)+C3+C4)
      B(1,2)=-(C1-C2)*F1
      B(1,3)=C8*F5
      B(1,4)=C8*F3
      DX(2)=(C5*F4+C7*F3*F4-C5*FOI*F2-C2*F1-C1*F1*F2+C8*F3*F5)
      B(2,1)=(C7*F3+C6-C3-C1*F2)
      B(2,2)=-(C1*F1+C5*FOI+C5+C7*F3)
      B(2,3)=-(C7*F4-C8*F5)
      B(2,4)=C8*F3
      DX(3)=(C1*F1*F2+C2*F1*F4+(C3+C4)*F1-C7*F3*F4-C8*F3*F5)
      B(3,1)=(C1*F2+C2*(F1+F4)+C3+C4-C7*F3)
      B(3,2)=((C1-C2)*F1+C7*F3)
      B(3,3)= (C7*F4-C8*F5)
      B(3,4)=-C8*F3
      DX(4)=(C1*F1*F2-C8*F3*F5+C3*F1)
      B(4,1)=C1*F2 +C3
      B(4,2)=C1*F1
      B(4,3)=-C8*F5
```

```
                B(4,4)=-DA*F3
                QX(1)=QX(1)*ADSM+RUAI*((RUF1EI-RUEI*F1)*DAE-F1*PHADS)
                QX(2)=QX(2)*ADSM+RUAI*((RUF2EI-RUEI*F2)*DAE-F2*PHADS)
                QX(3)=QX(3)*ADSM+RUAI*((RUF3EI-RUEI*F3)*DAE-F3*PHADS)
60              QX(4)=QX(4)*ADSM+RUAI*((RUF5EI-RUEI*F5)*DAE-F5*PHADS)
                DO 2 I=1,4
                DO 2  J=1,4
                B(I,J)=-B(I,J)*ADSM
                IF (I .EQ. J) B(I,J)=1.0+B(I,J)
65            2 CONTINUE
                IF (IBUG.EQ.0) GO TO 6
                DO 4 I=1,4
                WRITE(6,100) (B(I,J),J=1,4),QX(I)
              4 CONTINUE
70            6 CONTINUE
                CALL SLOP(QX,B,4)
                IF (IBUG.EQ.0) GO TO 7
                DO 5 I=1,4
                WRITE(6,100) (B(I,J),J=1,4),QX(I)
75            5 CONTINUE
              7 CONTINUE
        C           QX(I) IS NOW IN MOLE/GM UNIT
                DO 3 I=1,3
              3 DF(I)=QX(I)*WI(I)
80      C       ----------> CHARGE BALANCE IMPOSED (----------
                DF(4)=QX(1)-QX(2)*WI(4)
                DF(5)=QX(4)*WI(5)
                DF(6)= RUAI*((RUF6EI-RUEI*F6)*DAE -F6*PHADS)*WI(6)
                DF(7)= RUAI*((RUF7EI-RUEI*F7)*DAE -F7*PHADS)*WI(7)
85              DF(8)= RUAI*((RUF8EI-RUEI*F8)*DAE -F8*PHADS)*WI(8)
        C        DF(I) NOW  IN MASS FRACTION UNIT
          100 FORMAT( 2X, 1P16E12.3)
                RETURN
                END
```

```
      SUBROUTINE GLSOLV(A,X,N)
C     THIS PROGRAM SOLVES THE SOLUTION TO A SET OF N SIMULTANEOUS LINEAR
C     EQUATIONS BY USING THE GAUSS-JORDAN REDUCTION ALGORITHM WITH THE
C       DIAGONAL PIVOT STRATEGY
C          DESIGNED FOR NON-SINGULAR FOR IMPLICIT UNEMPLOYMENT ---CJ
      DIMENSION A(4,4),X(4)
      DO 9 K=1,N
      IF (ABS(A(K,K)) .GT. 1.E-10) GO TO 5
      WRITE (6,101)   K,A(K,K)
      DO 10 IP=1,N
      WRITE(6,100)(A(I,JP),JP=1,N),X(IP)
   10 CONTINUE
  100 FORMAT(1X,   1P10E12.3)
  101 FORMAT( * ERROR--- SMALL PIVOT *,I5,1PE12.5)
      STOP
    5 KP1= K+1
      DO 6 J= KP1, N
    6 A(K,J)= A(K,J)/A(K,K)
      X(K)= X(K)/A(K,K)
      A(K,K)= 1.0
      DO 9 I=1,N
      IF (I.EQ.K .OR. A(I,K).EQ.0.) GO TO 9
      DO 8 J=KP1,N
    8 A(I,J)= A(I,J)- A(I,K)*A(K,J)
      X(I)= X(I)- A(I,K)*X(K)
      A(I,K)=0.
    9 CONTINUE
   99 CONTINUE
      RETURN
      END
```

```
*DECK.BREAK
      SUBROUTINE BREAK
      DIMENSION ID(6)
      COMMON CPA(40),CPV(40),WA(40),RHOF(40),PSIV(40),HSE(40),UE(40),
     1 S(40),TB(40),PTB(40)
     2 ,RUE(40),RU2E(40),RUHSE(40),Y(40),RUF5E(20)
     3 ,SO,DS,SMAX,RHO,FV,U,T,HS,ATD  ,P,PR,USP,CTE,HR1,HR2,AJ,C,AI,YE
     4 ,WM,SE,AE,RPO,TP,RHOP,EP,DEP,CAE,DTS,TS,DRP,DRHOP,DSE,DYE,DT,DHS
     5 ,DU,DUP,DFV,DRHO,DP,DA,ADS,ARHO2,UM,SI,SXO,BETA
     6 ,RUAI,RUEI,RUF1EI,RUF2EI,RUF3EI,RUF4EI,RUF5EI,RHAUS
      COMMON RUF4E(20),D32(20),WDOT(8),RKI(8),WDOTN(8),UL(20),RUF1E(20),
     1 RUF2E(20),RUF3E(20),FOI, FE(8,20),PE(20),TE(20)
     2,      F(9),DF(9),D32I,D32II,XPLI,XMDU,ETA,ALD,ALT,DE,ULI,THETA
     3 ,F1,F2,F3,F4,F5,PI,AI1,BA,KNF8,CF8,UF,VP,GAMA,C1,C2,C3,C4,C5,C6,
     4 C7,C8 ,DF,A,RF ,XMA,XMAP,SS,UR,DUR,HSR,DHSR,XMLT
     5 ,RUF6E(20),RUF7E(20),RUF8E(20)
     6 ,RUF6EI,RUF7EI,RUF8EI,F6,F7,F8 ,F9 ,FFPL,FFTL,FFAL
     7 ,FFF,FFEV ,CF1,CF2,CF5,CF6,CF7,XNF1,XNF2,XNF5,D5,P7,FF3,FF4,XNPT
     8,XBK,YBK,TBK,PBK,RU2BK,RHOXY,SDP,NSD,NMCR,DEGP,B15D
      COMMON STB(30),TTB(30),RHOTB(30),UTB(30),FTB(8,30)
      COMMON /HEAT/ XL(5,9),WI(9)
      COMMON/LIQUID/ CPL,TBP,DHV,RHOL,WV,TBPO,SIG,TLO,UML,DO,HECP,
     1 FFVI,AK,BK,WE,ITBK,FFV,IPPY
      COMMON/INTEG/NPS,NPT,IDD(20),NSL,IOPT,ND,NS,NS1,IPUN,IO
      COMMON /SHOCK/ YO(20),PTBO(20),UTBO(20),TTBO(20),F1TBO(20),
     1              F2TBO(20),F3TBO(20),F4TBO(20),F5TBO(20),F6TBO(20),
     2              F7TBO(20),F8TBO(20)
      CD=1.2
C     ESTABLISHING SHOCK FRONT CONDITIONS
      DO 42 ID=2,NPS
      IF (SO .GE. S(ID-1) .AND. SO.LT.S(ID)) GO TO 43
   42 CONTINUE
      WRITE (6,200) ID, S(ID),SO
      STOP
  200 FORMAT (2X,*--- OUT OF RANGE ID=*,I5,2X,*SI=*,E10.3,2X,*SO=*,E10.3
     1 )
   43 CONTINUE
      CALL LIPLN (SO,PTB,S,PX,ID)
      CALL LIPLN (SO,WA,S,WAX,ID)
      CALL LIPLN(SO,TTB,S,TX,ID)
      CALL LIPLN(SO,RUE,S,RUEX,ID)
      CALL LIPLN (SO,RU2E,S,RU2EX,ID)
      CALL LIPLN(SO,RUF1E,S,F(1),ID)
      CALL LIPLN(SO,RUF2E,S,F(2),ID)
      CALL LIPLN(SO,RUF3E,S,F(3),ID)
      CALL LIPLN(SO,RUF4E,S,F(4),ID)
      CALL LIPLN(SO,RUF5E,S,F(5),ID)
      CALL LIPLN(SO,RUF6E,S,F(6),ID)
      CALL LIPLN(SO,RUF7E,S,F(7),ID)
      CALL LIPLN(SO,RUF8E,S,F(8),ID)
      CALL LIPLN (SO,RUHSE,S,HSX,ID)
      F(NS1)=0.0
C     ----- F(I) ARE IN MOLE/GM. -----
      UX=RU2EX/RUEX
      DO 44 I=1,NS
```

```
      F(I)=F(I)*WI(I)/RUEX
      PSIV(I)=F(I)
   44 CONTINUE
C     ----- F(I) IS NOW IN MASS FRACTIONS -----
      HSX=HSX/RUEX
      UX2=UX**2
      RHOX=RUEX/TX
      HX=HSX-UX2/(2.0*GTE)
C     ----- CALCULATING GAS PROPERTIES BEHIND JET SHOCK -----
      ITRK=0
      RHOXY=0.75
      RHOY=RHOX/RHOXY
   50 CONTINUE
      WRITE(6,121) PX,UX,HSX,RHOX,TX,WAX,(F(I),I=1,NS1)
      DO 40 IT=1,100
      PY=PX+R*UX2*(1.0-RHOXY)
      HY=HSX-UX2*(RHOXY*RHOXY)/(2.0*GTE)
      TBPY=TBPO
      TI=TX*PY/PX*RHOXY
      CALL TIN(HY,TY,TI,F,NS1,CPY)
      RHO=PY*WAX/RR2/TY
      IF (IBUG.NE.0)
     1WRITE (6,101)   RHOX,RHOY,RHOXY,RHO,PY,HY ,TY
      IF ( ABS((RHO/RHOY)-1.0).LT. 0.001) GO TO 41
      RHOY=0.5*(RHOY+RHO)
      RHOXY=RHOX/RHOY
   40 CONTINUE
      IF (IBUG.NE.0) WRITE(6,128) RHOX,RHOY,RHOXY,RHO,PY,HY
  128 FORMAT (/2X,* --- SHOCK CALCULATION DIVERGED*/1P10E12.3/)
   41 CONTINUE
      UY=UX*RHOXY
      ROHV=RR1/(CHV*HV)
      TBPOI=1.0/TBPO
      PW=PY/ATO
      TBPY=1.0/(TBPOI -ROHV*ALOG(PV))
      WRITE (6,122) PY,UY,HY,RHOY,TY ,TBPY
C     ----- COMPUTE FLASH VAPORIZATION AT SHOCKED PRESSURE -----
      UM=1.21E-5*(TY**1.5)/(TY+113)
      FFV=0.0
      IF (TBPY .LT. TLO) FFV=CPL*(TLO-TBPY)/CHV
      IF (FFV.GT.1.0) FFV=1.0
C     ----- JET TRACK-UP -----
      ULI=VLI* SIN(THETA)
      WE=RHOY* UY*UY*6.5*DE/SIG
      IF (WE..LT.WECR) WRITE(6,126) WE
      REJ=RHOY*UY*6.5*DE/UM
      XXX=REJ/(1.0+2.0*WE/ SQRT(REJ))
      XXX= SQRT(XXX)
      IF (IBUG.NE.0)
     1WRITE(6,101) RHOL,RHOY,UW,UAL,DE,UY,XXX,TY
      TBK=3.53*(RHOL/RHOY)**(3.0536)*(UM/UML)**(0.3333)*0.5*DE/UY*XXX
      XXX1=RHOY*CD*(UY-ULI)**2/DE/RHOL
      UBK=2.0*XXX1*TBK+ULI
      TBK=UB*TBK
      DBK=(AXXL*TBK+ULI)*TBK
```

```
      IF(DBK.LT.DE) DBK=DE
      XBK=DBK+SO
C     ----- CALCULATING DROPLET SIZE -----
      WEL=DE*UY*UY*RHOL/SIG
      GAMA=CPY/(CPY-RG1/WAX)
      SS= SQRT(GAMA*RG2*TY/WAX)
      XMA=UY/SS
      D30=48.3*(WEL**(-0.375))*(REJ/XMA)**(-0.25)*DE
      D32I=1.23*D30
      DMAX=D30*4.6*(D30/DE)**(0.16)
      IF(NWCR.EQ.0)  GO TO 62
C*********** VAPOR PRESSURE BREAK UP
   61 XEPS=0.1
      TSH=TREY/(1.0-XEPS)
C******    TSH= SHATTER TEMPERATURE
      IF (TLO.GT.TSH) GO TO 63
      AXX1= ((UY-VLI* SIN(THETA))**2 +VP**2)
      UR= SQRT(AXX1)
      HSRY=HY+UR*UR/(2.0*GTC)
      TI=TY
      CALL TINV(HSRY,TSY,TI,F,NS1,CPSY)
      XX2= ALD*UR*(TSY-TLO)
      V= SQRT(3.0*PY/RHOY)
      XX3=1.5+ALT*V*(TY-TLO)/XX2
C********** FREE MOLECULAR HEAT TRANSFER
      QP=0.5*XX2*PY*XX3/TY/GTC*PFEV
      TBK=CPL*(TSH-TLO)*RHOL*DE/(4.0*QP)
      XXX1=RHOY*CD*(UY-ULI)**2/DE/RHOL
      UBK=2.0*XXX1*TBK+ULI
      YBK=VP*TBK
      IF(YBK.GT.Y(NSL))  YBK=Y(NSL)
      XBK=(XXX1*TBK+ULI)*TBK+SO
      DMAX=0.0
      WEL=0.0
      D30=0.0
C********INPUT INITIAL PARTICLE SIZE
      READ(5,100) D32I
      GO TO 62
C********** VAPOR PRESSURE BREAK UP OCCUR INSTANTLY  INITIAL CONDITION
C*********** HAS TO BE INPUT
   63 READ(5,100) D32I,UBK,XBK,YBK
   62 CONTINUE
      WRITE (6,103) WE,REJ,TBK,UBK,XBK,YBK,WEL,D30,D32I,DMAX
      IF (ITBK.GT.0) GO TO 49
      ITBK=1
C******* MODIFYING SHOCK FRONT CONDITIONS
      DO 46 IJ=2,NSL
      IF (YBK.GT.Y(IJ-1).AND. YBK.LT.Y(IJ)) GO TO 47
   46 CONTINUE
      IJ=NSL
   47 CONTINUE
      PTBD(1)=PTBD(2)
      TTBD(1)=TTBD(2)
      UTBD(1)=0.0
      F1TBD(1)=F1TBD(2)
```

```
                F2T80(1)=F2T80(2)
                F3T80(1)=F3T80(2)
                F4T80(1)=F4T80(2)
                F5T80(1)=F5T80(2)
  170           F6T80(1)=F6T80(2)
                F7T80(1)=F7T80(2)
                F8T80(1)=F8T80(2)
                CALL LIPLN(Y3K,PT80,Y0,PX,I0)
                CALL LIPLN(Y3K,TT80,Y0,TX,I0)
  175           CALL LIPLN(Y3K,UT80,Y0,UX,I0)
                CALL LIPLN(Y3K,F1T80,Y0,F(1),I0)
                CALL LIPLN(Y3K,F2T80,Y0,F(2),I0)
                CALL LIPLN(Y3K,F3T80,Y0,F(3),I0)
                CALL LIPLN(Y3K,F4T80,Y0,F(4),I0)
  180           CALL LIPLN(Y3K,F5T80,Y0,F(5),I0)
                CALL LIPLN(Y3K,F6T80,Y0,F(6),I0)
                CALL LIPLN(Y3K,F7T80,Y0,F(7),I0)
                CALL LIPLN(Y3K,F8T80,Y0,F(8),I0)
              C********** F(I) ARE IN MOLE/GM
  185           WAX=0.0
                DO 48 II=1,NS
                WAX=WAX+F(II)
             48 CONTINUE
                WAX=1.0/WAX
  190           RHOX=PX*WAX/(R2*TX)
                WA(1)=WAX
                PT8(1)=PX
                UT8(1)=UX
                TT8(1)=TX
  195           RHOT8(1)=RHOX
                FT8(1,1)=F(1)
                FT8(2,1)=F(2)
                FT8(3,1)=F(3)
                FT8(4,1)=F(4)
  200           FT8(5,1)=F(5)
                FT8(6,1)=F(6)
                FT8(7,1)=F(7)
                FT8(8,1)=F(8)
                DO 31 JJ=1,5
  205           DD(JJ)=0.0
                DO 32 II=1,NS
                DD(JJ)=DD(JJ)+XL(JJ,II)*FT8(II,1)
             32 CONTINUE
             31 CONTINUE
  210           T10=TT8(1)/1000.0
                HX=1000.*(-DD(6)/T10+DD(5)+T10*(DD(1)+T10*(DD(2)/2.0+T10*(DD(3)/3.
               1 +T10*DD(4)/4.0))))
                HE = HX
                HSX =HX  +0.5*UT8(1)*UT8(1)/GTE
  215           HSE(1)=HSX
                XXX1=RHOT8(1)*UT8(1)
                RUE(1)=XXX1
                RUPE(1)=XXX1*UT8(1)
                RUHSE(1)=XXX1*HSE(1)
  220           RUFIE(1)=XXX1*FT8(1,1)
```

```
      RUF2E(1)=XXX1*FT3(2,1)
      RUF3E(1)=XXX1*FT3(3,1)
      RUF4E(1)=XXX1*FT3(4,1)
      RUF5E(1)=XXX1*FT3(5,1)
      RUF6E(1)=XXX1*FT3(6,1)
      RUF7E(1)=XXX1*FT3(7,1)
      RUF8E(1)=XXX1*FT3(8,1)
      WRITE(6,120)
      I=1
      WRITE(6,108)
      WRITE(6,106)    S(I),FT3(I),TT3(I),UT3(I), (FT3(II,I),II=1,NS)
      WRITE(6,107)
      WRITE(6,103) I,WA(I),HE,HSE(I),    RUE(I),RU2E(I),
     1 RUMSE(I),RUF1E(I),RUF2E(I),RUF3E(I),RUF4E(I),RUF5E(I)
     2,RUF6E(I), RUF7E(I),RUF8E(I)
      DO 49 II=1,NS
      F(II)=F(II)*WI(II)
      PSIV(II)=F(II)
   49 CONTINUE
C*********** F(II) NOW IS IN MASS FRACTION
      UX2=UX*UX
      GO TO 50
   45 CONTINUE
      RPO=0.5*3321
      S150 = 1.05*DEOP*DEOP/R2D
      SE = SOP + S150 *((XBK/(150. * DEOP))**AI)
      IF(XBK .LE. (70.*DEOP))  SE = SOP + S150*((70./150.)**AI)*XBK/(70.
     1      *DEOP)
      SE=FFAE*SE
      YE=YBK
      AE=0.5*PI*YE*SE
C     ----- RELAX TO EXTERNAL PRESSURE RAPIDLY -----
      DO 52 ID=2,NPS
      IF (XBK.GE. S(ID-1) .AND.XBK.LT.S(ID)) GO TO 53
   52 CONTINUE
      WRITE (5,280) ID, S(ID),XBK
      STOP
   53 CONTINUE
      XMV=FFV*XMLI
      XML=(1.0-FFV)*XMLI
      CALL LIPLN (XBK,PTE,S,PEBK,ID)
      CALL LIPLN(XBK,RU2E,S,RU2BK,ID)
      BETA=0.5*PI
      A=AE
      P=PEBK+RU2BK*( SIN(BETA)**2)*(1.0-RHOXY)
      P=P*FFPE
C     ----- MIXING OF SHOCKED AIR WITH FLASH VAPOR -----
      XMG=RHOX*UX*A
      XMM=XMG+XMV
      WRITE(6,124) XMV,XML,XMG,XMM,AE
      F(NS1)= XMV/XMM
      U=(XMG*UY+XMV*UBK+(PY-P)*A)/XMM
C     U=(XMG*UX+XMV*UBK (PX-P)*A)/XMM
      HSV=CPL*TEFV+3HV+(UBK*UBK)/(2.0*GT+)
      HS=(XMG*HSX+XMV*HSV)/XMM
```

```
      DO 24 I=1,NS
   24 F(I)= PSIV(I)*(1.0-F(NS1))
C********** NORMALIZED MASS FRACTION
      WM=0.0
      DO 29 I=1,NS1
C     F(I) ARE IN MASS FRACTION
      WM=WM+F(I)/WI(I)
   29 CONTINUE
      WM=1.0/WM
      H=HS-(U*U)/(2.0*GE)
      II=TX
      CALL TINV(H,I,II,F,NS1,GR)
      RHO=P *WM/GR2/T
C********** INITIAL DUCT TUBE AREA AFTER MIXING
      A=XMM/(RHO*U)
C     DA=A-AE
      RP=RPO
      TP=TRPY
      UP=URK
      SI=XSK
      XMLO=XML
      IF (FFV.GE.  1.0) PP=0.0
      IF (FFV.GE.  1.0) UP=U
C********** CALCULATING INITIAL RELATIVE STAGNATION TEMPERATURE
      AXX1=((U-UP )**2+VP**2)
      UR = SQRT(AXX1)
      HSR=HS-(U*U-UR*UR  )/(2.0*GE)
      II=TY
      CALL TINV(HSR,TS ,TI,F,NS1,GPSR)
      WRITE (6,129) SI,U,HSV,HSR,T,TS ,T,PHO,A
      WRITE(6,108) (F(I),I=1,NS1)
  100 FORMAT(9E10.3)
  101 FORMAT(2X,10E12.8)
  102 FORMAT(2A,I5,1P10E12.4)
  103 FORMAT(14 ,I5,1P9E12.3/3X,8E12.3)
  105 FORMAT(24,*MASS FRACTIONS OF SPECIES*/1X,*NU=*,1PE10.3,1X,*E-=*
     1,E10.3,1X,*O=*,E10.3,1X,*F-=*,E10.3,1X,*H=*,E10.3,1X,*O2=*,E10.3,1
     2X,*N2=*,E10.3,1X,*NO=*,E10.3,* FV=*,E10.3)
  106 FORMAT(1X,*AV=*,F6.2,2(1P11E11.3/))
  107 FORMAT(/ 5X, *I*, 6X,*HA*,10X, *HE*,10A,*HSE*,
     1 8X,*REJE*, 7X,*REUF2*,7X,*REUEHSE*,7X,*RUF1Z*,7X,*RUF2I*,7X,*RUF7
     2E*/3X,*RUF4E*,7X,*RUF5E*,7X,*RUF6E*,7X,*RUF7E*,7X,*RUF8E*)
  108 FORMAT(/          4X,*S*,10X,*PE*,8X,*TE*,8X,*UE*
     1,4X,*FF(I) (MOLE/GM)=*)
  120 FORMAT(1X,*---------- MODIFIED FREE STREAM CONDITIONS IN SHOCK FR
     1ONT BY SINGLE ITERATION -----*)
  121 FORMAT(/2X,* CONDITIONS IN FRONT OF SHOCK */2X,*PX=*,1PE10.3,2X,
     1 *UX=*,E10.3,2X,*HSX=*,E10.4,2X,*RHOX=*,E10.3,2X,*TX=*,E10.3
     2 ,2X,*WAX=*,E10.3/ 2X,
     2*MASS FRACTIONS F(I)=*,8E12.3/)
  122 FORMAT(/2X,* CONDITIONS BEHIND SHOCK*/2X,*PY=*,1PE10.3,2X,*UY=*,
     1 E10.3,2X,*HY=*,E10.3,2X,*RHOY=*,E10.3,2X,*TY=*,E10.3,2X,*TSPY=*,
     2 E10.3/)
  123 FORMAT(2X,* JET ASPARK-UP INFORMATION */2X,*WE=*,1PE10.4,2X,
     1 *REJ=*,E10.3,2X,*TJK=*,E10.3,2X,*UJK=*,E10.3,2X,*XJK=*,E10.3,2X,
```

```
     2 *YBK=*,E10.3/2X,*HEL=*,E10.3,2X, *D3L=*,E10.3,2X,*D32=*,E10.3,2X,
     3 *D44X=*,E10.3/)
  124 FORMAT(2X, *INITIAL FLOW RATE(G/SEC)*/2X,*XMV=*,1PE10.3,2X,*XML=*,
     1 E10.3,2X,*XMA=*,E10.3,2X,*X44=*,E10.3,2X,*AL=*,E10.3/)
335 125 FORMAT(2X,*------  CONDITIONS OF THE INITIAL MIXTURE AT S=*,F10.4
     1      /3X,*U=*,1PE10.3,2X,*HSV=*,E10.3,2X,*HSK=*,E10.3,2X,*H=*,
     1E10.3,2X,*TSR=*,E10.3,2X,*T=*,E10.3,2X,*RHO=*,E10.3,2X,*A=*,E10.3)
  126 FORMAT(/2X ,* --- AERODYNAMIC BREAK-UP IS IMPOSSIBLE, WE=*,1PE10.3
     1/)
340 127 FORMAT(2X, * -- INITIAL MIXING CALCULATION DOES NOT CONVERGE TO
     1CORRECT SOLUTION*,I5/1P11E11.3)
      RETURN
      END
```

```
*DECK,LIPLN
      SUBROUTINE LIPLN (SX,A,S,RA,K)
C     A SCHEME FOR LINEAR INTERPOLATION
      DIMENSION A(20),S(20)
   22 RA= (A(K-1)*(S(K)-SX) + A(K)*(SX-S(K-1)))/(S(K)-S(K-1))
      RETURN
      END
```

```
*DECK,DATA
      BLOCK DATA
      COMMON /HEAT/ XL(5,9),WI(9)
C*******  COEFFICIENTS FOR CP AND H POLYNOMIALS
C**********  FROM JANNAF CURVE FITTING
C******* XL(1,I) ARE IN (CAL/MOLE-K) AND XL(6,I) ARE IN (KCAL/MOLE)
      DATA XL/
     1  6.2601E+0, 1.4268E+0,-4.5701F-1, 3.6333E-2, 9.7635E-3, 2.3473E+2
     2, 4.9634E+0,-3.1704E-4, 7.4172E-5,-6.6372E-6,-1.7091E-5,-1.4813E+0
     3, 5.9617E+0,-1.1730E-1, 3.9405E-2,-2.0531E-3, 1.8127E-2, 5.6115E+1
     4, 4.9682E+0,-7.2226E-5, 2.2405F-5,-2.7745E-6,-1.0450E-5,-6.3081E+1
     5, 5.3462E+0,-8.6136E-2, 4.9520E-3, 6.1333E-3,-5.9068E-3, 1.1140E+2
     6, 7.2419E+0, 1.2395E+0,-1.5440E-1, 1.0565E-2,-5.4600E-2,-2.4210E+0
     7, 6.2640E+0, 1.4320E+0,-4.6159E-1, 3.7080F-2, 9.1659E-3,-1.9240E+0
     8, 6.7520E+0, 1.7000E+0,-4.1765E-1, 3.4120E-2,-1.6770E-2, 1.9420E+1
     9, 2.1523E+2,       0.0,       0.0,       0.0,       0.0, 0.0/
C******* WI(I) ARE MOLECULAR WEIGHT FOR EACH SPECIES
      DATA WI/39.8,5.487E-4,15.9,15.99,14.0,32.0,28.0,36.0,613.0/
      END
```

```
*DECK,ERF
      FUNCTION ERF(X)
C     ----- THIS CALCULATES THE ERROR FUNCTION AND ITS COMPLEMENT -----
      DATA EPSILN/1.0E-10/,N/100/,CONST/1.128379167955/
 5    KOMPL=+1
      GO TO 5
      ENTRY ERFC
      KOMPL=-1
    5 IF (X) 10,55,15
10  10 Z=-X
      GO TO 20
   15 Z= X
   20 IF (Z-5.) 25,25,45
   25 ZSQ=Z*Z
15    TERM=CONST*Z*EXP(-ZSQ)
      ERF=TERM
      I=0
      R=1.0
   30 I=I+1
20    R=R+2.0
      TERM=2.0*ZSQ*TERM/R
      ERF=ERF+TERM
      IF (I-N) 35,40,40
   35 IF (TERM-EPSILN*ERF) 40,30,30
25 40 IF (ERF-1.0) 50,50,45
   45 ERF=1.0
   50 IF (X) 60,55,65
   55 ERF=0.0
      GO TO 85
30 60 ERF=-ERF
   65 IF (KOMPL) 70,80,80
C     ----- COMPUTE COMPLEMENTARY ERROR FUNCTION ERF -----
   70 ERF=1.0-ERF
   80 RETURN
35    END
```

```
*DECK,TINV
      SUBROUTINE TINV (H,T,TI,F,NS1,CP)
C     ----- THIS SUBPROGRAM WILL INVERT TEMPERATURE FROM ENTHALPY BY THE
C                 NEWTON METHOD -----
      DIMENSION DD(6),F(9)
      COMMON /HEAT/ XL(9,9),WI(9)
      COMMON/LIQUID/ CPL,TBP,DHV,PHOL,HV,TBPC,SIG,TLO,DML,CO,ALCP,
     1 FFVI,AK,BK,WE,ITBK,FFV,TADV
      1 CONTINUE
      DO 10 J=1,6
      DD(J)=0.0
      DO 11 I=1,NS1
C       F(I) ARE IN MASS FRACTION
      DD(J)=DD(J)+XL(J,I)*F(I)/WI(I)
   11 CONTINUE
   10 CONTINUE
      EPS=1.0D-6*H
      T=TI
      DO 12 IT=1,100
      T10=T/1000.
      G=1000.*(-DD(6)/T10+DD(5)+T10*(DD(1)+T10*(DD(2)/2.+T10*(DD(3)/
     * 3.0+T10*DD(4)/4.0))))-H
      CP=         (DD(6)/(T10*T10)+DD(1)+T10*(DD(2)+T10*(DD(3)+T10*DD(4)
     1 )))
      IF( ABS(G).LT. EPS) GO TO 999
      T=T-G/CP
   12 CONTINUE
      WRITE (6,119) IT ,H,T,CP,TI ,G ,EPS
      STOP
   20 CONTINUE
      FAA=1.0-F(NS1)
      PC=XL(1,NS1)*F(NS1)/WI(NS1) +(XL(1,6)*0.251/WI(6)+XL(1,7)*0.749/
     1 WI(7))*FAA
      CP=PC
      T=H/CP
  999 CONTINUE
  119 FORMAT(12X, *--ITERATION DOES NOT CONVERGED TO THE CORRECT TEMPERA
     1TURE *,I5/2X,1P10E12.3)
      RETURN
      END
```

```
*DECK.MAIN
      PROGRAM J108(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE4)
C     ----- 12/16/73 -----
C      -----   THIS IS VERSION D -----
C     ----- THIS DECK FOR CDC USE -----
C*****************************************************************
C
C     ONE DIMENSIONAL REACTING DROPLET-VAPOR-AIR TUBE ANALYSIS
C          A SELF-INITIALIED REACTING D/A TUBE  (8/8/73)
C
C******* MODIFIED TUBE PRESSURE ((9/30/73)
C******** ITERATED SHOCK FRONT CONDITIONS (9/13/73)
C*************** GENERALIZED REACTION TYPE AND SPECIES (9/24/73)
C*****************************************************************
      COMMON CPA(40),CPV(40),WA(40),RHOE(40),PSIV(51),HSE(40),UE(40),
     1 S(40),T8(40),PTB(40)
     2 ,RJE(40),RUZE(40),RUHSE(40),Y(40),RUF5E(20)
     3 ,SO,DS,SMAX,RHO,FV,U,T,HS,ATO  ,P,RK,USP,CTE,RR1,RR2,AV,C,AI,YE
       ,HM,SE,AE,RPO,TP,RHOP,EP,DEP,DAE,DTS,TS,URP,DRHOP,DSE,DYE,DT,D45
     5 ,DU,DUP,DFV,DRHO,DP,DA,ADS,ARHO2,UM,SI,SXO,BETA
     6 ,RUA1,RUE1,RUF1EI,RUF2EI,RUF3EI,RUF4EI,RUF5EI,PHADS
      COMMON RUF4E(20),D32(2 ),          RKI(8),WDOTN(5),J.(20),RUF1E(20),
     1 RUF2E(20),RUF3E(20),FQI, FE(8,20),PE(20),TE(20)
     2,    F(51),DF(51),D32I,D32II,XML1,XMDU,ETA,ALD,A.T,JI,VLI,THETA
     3 ,F1,F2,F3,F4,F5,PI,AI1,BB,XNFE,CFE,UP,VP,GAMA,C1,C2,C3,C4,C8,C5,
     4 C7,C8 ,CP,A,RP  ,XMA,XMAP,SS,UR,DUR,HSR,DHSR,XMLO
       ,RUF6E(20),RUF7E(20),RUF8E(20)
     5 ,RUF6EI,RUF7EI,RUF8EI,F5,F7,F8  ,F9  ,FFPE,FFTE,FFAE
     7 ,FFF,FFEV  ,CF1,CF2,CF5,CF6,CF7,XNF1,XNF2,XNF5,B5,B7,FF3,FF4,XNFT
     8,XBK,YBK,TBK,PEBK,RU2BK,RHOXY,SUP,HSO,NHOR,DEQP,S1 2
      COMMON ST8(3,),TT8(3 ),RHOT8(3 ),UT8(3 ),FT8(8,3 )
      COMMON /HEAT/ XL(6,51),WI(51)
      COMMON/LIQUID/ CPL,TBP,DHV,RHOL,WV,TB=0,SIG,TLO,JM.,JO,HEQP,
     . FFVI,AK,BK,HE,ITBK,FFJ,TBPY
      COMMON/INTEG/NPS,NPT,IOO(20),NSL,IDPT,NO,NS,NS1,IBJG,IO,IKINE
      COMMON /SHOCK/ YO(20),PTBO(2 ),UTBO(20),TTBO(2 ),F1TBO(20),
     1               F2TBO(20),F3TBO(2 ),F4TBO(20),F5TBO(20),F6TBO(20),
     2               F7TBO(2 ),F8TBO(20)
      COMMON/CHEM2/CM(51,51),FI(51),WP(51),WM1(51),WDOT(51),DX(51)
     1 ,RC(100,5)
      COMMON /SPIO/ IZH,IZ1,IZ2,IZ3,IZ4,IZ5,   I4,INDP,I14,IOX,IF4,IN
      COMMON/CHEM1/IRR(1  ),IRT(1  ),IRRR(1   ,8),IZO(8),IDENT(51)
 1000 CONTINUE
      ITBK=0
      GO TO 1002
 1001 ITBK=2
 1002 READ (5,100) (IOO(I),I=1,20)
      IF( EOF(5) )  99, 3
    3 CONTINUE
      WRITE(6,99)
      WRITE(6,100) (IOO(I),I=1,20)
      READ (5,102) FFAE,FFPE,FFEV,FFF,FF3,FF4 ,PRXL,FFVI
      WRITE(6,102) FFAE,FFPE,FFEV,FFF,FF3,FF4,PRXL,FFVI
C******  CONSTANTS
      PI=3.141 9
```

```
                      SQTPI= SQRT(PI)
                      AV=6.02E23
                      RR=82.06
                      RR1= 1.987
                      RR2= 8.313E7
                      CTE= 4.186E7
                      ATO=1.013E6
                      IUK=0
                      XDK=1.0
                      DFV=0.0
                      DFQ=0.0
                      DU=0.0
                      DP=1.0
                      DRHO=0.0
                      DT=0.0
                      DHS=0.0
                      DTS=1.0
                      DRHOP=0.0
                      DUP=0.0
                      DRP=0.0
                      DEP=1.0
                      DA=0.0
                      DSE=0.0
                      DYE=0.0
                      DAE=1.0
                      ETA=1.0
                C***   RR IN CM3-ATM/G-MOLE-K
                      CALL PUTIN
                      DO 35 I=1,NS1
                      DF(I)=0.0
                      FI(I)=F(I)/WI(I)
                   35 CONTINUE
                      YPEN=YE
                      SEO=SE
                      EP= CPL*TP
                      HPS= EP+UP*UP/(2.0*CTE)
                      DS1=DS
                      DSMAX=5.0*DS
                      DSMIN=DS/10.0
                      WRITE(6,39)
                      WRITE(6,100) (IDD(I),I=1,20)
                      IPS=DSP
                      IS=-1
                    1 CONTINUE
                      DS=DS1
                      AXX1=((U-UP)**2+VP**2)
                      UR = SQRT(AXX1)
                      HSP=HS-(U*U-UR*UR  )/(2.0*CTE)
                      TI=TS
                      CALL TINV(HSP,TS ,TI,F,NS1,CPSP)
                      RHOP=1.0
                      XNP=0.0
                      IF (RP.LT.1.0E-9) GO TO 40
                      RHOP= (X1LI-RHO**(NS1)*U*A)/(UP*A)
                      XNP= 3.0*RHOP*UP*A/( 1.0*PI*RP**2*(
```

```
      XX1=RHOL*DH/*.5
      XX2=ALD*UR*(TS-TP)
      V= SQRT(3.0*P/RHO)
C****** V IS MEAN THERMAL VELOCITY OF MIXTURE BY KINETIC THEORY
      XX3=1.0+ALT*V*(T-TP)/XX2
      DP=0.5*XX2*P*XX3/T/DTE *FFEV
      DDDT=-DP/XX1
      PHIV=-1.5*RHO*P*DDDT/RP
      IF (PHIV.GT. 1.0E-5)  DS=DS1/(PHIV*A)
      IF ((IS..T.10).AND.(DS.GT.DSMIN)) DS=DSMIN
      IF (DS.GT.DSMAX) DS=DSMAX
   41 CONTINUE
      SI=SI+DS
      IF((SI.GT. S(NPS)).OR.(SI.LT.S(1))) GO TO 999
      DO 21 ID=2,NPS
      IF (SI.GE.S(ID-1) .AND. SI.LT.S(ID)) GO TO 22
   21 CONTINUE
      WRITE(6,200)ID,S(ID),SI
      STOP
  200 FORMAT (1H ,*    OUT OF RANGE    ID=*,I5, *  S=*,2F8.3/)
   22 CONTINUE
      CALL LIPLN(SI,RUE ,S,RUEI ,ID)
      CALL LIPLN(SI,RU2E,S,RU2EI,ID)
      CALL LIPLN(SI,RUH2E,S,RUH2EI,ID)
      CALL LIPLN(SI,RUF1E,S,RUF1EI,ID)
      CALL LIPLN(SI,RUF2E,S,RUF2EI,ID)
      CALL LIPLN(SI,RUF3E,S,RUF3EI,ID)
      CALL LIPLN(SI,RUF4E,S,RUF4EI,ID)
      CALL LIPLN(SI,RUF5E,S,RUF5EI,ID)
      CALL LIPLN(SI,RUF6E,S,RUF6EI,ID)
      CALL LIPLN(SI,RUF7E,S,RUF7EI,ID)
      CALL LIPLN(SI,RUF8E,S,RUF8EI,ID)
      CALL LIPLN(SI,PTE,S,PEI ,ID)
      XXXX=(SI-X8K)/PRXL
      IF(XXXX.GT.+.0.) XXXX=+.0.
      P1= PEI +RU2EI*(1.0-RHOXY)* EXP(-XXXX)
      P1=P1*FFPE
      IF (IBUG .NE. 0) WRITE(6,101) RUEI,RU2EI,RUH2EI,RUF1EI,RUF2EI,
     1 RUF3EI,RUF4EI,RUF5EI,RUF6EI,RUF 7EI,RUF8EI,P1
      DP=P1-P
      ADS=A*DS
      SP = SE
      SE=SOP+S15.*((SI/(15.*DEQP))**AI)
      IF (SI.LE.(75.*DEQP)) SE=SOP+S15.*((75./15.)**AI)*SI/(75.*DEQP)
      YPEN=YPEN+VP/UP*DS
      YE = YPEN+(SE-SP)
      SE=FFAE*SE
      DAE= 0.5*PI*SE*YE -AE
      IF(IBUG.NE.0) WRITE(6,1.1) AE,SE,YE,YPEN,C,AI,SI,DAE
      SQGAM= SQRT(GAMA)
      XMAP=XMA* UR/U
C*********      VISCOSITY FOR AIR IN (G/CM-SEC) BY SUTHERLAND LAW
      UM=1.21E-5*(T**1.5)/(T+117.)
      REP=RHO* UR*RP/UM
      PHADS=0.0
```

```
                      DFP=...
                      DRP=...
                      DQ=...
                      IF(RP.LT. 1.0E-9 ) GO TO 7
170.          C         CALCULATE DRAG COEFFICIENT
                      CDO=24./REP
                      CDI=0.44
                      CDB=1.0
                      CD=CDI
175                   AMK=XMAP/REP
                      XKN=1.26 * SQGAM*RMR
                      IF (XKN .GT.  2.00) GO TO 4
                      IF (XKN .LT. 1.E-6) GO TO 5
                      XX1=XKN**(-.8)
1 0                   XX2= EXP(1.2* XKN**(-.5))
                      GKN=XX1*XX2/(1.0+XX1*XX2)
                      XX3=XKN**0.7
                      XX4= EXP(XKN)
                      DRE=1.0- EXP(-XX3*XX4*(CDO-.48)*REP/8.)
1 5                   CDB=GKN*DRE
                    4 CONTINUE
                      S1= SQRT(.5*GAMA)*XMAP
                      S2=S1*S1
                      S3=S2*S1
1 0                   S4=S3*S1
                      S32=S2*..5
                      SQ=S1* SQRT(PI/TP)
                      CDFM=  EXP(-S32)*(1.0+2.0*S2)/SQTPI/S3
                     1     +(4.0*(S4+S2)-1..)/2.0/S4* ERF(S1)
 95                  2    +..667*SQTPI/SQ
                      CD=CDB*(CDFM-CDI)+CDI
                    5 FP=CD/24.*REP*FFF
                      DFP=4.5*RHOP*FP*U4 *(U-UP)*ADS/RHOL/FP/RP
                      DRP= .5*DOOT*DS/UP
1.0                   DQ=3.0*RHOP*DP*AUS*DS/(RP*RHOL*UP)
                      IF (IBUG.NE.0) WRITE(6,101) XKN,GKN,DRE,CDFM,CD,FP,S1,SQ
                      PHADS=PHIV*ADS
                    7 CONTINUE
                      RUA=RHO*U*A
2 5                   RUAI=1.0/RUA
                      RUAP=RHOP*UP*A
                      DUP=1.0
                      IF (FFV.EQ.1.0) GO TO 55
                      DUP = DFP / RUAP
210                55 IF (IBUG.NE.0)
                     .WRITE(6,101) RUAI,UP,U,PHADS,RUZEI,RUEI,DAE,A,DP,DFP
                      DU=RUAI*((UP-U)*PHADS+(RUZEI-RUEI*U)*DAE-A*DP+DFP)
                      DHPS= EP+(UP+DUP)*(UP+DUP)/(2.0*CTE) -HPS
                      DHS=RUAI*((HPS-HS)*PHADS+(RUHSEI-RUEI*HS)*DAE-RUEI*DHPS)
 .5                   DF(NS1)= RUAI*((1.0-F(NS1))*PHADS-F(NS1)*RUEI*DAE)
                      CALL CHEMF
                    3 CALCULATING DFI
                      F(NS1)=F(NS1)+DF(NS1)
                      DO 33 I=1,NS1
220                   IF ((F(I)       ) .LT. ...) GO TO 998
```

```
   33 CONTINUE
      DO 30 I=1,NS1
      FI(I)=F(I)/WI(I)
   30 CONTINUE
      HS=HS+DHS
      H=HS-(U+DU)*(U+DU)/(2.0*CTE)
      TI=T
      IF (IBUG.NE.0)
     .WRITE(6,101) DP,DU,DHS,DF(NS1),BETA,DUP,HS,H,DS
      CALL  TINV(H,T,TI,F,NS1,CP)
      WM=0.0
      DO 29 I=1,NS1
      WM=WM+FI(I)
   29 CONTINUE
      WM=1.0/WM
C      CALCULATE LOCAL SPECIFIC HEAT
      GAMA=CP/(CP-RR1/WM)
C          LOCAL SPEED OF SOUND
      SS=  SQRT(GAMA*RR2*T/WM)
C         LOCAL MACH NUMBER
      XMA=U/SS
      DRHO=P1*WM/RR2/T-RHO
C     DA=(PHADS+RUEI*DAE-A*U*DRHO-A*RHO*DU)/(RHO*U)
      DA=(PHADS+RUEI*DAE+RUA)/((RHO+DRHO)*(U+DU)) -A
      AE=AE+DAE
      RP=RP+DRP
      IF (RP.LT.0.0) RP=0.0
      UP=UP+DUP
      U=U+DU
      HPS=HPS+DHPS
      RHO=RHO+DRHO
      A=A+DA
      P=P1
      IS=IS+1
      IF ((SI+DS) .GT. SMAX ) GO TO 9
      IF(((IS/IPS)*IPS).NE. IS) GO TO 2
    9 CONTINUE
      EDEN= RHO*AV*FI(IEM)
      WRITE(6,103) SI,T,P,RHO,U,HS,F(NS1),WM
      WRITE (6,110) A,UP,TP,RP,RHOP,AE,TS,H
      WRITE(6,135)
      DO 42 I=1,NS1
      WRITE(6,119) IDENT(I),F(I),FI(I),WDOT(I)
   42 CONTINUE
      WRITE(6,105) EDEN
      WRITE(6,104) DS,   DP,DRHO,DU,DHS,DF(NS1),PHADS
      WRITE(6,111) DA,DAE,DUP    ,DRP,QP,PHIV,DFP,DQ
      WRITE(6,118) GAMA,CP,SS,XMA ,XMAP,REP,XNP
      WRITE(6,101) DS,ETA,SE,VE,VP,C,AI,SXO ,BETA
     .,BETA1
      IF ((SI+DS) .GT. SMAX ) GO TO 999
    2 CONTINUE
      GO TO 1
   91 WRITE(6,109)
  998 CONTINUE
```

```
      DO 34 I=1,NS1
      F(I)=FI(I)*WI(I)
   34 CONTINUE
      SI=S1-DS
      YPEN=YPEN-DP/UP*DS
      DS1=DS1*0.5
      IKT=1
  999 CONTINUE
      IF(ITBK.GT.2) CALL EXIT
      IF(WE.GE.WECR) CALL EXIT
      WRITE (6,126) WE
      GO TO 1001
   99 FORMAT(1H1)
  100 FORMAT(26A )
  101 FORMAT (2X,10E12.3)
  102 FORMAT (8E10.3)
  103 FORMAT(///*  S(CM)=*,F9.4/1X,*T(K)=*,F8.2,1X,*P(DYNE/CM2)=*,1PE1 .3
     1,1X,*RHO(GM/ML)=*,E10.3,1X,*U(CM/SEC)=*,E1..3,1X,*HS(CAL/GM)=*,E10
     2.3,1X,*FV=*,E10.3,1X,*MM=*,E10.3)
  104 FORMAT(2X,*DS=*,E10.3,  2X,*D2=*,E1..3,2X,*DRHO=*,E10.3,2X,*DU=*,
     1E1..3,2X,*DHS=*,E1..3,2X,*DFV=*,E..3,2X,*PHADS=*,E1..3)
  105 FORMAT (2X,* ----- ELECTRON DENSITY=*,E10.3)
  106 FORMAT(2X,*PRODUCTION RATES FOR EACH REACTION (MOL/SEC-CM3)*/2X,1P
     110E12.3)
  107 FORMAT(/2X,*PRODUCTION RATES FOR EACH SPECIE*,/2X,1P8E12.3)
  108 FORMAT(/*  CHANGES OF MASS FRACTION OVER DS=*,1PE1..3/4X,1P10E12.3
     1)
  109 FORMAT(1X ,*----- REACHING THE LOCAL SONIC SPEED  ------*)
  11  FORMAT (2X,*A=*,1PE1..3,2X,*UP=*,E1..3,2X,*TP=*,E1..3,2X,*RP=*,
     *  E10.3,2X,*RHOP=*,E10.3,2X,*AE=*,E10.3,2X,*TSR=*,E1..3,2X,*M=*,
     3E1..3/)
  111 FORMAT(2X,*DA=*,1PE10.3,2X,*DAE=*,E10.3 ,2X,*DUP=*
     ., E1..3,2X,*DRP=*,E1..3,2X,*DP=*,E1..3,2X,*PHIV=*,E1..3/ 2X,*DFP=*
     2,E10.3,2X,*D1=*,E10.3/)
  112 FORMAT(/2X, *  LOCAL   THERMODYNAMIC INFORMATION */ 2X,*GAMA=*
     1 F6.3,2X,* CP(CAL/G)=*,1PE1..3,2X,*SS=*,E1..3,2X,*M1=*,E10.3,2X,
     2*MAP=*,E10.3,2X,*REP=*,E10.3,2X,*DP/SEC=*,E10.3/)
  126 FORMAT(/2X ,* --- AERODYNAMIC BREAK-UP IS IMPOSSIBLE, WE=*,1PE10.3
     1/)
  119 FORMAT(9X,A4,3X,1P8E12.3)
  130 FORMAT(7X,*SPECIES*,5X, *F(I)*,5X,*FI(I)*,5X,*WDOT(I)*)
      REWIND 4
      STOP
      END
```

```
*DECK,PUTIN
      SUBROUTINE PUTIN
      DIMENSION DD(6),YB(2.)
      DIMENSION YOMAX(1,40)
      COMMON CPA(40),CPV(40),WA(40),RHOE(40),PSIV(51),HBE(40),DE(40),
     1 S(40),TB(40),PTB(40)
     2 ,RUE(40),RU2E(40),RUHSE(40),Y(40),RUF5E(2 )
     3 ,SO,DS,SMAX,RHO,FV,U,T,HS,ATD  ,P,RP,DSP,DTS,RR1,RR2,AV,C,AI,VE
     4 ,WM,SE,AE,RPO,TP,RHOP,EP,DEP,DAE,DTS,TS,DRP,DRHOP,DSE,DVE,DT,DHS
     5 ,DU,DUP,DFV,DRHO,DP,DA,ADS,ARHO2,DH,SI,SXO,BETA
     6 ,RUAI,RJEI,RUF1EI,RUF2EI,RUF3EI,RUF4EI,RUF5EI,PHOB
      COMMON RJF E(20),D32(20),        RKI(8),WDOTN(8,.),.(20),RUF1E(20),
     1 RUF2E(20),RUF3E(20),FQI, FE(8,20),PE(20),TE(20)
     2,    F(51),DF(51),D32I,D32II,XMLI,XMDO,ETA,ALO,AL1,JE,VLI,THETA
     3 ,F1,F2,F3,F4,F5,PI,AI1,B8,XNF8,CF8,UP,VP,GAM4,C1,C3,C4,C.,C9,
     4 C7,C8 ,CP,A,RP ,XMA,XMAP,SS,UR,DUR,HSM,DHSA,XMLO
     5 ,RUF6E(20),RUF7E(20),RUF8E(20)
     6 ,RUF6EI,RUF7EI,RUF8EI,F6,F7,F8 ,F9 ,FFPE,FFTE,FFEE
     7 ,FFF,FFEV ,CF1,CF2,CF5,CF6,CF7,XNF1,XNF2,XNF.,BE,B7,FF3,FF4,XNRT
     8,XBK,YBK,TBK,PEBK,RJ2BK,RHOXY,SOP,NSO,NWCR,DECP,BISO
      COMMON STB(30),TTB(30),RHOTB(30),UTB(30),FTB(6,30)
      COMMON /HEAT/ XL(6,51),WI(51)
      COMMON/LIQUID/ CPL,TBP,DHV,RHOL,WV,TBPO,SIG,TLO,UML,DD,WECR,
     1 FFVI,AK,BK,WE,ITBK,FFV,TBPY
      COMMON/INTEG/NPS,NPT,IDD(20),NSL,IOPT,KO,NS,NS1,IBUG,IO,IKINE
      COMMON /SHOCK/ YO(20),PTBO(20),UTBO(2.),TTBO(2.),FTBO(2 ),
     1               F2TBO(20),F3TBO(20),F.TBO(2.),F5TBO(20),F6TBO(20),
     2               F7TBO(20),F8TBO(20)
      COMMON/CHEM2/CM(51,51),FI(51),WP(51),WM1(51),WDOT(51),DX(51)
     1 ,RC(100,5)
      COMMON /SPID/ IZ4,IZ1,IZ2,IZ3,IZ-,IZ..   IH,INDP,IEM,IDX,IFM,IN
      COMMON/CHEM1/IRR(100),IRT(100),IRR(100,3),IID(6),IDENT(51)
      READ(5,100) WV,CPL,TBPO,DHV,RHOL,XMLI,VLI,THETA
     1 ,TLO,SIG,UML,DD,AK,BK
      THETA=THETA*PI/180.
      VP=VLI* COS(THETA)
      WRITE(6,115)WV,CPL,TBPO,DHV,RHOL,XMLI,VLI,THETA
     1 ,TLO,SIG,UML,DD,AK,BK
      READ(5,1.1) NPS,NSL,NOS,IBUG,IKINE,NS1,NSO,NWCR
      WRITE(6,117)NPS,NSL,NOS,IBUG,IKINE,NS1,NSO,NWCR
      NS=NS1-1
      DO 27 I=1,NS1
      F(I)=0.0
      FI(I)=0.0
      WDOT(I)=0.0
   27 CONTINUE
      WI(NS1)=WV
      READ(5,100) SO,DS,SMAX,DSP
      WRITE(6,100) SO,DS,SMAX,DSP
      READ (5,100) ALO,ALT,SOP,AI ,WECR
      WRITE(6,1. ) ALO,ALT,SOP,AI ,WECR
      AI1=AI-1.0
      XNOS=NOS
      DE= SQRT(XNOS) *DD
      XNSO=NSO
```

```
      UEQP=SQRT(XNSO)
      CALL CPUTIN(IKINE,NS1)
C ------> F(I) INPUT AS MOLE/GM OF MIXTURE <------
C       ASSUME ALL POSITIVE IONS ARE NO+ I.E. XNRT=1.0
      XNRT=1.0
C         CALCULATE MOLECULAR WEIGHT OF THE INITIAL MIXTURE
      DO 5 I=1,NPS
      READ(5,100) S(I)
C           COMPUTE AVERAGED FLUX OF ENTRAINMENT
      TTB(I)=0.0
      PTB(I)=0.0
      UTB(I)=0.0
      DO 11 II=1,NS
      FTB(II,I)=...
   11 CONTINUE
      Y(1)=0.0
      YO(1)=0.0
      UE(1)=...
      WRITE(6,105)
      DO 1 J=2,NSL
      READ(5,100)  Y(J),PE(J),TE(J),UE(J),(FE(II,J),II=1,NS)
C********  FE(I) ARE IN MOLE/GM-OF-MIXTURE
      PE(J)= 1.013E6*PE(J)
C****** PE(J) INPUT AS ATM AND CONVERTED TO DYNE/CM2
      WRITE(6,106) J,Y(J),PE(J),TE(J),UE(J)
     1, (FE(II,J),II=1,NS)
      IF(I.GT.1) GO TO 1
      YOMAX(I,J)=Y(J)
    1 CONTINUE
      DO 3 J=2,NSL
      J1=J
      DY= Y(J)-Y(J-1)
      DY5= 0.5*DY
      PTB(I)=PTB(I)+DY*PE(J)
      TTB(I)=TTB(I)+DY*TE(J)
      UTB(I)= UTB(I)+DY5*(UE(J)+UE(J-1))
      DO 10 II=1,NS
      FTB(II,I)= FTB(II,I)+DY*FE(II,J)
   10 CONTINUE
      IF (I.GT.1) GO TO 3
      YO(J)=Y(J)
      PTBO(J)= PTB(I)/Y(J)
      TTBO(J)= TTB(I)/Y(J)
      UTBO(J)= UTB(I)/Y(J)
      F1TBO(J)= FTB(1,I)/Y(J)
      F2TBO(J)= FTB(2,I)/Y(J)
      F3TBO(J)= FTB(3,I)/Y(J)
      F4TBO(J)= FTB(4,I)/Y(J)
      F5TBO(J)= FTB(5,I)/Y(J)
      F6TBO(J)= FTB(6,I)/Y(J)
      F7TBO(J)= FTB(7,I)/Y(J)
      F8TBO(J)= FTB(8,I)/Y(J)
    3 CONTINUE
    4 UTB(I)= UTB(I)/Y(J1)
      PTB(I)=PTB(I)/Y(J1)
```

```
                  FTB(I)=TTB(I)/Y(J1)
                  SUM=0.0
                  DO 12 II=1, NS
                  FTB(II,I)= FTB(II,I)/Y(J1)
      110         SUM=SUM+FTB(II,I)*WI(II)
                12 CONTINUE
                  DO 14 II=1,NS
                  FTB(II,I)=FTB(II,I)/SUM
                14 CONTINUE
      120     C****** NORMALIZED IN MOLE/GM OF MIXTURE
                  WA(I)=0.0
                  DO 3. II=1,NS
                  WA(I)=WA(I)+FTB(II,I)
                36 CONTINUE
      125         WA(I)= 1.0/WA(I)
                  RHOTB(I)= PTB(I)*WA(I)/(RR2*TTB(I))
                  DO 31 JJ=1,6
                  DD(JJ)=0.0
                  DO 32 II=1,NS
      13.         DD(JJ)= DD(JJ)+ XL(JJ,II)*FTB(II,I)
                32 CONTINUE
                31 CONTINUE
                  T1=TTB(I)/ 1000.0
                  HE=1000.*(-DD(5)/T1.+DD(6)+T1.*(DD(1)+T1.*(DD(2)/2.+T1.*(DD(3)/3.
      135        1 +T1*DD(4)/4.0))))
                  HSE(I)=HE+0.5*UTB(I)*UTB(I)/CTE
                  XXX1=RHOTB(I)*UTB(I)
                  RUE(I)=XXX1
                  RU2E(I)=XXX1*UTB(I)
      140         RUHSE(I)=XXX1*HSE(I)
                  RUF1E(I)=XXX1*FTB(1,I)
                  RUF2E(I)=XXX1*FTB(2,I)
                  RUF3E(I)=XXX1*FTB(3,I)
                  RUF4E(I)=XXX1*FTB(4,I)
      145         RUF5E(I)=XXX1*FTB(5,I)
                  RUF6E(I)=XXX1*FTB(6,I)
                  RUF7E(I)=XXX1*FTB(7,I)
                  RUF8E(I)=XXX1*FTB(8,I)
                  WRITE(6,126)   S(I),PTB(I),TTB(I),UTB(I), (FTB(II,I),II=1,NS)
      15.         WRITE(6,132)
                  WRITE(6,133) I,WA(I),HE,HSE(I),   RUE(I),RU2E(I),
                 1 RUHSE(I),RUF1E(I),RUF2E(I),RUF3E(I),RUF4E(I),RUF5E(I)
                 2,RUF6E(I), RUF7E(I),RUF8E(I)
                 5 CONTINUE
      1 5         YMAX=YOMAX(1,NSL)
                  CALL BREAK(YMAX)
                  GAMA=CP/(CP-RR1/AM)
                C      CALCULATE INITIAL SPEED OF SOUND
                  SS=  SQRT(GAMA*RR2*T/WM)
      150       C        CLACULATE INITIAL MACH NUMBER
                  XMA=U/SS
                  AXX1=((U-UP)**2+VP**2)
                  UR = SQRT(AXX1)
                  AM=1.21E-5*(T**1.5)/(T+110)
      155         REP=RHO* UR*RP/UM
```

```
      XMAP=XMA* UR/U
      WRITE(6,116)P,WM,RHO,HS,F(NS1),UP,VP      ,TP,RP,SE,YE
      WRITE(6,118) GAMA,CP,SS,XMA ,XMAP,REP
  999 CONTINUE
  170 100 FORMAT(8E10.3)
      101 FORMAT(10I5)
      1 2 FORMAT(/ 5X, *I*, 6X,*WA*,10X, *HE*,10X,*HSE*,
     1 9X,*REUE*, 7X,*REUE2*,7X,*REUEHSE*,7X,*RUF1E*,7X,*RJF2E*,7X,*RUF3
     2E*/9X,*RUF4E*,7X,*RJF5E*,7X,*RUF6E*,7X,*RUF7E*,7X,*RJF8E*)
  175 103 FORMAT(1H ,I5,1P9E12.3/5X,8E12.3)
      104 FORMAT( // 3X,*T(K)*,7X,*CPA*, 7X,*CPV*)
      105 FORMAT(/ 2X,*J*, 4X,*Y*,10X,*PE*,8X,*TE*,8X,*UE*
     1,4X,*FE(1) (MOLE/GM)=*)
      106 FORMAT(1X,I2,1X,F6.2,2(1P11E11.3/))
   10 107 FORMAT(1H ,*NPS=*,I5,3X,*NSL=*,I ,3X,*NOS=*,I5,3X,*IBUG=*,I5,3X,
     1 *NO. OF REACTIONS=*,I5,3X,*NO. OF SPECIES=*,I5,3X,
     2   *NSO=*,I5,3X,*BREAK-UP PARAMETER=*,I2/)
      108 FORMAT(1H ,*INITIAL S=*,F7.3,3X,* J.R. STEP SIZE(GM/SEC)=*,1PE1..3
     1 ,3X,*FINAL DISTANCE=*,E10.3,3X,
  105 + *PRINT INCREMENT=*,E10.3)
      109 FORMAT(/2X,*  C1=*,1PE10.3,2X,*C2=*,E1..3,2X,*C5=*,E10.3,2X,*C6=*,
     1E1..3,2X,*C7=*,E1..3,2X,*C8=*,E10.3,2X,*FF3=*,E10.3,2X,*FF4=*,E10.
     223)
      110 FORMAT(1H ,*  N1=*,1PE10.3,2X,*N2=*,E10.3,2X,*N5=*,E10.3,2X,*N6=*,
  1,0 1E10.3,2X,*B6=*,E1..3,2X,*B7=*,E1..3,2X,*B8=*,E10.3)
      111 FORMAT(1H ,*  NNO+/N+=*,1PE1..3,2X,*FNO+=*,E10.3,2X,*FE-=*,E10.3,2
     1X,*FO=*,E10.3,2X,*FF-=*, E10.3,2X,*FN=*,E1..3,2X,*FO2=*,E10.3/
     2 3X,*FN2=*,E10.3,2X,*FNO=*,E10.3)
      112 FORMAT(1H ,* -------- KINETIC CALCULATION ONLY   -------*/)
  195 115 FORMAT(8X,*   --- PROPERTIES OF THE INJECTED LIQUID ------ */
     1 20X,*MOLECULAR WT.=*,F1..2/20X,*SPECIFIC HEAT(CAL/G-K)=*,1PE10.3/
     2 20X,*BOILING PT. (K)=*,E10.3/20X,*HEAT OF VAPORIZATION(CAL/G)=*,E
     31..3  /2.X,*DENSITY (G/CM3)=*,E1..3/2 X,*MASS FLUX(G/SEC)=*,E1..3,
       /20X,*JET VELOCITY(CM/SEC)=*,E10.3/20X,*JET ANGLE(RAD.)=*,E10.3/
  2.0 5 20X,*TEMPERATURE(K)=*,E10.3/20X,*SURFACE TENSION(DYNE/CM)=*,E10.3
     5 /20X,*VISCOSITY(GM/CM-SEC)=*,E10.3  / 20X,*ORIFICE DIAMETER(CM)=*
     7,E1..3/2.X,*LIQUID DROP COEFFICIENTS*,/20X,*AK=*,E10.3/2.X,
     8  *BK=*,E10.3/)
      116 FORMAT (/2X,  *P=*,1PE10.3
  2.5 1,3X,*WM=*,E10.3,3X,*RHO=*,E10.3,3X,*HS=*,E10.3,3X,*F..=*,E10.3,3X,
     2 *UP=*,E10.3,2X,*VP=*,E10.3/ 2X,                          *TP=*
     2,E10.3,3X,*RP=*,E10.3,3X,*SE=*,E10.3,3X,*YE=*,E10.3)
      118 FORMAT(/2X, *  INITIAL THERMODYNAMIC INFORMATION */ 2X,*GAMA=*,
     1 F6.3,2X,* CP(CAL/G)=*,1PE10.3,2X,*SS=*,E1..3,2X,*XA=*,E10.3,2X,
  210 1*MAP=*,E10.3,2X,*RE=*,E10.3)
      119 FORMAT (/2X,*---- IS CALCULAATION DOES NOT CONVERGE IN IT=*,I5/)
      126 FORMAT(1X,*AV=*,F6.2,2(1P11E11.3/))
          RETURN
          END
```

```
*DECK.CPUTIN
      SUBROUTINE CPUTIN (IKINE,NS1)
C     ------------------------------------------------------------------
      COMMON /HEAT/ XL(6,51),WI(51)
      COMMON/CHEM2/CM(51,51),FI(51),WP(51),WM1(51),WDOT(51),QX(51)
     1 ,RC(100,5)
      COMMON /SPID/ IZH,IZ1,IZ2,IZ3,IZ4,IZ5,   IH,INOP,IEM,IOX,IFM,IN
      COMMON/CHEM1/IRR(100),IRT(100),IRRR(100,8),IZD(8),IDENT(51)
      AV=6.03E23
      IH=NS1+1
      INOP=NS1+1
      IEM=NS1+1
      IOX=NS1+1
      IFM=NS1+1
      IN=NS1+1
      DO 10 L=1,NS1
      READ(5,102) IDENT(L),WI(L),(XL(II,L),II=1,6)
      WRITE(6,103)IDENT(L),WI(L),(XL(II,L),II=1,6)
      IF (IDENT(L).EQ.IZH) IH=L
      IF (IDENT(L).EQ.IZ1) INOP=L
      IF (IDENT(L).EQ.IZ2) IEM=L
      IF (IDENT(L).EQ.IZ3) IOX=L
      IF (IDENT(L).EQ.IZ4) IFM=L
      IF (IDENT(L).EQ.IZ5) IN=L
   10 CONTINUE
      DO 2 I=1,IKINE
      READ (5,100) (IZD(J),J=1,8),IRR(I),IRT(I),(RC(I,KR),KR=1,5)
      WRITE(6,101) I,  (IZD(J),J=1,6),IRR(I),IRT(I),(RC(I,KR),KR=1,5)
      DO 5 J=1,8
      IRRR (I,J)=NS1+1
      DO 3 L=1,NS1
      IF (IZD(J)-IDENT(L)) 3,4,3
    4 IRRR(I,J)=L
    3 CONTINUE
    5 CONTINUE
      RC(I,1)= AV*RC(I,1)
    2 CONTINUE
  100 FORMAT(8(A4,1X),2I2, E9.2,F5.2,E8.1,2E7.1)
  101 FORMAT(2X,I2,2X,3(1X,A4,1X,"+"),1X,  A4,1X,"=",3(1X,A4,1X,"+"),
     1 1X,A4,1X,2I4,1P5E11.2)
  102 FORMAT (A4,6X,7E10.3)
  103 FORMAT (1X,A4,6X,7E10.3)
      RETURN
      END
```

```
*DECK.HRATE
      SUBROUTINE HRATE
      COMMON CPA(40),CPV(40),HA(40),RHOE(40),PSIV(51),HSE(40),UE(40),
     1 S(40),TB(40),PTB(40)
     2 ,RUE(40),RU2E(40),RUHSE(40),Y(40),RUF1E(20)
     3 ,SO,DS,SMAX,RHO,FV,U,T,HS,ATD  ,P,RR,DSP,CTE,RR1,RR2,AV,C,AI,YE
     4 ,WM,SE,AE,RPO,TP,RHOP,EP,DEP,DAE,DTS,TS,DRP,DRHOP,DSE,DYE,DT,DHS
     5 ,DU,DUP,DFV,DRHO,DP,DA,ADS,ARHO2,UM,SI,SXO,BETA
     6 ,RUAI,RUEI,RUF1EI,RUF2EI,RUF3EI,RUF4EI,RUF5EI,PHADS
      COMMON RUF4E(20),D32(20),          RKI(8),WDOTN(5),U_(20),RUF1E(20),
     1 RUF2E(20),RUF3E(20),FQI, FE(8,20),PE(20),TE(20)
     2,    F(51),DF(51),D32I,D32II,XMLI,XMDU,ETA,ALD,A_T,DE,VLI,THETA
     3 ,F1,F2,F3,F4,F5,PI,AI1,B8,XNF8,CF8,UP,VP,GAMA,C1,C2,C3,C4,C5,C6,
     4 C7,C8 ,CP,A,RP ,XMA,XMAP,SS,UR,DUR,HSR,DHSR,XMLO
     5 ,RUF6E(20),RUF7E(20),RUF8E(20)
     6 ,RUF6EI,RUF7EI,RUF8EI,F6,F7,F8 ,F9 ,FFPE,FFTE,FFAE
       ,FFF,FFEV ,CF1,CF2,CF5,CF6,CF7,XNF1,XNF2,XNF5,B6,B7,FF3,FF4,XNRT
     8,XBK,YBK,TBK,PEBK,RU2BK,RHOXY,SOP,NSO,NWCR,DEQP,S150
      COMMON STB(30),TTB(30),RHOTB(30),UTB(30),FTB(8,30)
      COMMON /HEAT/ YL(6,51),WI(51)
      COMMON/LIQUID/ CPL,TBP,DHV,RHOL,WV,TBPO,SIG,TLO,UML,DD,WECR,
     1 FFVI,AK,BK,WE,ITBK,FFV,TBPY
      COMMON/INTEG/NPS,NPT,IDD(20),NSL,IOPT,KO,NS,NS1,IBDS,ID,IKIN
      COMMON/CHEM2/CM(51,51),FI(51),WP(51),WM1(51),WDOT(51),QX(51)
     1 ,RC(100,5)
      COMMON /SPID/ IZH,IZ1,IZ2,IZ3,IZ4,IZ5,   IH,INOP,IEM,IOX,IFM,IN
      COMMON/CHEM1/IRR(100),IRT(100),IRRR(100,8),IZD(8),IDENT(51)
      F1=FI(INOP)
      F2=FI(IEM)
      F3=FI(IOX)
      F4=FI(IFM)
      F5=FI(IN)
      RKI(3)=0.0
      RKI(4)=0.0
      IF(RP   .LT. 1.0E-9) GO TO 25
      ULI=  SQRT(UP*UP+VP*VP)
      XMDU=0.5*XMLO*RP*RP/(ULI*A*RPO**3)
      TI50= T /5000.
      VPLUS= 1.88E5* SQRT(TI50)
      VEMIUS= 4.4E7* SQRT(TI50)
      VMIUS= 2.36E5* SQRT(TI50)
      DNM= (VEMIUS*RHO *F2   + (VMIUS+U -ULI)*RHO *F4  )
      CC= (VPLUS+U -ULI)*RHO *F1  /DNM
      CALL ETAGT(ETA,CC,SI)
      RKS    = 1.5*(1.0+ETA)*XMDU *(VPLUS+U -ULI)/ RHO
      RKI(3)=FF3*RKS   *VEMIUS*RHO *F2  /DNM
      RKI(4)=FF4*RKS   *(VMIUS+U -ULI)*RHO *F4   /DNM
   25 CONTINUE
      W3=RKI(3)*RHO*FI(INOP)
      W4=RKI(4)*RHO*FI(INOP)
      QX(INOP)=-W3-W4
      QX(IEM)=-W3
      QX(IFM)=-W4
      QX(IOX)=W3+W4
      QX(IN)=W3
```

```
      RETURN
      END
```

```
*DECK.ETAGT
      SUBROUTINE ETAGT(ETA,CC,SI)
      IF ((CC.LT.1.0) .AND. (CC.GT.0.0)) GO TO 4
    5 CONTINUE
      WRITE(6,100) CC,SI
      STOP
  100 FORMAT(1H ,*------  CC=*, 5E10.3)
    4 CONTINUE
      EP1=1.0E-1
      DETA=0.5*ETA
      ETA=1.0E-5-DETA
      DEL1=1.0
    1 CONTINUE
      ETA= ETA  +DETA
      XLHS= EXP(-ETA)
      XRHS= CC*(1.0+ETA)
      DEL= XLHS-XRHS
      EPS= ABS(XLHS*EP1)
      IF( ABS(DEL).LE.EPS) GO TO 3
      IF ((DEL*DEL1).GE.0.0) GO TO 2
      ETA= ETA-DETA
      DETA= 0.5*DETA
      GO TO 1
    2 DEL1= DEL
      GO TO 1
    3 CONTINUE
      RETURN
      END
```

```
*DECK,CHEMF
      SUBROUTINE CHEMF
      COMMON CPA(40),CPV(40),WA(40),RHOE(40),PSIV(51),HSE(40),UE(40),
     1 S(40),TB(40),PTB(40)
     2 ,RUE(40),RU2E(40),RUHSE(40),Y(40),RUF1E(20)
     3 ,SO,DS,SMAX,RHO,FV,U,T,HS,ATO   ,P,RR,DSP,CTE,RR1,RR2,AV,C,AI,YE
     4 ,WM,SE,AE,RPO,TP,R1OP,EP,DEP,DAE,UTS,TS,DRP,DRHOP,D3E,DYE,DT,DHS
     5 ,DU,DUP,DFV,DRHO,D2,DA,ADS,ARHO2,UM,SI,SXO,BETA
     6 ,RUAI,RUEI,RUF1EI,RUF2EI,RUF3EI,RUF4EI,RUF5EI,P1A35
      COMMON RUF4E(20),D32(20),        RKI(8),WDOTN(5),U.(20),RUF1E(20),
     1 RUF2E(20),RUF3E(20),FQI, FE(8,20),PE(20),TE(20)
     2,    F(51),DF(51),D32I,D32II,XMLI,XMDU,ETA,ALO,A_T,DE,VLI,THETA
     3 ,F1,F2,F3,F4,F5,PI,AI1,B6,XMF8,CF5,UP,VP,GAMA,C1,C2,C3,C4,C5,C6,
     4 C7,C8 ,CP,A,RP  ,XMA,XMAP,SS,UR,DUR,HSR,DHSR,XMLO
     5 ,RUF6E(20),RUF7E(20),RUF8E(20)
     6 ,RUF6EI,RUF7EI,RUF8EI,F6,F7,F8  ,F9  ,FFPE,FFTE,FFAE
     7 ,FFF,FFEV  ,CF1,CF2,CF3,CF6,CF7,XNF1,XNF2,XNF3,B5,B7,FF3,FF4,XNRT
     8 ,XBK,YBK,TBK,PEBK,RUEBK,RHOXY,SOP,NSO,NWCR,DEQP,S151
      COMMON STB(30),TTB(30),RHOTB(30),UTB(30),FTB(8,30)
      COMMON/HEAT/ XL(6,51),WI(51)
      COMMON/LIQUID/ CPL,TBP,DHV,RHOL,WV,TBPO,SIG,TLO,JM.,JO,WECR,
     1 FFVI,AK,BK,WE,ITBK,FFV,TBPY
      COMMON/INTEG/NPS,NPT,IDO(20),NSL,IOPT,KO,NS,NS1,IBJS,ID,IKINE
      COMMON/CHEM2/CM(51,51),FI(51),WP(51),WM1(51),WDOT(51),QX(51)
     1 ,RC(100,5)
      COMMON /SPID/ IZH,IZ1,IZ2,IZ3,IZ4,IZ5,   IH,INOP,IE4,IOX,IFM,IN
      COMMON/CHEM1/IRR(100),IRT(100),IRRR(100,8),IZD(8),IDENT(51)
      DIMENSION RO(80),RM(80)
      RRT=1.987*T
C     GAS CONSTANT IN 82.06 CM3-ATM/G-MOLE-K
      RRT1=82.06*T
      XLOGT=ALOG(T)
      DO 3 IR=1,NS1
      QX(IR)=0.0
      WP(IR)=0.0
      WM1(IR)=0.0
      WDOT(IR)=0.
      DO 4 JR=1,NS1
    4 CM(IR,JR)=0.0
    3 CONTINUE
      CALL HRATE
      DO 1 IR=1,IKINE
      J1=NS1+1
      J2=NS1+1
      J3=NS1+1
      J4=NS1+1
      J5=NS1+1
      J6=NS1+1
      J7=NS1+1
      J8=NS1+1
      KIRT=IRT(IR)
      GO TO (841,842,843,844,845,846,847,848,849),KIRT
  841 RKF=RC(IR,1)
      GO TO 850
  842 RKF=RC(IR,1)/T
```

```
      GO TO 850
  843 KKF=RC(IR,1)/T/T
      GO TO 85.
  844 KKF=RC(IR,1)/ SQRT(T)
      GO TO 850
  845 KKF=RC(IR,1)* EXP(RC(IR,3)/RRT)
      GO TO 850
  846 KKF=RC(IR,1)* EXP(RC(IR,3)/RRT)/T
      GO TO 850
  847 KKF=RC(IR,1)/T  / SQRT(T)
      GO TO 850
  848 KKF=RC(IR,1)*(T   **RC(IR,2))* EXP(RC(IR,3)/T   )
      GO TO 850
  849 XK=RC(IR,4)
      KKF=RC(IR,1)*(T**RC(IR,2))*(XK/T+1.0)* EXP(RC(IR,3)/T)
      GO TO 85.
  850 CONTINUE
      KIRR=IRR(IR)
      GO TO (851,852,853,854,855,856,857,858,859,860,851),KIRR
  851 J1=IRRR(IR,1)
      J2=IRRR(IR,2)
      J5=IRRR(IR,5)
      J6=IRRR(IR,6)
      CRR=RKF*RHO*RHO
      RQ(IR)=CRR*FI(J1)*FI(J2)
      RM(IR)=0.0
      DO 778 J=1,6
      SIGN=1.0
      IF (J .GT. 4) SIGN=-1.0
      IROW=IRRR(IR,J)
      CM(IROW,J1)=CM(IROW,J1)+SIGN*CRR*FI(J2)
      CM(IROW,J2)=CM(IROW,J2)+SIGN*CRR*FI(J1)
      QX(IROW)=QX(IROW)+SIGN*RQ(IR)
  778 CONTINUE
      GO TO 880
  852 J1=IRRR(IR,1)
      J2=IRRR(IR,2)
      J5=IRRR(IR,5)
      CRR=RKF*(RHO**3)/WM*AV
      RQ(IR)=CRR       *FI(J1)*FI(J2)
      RM(IR)=0.0
      DO 779 J=1,5
      SIGN=1.0
      IF (J .GT.4) SIGN=-1.
      IROW=IRRR(IR,J)
      CM(IROW,J1)= CM(IROW,J1)+SIGN*CRR       *FI(J2)
      CM(IROW,J2)= CM(IROW,J2)+SIGN*CRR       *FI(J1)
      QX(IROW)=QX(IROW)+SIGN*RQ(IR)
  779 CONTINUE
      GO TO 880
  853 J1=IRRR(IR,1)
      J2=IRRR(IR,2)
      J5=IRRR(IR,5)
      J6=IRRR(IR,6)
      J7=IRRR(IR,7)
```

```
                      CRR =RKF*RHO*RHO
                      RQ(IR)=CRR *FI(J1)*FI(J2)
                      RM(IR)=0.0
                      DO 780 J=1,7
115                   SIGN=1.0
                      IF (J .GT.4)  SIGN=-1..
                      IROW=IRRR(IR,J)
                      CM(IROW,J1)=CM(IROW,J1)+SIGN*CRR*FI(J2)
                      CM(IROW,J2)=CM(IROW,J2)+SIGN*CRR*FI(J1)
120                   QX(IROW)=QX(IROW)+SIGN*RQ(IR)
                  780 CONTINUE
                      GO TO 880
                  854 J1=IRRR(IR,1)
                      J2=IRRR(IR,2)
125                   J5=IRRR(IR,5)
                      CRR=RKF*RHO*RHO
                      RQ(IR)=CRR        *FI(J1)*FI(J2)
                      RM(IR)=0.0
                      DO 776 J=1,6
130                   SIGN=1.0
                      IF (J .GT. 4) SIGN =-1.0
                      IROW = IRRR(IR,J)
                      CM(IROW,J1)=CM(IROW,J1)+SIGN*CRR        *FI(J2)
                      CM(IROW,J2)=CM(IROW,J2)+SIGN*CRR        *FI(J1)
135                   QX(IROW)=QX(IROW)+SIGN*RQ(IR)
                  776 CONTINUE
                      GO TO 88.
                  85! J1=IRRR(IR,1)
                      J5=IRRR(IR,5)
140                   J6=IRRR(IR,6)
                      CRR=RKF*RHO*RHO/WM
                      RQ(IR)=CRR*FI(J1)
                      RM(IR)=0.0
                      DO 777 J=1,6
145                   SIGN=1..
                      IF (J .GT. 4) SIGN=-1.0
                      IROW = IRRR(IR,J)
                      CM(IROW,J1)=CM(IROW,J1)+SIGN*CRR
                  777 CONTINUE
1 0                   GO TO 880
                  856 J1=IRRR(IR,1)
                      J2=IRRR(IR,2)
                      J3=IRRR(IR,3)
                      J5=IRRR(IR,5)
155                   CRR=RKF*(RHO**4)*AV*AV
                      RQ(IR)=CRR*FI(J1)*FI(J2)*FI(J3)/WM
                      RM(IK)=0.0
                      DO 781 J=1,5
                      SIGN=1.0
160                   IF (J .GT. 4) SIGN=-1.0
                      IROW=IRRR(IR,J)
                      CM(IROW,J1)=CM(IROW,J1)+SIGN*CRR*FI(J2)*FI(J3)/WM
                      CM(IROW,J2)=CM(IROW,J2)+SIGN*CRR*FI(J1)*FI(J3)/WM
                      CM(IROW,J3)=CM(IROW,J3)+SIGN*CRR*FI(J1)*FI(J2)/WM
1 0                   QX(IROW)=QX(IROW)+SIGN*2.0*RQ(IR)
```

```
      781 CONTINUE
          GO TO 880
      857 J1=IRRR(IR,1)
          J5=IRRR(IR,5)
          J6=IRRR(IR,6)
          J7=IRRR(IR,7)
          CRR=RKF*RHO*RHO
          RQ(IR)=CRR*FI(J1)/WM
          KM(IR)=0.0
          DO 782 J=1,7
          SIGN=1.0
          IF (J.GT. 4) SIGN=-1.0
          IROW=IRRR(IR,J)
          CM(IROW,J1)=CM(IROW,J1)+SIGN*CRR
      782 CONTINUE
          GO TO 880
      858 J1=IRRR(IR,1)
          J2=IRRR(IR,2)
          J3=IRRR(IR,3)
          J5=IRRR(IR,5)
          J6=IRRR(IR,6)
          CRR=RKF*(RHO**3)*AV
          RQ(IR)=CRR*FI(J1)*FI(J2)*FI(J3)
          KM(IR)=0.0
          DO 783 J=1,6
          SIGN=1.0
          IF (J .GT. 4) SIGN=-1.0
          IROW=IRRR(IR,J)
          CM(IROW,J1)=CM(IROW,J1)+SIGN*CRR*FI(J2)*FI(J3)
          CM(IROW,J2)=CM(IROW,J2)+SIGN*CRR*FI(J1)*FI(J3)
          CM(IROW,J3)=CM(IROW,J3)+SIGN*CRR*FI(J1)*FI(J2)
          QX(IROW)=QX(IROW)+SIGN*2.0*RQ(IR)
      783 CONTINUE
          GO TO 880
      859 J1=IRRR(IR,1)
          J2=IRRR(IR,2)
          J3=IRRR(IR,3)
          J4=IRRR(IR,4)
          J5=IRRR(IR,5)
          J6=IRRR(IR,6)
          CRR=RKF*(RHO**4)*AV*AV
          RQ(IR)=CRR*FI(J1)*FI(J2)*FI(J3)*FI(J4)
          KM(IR)=0.0
          DO 784 J=1,6
          SIGN=1.0
          IF (J.GT.4) SIGN=-1.0
          IROW=IRRR(IR,J)
          CM(IROW,J1)=CM(IROW,J1)+SIGN*CRR*FI(J2)*FI(J3)*FI(J4)
          CM(IROW,J2)=CM(IROW,J2)+SIGN*CRR*FI(J1)*FI(J3)*FI(J4)
          CM(IROW,J3)=CM(IROW,J3)+SIGN*CRR*FI(J1)*FI(J2)*FI(J4)
          CM(IROW,J4)=CM(IROW,J4)+SIGN*CRR*FI(J1)*FI(J2)*FI(J3)
          QX(IROW)=QX(IROW)+SIGN*3.0*RQ(IR)
      784 CONTINUE
          GO TO 880
      860 J1=IRRR(IR,1)
```

```
      J2=IRRR(IR,2)
      J5=IRRR(IR,5)
      J6=IRRR(IR,6)
      J7=IRRR(IR,7)
      J8=IRRR(IR,8)
      CKR=CKF*RHO*RH)
      RD(IR)=CKR*FI(J1)*FI(J2)
      RM(IR)=0.0
      DO 745 J=1,8
      SIGN=1.0
      IF (J.GT.4)SIGN=-1.
      IROW=IRRR(IR,J)
      DM(IROW,J1)=DM(IROW,J1)+SIGN*CKR*FI(J2)
      DM(IROW,J2)=DM(IROW,J2)+SIGN*CKR*FI(J1)
      DX(IROW)=DX(IROW)+SIGN*RD(IR)
  745 CONTINUE
      GO TO 850
  751 J1=IRRR(IR,1)
      J2=1H
      DEL=RC(IR-5)
      CKR=DEL*CKF*RHO*RHO
      RD(IR)=CKR*FI(J1)*FI(IH)
      RM(IR)=0.0
      DO 746 J=1,8
      SIGN=1.0
      IF (J.GT.4)SIGN=-1.0
      IROW=IRRR(IR,J)
      DM(IROW,J1)=DM(IROW,J1)+SIGN*CKR*FI(J2)
      DM(IROW,J2)=DM(IROW,J2)+SIGN*CKR*FI(J1)
      DX(IROW)=DX(IROW)+SIGN*RD(IR)
  746 CONTINUE
  850 CONTINUE
      WP(J8)=WP(J8)+RD(IR)
      WM1(J8)=WM1(J8)+RM(IR)
      WP(J7)=WP(J7)+RD(IR)
      WM1(J7)=WM1(J7)+RM(IR)
      WP(J6)=WP(J6)+RD(IR)
      WM1(J6)=WM1(J6)+RM(IR)
      WP(J5)=WP(J5)+RD(IR)
      WM1(J5)=WM1(J5)+RM(IR)
      WP(J4)=WP(J4)-RD(IR)
      WM1(J4)=WM1(J4)-RM(IR)
      WP(J3)=WP(J3)-RD(IR)
      WM1(J3)=WM1(J3)-RM(IR)
      WP(J2)=WP(J2)-RD(IR)
      WM1(J2)=WM1(J2)-RM(IR)
      WP(J1)=WP(J1)-RD(IR)
      WM1(J1)=WM1(J1)-RM(IR)
    1 CONTINUE
      DO 857 J=1,NS
C     PRODUCTION RATE IN MOLE/GM-CM
      WDOT(J)=(WP(J)-WM1(J))[illegible]
  857 CONTINUE
      ADUM=A*DS*RUAT
      DX(1)=DX(1)*ADS+[illegible] ((RUF1(1)-RUB1*FI(1))*D4L-FI(1)*RHS[illegible]
```

```
      QX(2)=QX(2)*ADSM+RUAI*((RUF2E1-RUE1*FI(2))*D4E-FI(2)*PHADS)
      QX(3)=QX(3)*ADSM+RUAI*((RUF3E1-RUE1*FI(3))*D4E-FI(3)*PHADS)
      QX(5)=QX(5)*ADSM+RUAI*((RUF5E1-RUE1*FI(5))*D4E-FI(5)*PHADS)
      QX(6)=QX(6)*ADSM+RUAI*((RUF6E1-RUE1*FI(6))*D4E-FI(6)*PHADS)
      QX(7)=QX(7)*ADSM+RUAI*((RUF7E1-RUE1*FI(7))*D4E-FI(7)*PHADS)
      QX(8)=QX(8)*ADSM+RUAI*((RUF8E1-RUE1*FI(8))*D4E-FI(8)*PHADS)
      DO 2 I=1,NS
      QX(I)=QX(I)+FI(I)
      DO 2  J=1,NS
      CM(I,J)=CM(I,J)*ADSM
      IF(I.EQ.J) CM(I,J)=1.0+CM(I,J)
    2 CONTINUE
      IF (QX(4) .GT. 0.0) GO TO 6
      IF (IBUG.EQ.0) GO TO 6
      DO 24 I=1,NS
      WRITE(6,100) (CM(I,J),J=1,NS),QX(I)
   24 CONTINUE
    6 CONTINUE
      CALL SLOP(QX,CM,NS)
      IF (IBUG.EQ.0) GO TO 7
      DO 5 I=1,NS
      WRITE(6,100) (CM(I,J),J=1,NS),QX(I)
    5 CONTINUE
    7 CONTINUE
C           QX(I) IS NOW IN MOLE/GM UNIT
      DO 23 I=1,NS
      F(I)= QX(I)*WI(I)
   23 CONTINUE
C       F(I) NOW  IN MASS FRACTION UNIT
  100 FORMAT( 2X, 1P10E12.3)
      RETURN
      END
```

```
*DECK.SLOP
      SUBROUTINE SLOP(X,A,N)
C     THIS PROGRAM FINDS THE SOLUTIONS TO A SET OF N SIMULTANEOUS LINEAR
C     EQUATIONS BY USING THE GAUSS-GORDAN REDUCTION ALGORITHM WITH THE
C       DIAGONAL PIVOT STRATEGY
C          DESIGNED PARTICULARLY FOR IMPLICIT CHEMISTRY ---CJK
      DIMENSION A(51,51),X(51)
      DO 9 K=1,N
      IF( ABS(A(K,K)) .GT. 1.0D-1 ) GO TO 5
      WRITE (6,101)   K,A(K,K)
      DO 10 IR=1,N
      WRITE(6,100)(A(IR,JR),JR=1,N),X(IR)
   10 CONTINUE
  100 FORMAT(1X,   1P10E12.3)
  101 FORMAT( * ERROR--- SMALL PIVOT *,I5,1PE12.5)
      STOP
    5 KP1= K+1
      DO 6 J= KP1, N
    6 A(K,J)= A(K,J)/A(K,K)
      X(K)= X(K)/A(K,K)
      A(K,K)= 1.0
      DO 9 I=1,N
      IF (I.EQ.K .OR. A(I,K).EQ.0.) GO TO 9
      DO 8 J=KP1,N
    8 A(I,J)= A(I,J)- A(I,K)*A(K,J)
      X(I)= X(I)- A(I,K)*X(K)
      A(I,K)=0.
    9 CONTINUE
   99 CONTINUE
      RETURN
      END
```

```
*DECK,BREAK
      SUBROUTINE BREAK(YMAX)
      DIMENSION DD(6)
      COMMON CPA(40),CPV(40),WA(40),RHOE(40),PSIV(40),HEL(40),UE(40),
     1 S(40),TB(40),PTB(40)
     2 ,RUE(40),RU2E(40),RUHSE(40),Y(40),RUF8E(20)
     3 ,S0,DS,SMAX,RHO,FV,U,T,HS,ATD   ,P,RK,USP,CTE,RN1,RR2,AV,C,A1,YE
     ,WM,SE,AE,RPJ,TP,RHOP,EP,DEP,DAE,DTS,TS,DRP,DRHOP,DSE,DYE,DT,DHS
     5 ,DU,DUP,DFV,DRHO,DP,DA,ADS,ARHOZ,JM,S1,SXD,BETA
     3 ,RUAI,RUEI,RUF1EI,RUF2EI,RUF3EI,RUF4EI,RUF5EI,PHAS
      COMMON RUF4E(20),D32(20),          RKI(8),WDOTN(5),UL(10),RUF1E(20),
     1 RUF2E(20),RUF3E(20),FD1, FE(8,20),PE(20),TE(20)
     2,     F(51),DF(51),D321,D32II,XML1,XMOU,ETA,ALD,ALT,DE,VL1,THETA
     3 ,F1,F2,F3,F4,F5,PI,AI1,BB,XNF6,CF3,UP,VP,GAMA,C1,C2,C3,C4,C5,C6,
     + C7,C8 ,CP,A,RP ,XMA,XMAP,SS,UR,DUK,HSR,DHSR,XMLD
     ,RUF6E(20),RUF7E(20),RUF8E(20)
     5 ,RUF6EI,RUF7EI,RUF8EI,F6,F7,F8 ,F9 ,FFPE,FFTE,FFAE
     7 ,FFF,FFEV ,CF1,CF2,CF5,CF6,CF7,XNF1,XNF2,XNF5,B6,B7,FF3,FF4,XNRT
     8,XBK,YBK,TBK,PEBK,RU2BK,PHOXY,SDP,NSO,NHCR,DEQP,S15
      COMMON STB(30),TTB(30),RHOTB(30),UTB(30),FTB(8,30)
      COMMON /HEAT/ XL(5,51),WI(51)
      COMMON/LIQUID/ CPL,TBP,DHV,RHOL,WV,TBP0,SIG,TLO,JML,JJ,WECP,
     1 FFV1,AK,BK,WE,ITBK,FFV,TBPY
      COMMON/INTEG/NPS,NPT,IDD(20),NSL,IOPT,KO,NS,NS1,ISJS,IO,IKINE
      COMMON /SHOCK/ YD(20),PTBD(20),UTBD(20),TTBD(20),F1TBD(20),
     1               F2TBD(20),F3TBD(20),F4TBD(20),F5TBD(20),F6TBD(20),
     2               F7TBD(20),F8TBD(20)
      COMMON/CHEM2/CM(51,51),FI(51),WP(51),WM1(51),WDOT(51),DX(51)
     1 ,RC(100,5)
      COMMON /SPID/ IZH,IZ1,IZ2,IZ3,IZ4,IZ5,   I4,INOP,IE4,IOX,IF4,IN
      COMMON/CHEM1/IRR(10 ),IRT(10 ),IRRK(10 ,8),IZD(9),IDENT(51)
      SO=1.2
C     ESTABLISHING SHOCK FRONT CONDITIONS
      DO 42 ID=2,NPS
      IF (SO .GE. S(ID-1) .AND. SO.LT.S(ID)) GO TO 43
   42 CONTINUE
      WRITE (6,200) ID, S(ID),SO
      STOP
  200 FORMAT (2X,*--- OUT OF RANGE ID=*,I5,2X,*SI=*,E11.3,2X,*SO=*,E11.3
     1 )
   43 CONTINUE
      CALL LIPLN (SO,PTB,S,PX,ID)
      CALL LIPLN (SO,WA,S,WAX,ID)
      CALL LIPLN(SO,TTB,S,TX,ID)
      CALL LIPLN(SO,RUE,S,RUEX,ID)
      CALL LIPLN (SO,RU2E,S,RU2EX,ID)
      CALL LIPLN(SO,RUF1E,S,F(1),ID)
      CALL LIPLN(SO,RUF2E,S,F(2),ID)
      CALL LIPLN(SO,RUF3E,S,F(3),ID)
      CALL LIPLN(SO,RUF4E,S,F(4),ID)
      CALL LIPLN(SO,RUF5E,S,F(5),ID)
      CALL LIPLN(SO,RUF6E,S,F(6),ID)
      CALL LIPLN(SO,RUF7E,S,F(7),ID)
      CALL LIPLN(SO,RUF8E,S,F(8),ID)
      CALL LIPLN (SO,RUHSE,S,HSX,ID)
```

```
      F(NS1)=0.0
C     ----- F(I) ARE IN MOLE/GM. -----
      UX=RU2EX/RUEX
      DO 44 I=1,NS
C     F(I)=F(I)*WI(I)/RUEX
      PSIV(I)=F(I)
   44 CONTINUE
C     ----- F(I) IS NOW IN MASS FRACTIONS -----
      HSX=HSX/RUEX
      UX2=UX*UX
      RHOX=RUEX/UX
      HX=HSX-UX2/(2.*CTE)
C     ----- CALCULATING GAS PROPERTIES BEHIND JET SHOCK -----
      RHOXY=0.25
      RHOY=RHOX/RHOXY
    5 CONTINUE
      WRITE(6,121) PX,UX,HSX,RHOX,TX,WAX,(F(I),I=1,NS1)
      DO 40 IT=1,100
      PY=PX+RHOX*UX2*(1.0-RHOXY)
      HY=HSX-UX2*(RHOXY*RHOXY)/(2.*CTE)
      TBPY=TBPO
      TI=TX*PY/PX*RHOXY
      CALL TINV(HY,TY,TI,F,NS1,CPY)
      RHO=PY*WAX/RR2/TY
      IF (IBUG.NE.0)
     1WRITE (6,101)   RHOX,RHOY,RHOXY,RHO,PY,HY ,TY
      IF ( ABS((RHO/RHOY)-1.0).LT. 0.001) GO TO 41
      RHOY=0.5*(RHOY+RHO)
      RHOXY=RHOX/RHOY
   40 CONTINUE
      IF (IBUG.NE.0) WRITE(6,128) RHOX,RHOY,RHOXY,RHO,PY,HY
  128 FORMAT (/2X,* --- SHOCK CALCULATION DIVERGED*/1P10E12.3/)
   41 CONTINUE
      UY=UX*RHOXY
      RDHV=RR1/(DHV*WV)
      TBPOI=1./TBPO
      PV=PY/ATO
      TBPY=1.0/(TBPOI -RD4V*ALOG(PV))
      WRITE (6,122) PY,UY,HY,RHOY,TY ,TBPY
C     ----- COMPUTE FLASH VAPORIZATION AT SHOCKED PRESSURE -----
      UM=1.21E-5*(TY**1.5)/(TY+110)
      FFV=0.0
      IF (TBPY .LT. TLO) FFV=CPL*(TLO-TBPY)/DHV
      IF (FFV.GE.FFVI) FFV=1.0
C     ----- JET BREAK-UP -----
      ULI=VLI* SIN(THETA)
      WE=RHOY*UY*UY*0.5*DE/SIG
      IF ((WE.LT.WECR).AND.(ITBK.NE.1)) GO TO 51
      REJ=RHOY*UY*0.5*DE/UM
      XXX=REJ/(1.0+2.0*WE/ SQRT(REJ))
      XXX= SQRT(XXX)
      IF (IBUG.NE.0)
     1WRITE(6,131) RHOL,RHOY,UM,UML,DE,UY,XXX,TY
      TBK=0.536*(RHOL/RHOY)**(0.6666)*(UM/UML)**(0.3333)*0.5*DE/UY*XXX
      XXX1=RHOY*CD*(UY-ULI)**2/DE/RHOL
```

```
      UBK=2.0*XXX1*TBK+ULI
      YBK=VP*TBK
      DBK=(XXX1*TBK+ULI)*TBK
      IF(DBK.LT.DE) DBK=DE
      XBK=DBK+SO
C     ----- CALCULATING DROPLET SIZE -----
      WEL=DE*UY*UY*RHOL/SIG
      GAMA=CPY/(CPY-RR1/WMX)
      SS=  SQRT(GAMA*RR2*TY/WMX)
      XMA=UY/SS
      D30=48.0*(WEL**(-0.375))*(REJ/XMA)**(-0.25)*DE
      D32I=1.26*D30
      DMAX=D30*4.6*(D30/DE)**(0.16)
      READ (5,100) FIM
      GO TO 62
C************ VAPOR PRESSURE BREAK UP
   61 XEPS=0.1
      TSH=TBPY/(1.-XEPS)
C******   TSH= SHATTER TEMPERATURE
      IF(TLO.GT.TSH) TLO=TBPY
      AXX1= ((UY-VLI* SIN(THETA))**2 +VP**2)
      UR= SQRT(AXX1)
      HSRY=HY+UR*UR/(2.0*CTE)
      TI=TY
      CALL TINV(HSRY,TSY,TI,F,NS1,CPSY)
      XX2= ALO*UR*(TSY-TLO)
      V= SQRT(3.0*PY/RHOY)
      XX3=1.0+ALT*V*(TY-T_O)/XX2
C********** FREE MOLECULAR HEAT TRANSFER
      QP=0.5*XX2*PY*XX3/TY/CTE*FFEJ
      TBK=CPL*(TSH-TLO)*RHOL*DE/(4.0*QP)
      XXX1=RHOY*CD*(UY-ULI)**2/DE/RHOL
      UBK=2.0*XXX1*TBK+ULI
      YBK=VP*TBK
      IF(YBK.GT.YMAX) YBK=YMAX
      XBK=(XXX1*TBK+ULI)*TBK+SO
      DMAX=0.0
      WEL=0.0
      D30=0.0
      D32I=(AK*EXP((-BK)*TLO))*00
   62 CONTINUE
      WRITE (6,123) WE,REJ,TBK,UBK,XBK,YBK,WEL,D30,D32I,DMAX
      IF ((ITBK.EQ.1).OR.(ITBK.EQ.3)) GO TO 45
      ITBK=ITBK+1
C     ----- MODIFYING SHOCK FRONT CONDITIONS -----
      DO 46 ID=2,NSL
      IF (YBK.GT.Y(ID-1).AND. YBK.LT.Y(ID)) GO TO 47
   46 CONTINUE
      ID=NSL
   47 CONTINUE
      PTBO(1)=PTBO(2)
      TTBO(1)=TTBO(2)
      UTBO(1)=0.0
      F1TBO(1)=F1TBO(2)
      F2TBO(1)=F2TBO(2)
```

```
                F3TB0(1)=F3TB0(2)
                F4TB0(1)=F4TB0(2)
                F5TB0(1)=F5TB0(2)
                F6TB0(1)=F6TB0(2)
1 0             F7TB0(1)=F7TB0(2)
                F8TB0(1)=F8TB0(2)
                CALL LIPLN(Y8K,PTB0,Y0,PX,ID)
                CALL LIPLN(Y8K,TTB0,Y0,TX,ID)
                CALL LIPLN(Y8K,UTB0,Y0,UX,ID)
175             CALL LIPLN(Y8K,F1TB0,Y0,F(1),ID)
                CALL LIPLN(Y8K,F2TB0,Y0,F(2),ID)
                CALL LIPLN(Y8K,F3TB0,Y0,F(3),ID)
                CALL LIPLN(Y8K,F4TB0,Y0,F(4),ID)
                CALL LIPLN(Y8K,F5TB0,Y0,F(5),ID)
1 0             CALL LIPLN(Y8K,F6TB0,Y0,F(6),ID)
                CALL LIPLN(Y8K,F7TB0,Y0,F(7),ID)
                CALL LIPLN(Y8K,F8TB0,Y0,F(8),ID)
              C********** F(I) ARE IN MOLE/GM
                WAX=0.0
1 5             DO 48 II=1,NS
                WAX=WAX+F(II)
             46 CONTINUE
                WAX=1.0/WAX
                RHOX=PX*WAX/(RR2*TX)
1 0             WA(1)=WAX
                PTB(1)=PX
                UTB(1)=UX
                TTB(1)=TX
                RHOTB(1)=RHOX
1 5             FTB(1,1)=F(1)
                FTB(2,1)=F(2)
                FTB(3,1)=F(3)
                FTB(4,1)=F(4)
                FTB(5,1)=F(5)
2 0             FTB(6,1)=F(6)
                FTB(7,1)=F(7)
                FTB(8,1)=F(8)
                DO 31 JJ=1,6
                DD(JJ)=0.0
2 5             DO 32 II=1,NS
                DD(JJ)= DD(JJ)+ XL(JJ,II)*FTB(II,1)
             32 CONTINUE
             31 CONTINUE
                T1.=TTB(1)/ 1[illegible]
210             HX=1000.*(-DD(5)/T10+DD(5)+T10*(DD(1)+T10*(DD(2)/2.0+T10*(DD(3)/3.
               1 +T10*DD(4)/4.0))))
                HE=HX
                HSX =HX  +0.5*UTB(1)*UTB(1)/CTE
                HSE(1)=HSX
215             XXX1=RHOTB(1)*UTB(1)
                RUE(1)=XXX1
                RU2E(1)=XXX1*UTB(1)
                RUHSE(1)=XXX1*HSE(1)
                RUF1E(1)=XXX1*FTB(1,1)
220             RUF2E(1)=XXX1*FTB(2,1)
```

```
      RUF3E(I)=XXXI*FTB(3,I)
      RUF4E(I)=XXXI*FTB(4,I)
      RUF5E(I)=XXXI*FTB(5,I)
      RUF6E(I)=XXXI*FTB(6,I)
      RUF7E(I)=XXXI*FTB(7,I)
      RUF8E(I)=XXXI*FTB(8,I)
      WRITE(6,120)
      I=1
      WRITE(6,106)
      WRITE(6,105)    S(I),PTB(I),TTB(I),UTB(I), (FTB(
      WRITE(6,107)
      WRITE(6,103) I,WA(I),ME,HSE(I),    RUE(I),RU2E(I),
     1 RU4SE(I),RUF1E(I),RUF2E(I),RUF3E(I),RUF4E(I),RUF5E(I)
     2,RUF6E(I), RUF7E(I),RUF8E(I)
      DO 49 II=1,NS
      F(II)=F(II)*WI(II)
      PSIV(II)=F(II)
   49 CONTINUE
C********** F(II) NOW IS IN MASS FRACTION
      U02=UBK*UX
      GO TO 50
   45 CONTINUE
      DP=0.5*D321
      S150=1.05*DEQP*DEQP/RPO
      SE=S0P+S150*((XBK/(150.*DEQP))**AI)
      IF(XBK.LE.(70.*DEQP)) SE=S0P+S15 *( (7 ./15 .)**AI)*XBK
      SE=FFAE*SE
      YE=YBK
      AE=0.5*PI*YE*SE
C----- RELAX TO EXTERNAL PRESSURE RAPIDLY -----
      DO 52 ID=2,NPS
      IF (XBK.GE. S(ID-1) .AND.XBK.LT.S(ID)) GO TO 53
   52 CONTINUE
      WRITE (6,200) ID, S(ID),XBK
      STOP
   53 CONTINUE
C       INITIAL MASS FRACTION OF H
      F(IH)=FIH
      XMV=FFV*XMLI
      XML=(1.0-FFV)*XMLI
      CALL LIPLN (XBK,PTB,S,PEBK,ID)
      CALL LIPLN(XBK,RU2E,S,RU2BK,ID)
      BETA=0.5*PI
      A=AE
      DO 30 IT=1,100
      P=PEBK+RU2BK*( SIN(BETA)**2)*(1.0-RHOX)
      P=P*FFPE
C----- MIXING OF SHOCKED AIR WITH FLASH
      XMU=RHOX*UY*A
      XMM=XMU+XMV
      WRITE(6,124) XMV,XMU,XMM
      F(NS1)=XMV/XMM
      U=(XMU*U+XMV*UBK+
      HSV=CP *FRPY+DHV+(U3*
      HS=(X   *  SX+XMV*HSV)
```

```
                  DO 24 I=1,NS
                24 F(I)= PSIV(I)*(1.0-F(NS1))
               C********** NORMALIZED MASS FRACTION
                  WM=0.0
2.0               DO 29 I=1,NS1
               C     F(I) ARE IN MASS FRACTION
                  WM=WM+F(I)/WI(I)
                29 CONTINUE
                  WM=1.0/WM
2.5               H=HS-(U*U)/(2.*CTE)
                  TI=TX
                  CALL TINV(H,T,TI,F,NS1,CP)
                  RHO=P *WM/RR2/T
               C********** INITIAL DVA TUBE AREA AFTER MIXING
3.0               A=XMM/(RHO*U)
               C     DA=A-AE
                  XP=RPO
                  TP=TBPY
                  UP=UBK
3.5               SI=XBK
                  XMLO=XML
                  IF (FFV.GE.  1.0) VP=0.0
                  IF (FFV.GE.  1.0) UP=U
               C********** CALCULATING INITIAL RELATIVE STAGNATION TEMPERATURE
4.0               AXX1=((U-UP )**2+VP**2)
                  UR = SQRT(AXX1)
                  HSR=HS-(U*U-UR*UR  )/(2.0*CTE)
                  TI=TY
                  CALL TINV(HSR,TS ,TI,F,NS1,CPSR)
4.5               WRITE (6,125) SI,U,HSV,HSR,H,TS ,T,RHO,A
                  WRITE(6,135)
                  DO 72 I=1,NS1
                  WRITE(6,119) IDENT(I),F(I),FI(I),WDOT(I)
                72 CONTINUE
5.0             100 FORMAT(8E1 .3)
                101 FORMAT(2X,10E12.3)
                102 FORMAT(2X,I5,1P10E12.4)
                103 FORMAT(1H ,I5,1P9E12.3/5X,6E12.3)
                105 FORMAT(2X,*MASS FRACTIONS OF SPECIES*/1X,*NO+=*,1PE1..3,1X,*E-=*
5.5                1,E10.3,1X,*O=*,E10.3,1X,*F-=*,E10.3,1X,*N=*,E10.3,1X,*O2=*,E10.3,1
                   2X,*N2=*,E10.3,1X,*NO=*,E10.3,* FV=*,E10.3)
                106 FORMAT(1X,*AV=*,F5.2,2(1P11E11.3/))
                107 FORMAT(/ 5X, *I*, 8X,*WA*,10X, *HE*,10X,*HSE*,
                   1 9X,*REUE*, 7X,*REUE2*,7X,*REUEHSE*,7X,*RUF1E*,7X,*RJF2E*,7X,*RJF3
6.0                2E*/9X,*RUF4E*,7X,*RJF5E*,7X,*RUF6E*,7X,*RUF7E*,7X,*RJF8E*)
                108 FORMAT(/          7X,*S*,10X,*PE*,8X,*TE*,8X,*UE*
                   1,/X,*FE(I) (MOLE/GM)=*)
                119 FORMAT(9X,A4,3X,1P8E12.3)
                120 FORMAT(1X,*---------   MODIFIED FREE STREAM CONDITIONS IN SHOCK FR
6.5                1ONT BY SINGLE ITERATION -----*)
                121 FORMAT(/2X,* CONDITIONS IN FRONT OF SHOCK */2X,*PX=*,1PE10.3,2X,
                   1 *UX=*,E10.3,2X,*HSX=*,E10.3,2X,*RHOX=*,E10.3,2X,*TX=*,E10.3
                   2 ,2X,*WAX=*,E10.3/ 2X,
                   2*MASS FRACTIONS F(I)=*,9E12.3/)
7.0             122 FORMAT(/2X,* CONDITIONS BEHIND SHOCK*/2X,*PY=*,1PE1..3,2X,*UY=*,
```

```
     1 E10.3,2X,*HY=*,E10.3,2X,*RHOY=*,E10.3,2X,*TY=*,E10.3,2X,*TBPY=*,
     2 E10.3/)
  123 FORMAT(2X,* JET BREAK-UP INFORMATION */2X,*WE=*,1PE1 .3,2X,
     1 *REJ=*,E10.3,2X,*TBK=*,E10.3,2X,*UBK=*,E10.3,2X,*KBK=*,E10.3,2X,
     2 *YBK=*,E10.3/2X,*WEL=*,E10.3,2X, *D30=*,E10.3,2X,*D32=*,E10.3,2X,
     3 *DMAX=*,E10.3/)
  124 FORMAT(2X, *INITIAL FLOW RATE(G/SEC)*/2X,*XMV=*,1PE10.3,2X,*XML=*,
     1 E10.3,2X,*XMA=*,E10.3,2X,*XMM=*,E10.3,2X,*AE=*,E10.3/)
  125 FORMAT(2X,*------  CONDITIONS OF THE INTIAL MIXTURE AT S=*,F10.4
     1       /2X,*J=*,1PE10.3,2X,*HSJ=*,E10.3,2X,*HSR=*,E10.3,2X,*H=*,
     1E10.3,2X,*TSR=*,E10.3,2X,*T=*,E10.3,2X,*RHO=*,E10.3,2X,*A=*,E10.3)
  127 FORMAT(2X, * -- INITIAL MIXING CALCULATION DOES NOT CONVERGE TO
     1CORRECT SOLUTION*,I3/1P11E11.3)
  135 FORMAT(7X,*SPECIES*,5X, *F(I)*,5X,*FI(I)*,5X,*WDOT(I)*)
      RETURN
      END
```

```
*DECK,ERF
      FUNCTION ERF(X)
C     ----- THIS CALCULATES THE ERROR FUNCTION AND ITS COMPLEMENT -----
      DATA EPSILN/1.0E-14/,N/100/,CONST/1.12837916795507/
      KOMPL=+1
      GO TO 5
      ENTRY ERFC
      KOMPL=-1
    5 IF (X) 10,55,15
   10 Z=-X
      GO TO 20
   15 Z= X
   20 IF (Z-5.) 25,25,45
   25 ZSQ=Z*Z
      TERM=CONST*Z*EXP(-ZSQ)
      ERF=TERM
      I=0
      R=1.0
   30 I=I+1
      R=R+2.0
      TERM=2.0*ZSQ*TERM/R
      ERF=ERF+TERM
      IF (I-N) 35,40,40
   35 IF (TERM-EPSILN*ERF) 40,30,30
   40 IF (ERF-1.0) 50,50,45
   45 ERF=1.0
   50 IF (X) 60,55,65
   55 ERF=0.0
      GO TO 65
   60 ERF=-ERF
   65 IF (KOMPL) 70,99,99
C     ----- COMPUTE COMPLEMENTARY ERROR FUNCTION ERF -----
   70 ERF=1.0-ERF
   99 RETURN
      END
```

```
*DECK.LIPLN
      SUBROUTINE LIPLN (SX,A,S,RA,K)
C     A SCHEME FOR LINEAR INTERPOLATION
      DIMENSION A(20),S(20)
   22 RA= (A(K-1)*(S(K)-SX) + A(K)*(SX-S(K-1)))/(S(K)-S(K-1))
      RETURN
      END
```

```
*DECK,TINV
      SUBROUTINE TINV (H,T,TI,F,NS1,CP)
C     ----- THIS SUBPROGRAM WILL INVERT TEMPERATURE FROM ENTHALPY BY THE
C                 NEWTON METHOD -----
      DIMENSION DD(6),F(51)
      COMMON /HEAT/ XL(6,51),WI(51)
      COMMON/LIQUID/ CPL,TBP,DHV,RHOL,WV,TBPO,SIG,TLO,UML,DO,WECR,
     1 FFVI,AK,BK,WE,ITBK,FFV,TBPV
    1 CONTINUE
      DO 10 J=1,6
      DD(J)=0.0
      DO 11 I=1,NS1
C       F(I) ARE IN MASS FRACTION
      DD(J)=DD(J)+XL(J,I)*F(I)/WI(I)
   11 CONTINUE
    1 CONTINUE
      EPS=1.0E-6*H
      T=TI
      DO 12 IT=1,100
      T1 =T/100.
      G=1000.*(-DD(5)/T10+DD(6)+T10*(DD(1)+T10*(DD(2)/2.+T10*(DD(3)/
     * 3.0+T10*DD(4)/4.0))))-H
      CP=        (DD(5)/(T10*T10)+DD(1)+T10*(DD(2)+T10*(DD(3)+T10*DD(4)
     1 )))
      IF( ABS(G).LT. EPS) GO TO 999
      T=T-G/CP
   12 CONTINUE
      WRITE (6,119) IT ,H,T,CP,TI ,G ,EPS
      STOP
   20 CONTINUE
      FAA=1.0-F(NS1)
      PC=XL(1,NS1)*F(NS1)/WI(NS1) +(XL(1,6)*.231/WI(6)+(.11,7)*(.769/
     1 WI(7)))*FAA
      CP=PC
      T=H/CP
  999 CONTINUE
  119 FORMAT(12X, *--ITERATION DOES NOT CONVERGE TO THE CORRECT TEMPERA
     1TURE *,I5/2X,1P10E12.3)
      RETURN
      END
```