

**ENGINEERING AND PROGRAMMING  
MANUAL**

**TWO-DIMENSIONAL KINETIC  
REFERENCE COMPUTER PROGRAM**

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REFERENCE COMPUTER PROGRAM (TLK) Final  
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**TDK**

**Final Report  
Contract No. NAS8-35931**

**April 1985**

**By: G. R. Nickerson**

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**Prepared For**

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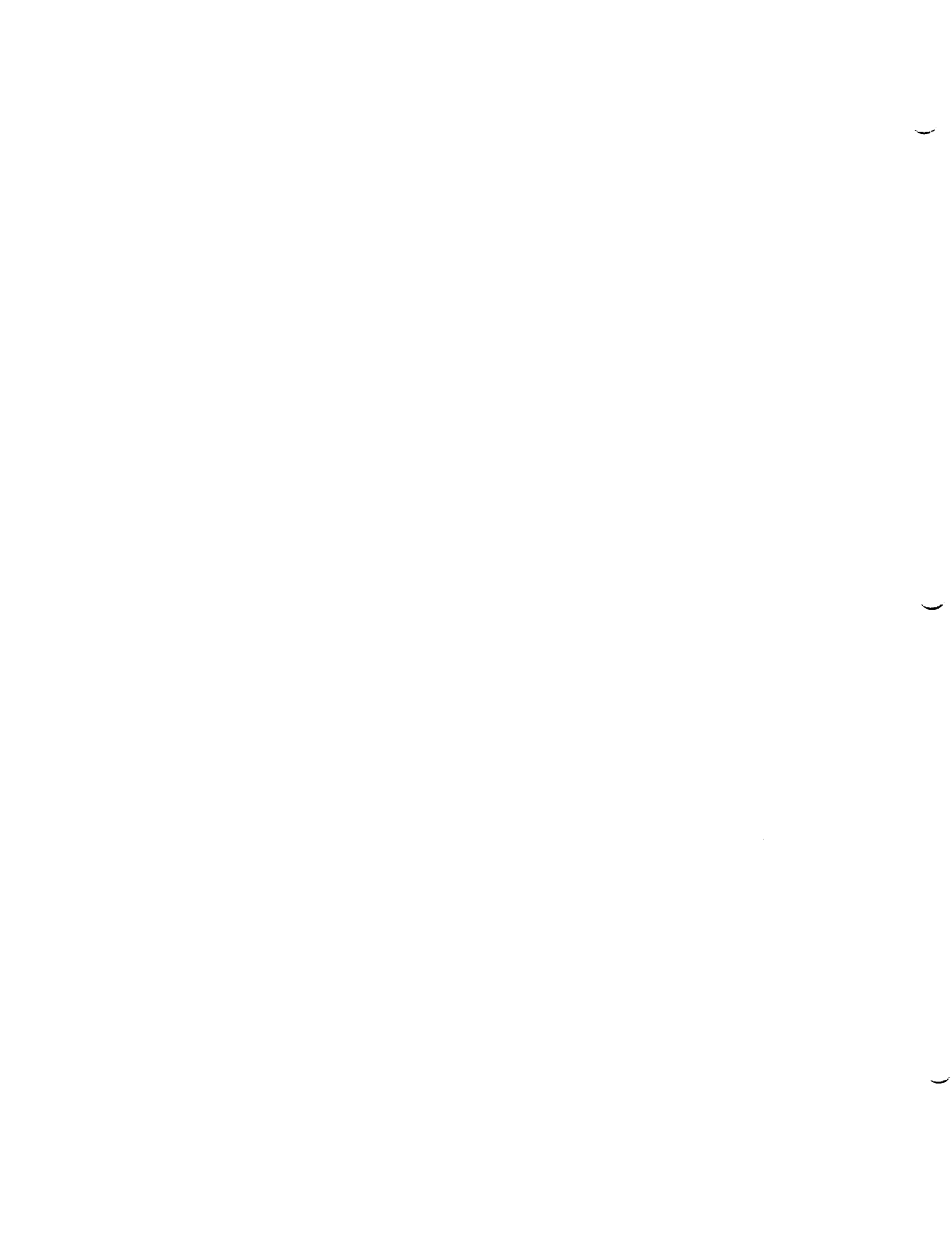
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## FOREWORD

This report contains an engineering and programming description for the revised April/85 version of the Two-Dimensional Kinetic Thrust Chamber Analysis Computer Program, TDK, developed by Software and Engineering Associates, Inc., Carson City, Nevada. Revision of the TDK Computer Program was performed under Contract Numbers NAS8-34974, NAS8-35046, and NAS8-35931. The work performed was monitored by Mr. Klaus Gross and Mr. A. Krebsbach of the NASA George C. Marshall Space Flight Center, Huntsville, Alabama.

The TDK Computer Program consists of the following computational modules:

MCM	Master Control Module
ODE	One-Dimensional Equilibrium Nozzle Analysis Module
ODK	One-Dimensional Kinetic Nozzle Analysis Module
TRANS	Transonic Analysis Module
MOC	Method of Characteristics Module for Equilibrium, Kinetic, or Frozen Nozzle Flow
BLM	Boundary Layer Module

The reference procedure which utilizes the above computer programs is given in the JANNAF Rocket Engine Performance Prediction and Calculation Manual, CPIA246, Reference 1.



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## NOMENCLATURE

<b>a</b>	Nozzle area ratio, also reaction rate parameter
$a_{ki}$	Gram atoms of the $k^{\text{th}}$ element in the $i^{\text{th}}$ species
<b>A</b>	Adiabatic heat addition term linking fluid dynamic and relaxation processes, also total mass reactant in ODE
<b>b</b>	Reaction rate parameter
<b>B</b>	Energy exchange term linking fluid dynamic and relaxation processes
<b>c</b>	Species mass fraction
$c_F$	Thrust coefficient
$C_p$	Frozen heat capacity
$C_{pe}$	Equilibrium heat capacity
$C^*$	Characteristic exhaust velocity
$\mathcal{G}_i$	Heat capacity per mole of $i^{\text{th}}$ species/R
<b>f</b>	Derivative
<b>F</b>	Free energy, also function defined by Equation (2.5-5)
$\mathcal{F}_i$	Free energy per mole of $i^{\text{th}}$ species/R
<b>G</b>	Function defined by Equation (2.5-6)
<b>h</b>	Enthalpy, also integration increment
<b>H</b>	Total enthalpy, also function defined by Equation (2.5-7)
$\Delta H_F$	Heat of formation
$\lambda_i$	Enthalpy per mole of $i^{\text{th}}$ species/RT
$I_{sp}$	Specific impulse
<b>k</b>	Variable increment, also reaction rate parameter
<b>K</b>	Equilibrium constant
<b>m</b>	Reaction rate ratio
$M_w$	Molecular weight
<b>M</b>	Mach number, also third body reaction term
<b>n</b>	Reaction rate parameter, also summation or iteration index
$n_i$	Moles of $i^{\text{th}}$ species
$N_e$	Average equilibrium pressure expansion coefficient
<b>P</b>	Pressure

## NOMENCLATURE (continued)

$r$	Radial distance coordinate, from axis
$r^*$	Nozzle throat radius
$R$	Gas constant
$R^*$	Nozzle wall radius of curvature at throat
$\mathcal{R}$	Universal gas constant
$S$	Entropy, also summation term
$s_1$	Entropy per mole of $i^{\text{th}}$ species/ $R$
$T$	Temperature
$u$	Velocity in x-direction
$v$	Velocity in r-direction
$V$	Velocity
$x$	Axial distance coordinate, from throat
$y$	Dependent variable
$Y_1$	Slipline height
$\alpha$	Mach angle, angle between streamline and Mach line characteristics
$\alpha_1$	Partial derivative, $\partial f_1 / \partial x$
$\beta_{1,j}$	Partial derivative, $\partial f_1 / \partial y_j$
$\gamma$	Frozen heat capacity ratio
$\gamma_e$	Equilibrium heat capacity ratio
$\delta_1$	Incremental error
$\delta_{1,j}$	Kronecker delta
$\epsilon$	Area ratio
$\rho$	Density
$\theta$	Nozzle cone angle
$\omega_1$	Net species production rate

**Subscripts:**

$c$	Refers to chamber conditions
$i$	Refers to $i^{\text{th}}$ species or equation
$j$	Refers to $j^{\text{th}}$ reaction or variable
$o$	Refers to reference conditions

**Superscript:**

$*$	Refers to throat conditions or sonic conditions
-----	-------------------------------------------------



## ABBREVIATIONS

BLIMP	Boundary Layer Integral Matrix Procedure, JANNAF computer program
BLM	Boundary Layer Module, computer program
JANNAF	Joint Army-Navy-NASA-Air Force
MØC	Method of Characteristics, module of SPP and TDK
ØDE	One-Dimensional Equilibrium, module of SPP and TDK
ODK	One-Dimensional Kinetics, module of SPP and TDK
OTV	Orbit Transfer Vehicle
PSS	Performance Standardization Subcommittee of JANNAF
SEA	Software and Engineering Associates, Inc.
SPP	Solid Performance Program, JANNAF computer program
TDE	Two-Dimensional Equilibrium, module of TDK
TDK	Two-Dimensional Kinetics, JANNAF computer program

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## 1. INTRODUCTION

The Two-Dimensional Kinetics (TDK) computer program is a primary tool in applying the JANNAF liquid rocket thrust chamber performance prediction methodology.<sup>1</sup> This computer program and the performance prediction methodology were originally developed under the auspices of the Performance Standardization Subcommittee (PSS) of the JANNAF. The goal of the PSS is the development of a methodology that includes all aspects of rocket engine performance from analytical calculation to test measurements, that is physically accurate and consistent, and that serves as an industry and government reference.

Recent interest in rocket engines that operate at high expansion ratio, such as most Orbit Transfer Vehicle (OTV) engine designs, has required an extension of the analytical methods used by the TDK computer program. Thus, the version of TDK that is described in this manual is in many respects different from the 1973 version of the program that is described in Reference 2. Although much material from the 1973 document is included in this manual, other material is entirely new. This new material reflects the new capabilities of the TDK computer program, the most important of which are described below.

---

Ref. 2: Nickerson, G. R., Coats, D. E., and Bartz, J. L., "The Two-Dimensional Kinetic (TDK) Reference Computer Program", Engineering and Programming Manual, Ultrasystems, Inc., December 1973, prepared for Contract No. NAS9-12652, NASA JSC.

- a) A Boundary Layer Module (BLM) has been included within the TDK program. The BLM can be used to automatically calculate the wall boundary layer after execution of the Method of Characteristics (MOC). The resulting wall displacement and the heat transferred through the wall are computed. The ODE-ODK-TRANS-MOC series of calculations can then be automatically repeated with the appropriate parameters (wall contour and propellant enthalpy) updated. This feature allows the "rigorous analytical procedure" of the JANNAF rocket engine performance prediction methodology<sup>1</sup> to be carried out with a single computer run for a regeneratively cooled engine.
- b) The ODE module of TDK has been modified so that it will compute transport properties for the nozzle exhaust composition. This information is required by the BLM.
- c) The ODE module of TDK has been modified so that it will provide tables of gas properties versus temperature for the stream tube mixture ratio adjacent to the nozzle wall. This information is required by the BLM.
- d) New nozzle wall geometry options have been added to the program.
- e) The ODK and MOC modules can contain condensed phases that are in thermal and velocity equilibrium with the gas.
- f) The transonic flow module (TRANS) has been modified to analyze flow with variable mixture ratio.

- g) The MOC module has been rewritten to allow for the presence of a shock wave in the flow. The shock can be either attached to the nozzle wall, or induced by the nozzle wall curvature. Regular reflections from the nozzle axis and the nozzle wall can be computed. The shock option can be used for flows with gas properties along streamlines that are either:
- 1) constant,
  - 2) chemically frozen (i.e., fixed composition, but properties varying with temperature), or
  - 3) governed by finite rate kinetics.
- h) The thermodynamic data and kinetic rate data (see Appendix A) for the program have been updated.

The TDK Computer Program is designed for engineering use and is specified and programmed in a straight forward manner to facilitate its application. The FORTRAN IV programming language has been used in an attempt to make the computer program as machine independent as possible. A complete engineering and programming description of the TDK Computer Program is contained in this report.

Section 2 of this report contains a description of the methods of analysis used in the computer program.

Section 3 contains a description of the numerical methods used to integrate the fluid dynamic and chemical relaxation equations in the computer program.

Section 4 contains a description of the program structure.

Section 5 contains a detailed engineering and programming description of the program subroutines.

Section 6 contains a program user's manual describing the use of the computer program with an explanation of the program input and output.

Section 7 contains input and output for a sample case using the TDK option of the program.

Section 8 contains a discussion of program usage and error diagnostics.

## 2. ANALYSIS

The TDK Computer Program has been written for the purpose of evaluating two-dimensional effects on the performance of liquid propellant exhaust nozzles. An important feature of the TDK program is its ability to consider nonequilibrium chemical processes. The basic method of analysis used by TDK is the method of characteristics. The program constructs a finite-difference mesh by tracing gas streamlines and characteristic surfaces. The mesh points are located at the intersections of these surfaces. Systems of large size can be considered by the program as is indicated by Table 2-1 which gives maximum dimensions for the program.

The method of characteristics calculation is capable of considering either continuous mixture ratio variation, or flow striations. Striated regions are separated by slipline conditions, i.e., adjacent streamlines with matched pressure and gas streamline angle, but at different mixture ratio, temperature, etc. Mixing between striated zones, is not considered. The initial data line required to start the method of characteristics is calculated using a transonic analysis provided for this purpose. The characteristic equations governing the fluid dynamic variables are integrated using a second order (modified Euler) explicit integration method while the chemical relaxation equations are integrated using a first order implicit integration method to insure numerical stability in near equilibrium flows.

In order to start the method of characteristics calculation, it is necessary to approximate an initial data line across the nozzle throat. This initial data line must be supersonic and

TABLE 2-1 MAXIMUM DIMENSIONS FOR TDK

Number of defined elements provided	102
Number of possible species per case	40
Number of species in the Master Thermodynamic Data File	1000
Number of possible reactions	150
Number of possible reactions with implied third body	50
Number of reactants per reaction	10
Number of products per reaction	10
Maximum stoichiometric coefficient total	600
Number of possible third body efficiencies to be considered	2000
Maximum number of streamlines (i.e. mesh points per left running characteristic)	275
Maximum number of zones (i.e. striations)	50

must be compatible with the mesh construction methods used by TDK. The calculations performed by TDK to generate this initial data line are carried out in two stages. First chemical information is computed by use of the ODK module as described in Section 2.1. Chemical and fluid properties, obtained from this calculation are retained in the form of tables. The second stage of the calculation makes use of this information and employs a perturbation method to estimate two dimensional effects in the transonic region of the nozzle throat. Variable mixture ratio flows and striated flows are treated by means of a straight forward extension of the procedure described above.

The description given above is shown schematically in Figure 2-1a. The TDK Computer Program is divided into modules as shown in the figure. The modules are illustrated in the master flow chart presented in Figure 2-1b. For a description of the analysis used by ODE, Reference 3 should be used.



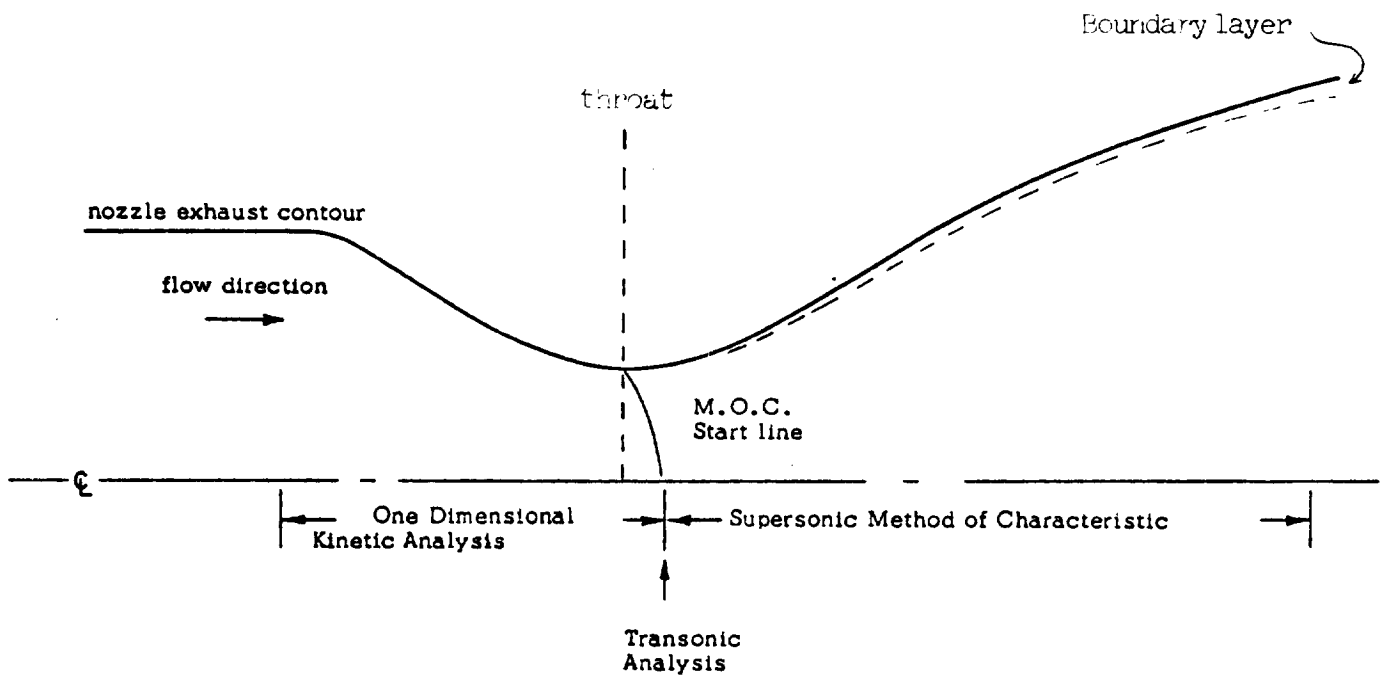


Figure 2-1a. Schematic for TDK Analysis

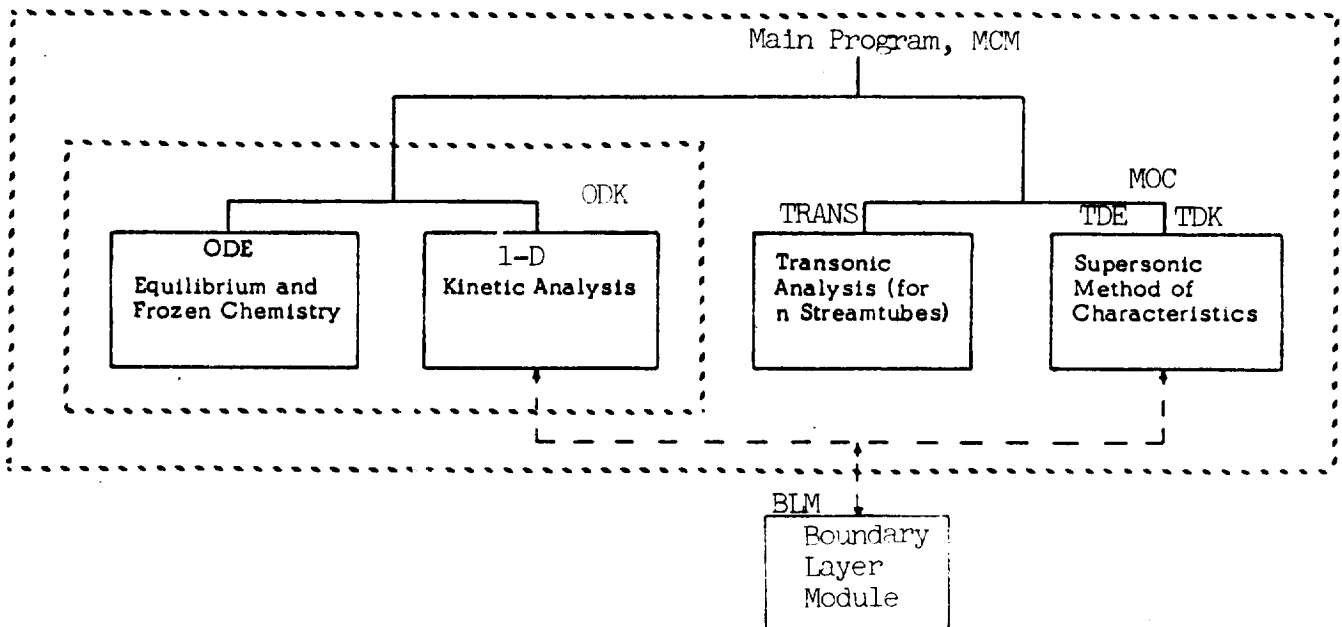


Figure 2-1b. Master Flow Chart for TDK

In Section 2.1 of this report the analysis for the ODK computer program is given. In Section 2.2 a discussion of the finite rate chemistry used by both ODK and TDK is presented. In Section 2.3 the conservation equations governing two dimensional axisymmetric inviscid flow are presented. In Section 2.4 the transonic flow method used to construct an initial data line for the method of characteristics solution is presented. The method of characteristics relations are presented in Section 2.5. The boundary layer solution is presented in Section 2.6.

### PERFORMANCE PREDICTION METHODOLOGY

The JANNAF thrust chamber performance prediction methodology is defined in Reference 1. In this methodology the predicted delivery specific impulse for the thrust chamber can be expressed as:

$$I_{sp_{deliv}} = \eta_{DER} I_{sp_{TDK'}} - \Delta F_{BLM}' / \dot{M}_{TDK'}$$

The factor  $\eta_{DER}$  in the above expression represents the distributed energy release of the combustion process. The terms

$I_{sp_{TDK'}}$ ,  $\dot{M}_{TDK'}$ , and  $\Delta F_{BLM}'$  represent the values predicted by TDK for nozzle specific impulse and mass flow, and by the BLM for boundary layer thrust deficit. The prime denotes that these quantities have been corrected using the Prandtl procedure. Thus, a second TDK calculation has been made with the nozzle wall displaced inwards a distance equal to the boundary layer displacement thickness. Also, in this calculation the heat picked up by the regen cooling circuits has been returned to the thrust chamber as increased propellant enthalpy. Care is taken

in the procedure to assure that a complete energy balance is maintained.

The boundary layer thrust deficit is evaluated by integrating across the boundary layer at the nozzle exit for momentum thickness,  $\theta$ , and displacement thickness,  $\delta^*$ , and applying the results as follows:

$$F_{BLM} = 2\pi r_e \cos \alpha_e \rho_e U_e^2 \theta_{BLM} \\ - 2\pi r_e \cos \alpha_e (P_e - P_{BLM}) \delta_{BLM}^*$$

The first term in the above expression represents the momentum deficit in the boundary layer and includes the effects of wall skin friction and heat transfer. The second term represents the pressure force acting on the annular portion of the nozzle exit plane that is between the real wall and the inviscid edge of the boundary layer. The quantities  $r_e$ ,  $\rho_e$ ,  $P_e$ , and  $U_e$ , are boundary layer edge properties obtained from the second TDK calculation.

## 2.1 ANALYSIS FOR THE ØDK COMPUTER PROGRAM

The One Dimensional Kinetic nozzle analysis computer program (ØDK) described in this section has been developed for performing reference liquid propellant thrust chamber performance calculations. The ODK computer program calculates the inviscid one dimensional equilibrium, frozen and nonequilibrium nozzle expansion of gaseous propellant exhaust mixtures. The ØDK program is also used as a subprogram by TDK. The ØDE computer program, which is described in Reference 3, is used to perform the equilibrium composition computations. The ØDE program computations are based on the assumption that species compositions at any pressure and enthalpy point will be distributed such that the free energy of the system is minimized. Solid and liquid phases can be included in ØDE computations, and to a certain extent in the ØDK and TDK computations.

The ODK one dimensional nonequilibrium calculation is performed beginning at the converging section of the nozzle and ending at an axial station located beyond the throat plane. In this calculation pressure defined relations are used to integrate the differential equations for a one dimensional streamtube until the flow becomes supersonic. This pressure profile is obtained by computing an average value of expansion coefficient based on a chemical equilibrium gas composition at the nozzle chamber and throat. These parameters are supplied automatically by ODE. Pressure and its axial derivative are then obtained for the exact prescribed inlet geometry from the relations for isentropic expansion. Once the pressure profile has been determined the one dimensional nonequilibrium flow relations are integrated starting with an equilibrium calculation obtained at the thrust chamber contraction ratio. The advantage of using the pressure defined boundary condition is that the differential equations are not singular at Mach one so that no difficulties are encountered when integrating through the nozzle throat region. The throat (minimum area) occurs when the product of density and velocity maximizes and thus determines the mass flux corresponding to the choke flow condition. Using this mass flux, the nozzle area profile can then be determined. Experience has shown good agreement between this area profile and the original input geometry. Once supersonic conditions are reached the program automatically changes over to area defined differential equations.

### 2.1.1 Conservation Equations for One Dimensional Kinetic Expansions

The conservation equations governing the inviscid one dimensional flow of reacting gas mixtures have been given by Hirschfelder, Curtiss and Byrd,<sup>4</sup> Penner<sup>5</sup> and others. The basic assumptions made in the derivation of these equations are:

- o There are no mass or energy losses from the system
- o The gas is inviscid
- o Each component of the gas is a perfect gas
- o The internal degrees of freedom (translational, rotational and vibrational) of each component of the gas are in equilibrium.

The conservation equations are presented here in the form used in the present analysis.

For each component of the gas the continuity equation is

$$\frac{d}{dx} (\rho_i V \bar{a}) = \omega_i r^* \bar{a}$$

where the axial coordinate ( $x$ ) has been normalized with the throat radius. Summing over all components of the mixture, the overall continuity equation is obtained

$$\frac{d}{dx} (\rho V \bar{a}) = 0$$

Combining the above two equations gives

$$\frac{dc_i}{dx} = \frac{\omega_i r^*}{\rho V}$$

The momentum equation is

$$\rho V \frac{dV}{dx} + \frac{dP}{dx} = 0$$

The energy equation is

$$h + \frac{1}{2} V^2 = H_c$$

where

$$h = \sum_{i=1} c_i h_i$$

and

$$h_i = \int_0^T C_{pi} dT + h_{i0}$$

For each component of the gas, the equation of state is

$$P_i = \rho_i R_i T$$

Summing over all components of the mixture, the overall equation of state is obtained

$$P = \rho R T$$

where

$$R = \sum_{i=1} c_i R_i$$

Since the expansion through a nozzle can be specified either by the expansion process or by the nozzle geometry, two forms of the above equations are of interest.

If the expansion process is specified and the pressure is known as a function of distance through the nozzle, the above equations become

$$\frac{dc_1}{dx} = \frac{\omega_1 r^*}{\rho V}$$

$$\frac{dV}{dx} = - \frac{1}{\rho V} \frac{dP}{dx}$$

$$\frac{d\rho}{dx} = \left[ \frac{1}{\gamma P} \frac{dP}{dx} - A \right] \rho$$

$$\frac{dT}{dx} = \left[ \frac{\gamma - 1}{\gamma} \frac{1}{P} \frac{dP}{dx} - B \right] T$$

while if the nozzle geometry is specified, the above equations become

$$\frac{dc_i}{dx} = \frac{\omega_i r^*}{\rho V}$$

$$\frac{dV}{dx} = \left[ \frac{1}{\bar{a}} \frac{d\bar{a}}{dx} - A \right] \frac{V}{M^2 - 1}$$

$$\frac{d\rho}{dx} = - \left\{ \left[ \frac{1}{\bar{a}} \frac{d\bar{a}}{dx} - A \right] \frac{M^2}{M^2 - 1} + A \right\} \rho$$

$$\frac{dT}{dx} = - \left\{ \left[ \frac{1}{\bar{a}} \frac{d\bar{a}}{dx} - A \right] \frac{(\gamma - 1)M^2}{M^2 - 1} + B \right\} T$$

$$P = \rho RT$$

where

$$A = \frac{r^*}{PV} \left[ \sum_{i=1} \omega_i R_i T - \frac{\gamma - 1}{\gamma} \sum_{i=1} \omega_i h_i \right]$$

$$B = \frac{\gamma - 1}{\gamma} \frac{r^*}{PV} \sum_{i=1} \omega_i h_i$$

$$M = \frac{V}{\sqrt{\gamma RT}}$$

$$\gamma = \frac{C_p}{C_p - R}$$

and

$$C_p = \sum_{i=1} c_i C_{pi}$$

The first set of equations is completely specified at the sonic point while the second set of equations is singular. Thus, if the expansion through the nozzle is specified by the pressure distribution, the equations governing the expansion can be directly integrated through the sonic point without mathematical difficulty.



The expansion from the chamber through the sonic point is specified by the pressure distribution in the present program in order to eliminate numerical difficulties at the sonic point. In the expansion section downstream of the sonic point, however, the area variation is specified and the second set of equations is integrated through the supersonic expansion section.

In specifying the nozzle pressure distribution from the chamber through the sonic point, rather than the known area distribution, a question naturally arises regarding how accurately the calculation represents the flow through a specified nozzle geometry. It has been shown by Bray<sup>6</sup> and others that the pressure distribution through a nozzle is essentially identical with the equilibrium pressure distribution up to the freeze point which generally occurs downstream of the throat (or sonic point). Thus, the difference in the expansion and predicted performance caused by utilizing the equilibrium pressure distribution rather than the nozzle geometry to specify the expansion from the chamber to the sonic point is negligible. If a case does arise in which the equilibrium pressure distribution is not an adequate representation of the expansion, the pressure distribution can be iterated to obtain the correct pressure distribution. Experience has shown that this is rarely if ever required.

In the above analysis the chemistry is brought into the conservation equations through the net species production rates,  $\omega_i$ . The analysis pertaining to the chemistry is given in the following section.

## 2.2 CHEMISTRY

The method by which the net species production rate,  $\dot{\omega}_i$ , required by the preceding analysis is determined is described below.

A chemical reaction can be written in terms of its stoichiometric coefficients ( $\nu_{ij}$  and  $\nu'_{ij}$ ) as

$$\sum_{i=1} \nu_{ij} \bar{M}_i \rightleftharpoons \sum_{i=1} \nu'_{ij} \bar{M}_i$$

where  $\bar{M}_i$  represents the  $i^{\text{th}}$  chemical species name and  $j$  represents the  $j^{\text{th}}$  reaction.

Given a system of chemical reactions, the net species production rate  $\omega_i$  for each species (component) is calculated from

$$\omega_i = m_{w_i} \sum_{j=1} \rho \sum_{\ell=1}^{\lambda_j} \nu_{\ell j} (\nu'_{ij} - \nu_{ij}) X_j$$

where

$$X_j = [K_j \prod_{i=1} \bar{c}_i^{\nu_{ij}} - \rho^{\lambda_j} \prod_{i=1} \bar{c}_i^{\nu'_{ij}}] k_j M_j \quad (2.2-1)$$

The reaction rate,  $k_j$ , is from right to left (reverse) in the above equation and is represented by the Arrhenius form

$$k_j = a_j T^{-n_j} e^{(-b_j/RT)}$$

where

- $a_j$  is the pre-exponential coefficient
- $n_j$  is the temperature dependence of the pre-exponential factor
- $b_j$  is the activation energy

The term  $M_j$  is provided so that the reaction rate can be modified for reactions involving a third body, i.e.

$$M_j = \sum_{i=1} m_{j,i} \bar{c}_i \quad \text{for reactions requiring a third body}$$

$$M_j = 1 \quad \text{for all other reactions}$$

where the constants  $m_{j,i}$  are specified, and

$$\bar{c}_i = c_i / M w_i$$

The integer,  $\lambda_j$ , is determined for a given reaction from the stoichiometric coefficients

$$\lambda_j = \sum_{i=1} (\nu'_{ij} - \nu_{ij})$$

The equilibrium constant,  $K_j$ , is\*

$$K_j = e^{-\Delta F/RT} (RT)^{-\lambda_j}$$

where

$$\Delta F = \sum_{i=1} f_i \nu_{ij} - \sum_{i=1} f_i \nu'_{ij}$$

Reactions involving a third body have a distinct reaction rate for each particular third body, so that the net production rate should be calculated from

$$x_j = \sum_{k=1} \left[ K_j \prod_{i=1} \bar{c}_i^{\nu_{ij}} - \rho \prod_{i=1} \bar{c}_i^{\nu'_{ij}} \right] \bar{c}_k k_{kj} \quad (2.2-2)$$

rather than Equation (2.2-1). Benson and Fueno<sup>7</sup> have shown theoretically that the temperature dependence of recombination rates is approximately independent of the third body. Available experimental recombination rate data also indicates that the temperature dependence of recombination rates is independent of the third body within the experimental accuracy of the measurements. Assuming that the temperature dependence of recombination rates is independent of the third body, the recombination rate associated with the  $k^{\text{th}}$  species (third body) can be represented as

$$k_{kj} = a_{kj} T^{-n_j} e^{(-b_j/RT)} \quad (2.2-3)$$

where only the constant  $a_{kj}$  is different for different species (third bodies). From Equation (2.2-2) it can be shown that

$$\begin{aligned} x_j &= \left[ K_j \prod_{i=1} \bar{c}_i^{\nu_{ij}} - \rho \prod_{i=1} \bar{c}_i^{\nu'_{ij}} \right] \sum_{k=1} a_{kj} \bar{c}_k T^{-n_j} e^{-b_j/RT} \\ &= \left[ K_j \prod_{i=1} \bar{c}_i^{\nu_{ij}} - \rho \prod_{i=1} \bar{c}_i^{\nu'_{ij}} \right] \left[ \sum_{i=1} \frac{a_{ij}}{a_{kj}} \bar{c}_i \right] a_{kj} T^{-n_j} e^{-b_j/RT} \end{aligned}$$

\* $K_j$  is also the ratio of the forward to reverse reaction rates.

Thus the recombination rates associated with each third body can be considered as in Equation (2.2-1) by calculating the general third body term ( $M_j$ ) as

$$M_j = \sum_{i=1} m_{j,i} \bar{c}_i$$

where  $m_{j,i}$  is the ratio  $\left( \frac{a_{ij}}{a_{kj}} \right)$  of the recombination rate associated with the  $i^{\text{th}}$  species (third body) to the recombination rate associated with the  $k^{\text{th}}$  species (third body) which is the reference species (third body) whose rate in the form of Equation (2.2-3) is specified in the program input.

Chemical kinetic rate data is discussed in Appendix A.

## 2.3 CONSERVATION EQUATIONS FOR TWO DIMENSIONAL KINETIC EXPANSIONS

The conservation equations governing the axisymmetric inviscid flow of reacting gas mixtures have been given by Hirschfelder, Curtiss and Bird<sup>4</sup> Penner<sup>5</sup> and others. The basic assumptions made in the derivation of these equations are:

- o There are no mass or energy losses from the system
- o The gas is inviscid
- o Each component of the gas is a perfect gas
- o The internal degrees of freedom (translational, rotational, and vibrational) of each component of the gas are in equilibrium.

The conservation equations are presented here in the form used in the present analysis.

For each component of the gas, the continuity equation is

$$\left(\rho_i u\right)_x + \frac{1}{r} \left(r \rho_i v\right)_r = \omega_i r^* \quad (2.3-1)$$

where the coordinates  $(r, x)$  have been normalized with the throat radius. Summing over all components of the mixture, the overall continuity equation is obtained

$$(\rho u)_x + \frac{1}{r} (r \rho v)_r = 0 \quad (2.3-2)$$

Combining the above two equations gives

$$u \left(c_i\right)_x + v \left(c_i\right)_r = \frac{\omega_i r^*}{\rho} \quad (2.3-3)$$

The momentum equations are

$$\rho(uu_x + vv_r) + P_x = 0 \quad (2.3-4)$$

$$\rho(uv_x + vv_r) + P_r = 0 \quad (2.3-5)$$

The energy equation is

$$h + \frac{1}{2}(u^2 + v^2) = H_c \quad (2.3-6)$$

where

$$h = \sum_{i=1} c_i h_i \quad (2.3-7)$$

and

$$h_i = \int_0^T C_{pi} dT + h_{i0} \quad (2.3-8)$$

For each component of the gas, the equation of state is

$$P_i = \rho_i R_i T \quad (2.3-9)$$

Summing over all components of the mixture, the overall equation of state is obtained

$$P = \rho R T \quad (2.3-10)$$

where

$$R = \sum_{i=1} c_i R_i \quad (2.3-11)$$

## 2.4 INITIAL LINE CONSTRUCTION

The solution to equations 2.3-1 through 2.3-11 becomes highly complex in the subsonic-transonic domain. Because of the elliptic character of the partial differential equations for the case of steady-state, choked flow in a rocket nozzle, the known boundary conditions are improperly set. Thus, it is necessary to construct by approximate means an initial data line suitable for the calculation by method of characteristics of the flow field in the supersonic domain. The method used by the TDK Computer Program in constructing this initial line is summarized below.

### 2.4.1 Uniform Expansions

For the purpose of calculating a transonic solution in the region of the nozzle throat, an average expansion coefficient is determined. To accomplish this, a one-dimensional calculation is performed from the chamber to throat for the propellant system and nozzle geometry specified using the ODK subprogram.

Tables of flow properties ( $\rho, V, T, c_1$ ) are constructed as a function of pressure. These tables span the nozzle throat region. An average expansion coefficient is computed using these tables as\*

$$\gamma = \frac{\ln(P_\ell/P_1)}{\ln(\rho_\ell/\rho_1)}$$

where the subscripts 1 and  $\ell$  refer to the first and last table entries, respectively.

Using the above expansion coefficient and the throat wall geometry, the transonic flow field is constructed using the method of Sauer in a somewhat modified form as described in section 2.4.3. The initial line calculated by this method is an approximation to the constant pressure surface emanating from the throat minimum point. Along a constant property line it is a reasonable assumption that a constant value for expansion coefficient can be used.

---

$$* \quad \gamma \equiv \frac{d \ln P}{d \ln \rho} \doteq \frac{\ln P_\ell - \ln P_1}{\ln \rho_\ell - \ln \rho_1} = \frac{\ln(P_\ell/P_1)}{\ln(\rho_\ell/\rho_1)}$$

The TDK transonic analysis computes the pressure value at the throat minimum point, the location of the corresponding isobar, and the variation of streamline flow angle along this isobar. This particular surface has been chosen because it is advantageous from the standpoint of the assumptions made in the transonic analysis. It satisfies boundary conditions exactly at the wall, as well as at the axis and will yield a constant Mach number which is usually slightly greater than unity. If supersonic, this surface will be upstream of its characteristics, both left and right running. Should this surface be subsonic due to nonequilibrium effects, a provision exists for displacing the initial line downstream. Once the pressure surface described above has been calculated, all of the other gas dynamic properties are obtained by interpolation from the tables constructed by ODK.

#### 2.4.2 Zoned Expansions

Many rocket thrust chambers are designed to operate with a cool (fuel rich) barrier zone near the wall to help shield the wall from excessive heat transfer. In addition thrust chamber and injector design usually result in a mal-distribution of the fuel/oxidizer ratio so that the resultant flow is striated into numerous zones of varying mixture ratio. In order to obtain an estimate of the effect of these phenomena on engine performance, a zoned expansion capability is included in the TDK computer program. Each zone is assumed to have a distinct mixture ratio and to contain a specified fraction of the total nozzle mass flow rate. The zones are assumed to be axially symmetric and are distributed radially from the nozzle axis to the nozzle wall.

The procedure used in constructing an initial line for zoned expansions is analogous to that described above for uniform expansions. For the purpose of calculating a transonic solution in the region of the nozzle throat, an average expansion coefficient is determined for each zone. To accomplish this, a one dimensional calculation is performed from the chamber to throat for the propellant system and nozzle geometry specified using the ODK Computer Program. One such calculation is performed for each zone (i. e. for each mixture ratio).



Tables of flow properties ( $\rho, V, T, c_1$ ) are constructed as a function of pressure for each zone. These tables span the nozzle throat region. An average expansion coefficient,  $\bar{\gamma}_n$ , is computed for each of N zones using these tables as

$$\bar{\gamma}_n = \frac{\ln(P_\ell / P_1)_n}{\ln(\rho_\ell / \rho_1)_n} \quad n = 1, \dots, N$$

where the subscripts 1 and  $\ell$  refer to the first and last table entries, respectively.

Using the above expansion coefficient vector and the throat wall geometry, the transonic flow field is constructed using the method described in section 2.4.3. The initial line calculated by this method is an approximation to the constant pressure surface emanating from the throat minimum point. Along this line each zone is separated by a double point defining the properties on either side of the contact discontinuity.

These points, which have equal pressure and gas streamline angle, become dividing streamline points in the method of characteristics calculation (see subroutine DSPT, Section 5). Properties other than pressure and flow angle are discontinuous across a dividing streamline and these discontinuities may be large. Within a given zone only the gas streamline angle will vary with location ( $r, x$ ) along the start line. Properties other than pressure and flow angle are obtained by interpolation on pressure from the tables constructed as described above by use of the ODK subprogram.

### 2.4.3 Transonic Analysis

The basic assumptions made in carrying out the transonic analysis are summarized below (see Reference 9 for a more complete discussion):

- o The flow is inviscid and compressible
- o The flow is near the sonic speed and directed nearly along the nozzle axis
- o The flow is axially symmetric
- o The flow is divided into annular zones, each of which is characterized by a single adiabatic expansion coefficient,  $\gamma$ .
- o In the nozzle throat region the flow is dependent only on the local wall geometry

With the above assumptions equations 2.3-1 through 2.3-11 reduce to the equations governing the irrotational flow of a perfect gas, i.e.:

$$\frac{\partial v}{\partial x} - \frac{\partial u}{\partial r} = 0$$

and

$$(a^2 - u^2) \frac{\partial u}{\partial x} - 2uv \frac{\partial u}{\partial r} + (a^2 - v^2) \frac{\partial v}{\partial r} + \frac{a^2 v}{r} = 0$$

The method of analysis used to approximate a transonic solution to these equations is a small perturbation technique. For a one zone expansion the method reduces to that given by Sauer.<sup>8</sup> The method consists of normalizing the velocity to the critical speed of sound

$$\tilde{u} = \frac{u}{a^*}$$

$$\tilde{v} = \frac{v}{a^*}$$

Perturbation variables  $u'$  and  $v'$  (both of which are assumed of small magnitude with respect to unity) are then introduced.

$$\tilde{u} = 1 + u'$$

$$\tilde{v} = v'$$

It can be shown that substituting these relations into the governing equations and retaining only terms through first order gives\*

$$\frac{\partial v'}{\partial x} - \frac{\partial u'}{\partial r} = 0$$

$$(\gamma + 1) u' \frac{\partial u'}{\partial x} - \frac{\partial v'}{\partial r} - v'/r = 0$$

An exact solution for the above equations can be constructed and is found to be

$$u' = \frac{1}{4} (\gamma + 1) B_1^2 r^2 + C_1 \ln r + B_0 + B_1 x$$

$$v' = \frac{1}{16} (\gamma + 1)^2 B_1^3 r^3 + \frac{1}{2} (\gamma + 1) B_1 C_1 r (\ln r - \frac{1}{2})$$

$$+ \frac{1}{2} (\gamma + 1) B_1 B_0 r + C_2/r$$

$$+ \left[ \frac{1}{2} (\gamma + 1) B_1^2 r + C_1/r \right] x$$

where  $B_0$ ,  $B_1$ ,  $C_1$ , and  $C_2$  are constant coefficients which must be determined from boundary conditions. For the case of a nozzle throat with constant radius of curvature,  $R$ , (i.e. a circular arc, see Figure 2-2) these coefficients are found to be

$$B_0 = - \frac{1}{4R}$$

$$B_1 = + \left( \frac{2}{(\gamma + 1)R} \right)^{\frac{1}{2}}$$

$$C_1 = C_2 = 0$$

which is the classical solution given by Sauer.<sup>8</sup>

\*A complete derivation of the material presented here is given in Reference 9.

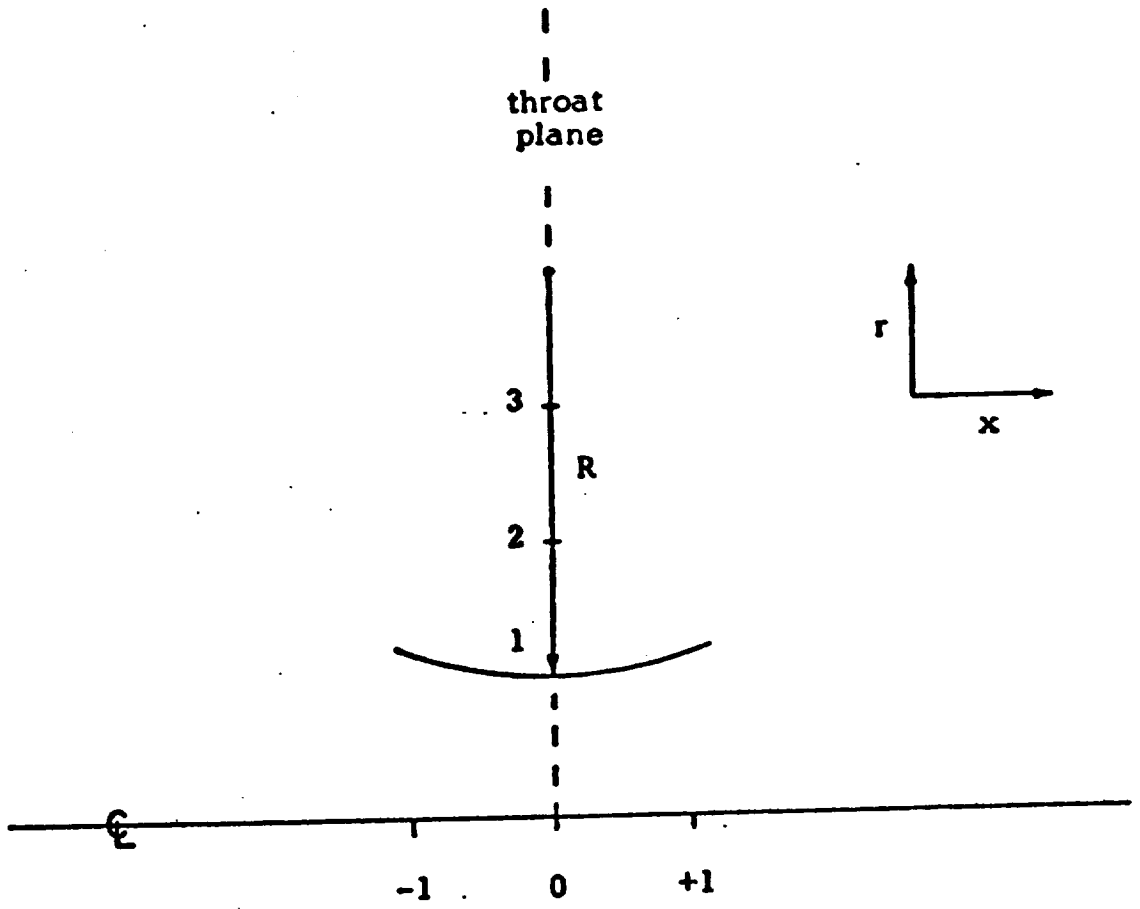


Figure 2-2 Nozzle Throat Geometry

Nearly all exhaust nozzles for engines using liquid propellants are constructed with a radius of curvature smaller than appropriate to the small perturbation methods of analysis. Fortunately a simple modification to the method yields results which compare favorably both with experimental measurement and with the results of other analysis when applied to throat geometries such as occur in rocket exhaust nozzles of practical interest. The basis for this modification is to bound the method such that the computed pressure proceeds to a physically reasonable limit for a zero radius of curvature throat. The bound is applied at the wall boundary condition and is chosen such that the ratio of pressure to sonic pressure be zero at this limit. This assumption leads to the result that

$$P/P^* \Big|_{\text{throat}} = 1 - (\gamma/4) / (R + \gamma/4)$$

rather than the usual result

$$P/P^* \Big|_{\text{throat}} = 1 - (\gamma/4) / R$$

which is divergent for  $R = 0$ . Results obtained from the transonic analysis (see Reference 8) have been found to compare favorably to both available experimental data and to the results of other, more complex, analytical methods.

To apply the small perturbation analysis to striated flow the analysis assumes that the nozzle flow is divided into  $N$  axially symmetric zones, each of which is characterized by a constant (i.e. average) specific heat ratio. These  $N$  zones are bounded by  $N-1$  sliplines, i.e. dividing streamlines, such that pressure and streamline angle are matched but other properties such as velocity, temperature, and Mach number are discontinuous. A first order method is used to determine the radial coordinate location,  $Y_n$ , of each slipline. Once these locations are known, boundary conditions are applied at the wall, axis, and each slipline to complete the solution.

The indices  $n = 0, 1, \dots, N$  identifying each zone and slipline boundary are taken numbered from nozzle axis to wall as shown in Figure 2-3. The sliplines are located at

$$Y_n ; n = 0, 1, \dots, N$$

The total mass flow rate for the nozzle is

$$\dot{M}$$

and for each zone the partial mass flow rate is

$$\dot{m}_n = \frac{\text{mass flow rate, zone } n}{\dot{M}} \quad , n = 1, 2, \dots, N$$

so that

$$\sum_{n=1}^N \dot{m}_n = 1 = \dot{m}_1 + \dot{m}_2 + \dots + \dot{m}_n$$

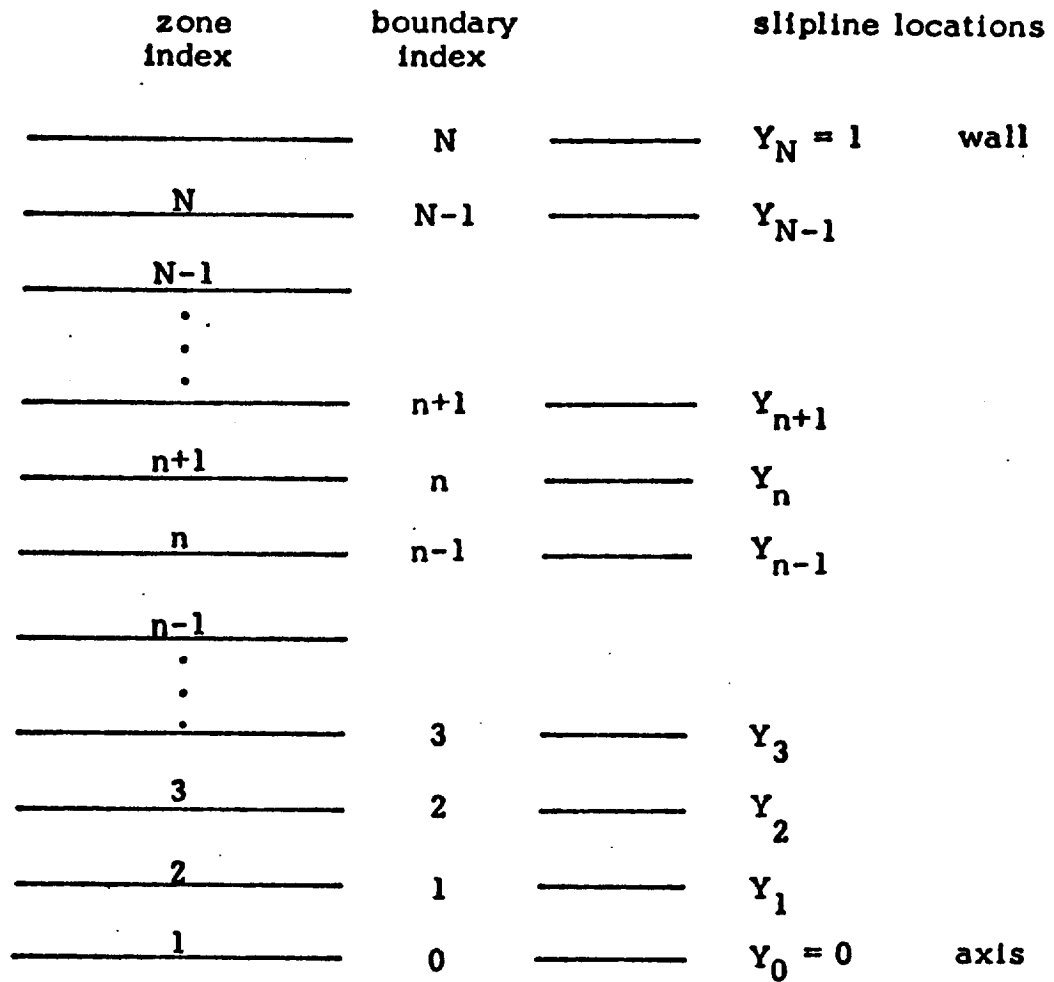


Figure 2-3    Nomenclature for the Numbering of Zones





at the wall;

the gas streamline follows the wall streamline through first order. These conditions require that the following relations be satisfied by the constant coefficients:

at the axis (for  $n=1$ );

$$C_{1_1} = C_{2_1} = 0$$

at the sliplines (for  $n=2, \dots, N=1$ );

$$\begin{aligned} \frac{1}{16} (\gamma_n + 1)^2 B_{1_n}^3 Y_n^3 &+ \frac{1}{2} (\gamma_n + 1) B_{1_n} C_{1_n} Y_n (\ln Y_n - \frac{1}{2}) \\ &+ \frac{1}{2} (\gamma_n + 1) B_{1_n} B_{0_n} Y_n + C_{2_n} Y_n^{-1} = \end{aligned}$$

$$\begin{aligned} \frac{1}{16} (\gamma_{n+1} + 1)^2 B_{1_{n+1}}^3 Y_n^3 &+ \frac{1}{2} (\gamma_{n+1} + 1) B_{1_{n+1}} C_{1_{n+1}} Y_n (\ln Y_n - \frac{1}{2}) \\ &+ \frac{1}{2} (\gamma_{n+1} + 1) B_{1_{n+1}} B_{0_{n+1}} Y_n + C_{2_{n+1}} Y_n^{-1} \end{aligned}$$

and

$$\frac{1}{2} (\gamma_n + 1) B_{1_n}^2 Y_n + C_{1_n} Y_n^{-1} = \frac{1}{2} (\gamma_{n+1} + 1) B_{1_{n+1}}^2 Y_n + C_{1_{n+1}} Y_n^{-1}$$

and

$$\begin{aligned} P_n^* \left\{ 1 - \gamma_n \left[ \frac{1}{4} (\gamma_n + 1) B_{1_n}^2 Y_n^2 + C_{1_n} \ln Y_n + B_{0_n} \right] \right\} = \\ P_{n+1}^* \left\{ 1 - \gamma_{n+1} \left[ \frac{1}{4} (\gamma_{n+1} + 1) B_{1_{n+1}}^2 Y_n^2 + C_{1_{n+1}} \ln Y_n + B_{0_{n+1}} \right] \right\} \end{aligned}$$

and

$$P_n^* \gamma_n B_{1_n} = P_{n+1}^* \gamma_{n+1} B_{1_{n+1}}$$

at the wall ( $n = N$ );

$$\frac{1}{16} (\gamma_N + 1)^2 B_{1N}^3 - \frac{1}{4} (\gamma_N + 1) B_{1N} C_{1N} + \frac{1}{2} (\gamma_N + 1) B_{1N} B_{0N} + C_{2N} = 0$$

and

$$\frac{1}{2} (\gamma_N + 1) B_{1N}^2 + C_{1N} = 1/R$$

The above equations form a system of  $4N$  non-linear equations in  $4N$  unknowns ( $B_{0n}, B_{1n}, C_{1n}, C_{2n}$ ). For given values of  $R$  and of the vectors  $\dot{m}_n, A_n, \gamma_n,$  and  $Y_n$  the above system of equations can be used to determine the  $4N$  unknown coefficients by employing standard numerical technique.

To apply a numerical method (such as the Newton method) to obtain a solution to the above system of equations requires an estimate for the solution vector ( $B_{0n}, B_{1n}, C_{1n}, C_{2n}$ ). The TDK program uses the one zone solution to provide a first estimate. A good estimate is obtained since if

$$\gamma_n = \gamma_{n+1} \quad n = 1, 2, \dots, N-1$$

the one zone solution satisfies the above system identically. The program also takes advantage of the banded property of the Jacobian,  $J$ , for the above system in using Newton's Method,  $x^{(k+1)} = x^{(k)} - J^{(k)^{-1}} f^{(k)}$ , to obtain solutions.

The method described above has also been bounded so as to give reasonable answers for nozzle geometries where  $R$  is small.

#### 2.4.4 Transonic Model with Mixture Ratio Variation

The transonic model used by TDK which is described in the preceding section divides the flow into regions of constant mixture ratio that are separated by sliplines. Each region contains a specified fraction of the total mass flow. This method, which is called the striated flow option, has been modified so that flows with continuous mixture ratio variation can be analyzed. This variable mixture ratio option is described below.

When the variable mixture ratio option is used, there are no sliplines in the flow. Instead, the flow mixture ratio,  $r$ , will vary from the axis ( $\Psi=0$ ) to the wall ( $\Psi=1$ ) as specified by an input table of  $r$  versus  $\Psi$ . The streamline function,  $\Psi$ , represents the mass flow between the streamline and the axis, divided by the total nozzle mass flow. An ODK calculation is done for each entry in the above table. Values along the initial data line for the MOC are obtained by interpolation in the ODK results using pressure and radial coordinate position,  $Y$ , as independent variables. The transonic analysis is used to provide a table of  $\Psi$  versus  $Y$ . The method used is described below.

The ODK program constructs tables of flow properties ( $\rho$ ,  $V$ ,  $T$ , and  $c_1$ ) as a function of pressure. These tables span the nozzle throat region. An average expansion coefficient is computed using these tables as

$$\bar{\gamma} = \ln(P_2/P_1) / \ln(\rho_2/\rho_1)$$

where the subscripts 1 and  $l$  refer to the first and last table entries, respectively. Values of  $Y$  are found from  $\bar{Y}$  and from input to the transonic analysis

$$Y_n = (\bar{Y}_n + \bar{Y}_{n-1})/2 \quad n = 1, 2, \dots, N$$

and also

$$P_{c_n} = (\bar{P}_{c_n} + \bar{P}_{c_{n-1}})/2$$

$$\xi_n = \psi_n - \psi_{n-1}$$

Using these values, the transonic analysis calculates

$$Y_0 = 0, Y_1, Y_2, \dots, Y_N = Y_{\text{wall}}$$

The above  $Y_n$  values represent the radial location at which the input mixture ratios

$$r_0, r_1, r_2, \dots, r_N$$

are located. In this way the input table of  $r$  versus  $\psi$  is converted to a table of  $r$  versus  $Y$ .

Next, the transonic analysis is used to compute the coefficients  $(B_0, B_1, C_1, C_2)$ . These are used to compute  $P(X, Y)$  and  $\theta(X, Y)$  in the transonic region (see Reference 9, pp.2-20) at points  $n=0, 1, \dots, N$ . Using each of these  $N + 1$  values of  $P$  as an independent variable, the corresponding values for  $\rho, V, T$ , and  $c_i$  are obtained by linear interpolation from the corresponding table that was computed by ODK. These tables are then used to linearly interpolate for  $P, \rho, V, \theta, T$ , and  $c_i$  at each MOC initial line point using  $\psi$  as the independent variable.

The program will not function properly if the spacing in the mixture ratio table,  $r_n$ , is too large. The required spacing depends on the chemical system. As a rule each entry must differ no more than 4 or 5% from its adjacent values, depending on the stoichiometry of the system.

The average engine mixture ratio,  $r_{ave}$ , is also calculated:

$$r_{ave} = \frac{\int_0^{Y_{wall}} \left(\frac{r}{r+1}\right) d\dot{m}}{\int_0^{Y_{wall}} \left(\frac{1}{r+1}\right) d\dot{m}}$$

where

$r$  is the mixture ratio at position  $Y$ , and

$$d\dot{m} = \rho V \frac{\sin(\phi-\theta)}{\sin\phi} Y dY.$$

## 2.5 METHOD OF CHARACTERISTICS FOR KINETIC EXPANSIONS

By standard methods the characteristic relationships for the conservation equations 2.3-1 through 2.3-11 can be shown to be (see Volume 2, Section 18-3, Zucrow and Hoffman<sup>10</sup>).

$$\frac{dr}{dx} = \tan \theta$$

$$d \frac{v^2}{2} + \frac{dP}{\rho} = 0$$

$$\frac{dP}{\gamma P} - \frac{d\rho}{\rho} = \frac{A}{\cos \theta} dx$$

$$\frac{\gamma - 1}{\gamma} \frac{dP}{P} - \frac{dT}{T} = \frac{B}{\cos \theta} dx$$

$$dc_i = \frac{\omega_i r^*}{\rho V \cos \theta} dx$$

along streamlines,

$$\frac{dx}{dr} = \cot(\theta + \alpha) \quad (2.5-1)$$

$$\frac{dP}{P} = G \left[ \left( A - \frac{\sin \theta}{r} \right) F dr - d\theta \right] \quad (2.5-2)$$

along left running characteristics, and

$$\frac{dr}{dx} = \tan(\theta - \alpha) \quad (2.5-3)$$

$$\frac{dP}{P} = -G \left[ \left( A - \frac{\sin \theta}{r} \right) H dx - d\theta \right] \quad (2.5-4)$$

along right running characteristics, where

$$A = \frac{r^*}{PV} \left( \sum_{i=1} \omega_i R_i T - \frac{\gamma - 1}{\gamma} \sum_{i=1} \omega_i h_i \right)$$

$$B = \frac{r^*}{PV} \frac{\gamma - 1}{\gamma} \sum_{i=1} \omega_i h_i$$

$$V = (u^2 + v^2)^{1/2}$$

$$\theta = \tan^{-1} \left( \frac{v}{u} \right)$$

$$\alpha = \sin^{-1} \left( \frac{1}{M} \right)$$

$$M = \frac{V}{(\gamma RT)^{1/2}}$$

$$\gamma = \frac{C_p}{C_p - R}$$

$$C_p = \sum_{i=1} c_i C_{pi}$$

$$F = \cos \theta - \sin \theta \cot (\theta + \alpha) \quad (2.5-5)$$

$$G = \frac{\gamma}{\sin \alpha \cos \alpha} \quad (2.5-6)$$

$$H = \cos \theta \tan (\theta - \alpha) - \sin \theta \quad (2.5-7)$$

The above form of the characteristic relationships remains determinant when the streamline is horizontal, when the left running characteristic is vertical, or when the right running characteristic is horizontal. Rarely (if ever) will the inverse of the three situations occur in nozzle flow field calculations.

In the analysis above the chemistry is brought into the conservation equations through the net species production rates,  $\omega_i$ . The analysis pertaining to the chemistry is identical to that used by the ODK program as presented in Section 2.2.



### 2.5.1 Method of Characteristics for Frozen Expansions (TDF)

The methods developed in the preceding section for kinetic expansions apply with the exception that

$$\dot{\omega}_1 = 0$$

so that

$$A = B = 0$$

and

$$dc_1/dx = 0$$

Ordinarily the TDF expansion assumes the chemical composition to be frozen at the equilibrium values at the chamber contraction ratio (ECRAT). However, initial species compositions and flow conditions can be input. This is the procedure that must be followed when analyzing hydrazine monopropellant thrusters.

## 2.5.2 Method of Characteristics for Equilibrium Expansions (TDE)

The supersonic expansion can be analyzed using the method of characteristics assuming that the process is in a state of shifting chemical equilibrium. This option is called a TDE analysis. It can be used both for striated flow, and flow with streamline to streamline mixture ratio variation. Like the TDF analysis, it is very much faster than a TDK analysis. The methods used by TDE are described below.

The conservation equations to be solved are:

continuity:  $(\rho u)_x + \frac{1}{r} (r\rho v)_r = 0$

momentum:  $\rho (uu_x + vu_r) + P_x = 0$

$$\rho (uv_x + vv_r) + P_r = 0$$

energy: The energy equation is not used explicitly. Instead, property distributions are provided in the form of tables by a separate equilibrium computation. The energy equation is then satisfied in an implicit manner as\*

$$V = (2h_0 - 2h)^{1/2}$$

where

$$h = h(P)$$

is supplied by the chemical equilibrium module, ODE, in the form of a table.

---

\*Entropy is a constant for the expansion so that a function of only one variable, P, is required.

state: The state equation is also satisfied in an implicit manner as

$$\rho = \frac{PM_w}{RT}$$

where  $T = T(P)$

and  $M_w = M_w(P)$

are supplied by the chemical equilibrium module, ODE, in the form of tables.

The above conservation equations have been transformed to the characteristic form and are solved numerically in the same manner as by TDK. For convenience tables of specific heat ratio and Mach number are also tabulated. The complete set of tables used are:

h	vs	log (P)	enthalpy
M	vs	log (P)	Mach number
$M_w$	vs	log (P)	molecular weight
T	vs	log (P)	temperature
$\gamma$	vs	log (P)	ratio of specific heats

where each of the above tables has been constructed for each zone (i.e., region of constant mixture ratio) of the expansion. The above choice of curve fit form (i.e., vs P or log P) was made after investigating the graphical form of the above functions for typical equilibrium expansions. A spline fit method is used to interpolate in the above tables.

### 2.5.3 METHOD OF CHARACTERISTICS FOR APPROXIMATE KINETIC EXPANSION (TTDK)

The supersonic expansion can be analyzed using the method of characteristics assuming that the gas properties are defined by a set of tables prepared by the ODK module. The procedures and tables are the same as presented in the preceding subsection describing TDE expansions, except that ODK is used to prepare the tables, not ODE.

An expression for the kinetic variable, A, is also required. It is found as (see the third equation in Section 2.5):

$$A = \left( \frac{1}{\gamma P} \frac{dP}{dX} - \frac{1}{\rho} \frac{d\rho}{dX} \right) \cos \theta$$

where  $dP/dX$  and  $d\rho/dX$  are found by numerical differencing.

The kinetic variable, B, is not required, since the gas temperature is found as a tabular function of the logarithm of the pressure.

A significant advantage of this option is that it gives an order of magnitude reduction in computer time for a given case. Although exact results can be obtained in the frozen and equilibrium limits, error can be introduced when the expansion is in chemical nonequilibrium.

### 2.5.4 SUPERSONIC FLOW WITH SHOCK WAVES

For the case of continuous variation (or no variation) in mixture ratio, the TDK computer program can calculate the effects of a single shock wave that is caused by the nozzle wall. The shock can either be attached to the wall, or induced by the wall. The latter case is the more difficult to treat. The program logic utilizes a series six of point calculation procedures to locate and compute the shock. These procedures are illustrated in Figures 2-4a through f. The flow direction

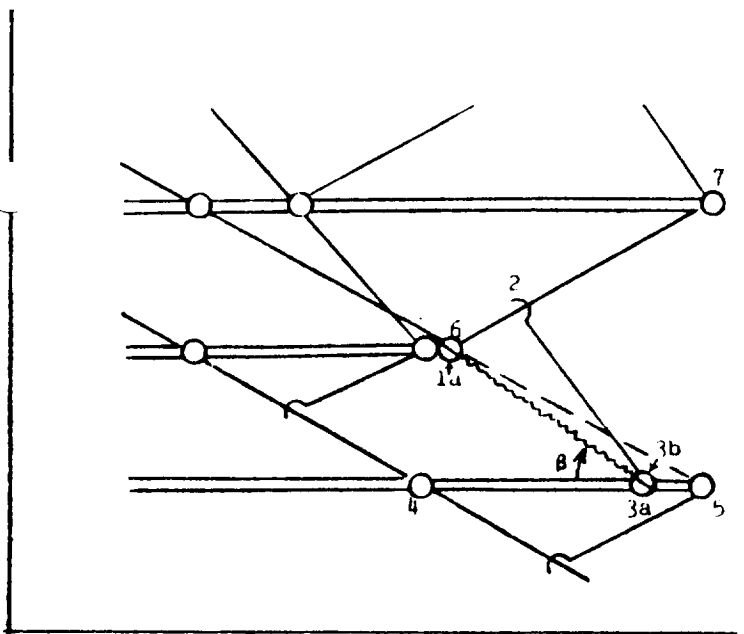


Fig. 2-4a: Right-Running Shock Point

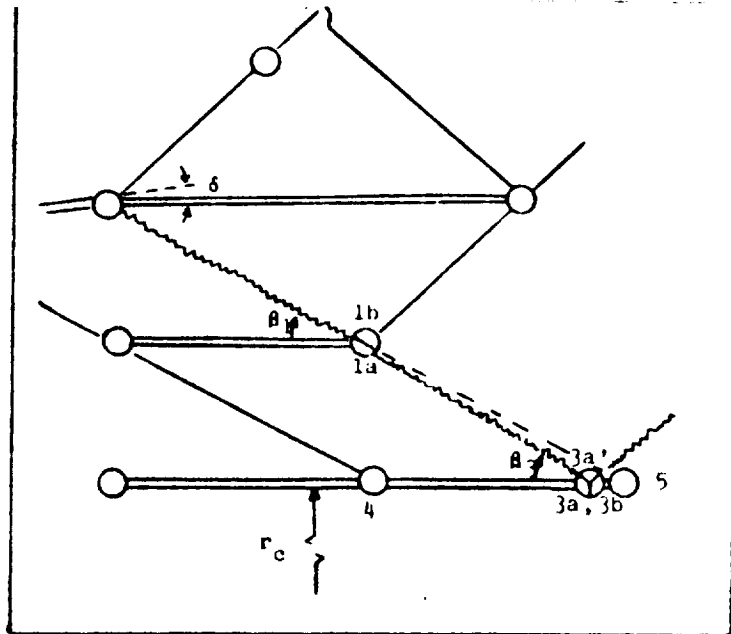


Fig. 2-4b: Shock Reflection Point at the Axis

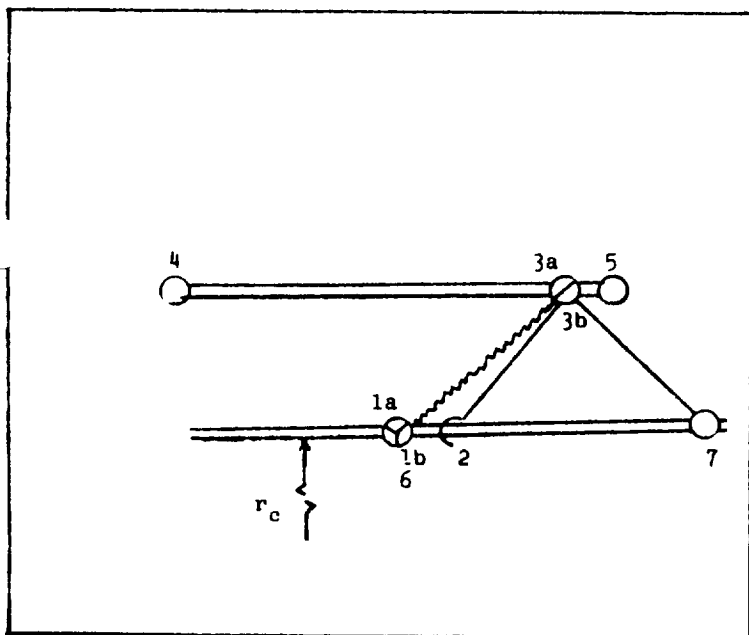


Fig. 2-4c: Left-Running Shock Point at the Axis

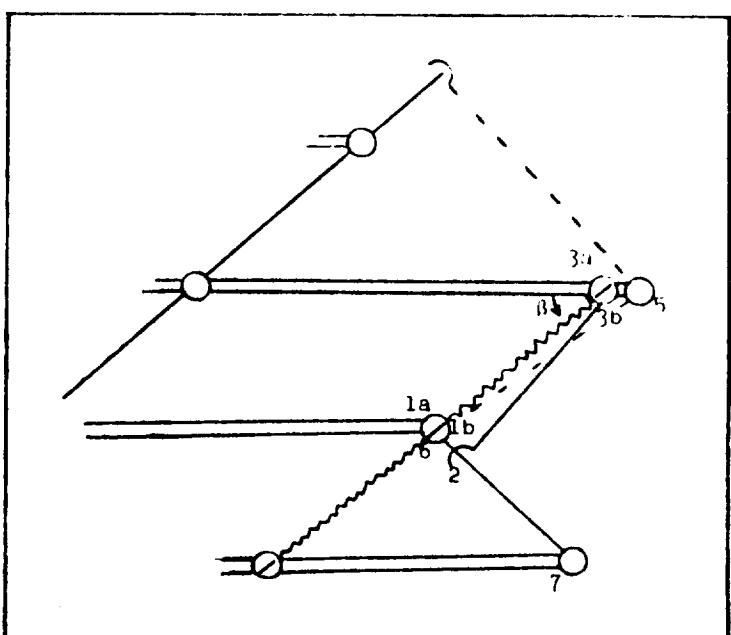


Fig. 2-4d: Left-Running Shock Point

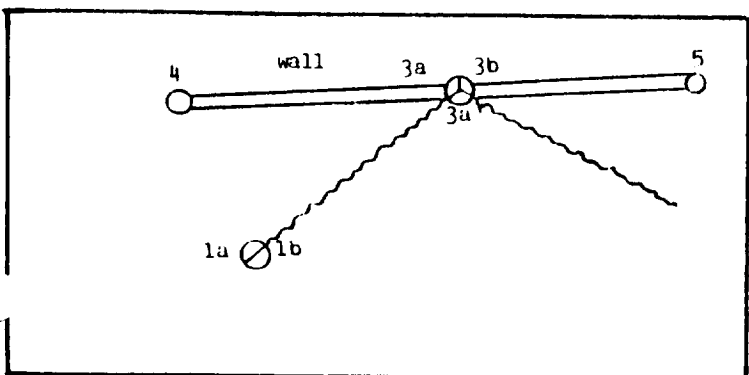


Fig. 2-4e: Shock Reflection Point at the Wall

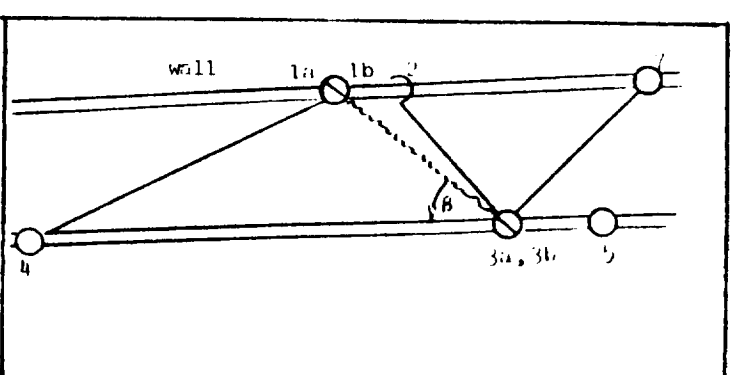


Fig. 2-4f: Right-Running Shock Point at the Wall

is left to right with streamlines shown as double lines. As shown in Fig. 2-4a the shock is initiated by a crossing of right-running characteristics. A shock point, labeled 3a (front) and 3b (back) is computed by iteration of the streamline, characteristic, and shock relations. When completed, the point location and the front and back side properties satisfy all of these relations. This right running shock is traced to the flow axis and reflected as a left running shock. The procedure for calculating the reflection is shown in Fig. 2-4b. If at any point in the shock tracing it is found that regular reflection is not possible, then a right regular cylinder of radius,  $r_c$ , is inserted centered along the flow axis. The shock is reflected from this cylinder, which is located so that regular reflection is still possible. In this way Mach shocks are removed from the flow. The first point off the axis (or cylinder) behind the shock reflection is calculated by the special procedure shown in Fig. 2-4c. Next, the shock is traced as a left running shock using the point calculation procedure shown in Fig. 2-4d. This procedure is the inverse of the right running shock point procedure shown in Fig. 2-4a. When the shock reaches the wall, it is reflected using the procedure shown in Fig. 2-4e. A special point calculation procedure is then required for the first point behind this reflection as shown in Fig. 2-4f. The resultant right running shock is then traced as before, etc. Thus, multiple reflections are allowed from the axis and the wall. In general the shock strengthens as it travels towards the axis (right running), and weakens as it travels away from the axis and towards the wall (left running).

The shock option is not applicable to the TDE and TTDK options.

## 2.6 THE BOUNDARY LAYER MODULE (BLM)

The purpose of the Boundary Layer Module (BLM) is to provide a method for computing compressible laminar and turbulent wall boundary layers in axisymmetric nozzles. The BLM can also be used to calculate two-dimensional and axisymmetric external flows. The method utilizes an efficient two-point finite difference method developed by Keller and Cebeci<sup>11</sup>. Turbulence modeling is achieved through the use of Cebeci-Smith eddy-viscosity formulation<sup>12</sup> which has been tested for a large class of flows with various boundary conditions.

In this section the method is described and the relevant equations, turbulence model, fluid properties and solution procedure are presented. Description of the numerical procedure is not presented, since it has already been described in several sources, for example Reference 13.

The computer program on which the BLM is based was developed for SEA, Inc. by CBC Enterprises, Inc.

- Ref. 11 Keller, H. B., and Cebeci, T.: Accurate Numerical Methods for Boundary Layer Flows, Pt. 2, Two-Dimensional Turbulent Flows. AIAA J., 10, 1972, pg. 1193.
- Ref. 12 Cebeci, T., and Smith, A. M. O.: Analysis of Turbulent Boundary Layers, Academic Press, N.Y., 1974.
- Ref. 13 Bradshaw, P., Cebeci, T., and Whitelaw, J. H.: Engineering Calculation Methods for Turbulent Flows. Academic Press, London, 1981.

### 2.6.1 Boundary-Layer Equations

For a compressible boundary-layer flow in a symmetric nozzle, the governing equations are well known and can be written as

Continuity

$$\frac{\partial}{\partial x} (\rho u r^k) + \frac{\partial}{\partial y} (\rho v r^k) = 0 \quad (2.6-1)$$

Momentum

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} = \rho_e u_e \frac{du_e}{dx} + \frac{1}{r^k} \frac{\partial}{\partial y} [r^k (\mu \frac{\partial u}{\partial y} - \rho \overline{u'v'})] \quad (2.6-2)$$

Energy

$$\rho u \frac{\partial H}{\partial x} + \rho v \frac{\partial H}{\partial y} = \frac{1}{r^k} \frac{\partial}{\partial y} \left\{ r^k \left[ \frac{\mu}{Pr} \frac{\partial H}{\partial y} + \mu \left( 1 - \frac{1}{Pr} \right) u \frac{\partial u}{\partial y} - \rho \overline{H'v'} \right] \right\} \quad (2.6-3)$$

where  $k$  denotes the flow index which is zero for a two-dimensional flow and is unity for an axisymmetric flow, and

$$\begin{aligned} \overline{\rho v} &= \rho v + \overline{\rho'v'} \\ r &= r_0 - y \cos\phi \end{aligned}$$

The boundary conditions for Eqs. (7-1) to (7-3) are

$$\text{at } y = 0, \quad u = 0, \quad v = v_w(x),$$

$$T = T_w(x) \quad \text{or} \quad \dot{q}_w(x) \text{ (heat transfer specified)} \quad (2.6-4a)$$

$$\text{at } y = \delta, \quad u = u_e, \quad H = H_e \quad (2.6-4b)$$

The above equations require initial conditions and a turbulence model for Reynolds shear stress and heat flux terms,  $-\rho \overline{u'v'}$  and  $-\rho \overline{H'v'}$ , respectively. Here we use the concepts of eddy viscosity and turbulent Prandtl number and define



$$-\rho \overline{u'v'} = \rho \epsilon_m \frac{\partial u}{\partial y}, \quad -\rho \overline{H'v'} = \rho \frac{\epsilon_m}{Pr_t} \frac{\partial H}{\partial y} \quad (2.6-5)$$

We also use transformed variables to provide the initial conditions for a stagnation point flow and to reduce the sensitivity of the solutions to the  $\Delta x$ -spacing. They are defined by

$$d\xi = \left(\frac{r_0}{L}\right)^{2k} dx \quad (2.6-6a)$$

$$d\eta = \left(\frac{u_e}{\rho_e \mu_e \xi}\right)^{1/2} \rho \left(\frac{r_0}{L}\right)^k dy \quad (2.6-6b)$$

We also use a dimensionless stream function  $f(\xi, \eta)$  defined by

$$\psi = (u_e \rho_e \mu_e \xi)^{1/2} L^k f(\xi, \eta) \quad (2.6-7)$$

where

$$\rho u r^k = \frac{\partial \psi}{\partial y}, \quad \rho v r^k = (\rho v)_w r_0^k - \frac{\partial \psi}{\partial x} \quad (2.6-8)$$

With these transformations and with the definition of the relations given by Eqs (2.6-6 to 8) it can be shown that the momentum and energy equations can be written as

$$(bf'')' + m_1 f f'' + m_2 [c - (f')^2] - m_3 f'' = \xi \left( f' \frac{\partial f'}{\partial \xi} - f'' \frac{\partial f}{\partial \xi} \right) \quad (2.6-9)$$

$$(eg')' + (df'f'')' + m_1 f g' - m_3 g' = \xi \left( f' \frac{\partial g}{\partial \xi} - g' \frac{\partial f}{\partial \xi} \right) \quad (2.6-10)$$

Here primes denote differentiation with respect to  $\eta$  and

$$f' = u/u_e, \quad g = H/H_e \quad (2.6-11)$$

The parameters  $b, e, d$  denote parameters defined by

$$b = (1 + \epsilon_m^+) C (1 - t)^{2k}, \quad e = \frac{C}{Pr} \left(1 + \epsilon_m^+ \frac{Pr}{Pr_t}\right) (1 - t)^{2k} \quad (2.6-12)$$

$$d = \frac{Cu_e^2}{H_e} \left(1 - \frac{1}{Pr}\right) (1 - t)^{2k}$$

where

$$C = \frac{\rho u}{\rho_e \mu_e}, \quad c = \frac{\rho_e}{\rho}$$

The parameters below denote dimensionless pressure gradients

$$m_1 = \frac{1 + m_2 + m_4}{2}, \quad m_2 = \frac{\xi}{u_e} \frac{du_e}{d\xi}, \quad m_4 = \frac{\xi}{\rho_e \mu_e} \frac{d}{d\xi} (\rho_e \mu_e) \quad (2.6-13)$$

and  $m_3$  denotes dimensionless mass transfer parameter

$$m_3 = \frac{(\rho v)_w}{\rho_e u_e} R_\xi^{1/2} \left(\frac{L}{r_0}\right)^k \quad (2.6-14)$$

The boundary conditions given by (2.6-4) can be written in the following form

$$\begin{aligned} \text{at } \eta = 0, \quad f = f' = 0, \quad g = g_w(\xi) \text{ given} \\ \text{or} \\ g'_w(\xi) = \text{given} \end{aligned} \quad (2.6-15a)$$

$$\text{at } \eta = \eta_e, \quad f' = 1, \quad g = 1 \quad (2.6-15b)$$

Note that the wall mass transfer quantity  $(\rho v)_w$  does not appear in the above boundary conditions, instead it appears in the differential equations through  $m_3$ . This is a useful convenient form when dealing with mass transfer (suction or blowing) problems.

### 2.6.2 Turbulence Model

Here we use the eddy-viscosity formulation due to Cebeci and Smith to model the Reynolds shear stress term. We assume a constant turbulent Prandtl number and take it equal to 0.9.

According to the Cebeci and Smith eddy-viscosity formulation, the dimensionless eddy-viscosity  $\epsilon_m^+$  is defined by two separate formulas: in the inner region of the boundary layer,  $\epsilon_m^+$  is defined by a modified mixing-length expression and in the outer region by an expression based on the velocity defect. This formulation is defined by the following expressions:

$$\epsilon_m^+ = \begin{cases} \frac{L^2}{\nu} \frac{\partial u}{\partial y} \gamma \gamma_{tr} & y \leq y_c \text{ , inner} \\ \frac{0.0168}{\nu} \int_0^\infty |(u_e - u)| dy \gamma \gamma_{tr} & y > y_c \text{ , outer} \end{cases} \quad (2.6-16)$$

Here  $y_c$  is obtained from the continuity of eddy-viscosity expression. The definition of  $L$  is:

$$L = 0.4y[1 - \exp(-y/A)] \quad (2.6-17)$$

where

$$A = 26 \left( \frac{\rho_e}{\rho_w} \right)^{1/2} \frac{\nu}{N} u_\tau^{-1} \quad u_\tau = \left( \frac{\tau_w}{\rho_w} \right)^{1/2}$$

$$N^2 = \frac{\mu}{\mu_e} \left( \frac{\rho_e}{\rho_w} \right)^2 \frac{p^+}{v_w^+} [1 - \exp(11.8 \frac{\mu_w}{\mu} v_w^+)] + \exp(11.8 \frac{\mu_w}{\mu} v_w^+) \quad (2.6-18)$$

$$p^+ = \frac{v_e u_e}{u_\tau^3} \frac{du_e}{dx}, \quad v_w^+ = \frac{v_w}{u_\tau}, \quad R_\xi = \frac{u_e \xi}{\nu_e}, \quad \frac{\mu}{\mu_e} \left( \frac{\rho_e}{\rho_w} \right)^2 = C_{cc}^2 C_w^2$$

When there is no mass transfer,

$$N^2 = 1 - 11.8 \frac{\mu_w}{\mu_e} \left( \frac{\rho_e}{\rho_w} \right)^2 p^+ = 1 - 11.8 C_w C_w^3 p^+$$

The parameter  $\gamma$  is an intermittency term defined by

$$\gamma = \frac{1}{1 + 5.5(y/\delta)^6} \quad (2.6-19a)$$

and  $\gamma_{tr}$  is a parameter which accounts for the transitional region which exists between a laminar and turbulent flow. At high Reynolds number flows, though the transition region is small and  $\gamma_{tr}$  has negligible effect on the results, this expression is still useful because it avoids a jump from laminar to turbulent flow calculations by allowing  $\epsilon_m^+$  to change gradually. It is given by:

$$\gamma_{tr} = 1 - \exp[-Gr_0^k(x_{tr}) \left( \int_{x_{tr}}^x \frac{dx}{r_0^k} \right) \left( \int_{x_{tr}}^x \frac{dx}{u_e} \right)] \quad (2.6-19b)$$

where  $G$  is a spot-formation-rate parameter

$$G = (3/C_1^2)(u_e^3/\nu_e^2)R_{\xi_{tr}}^{-1.34}$$

$$C_1 = 60 + 4.86M_e^{1.92}$$

In terms of transformed variables, the eddy-viscosity formulas become:

$$\epsilon_m^+ = \begin{cases} \varphi_1 f'' & 0 < \eta < \eta_c \\ \varphi_2 \left| \int_0^{\eta} \frac{c}{(1-t)^k} (1-f') d\eta \right| & \eta_c \leq \eta < \eta_e \end{cases} \quad (2.6-20)$$

Here

$$\varphi_1 = \frac{0.16}{c^2} \left(\frac{L}{r_0}\right)^k (1-t)^k \frac{u_e}{\mu} R_{\xi}^{1/2} I_1^2 [1 - \exp(-y/A)]^2 \gamma_{tr}$$

$$\varphi_2 = \frac{0.0168}{c} \frac{u_e}{\mu} \left(\frac{L}{r_0}\right)^k R_{\xi}^{1/2} \gamma_{tr}$$

(2.6-21)

$$\frac{y}{A} = \frac{N}{26} c^{-3/2} \left(\frac{L}{r_0}\right)^{k/2} \frac{C_w^{1/2}}{c} R_{\xi}^{1/4} I_1 (f_w'')^{1/2}, \quad I_1 = \int_0^{\eta} \frac{c}{(1-t)^k} d\eta$$

$$p^+ = \left(\frac{u_e}{u_{\tau}}\right)^3 \frac{m_2}{R_{\xi}} \left(\frac{r_0}{L}\right)^{2k}$$

$$u_{\tau} = \frac{u_e}{R_{\xi}^{1/4}} \sqrt{c_w f_w'' C_w (r_0/L)^k}$$

### 2.6.3 Fluid Properties

Values of specific heat at constant pressure,  $C_p$ , and ratio of specific heats,  $\gamma$ , static enthalpy,  $h$ , and the gas constant  $R$ , are required by BLM. These properties are evaluated along the wall streamline as a function of temperature using the ODE module. The tables are prepared using a series of (T,S) equilibrium calculations, where  $T$  varies from  $600^\circ\text{R}$  to  $7000^\circ\text{R}$  at  $200^\circ\text{R}$  increments. The chamber entropy value is used for  $S$ . Values at  $100^\circ\text{R}$  are then extrapolated and added to the table. The table is printed with the BLM output. An example of this output is presented in Figure 2-5.

Since the ODE module did not contain a (T,S) option, it was added using the following procedure. Using known values of  $P_a$ ,  $T_a$ , and  $\gamma_a$ , and the given value of temperature,  $T$ , a first estimate for pressure  $P^{(1)}$  was found as

$$P^{(1)} = P_a (T/T_a)^{\gamma_a/(\gamma_a-1)}$$

The (T,P) option of ODE is used to obtain  $S^{(1)}$  as a function of  $P^{(1)}$ . The procedure is iterated using the secant method (subroutine ITER plus a driver) to find  $P^{(1)}$  such that

$$|(S^{(1)} - S_c)/S_c| < 5 \text{ E-}5$$

where  $S_c$  is the chamber entropy. The procedure is repeated for each temperature in these tables. The procedure is internal to the program and not callable through the ODE input.

If the chemical system contains a condensed phase, then equilibrium solutions made during phase change can yield values for  $\gamma$  that are unacceptable to BLM, e.g., values of  $\gamma < 1$ .

Figure 2-5: Tables of h,  $\mu$ , k, C<sub>p</sub>,  $\gamma$ , and R versus T<sup>0</sup>R for use by the BLM

T DEG R	HS FT2/SEC2	MU LBM/FT-SEC	K LBM=FT/S3=DEGR	CP FT2/SEC2=DEGR	GAMMA	RGAS LBF=FT/LBM=DEGR
1.0000E+02	-1.4650E+08	2.1240E-06	4.5618E-02	1.3210E+04	1.3391E+00	1.0396E+02
6.0000E+02	-1.3989E+08	9.3635E-06	2.0110E-01	1.3210E+04	1.3391E+00	1.0396E+02
8.0000E+02	-1.3722E+08	1.1882E-05	2.6108E-01	1.3514E+04	1.3289E+00	1.0396E+02
1.0000E+03	-1.3448E+08	1.4293E-05	3.2270E-01	1.3887E+04	1.3173E+00	1.0396E+02
1.2000E+03	-1.3167E+08	1.6622E-05	3.8664E-01	1.4307E+04	1.3052E+00	1.0396E+02
1.4000E+03	-1.2876E+08	1.8885E-05	4.5315E-01	1.4759E+04	1.2931E+00	1.0396E+02
1.6000E+03	-1.2576E+08	2.1092E-05	5.2228E-01	1.5230E+04	1.2815E+00	1.0396E+02
1.8000E+03	-1.2267E+08	2.3253E-05	5.9399E-01	1.5711E+04	1.2705E+00	1.0396E+02
2.0000E+03	-1.1947E+08	2.5372E-05	6.6906E-01	1.6219E+04	1.2598E+00	1.0396E+02
2.2000E+03	-1.1618E+08	2.7456E-05	7.4517E-01	1.6693E+04	1.2506E+00	1.0396E+02
2.4000E+03	-1.1280E+08	2.9506E-05	8.2215E-01	1.7137E+04	1.2425E+00	1.0396E+02
2.6000E+03	-1.0933E+08	3.1528E-05	8.9997E-01	1.7557E+04	1.2354E+00	1.0396E+02
2.8000E+03	-1.0578E+08	3.3523E-05	9.7888E-01	1.7960E+04	1.2290E+00	1.0397E+02
3.0000E+03	-1.0215E+08	3.5494E-05	1.0596E+00	1.8361E+04	1.2231E+00	1.0397E+02
3.2000E+03	-9.8436E+07	3.7442E-05	1.1435E+00	1.8783E+04	1.2174E+00	1.0397E+02
3.4000E+03	-9.4642E+07	3.9370E-05	1.2327E+00	1.9258E+04	1.2118E+00	1.0399E+02
3.6000E+03	-9.0754E+07	4.1277E-05	1.3304E+00	1.9824E+04	1.2058E+00	1.0401E+02
3.8000E+03	-8.6755E+07	4.3167E-05	1.4409E+00	2.0530E+04	1.1995E+00	1.0405E+02
4.0000E+03	-8.2623E+07	4.5040E-05	1.5692E+00	2.1429E+04	1.1926E+00	1.0411E+02
4.2000E+03	-7.8330E+07	4.6897E-05	1.7215E+00	2.2578E+04	1.1853E+00	1.0420E+02
4.4000E+03	-7.3842E+07	4.8738E-05	1.9036E+00	2.4023E+04	1.1777E+00	1.0433E+02
4.6000E+03	-6.9128E+07	5.0565E-05	2.1210E+00	2.5799E+04	1.1703E+00	1.0452E+02
4.8000E+03	-6.4157E+07	5.2379E-05	2.3775E+00	2.7917E+04	1.1632E+00	1.0476E+02
5.0000E+03	-5.8909E+07	5.4180E-05	2.6735E+00	3.0350E+04	1.1569E+00	1.0507E+02
5.2000E+03	-5.3376E+07	5.5968E-05	3.0056E+00	3.3030E+04	1.1516E+00	1.0544E+02
5.4000E+03	-4.7567E+07	5.7744E-05	3.3664E+00	3.5857E+04	1.1475E+00	1.0589E+02
5.6000E+03	-4.1503E+07	5.9509E-05	3.7456E+00	3.8712E+04	1.1445E+00	1.0639E+02
5.8000E+03	-3.5216E+07	6.1264E-05	4.1324E+00	4.1487E+04	1.1425E+00	1.0694E+02
6.0000E+03	-2.8754E+07	6.3008E-05	4.5145E+00	4.4068E+04	1.1414E+00	1.0754E+02
6.2000E+03	-2.2138E+07	6.4742E-05	4.8870E+00	4.6427E+04	1.1410E+00	1.0817E+02
6.4000E+03	-1.5411E+07	6.6466E-05	5.2427E+00	4.8514E+04	1.1411E+00	1.0883E+02
6.6000E+03	-8.6044E+06	6.8181E-05	5.5780E+00	5.0319E+04	1.1417E+00	1.0950E+02
6.8000E+03	-1.7450E+06	6.9888E-05	5.8911E+00	5.1845E+04	1.1427E+00	1.1019E+02
7.0000E+03	5.1455E+06	7.1585E-05	6.1813E+00	5.3109E+04	1.1439E+00	1.1087E+02

Since condensation is an isothermal process, using (T,S) solutions avoid this problem. It also avoids the "temperature out of range" problem that can occur had other, existing options been used.

The fluid properties shown in Fig. 2-5 are  $h, \mu, \kappa, C_p, \gamma,$  and  $R$  versus  $T^{\circ}R$ . The values of  $\mu$  and  $\kappa$  are prepared as described in Section 2.6.4. The values for  $h, C_p, \gamma,$  and  $R$  are prepared as described above, i.e., they are equilibrium properties including condensed phases (no gas particle lag).

The gas constant,  $R$ , is the universal gas constant divided by the molecular weight of the equilibrium mixture.

If the inviscid core flow is frozen, it is more appropriate to use gas properties prepared using a frozen expansion of the chemical species. The program will prepare frozen tables that are analogous to the equilibrium tables described above when the TDF option is used, or if requested.

#### 2.6.4 Near Wall Gas Transport Properties.

Values of gas viscosity,  $\mu$ , gas conductivity,  $\kappa$ , Prandtl number, Pr, are required by BLM. These transport properties are evaluated along the wall streamline as a function of temperature using the ODE module. It is assumed that the expansion is in equilibrium, including condensed species. In the model these properties are then computed as "frozen" properties using the local gas composition with condensed phases included.

The viscosity and thermal conductivity of the individual gaseous species are calculated from formulas given in Reference 14 as follows:

$$\mu_i = \frac{4.15822 \times 10^{-8} \sqrt{M_{w_i} T}}{\sigma_i^2 \Omega_i}$$

$$\kappa_i = \frac{\mu_i R}{M_{w_i}} \left( .45 + 1.32 \frac{C_{p_i}}{(\kappa/M_{w_i})} \right)$$

The required Lennard Jones parameters,  $(\sigma_i, \Omega_i)$  are internally stored in the computer program for 206 gas phase species. (See Subroutine MUK in Section 5 of this report, for a list of the species.) The viscosity of the mixture is calculated from Wilke's semi-empirical formula<sup>15</sup>.

$$\mu = \sum_{i=1}^N \left[ \mu_i \left( 1 + \sum_{\substack{j=1 \\ j \neq i}}^N \phi_{ij} \frac{x_j}{x_i} \right)^{-1} \right]$$

where N is the number of species,  $x_i$  the mole fraction of species i, and  $\phi_{ij}$  is defined by:

Ref. 14. Svehla, R. A., "Estimated Viscosities and Thermal Conductivities of Gases at High Temperatures," NASA TR-132, 1962.

Ref. 15. Bird, R. B., Stewart, U. E., and Lightfoot, E. N., Transport Phenomena, John Wiley & Sons, 1960.



$$\phi_{ij} = \frac{1}{2^{3/2}} \left[ 1 + \frac{M_i}{M_j} \right]^{-1/2} \left[ 1 + \left( \frac{u_i}{u_j} \right)^{1/2} \left( \frac{M_j}{M_i} \right)^{1/4} \right]^2$$

The thermal conductivity,  $\kappa$ , is based on the equation given by Mason and Saxena<sup>16</sup> which is a slight modification of Eucken's relation,

$$\kappa = \sum_{i=1}^N \kappa_i \left[ 1 + 1.065 \sum_{\substack{j=1 \\ j \neq i}}^N \phi_{ij} \frac{x_j}{x_i} \right]^{-1}$$

The results calculated as described above are used to provide the BLM with properties using the following procedure.

The viscosity at the nozzle throat,  $\mu^*$ , and the corresponding temperature,  $T^*$ , are calculated. Using these values, an exponent,  $\omega$ , is computed such that the expression

$$\mu = \mu^* (T/T^*)^\omega$$

provides a best fit in a least square manner to the chamber and exit values for viscosity. Next, a constant value for Prandtl number is computed as

$$Pr^* = \left( \frac{\mu C_p}{\kappa} \right)^*$$

where  $\mu$ ,  $\kappa$ , and  $C_p$  are evaluated at the nozzle throat. The "frozen"  $C_p$  value is used. The values transmitted to BLM are then  $\mu^*$ ,  $T^*$ ,  $\omega$ , and  $Pr^*$ . Actually, BLM only uses the ratio  $Pr/\mu$ , and does not require  $\kappa$  or the frozen  $C_p$  versus  $T$ .

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Ref. 16. Mason, E. A., and Saxena, S. C., Physics of Fluids, Vol. 1, No. 5, pp. 361-369, 1958.

### 2.6.5 Use of Boundary Conditions and Gas Properties by BLM

In general, the flow properties at the boundary layer edge as computed by TDK are not isentropic. The TDK expansion is isentropic only if the flow is in a state of equilibrium, or if the flow is frozen in composition. When the TDK expansion is not isentropic, there are inconsistencies between TDK and BLM with respect to edge values and gas properties. Thus it is important to describe the methods by which these parameters are treated.

TDK supplies BLM with tables of  $V$ , and  $P$  vs  $X$ . Corresponding values of static enthalpy,  $h$ , are computed from the relation:

$$h = H_t - V^2/2$$

i.e., the BLM is given the condition that total enthalpy at the boundary layer edge is constant. In BLM enthalpy profiles and velocity profiles at constant pressure are used as state variables. Temperature and the gas constant,  $R$ , are obtained as a function of  $h$  by interpolation in the gas properties tables that were computed by the ODE module (see Section 2.6.3). Temperature is not a state variable, but together with the gas constant, it is used to obtain the gas density from the equation of state, i.e.,

$$\rho = P/RT.$$

Thus, in general the gas density used by BLM at the boundary layer edge does not match the TDK value, although the values of  $P$ ,  $V$ , and  $h$  do match.

The only other gas properties required by BLM are the Prandtl number,  $P_r$ , and the viscosity,  $\mu$ . A constant value is input for  $P_r$  and the viscosity,  $\mu$ , is computed (see Section 2.6.4) as

$$\mu = \mu^* (T/T^*)^\omega$$

where the reference values  $\mu^*$  and  $T^*$  are taken at the nozzle throat.

Values for  $C_p(T)$ ,  $\gamma(T)$ , and  $k(T)$  are made available to BLM for auxiliary calculations, but are not used in the boundary layer solution procedure.

#### 2.6.6 Solution Procedure

The solution procedure uses the numerical method described in Bradshaw et.al., Reference 13, to solve the governing equations presented in Section 2.6.1. This is an efficient two-point finite-difference method developed by Keller and Cebeci and extensively used by Cebeci for two-dimensional and three-dimensional flows. A detailed description is presented in Reference 13, and is not repeated here.

One of the advantages of this numerical method is that nonuniform net spacings can be used in the x-direction as well as across the boundary layer. In the latter case, the nonuniform grid is a geometric progression with the property that the ratio of lengths of any two adjacent intervals is a constant; that is,  $\Delta\eta_j = K\Delta\eta_{j-1}$ . The distance to the j-th line is given by the following formula:

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$$\eta_j = \Delta\eta_1(K^j - 1)/(K - 1) \quad K > 1$$

There are two parameters in the above equation: 1)  $\Delta\eta_1$ , the length of the first step, and: 2)  $K$ , the ratio of two successive steps. The total number of points,  $J$ , can be calculated from the following formula:

$$J = \frac{\ln[1 + (K - 1)(\eta_e/\Delta\eta_1)]}{\ln K} + 1$$

Default values used by the computer program for  $\Delta\eta_1$  and  $K$  are 0.01 and 1.14, respectively.

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NOMENCLATURE FOR SECTION 2.6, BLM

<u>Alphabetic Symbol</u>	<u>Definition</u>
A	damping length
c	density ratio, $\rho_e/\rho$
C	dimensionless density-viscosity ratio
$c_f$	local skin-friction coefficient, $\tau_w/(1/2)\rho_e u_e^2$
c	specific heat at constant pressure
$f^p$	dimensionless stream function
g	total emthalpy ratio, $H/H_e$
h	static enthalpy
H	total enthalpy
k	flow index, 0 for two dimensional flow, 1 for axisymmetric flow
L	reference length
M	Mach number
$M_w$	molecular weight
$P^w$	static pressure
Pr	molecular Prandtl number
$Pr_t$	turbulent Prandtl number
q	heat-transfer rate
r	radial distance from axis of revolution
$r_o$	local radius of body of revolution
$R^o$	gas constant
$R_\xi$	local Reynolds number, $u_e \xi / \nu_e$
S	entropy
t	transverse curvature term, $y \cos\phi / r_o$
T	static temperature
u, v	x and y components of velocity, respectively
$u_e$	velocity at the edge of the boundary layer
$u_\tau$	friction velocity $(\tau_w \rho_w)^{1/2}$
$x^\tau$	surface distance
X	axial distance
y	distance normal to the surface of the body

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NOMENCLATURE (Continued)

<u>Greek Symbol</u>	<u>Definition</u>
$\gamma$	ratio of specific heats, $C_p/C_v$
$\delta$	boundary-layer thickness
$\delta^*$	displacement thickness
$\epsilon_m^+$	eddy viscosity
$\eta$	similarity variable
$\theta$	momentum thickness
$\kappa$	gas conductivity
$\mu$	dynamic viscosity
$\nu$	kinematic viscosity
$\rho$	density
$\tau$	shear stress
$\phi$	angle of body slope, $\tan^{-1}(dr_o/dX)$
$\psi$	stream function

<u>Subscripts</u>	<u>Definition</u>
c	chamber (stagnation) conditions
e	edge of the boundary layer
r	reference conditions
tr	transition
w	evaluated at the wall
x	x-direction

<u>Superscripts</u>	<u>Definition</u>
*	nozzle throat conditions

Primes designate differentiation with respect to  $\eta$

### 3. NUMERICAL METHODS

In this Section numerical methods used by the ODK and TDK programs are discussed. The ODK subprogram integrates the system of differential equations presented in Section 2.1.1. Standard integration methods, such as Runge-Kutta, are impractical when applied to these differential equations because of the very small step sizes often required for stability. Consequently a fully stable integration method has been developed and applied as described in Section 3.1.

Solution of the characteristic differential equations presented in Section 2.5 also requires a numerically stable integration method. A highly stable implicit finite difference method is presented in Section 3.2 for integration of these characteristic relationships.

### 3.1 ODK NUMERICAL INTEGRATION METHOD

It has been shown by Tyson<sup>17</sup> that in the numerical integration of relaxation equations in near equilibrium flow regions (such as the chamber and nozzle inlet in rocket engines), explicit integration methods are unstable unless the integration step size is of the order of the characteristic relaxation distance of the relaxation equations. Since the characteristic relaxation distance is orders of magnitude smaller than the characteristic physical dimensions of the system of interest (such as the nozzle throat diameter and length) in near equilibrium flow regions, the use of explicit methods to integrate relaxation equations in these regions results in excessively long computation times. Implicit integration methods were shown to be inherently stable in integrating relaxation equations in all flow situations (whether near equilibrium or frozen) and can thus be used to integrate with step sizes of the order of the physical dimensions of the system of interest throughout the integration reducing the computation time per case several orders of magnitude. Since it has been demonstrated that there are significant advantages in using implicit rather than explicit integration of the relaxation equations, a second order implicit integration method has been chosen for use in the ODK computer program.



### 3.1.1 Stability Considerations

The numerical considerations leading to the above conclusions can be illustrated by considering the simple relaxation equation.

$$\frac{dy}{dx} = - \frac{y - y_e}{\tau} \quad (3.1-1)$$

which represents the relaxation toward equilibrium of chemical reactions, gas particle lags, etc. In this equation  $y_e$  is the equilibrium condition and  $\tau$  is the characteristic relaxation distance of the equation. In the equilibrium limit,  $\tau$  is very small compared to the physical dimensions of the system of interest while in the frozen limit,  $\tau$ , is very large compared to the physical dimensions of the system of interest. The mathematical behavior of solutions to the above equation can be found by considering the simple case where  $\tau$  is constant and

$$y_e = y_{e0} + a(x - x_0)$$

which is equivalent to terminating the Taylor series for  $y_e$  after the first term. The exact solution for this case can be shown to be

$$y(x_0 + h) = y(x_0) + [y_{e0} - y(x_0) - a\tau] [1 - e^{-h/\tau}] + ah$$

where  $y(x_0)$  is the initial value of  $y$  and  $h$  is the integration step.

It is seen that the solution consists of two parts, a term which varies slowly with  $x$  and a term which exponentially decays with a relaxation length of  $\tau$ , the characteristic relaxation length of Equation (3.1-1). Thus after a few relaxation lengths

$$y(x) \approx y_{e0} + ah, \quad h \gg \tau$$

which is independent of  $y(x_0)$  the initial condition. Since explicit integration methods construct the solution of Equation (3.1-1) as a Taylor series about the initial condition  $y(x_0)$ , the above example indicated that explicit integration methods should be limited to step sizes of the order of a few relaxation lengths.

That this is indeed the case can be shown by explicitly integrating Equation (3.1-1) using Euler's method. The explicit finite difference form is

$$\frac{y(x_0 + h) - y(x_0)}{h} = - \frac{y(x_0) - y_{e0}}{\tau}$$

which yields the truncated Taylor series

$$y(x_0 + h) = y(x_0) \left(1 - \frac{h}{\tau}\right) + y_{e0} \frac{h}{\tau}$$

when solved for  $y(x_0 + h)$ . After  $n$  integration steps, it is found that

$$y(x_0 + nh) = y(x_0) \left[1 - \frac{h}{\tau}\right]^n + \sum_{i=1}^n \left[y_{e0} + (i-1)ah\right] \left[1 - \frac{h}{\tau}\right]^{n-i} \frac{h}{\tau}$$

Examination of this equation shows that the independence on the initial condition  $y(x_0)$  will decay only if  $\left|1 - h/\tau\right| < 1$ , otherwise  $y(x_0 + nh)$  will oscillate with rapidly increasing amplitude. Hence the calculation will be stable only if  $h/\tau < 2$ . Similar results are obtained for other explicit integration methods. (The stable step size for Runge-Kutta integrations is  $h/\tau < 5.6$ .) Thus the stable step size for explicit integration of relaxation equations is of the order of the relaxation distance which explains the large computation times associated with explicit integration of relaxation equations in near equilibrium flow regions. As shown below, the use of implicit integration methods allows the integration of relaxation equations on a step size which is independent of the relaxation length.

Implicitly integrating Equation (3.1-1) using Euler's method, the finite difference form of Equation (3.1-1) is

$$\frac{y(x_0 + h) - y(x_0)}{h} = - \frac{y(x_0 + h) - y_{e0} - ah}{\tau}$$

which yields

$$y(x_0 + h) = \frac{y(x_0) + (y_{e0} + ah) \frac{h}{\tau}}{1 + \frac{h}{\tau}}$$

when solved for  $y(x_0 + h)$ . After  $n$  integration steps it is found that

$$y(x_0 + nh) = \frac{y(x_0)}{\left[1 + \frac{h}{\tau}\right]^n} + \sum_{i=1}^n \frac{y_{e0} + ia h}{\left[1 + \frac{h}{\tau}\right]^{n+1-i}} \frac{h}{\tau} \quad (3.1-2)$$

Examination of this equation shows that the dependence on the initial condition  $y(x_0)$  always decays, regardless of the step size. Hence the implicit calculation will always be stable. As an extreme example, consider one integration step,  $h = x - x_0$ . From Equation (3.1-2), it is seen that

$$y(x) \approx y_{e0} + ah \quad , \quad h \gg \tau$$

when the step size is large compared to the relaxation length and

$$y(x) = y(x_0) \left(1 - \frac{h}{\tau}\right) + y_{e0} \frac{h}{\tau} + \dots \quad , \quad h \gg \tau$$

when the step size is small compared to the relaxation length.

It is seen that in the equilibrium limit ( $\tau$  small,  $h/\tau$  large) the exact solution and the implicit integration of the relaxation equation go to the same limit which is independent of the relaxation distance and depends only on the rate of change of the equilibrium condition. In the frozen case ( $\tau$  large and  $h/\tau$  small) the implicit and explicit methods are essentially the same (truncated Taylor series). Thus, implicit numerical integration methods can be used to integrate relaxation equations using step sizes of the order of the physical dimensions of the system of interest in all flow situations whether near equilibrium or near frozen. For a complete discussion of the numerical integration of relaxation equations, see Reference 17.

In choosing a numerical integration method, the primary items of concern are the stability, accuracy and simplicity of the method. As shown by Tyson<sup>21</sup> and discussed above, implicit methods are to be preferred for numerically integrating relaxation equations due to their inherent stability. Having chosen the basic integration method for stability reasons, the order of the integration method is determined by accuracy and simplicity considerations. In general, the higher the order of the integration method, the more complex the method becomes requiring more information in the form of past value or past derivatives of the function being integrated.

Second order methods (accurate to  $h^2$  with error of order  $h^3$ ) have the advantage of simplicity and flexibility since they require only one past value of the function while retaining sufficient accuracy to allow the use of reasonably economical step sizes. For these reasons, a second order implicit numerical integration method was chosen for use in the present program. A complete derivation of this numerical integration method is given in the following section.

### 3.1.2 Derivation of the ODK Numerical Integration Method

Consider the coupled set of first order simultaneous differential equations.

$$\frac{dy_i}{dx} = f_i(x, y_1, \dots, y_N) \quad , \quad i = 1, 2, \dots, N$$

It will be assumed that the equations are not singular and that a solution exists which may be developed as a Taylor series about the forward point

$$k_{i, n+1} = \left. \frac{dy_i}{dx} \right|_{x_n+h} h - \left. \frac{d^2 y_i}{dx^2} \right|_{x_n+h} \frac{h^2}{2} + \left. \frac{d^3 y_i}{dx^3} \right|_{x_n+h} \frac{h^3}{6} - \left. \frac{d^4 y_i}{dx^4} \right|_{x_n+h} \frac{h^4}{24} + \dots$$

where  $k_{i, n+1}$  is the increment in  $y_i$  and  $h$  is sufficiently small. For equal integration steps

$$\begin{aligned} k_{i, n+1} + k_{i, n} &= 2 \left. \frac{dy_i}{dx} \right|_{x_n+h} h - 4 \left. \frac{d^2 y_i}{dx^2} \right|_{x_n+h} \frac{h^2}{2} + 8 \left. \frac{d^3 y_i}{dx^3} \right|_{x_n+h} \frac{h^3}{6} \\ &\quad - 16 \left. \frac{d^4 y_i}{dx^4} \right|_{x_n+h} \frac{h^4}{24} + \dots \end{aligned}$$

Solving these equations for the derivative at the forward point, it is found that

$$\left. \frac{dy_i}{dx} \right|_{x_n+h} = \frac{3k_{i, n+1} - k_{i, n}}{2h} + \left. \frac{d^3 y_i}{dx^3} \right|_{x_n+h} \frac{h^2}{3} - \dots$$

Expanding the function  $f_i(x, y, \dots, y_N)$  as a Taylor's series about the back point  $(x_n)$ , it is found that

$$\left. \frac{dy_i}{dx} \right|_{x_n+h} = f_{i, n} + \alpha_{i, n} h + \sum_{j=1}^N \beta_{i, j, n} k_{j, n+1} + \left. \frac{d^3 y_i}{dx^3} \right|_{x_n} \frac{h^2}{2} + \dots$$

where

$$f_i = f_i(x, y_1, \dots, y_N)$$

$$\alpha_i = \frac{\partial f_i}{\partial x}$$

$$\beta_{i,j} = \frac{\partial f_i}{\partial y_j}$$

and the subscript n refers to the functions  $f_i$ ,  $\alpha_i$  and  $\beta_{i,j}$  evaluated at the point  $x_n$ . Since

$$\left. \frac{d^3 y}{dx^3} \right|_{x_n} = \left. \frac{d^3 y}{dx^3} \right|_{x_n+h} - \left. \frac{d^4 y}{dx^4} \right|_{x_n+h} h + \dots$$

and

$$\left. \frac{d^4 y}{dx^4} \right|_{x_n} = \left. \frac{d^4 y}{dx^4} \right|_{x_n+h} - \dots,$$

Thus the formula for Taylor Series expansion about the back point can be written as

$$\left. \frac{dy_i}{dx} \right|_{x_n+h} = f_{i,n} + \alpha_{i,n} h + \sum_{j=1}^N \beta_{i,j,n} k_{j,n+1} + \left. \frac{d^3 y_i}{dx^3} \right|_{x_n+h} \frac{h^2}{2} - \dots$$

Equating the expressions for the derivative at the forward point and back point, it is found that

$$\frac{3k_{i,n+1} - k_{i,n}}{2h} = f_{i,n} + \alpha_{i,n} h + \sum_{j=1}^N \beta_{i,j,n} k_{j,n+1} + \left. \frac{d^3 y_i}{dx^3} \right|_{x_n+h} \frac{h^2}{6} + \dots$$

or

$$k_{i,n+1} = \frac{1}{3} \left[ k_{i,n} + 2 \left( f_{i,n} + \alpha_{i,n} h + \sum_{j=1}^N \beta_{i,j,n} k_{j,n+1} \right) h \right] + \left. \frac{d^3 y_i}{dx^3} \right|_{x_n+h} \frac{h^3}{9} + \dots$$

Neglecting the third order derivative term and solving the set of N linear nonhomogeneous algebraic equations

$$\left(1 - \frac{2}{3} \beta_{i, i, n} h\right) k_{i, n+1} - \sum_{j=1}^N (1 - \delta_{i, j}) \beta_{i, j, n} k_{j, n+1} = \frac{1}{3} \left[ k_{i, n} + 2(f_{i, n} + \alpha_{i, n} h) h \right]$$

where  $\delta_{i, j}$  is the Kronecker delta thus yields a second order implicit solution of the above coupled first order simultaneous differential equations.

For unequal step sizes, it can be similarly shown that solving the set of N linear nonhomogeneous algebraic equations

$$\left(1 - \frac{h_{n+1} + h_n}{2h_{n+1} + h_n} \beta_{i, i, n} h_{n+1}\right) k_{i, n+1} - \frac{h_{n+1}^2}{(2h_{n+1} + h_n)h_n} \sum_{j=1}^N (1 - \delta_{i, j}) \beta_{i, j, n} k_{j, n+1}$$

$$= \frac{h_{n+1}^2}{(2h_{n+1} + h_n)h_n} \left[ k_{i, n} + (f_{i, n} + \alpha_{i, n} h_{n+1}) \frac{h_n}{h_{n+1}} (h_{n+1} + h_n) \right]$$

yields a second order implicit solution of the above set of coupled first order simultaneous differential equations.

### 3.2 TDK NUMERICAL INTEGRATION METHOD

The reacting gas characteristic relationships given in Section 2.5 are usually integrated using second order explicit methods. It has been shown, however, that implicit integration methods are superior to explicit methods for integrating chemical relaxation equations<sup>17</sup>. Thus, in the present program the fluid dynamic equations are integrated using an explicit Euler method while the chemical relaxation equations are integrated using a first order implicit integration method.

In numerically calculating flow fields using the method of characteristics, only two (previously calculated) known points are directly usable in calculating a forward point. In equilibrium flows, only two known points are required to calculate a forward point and the calculation is straightforward and unambiguous. In nonequilibrium flows, however, more than two known points are required to calculate a forward point so that a choice must be made as to which points in the flow field will be used directly and which will be interpolated. Since even small interpolation errors in species concentrations are known to cause serious stability and accuracy problems in the numerical integration of the chemical relaxation equations, the back streamline point and one characteristic point were chosen as the known points. This choice avoids interpolation for the species concentrations in that only fluid dynamic properties (velocity, pressure, etc.) and the kinetic coupling terms (A and B) need be interpolated at one of the back characteristic points. Since these quantities are all slowly varying across the characteristics mesh, they can be accurately interpolated. Experience has shown that this choice of numerical integration methods and known data points is satisfactory for reacting gas characteristics calculations. A derivation of the numerical integration methods used in the program are given in Sections 3.2.1 and 3.2.2 below.

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### 3.2.1 Integration of the Fluid Dynamic Equations

Consider the flow field shown in Figure 3-1, below:

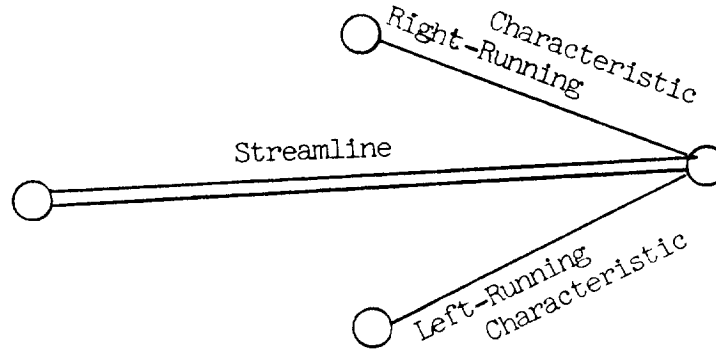


Figure 3-1. Flow Field Interior Point Calculation

Between points 3 and 4 the streamline characteristic relationships are integrated as:

$$r_3 = r_4 + (x_3 - x_4) \tan \theta_{34} \quad (3.2-1)$$

$$V_3 = \{V_4^2 - 4(P_3 - P_4) / (\rho_3 + \rho_4)\}^{1/2} \quad (3.2.2a)$$

or

$$V_3 = \{2(H_T - \sum c_i h_i)\}^{1/2} \quad (3.2.2b)$$

$$\rho_3 = \rho_4 \left(\frac{P_3}{P_4}\right)^{\frac{1}{\gamma}} \exp \left\{ -\left(\frac{A}{\cos \theta_{43}}\right)(x_3 - x_4) \right\} \quad (3.2-3)$$

$$T_3 = T_4 \left(\frac{P_3}{P_4}\right)^{\frac{\gamma-1}{\gamma}} \exp \left\{ -\left(\frac{B}{\cos \theta_{43}}\right)(x_3 - x_4) \right\} \quad (3.2-4)$$

where the double subscripts imply averaged values, e.g.:

$$\theta_{34} = (\theta_3 + \theta_4)/2 ,$$

$$\left(\frac{1}{\gamma}\right)_{43} = (1/\gamma_4 + 1/\gamma_3)/2 , \text{ etc.}$$

The integration formula (3.2-1) relating the coordinates of points 3 and 4 is exact if the streamline is a circular arc between points 3 and 4. Equation (3.2-2a) is the Bernoulli Equation and is used to obtain a first estimate for  $V_3$ . Successive estimates are made using the energy equation directly, i.e., equation 3.2-2b, so that energy is conserved exactly along streamlines. In integrating the energy equation and the perfect gas relationship to obtain Equations (3.2-3) and (3.2-4), the coefficients  $\gamma^{-1}$ ,  $A/\cos \theta$ ,  $(\gamma-1)/\gamma$ , and  $B/\cos \theta$  appearing in these equations were assumed to be equal to their average value between points 3 and 4.

Between points 1 and 3 the right running characteristics relationships are integrated as:

$$r_3 = r_1 + (x_3 - x_1) \tan (\theta - \alpha)_{31} \quad (3.2-5)$$

$$P_3 = P_1 + P_{13} \left\{ \left[ -(AGH)_{13} + (GH)_{13} \frac{\sin \theta_{13}}{r_{13}} \right] (x_3 - x_1) + G_{13} (\theta_3 - \theta_1) \right\} \quad (3.2-6)$$

The above equations are a finite difference form of equations (2.5-3) and (2.5-4), respectively.

If point 3 is an axis point then  $r_3$  and  $\theta_3$  are zero and the indeterminate quantity  $(\sin \theta_3)/r_3$  appearing in Equation (3.2-9) can be approximated by using the value obtained at point 1.

Between points 2 and 3 the left running characteristics relationships are integrated as:

$$x_3 = x_2 + (r_3 - r_2) / \tan(\theta + \alpha)_{32} \quad (3.2-7)$$

$$P_3 = P_2 + P_{23} \left\{ \left[ (AGF)_{23} - (GF)_{23} \frac{\sin \theta_{23}}{r_{23}} \right] (r_3 - r_2) - G_{23} (\theta_3 - \theta_2) \right\} \quad (3.2-8)$$

The above equations (3.2-7) and (3.2-8) are a finite difference form of equations (2.5-1) and (2.5-2), respectively.

If point 2 is an axis point, then  $r_2$  and  $\theta_2$  are zero and the indeterminate quantity  $(\sin \theta_2)/r_2$  appearing in Equation (3.2-8) can be approximated using the values estimated for point 3.

Equations (3.2-6) and (3.2-8) can be combined to yield:

$$\theta_3 = \left\{ P_2 - P_1 + P_{23} \left[ + (AGF)_{23} - (GF)_{23} \frac{\sin \theta_{23}}{r_{23}} \right] (r_3 - r_2) - P_{13} \left[ - (AGH)_{13} + (GH)_{13} \frac{\sin \theta_{13}}{r_{13}} \right] (x_3 - x_1) + P_{23} G_{23} \theta_2 + P_{13} G_{13} \theta_1 \right\} / \left\{ P_{23} G_{23} + P_{13} G_{13} \right\} \quad (3.2-9)$$

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The modified Euler iteration method is used by TDK to solve the above equations in the various point calculations. The implicit method used by TDK to integrate the chemical relaxation equations is presented next in Section 3.2.2.

### 3.2.2 Derivation of the TDK Numerical Integration Method

The chemical relaxation equations are a coupled set of first order simultaneous differential equations of the form

$$\frac{dc_i}{dx} = f_i(c_1, c_2, \dots, c_N, y_1, y_2, y_3, y_4) \quad i = 1, 2, \dots, N$$

along the streamline where  $y_1, y_2, y_3,$  and  $y_4$  refer to the fluid dynamic variables  $V, \rho, T,$  and  $\theta,$  respectively. Assuming that the equations are not singular and that a solution exists which may be developed as a Taylor series about the forward point, one obtains

$$k_i = \left. \frac{dc_i}{dx} \right|_{x_{n+h}} h$$

where  $k_i$  is the increment in  $c_i$  and  $h$  is sufficiently small. The first coefficient of the Taylor series may be calculated as

$$\left. \frac{dc_i}{dx} \right|_{x_n} = f_i(c_1, c_2, \dots, c_N, y_1, y_2, y_3, y_4)$$

Expanding as a Taylor series about the point  $x_n,$  it is found that

$$\left. \frac{dc_i}{dx} \right|_{x_{n+h}} = f_{i,n} + \sum_{j=1}^N \beta_{i,j,n} k_j + \sum_{j=1}^4 \phi_{i,j,n} \Delta y_j + O[h^2]$$

where

$$\beta_{i,j} = \frac{\partial f_i}{\partial c_j}$$

$$\phi_{i,j} = \frac{\partial f_i}{\partial y_j}$$

and the subscript  $n$  refers to the functions  $f_i$ ,  $\beta_{i,j}$ , and  $\phi_{i,j}$  evaluated at the point  $x_n$ .

Thus neglecting the second order error and derivative terms yields the integration formula for the increment  $k_i$

$$k_i = \left[ f_{i,n} + \sum_{j=1}^N \beta_{i,j,n} k_j + \sum_{j=1}^4 \phi_{i,j,n} \Delta y_j \right] h$$

### 3.3 SUMMARY OF THE TDK COMPUTATIONAL PROCEDURE

The steps below summarize the computational procedure used by the TDK Computer Program (ODE-ODK-TDK input option):

#### Step 1. (Zone 1, inner zone O/F ratio)

- 1.1 ODE is used to compute:
  - 1.1.1 P,H solution at stagnation (chamber  $V=0$ ) condition
  - 1.1.2 P,S solution at throat ( $\rho V$  maximum) condition. Entropy, S, is computed in step 1.1.1 above.
  - 1.1.3  $\epsilon_c, S$  solution at input contraction ratio.
- 1.2 An average expansion coefficient,  $N_e$ , is computed by Subroutine SUBNE. This expansion coefficient is the perfect gas expansion coefficient which would yield the throat pressure ratio computed in step 1.1.2.
- 1.3 A pressure table  $P(x)$  and its derivative  $dP(x)/dx$  are computed using the perfect gas relations,  $N_e$ , and the input thrust chamber geometry.
- 1.4 The ODK Computer Program is used to integrate the finite rate equations for one dimensional flow. The integration begins at  $\epsilon_c$ . So that the flow will not be singular at the throat,  $P(x)$  and  $dP(x)/dx$  are used until the flow is supersonic ( $M \leq 1.02$ ). For supersonic flow the area defined relations are used.

#### Step 2.

The sequence described in Step 1, above, is repeated for zones 2 through  $N \leq 50$ , the outer zone.

The following throat property tables are constructed during each of the above calculations:

$$\rho, V, T, c_1 \text{ vs. } P.$$

These tables begin at the ODK determined throat ( $\rho V$  maximum) and end when the flow attains a Mach number of 1.5.

### Step 3.

An average expansion coefficient,  $\gamma_n$ , is computed for each zone using the tables constructed in Step 2.

$$\gamma_n = \frac{\ln(P_\ell/P_1)}{\ln(\rho_\ell/\rho_1)} \quad n = 1, \dots, N \leq 50$$

The subscripts 1 and  $\ell$  refer to the first and last table entries (at the ODK throat and at  $M=1.5$ ). Thus if the flow through the throat is in equilibrium  $\gamma$  will attain the equilibrium value and if the flow is frozen  $\gamma$  will attain the frozen value.

### Step 4.

- 4.1 Using the above values of  $\gamma_n$  and the upstream radius of curvature at the nozzle throat,  $R_u$ , a two dimensional (axially symmetric) initial data line is constructed using a small perturbation method. The location of the initial data line across the nozzle throat region is determined. The location of the slipline positions is also determined by the small perturbation method (from the continuity relation). Pressure and flow angle are matched (through a first order of approximation) at the sliplines.
- 4.2 Flow properties of  $\rho$ ,  $V$ ,  $T$ , and  $c_1$  are interpolated from the tables constructed in Step 2 using the pressure determined in Step 4.1.

### Step 5.

A method of characteristics solution is computed for the nozzle. Boundary conditions are the initial data line and nozzle wall with a symmetry condition used along the nozzle axis and slip conditions (matched pressure and flow angle) used along the streamlines dividing zones of different O/F. The finite difference mesh is constructed at gas streamline and left running characteristic intersections.



#### 4. PROGRAM STRUCTURE

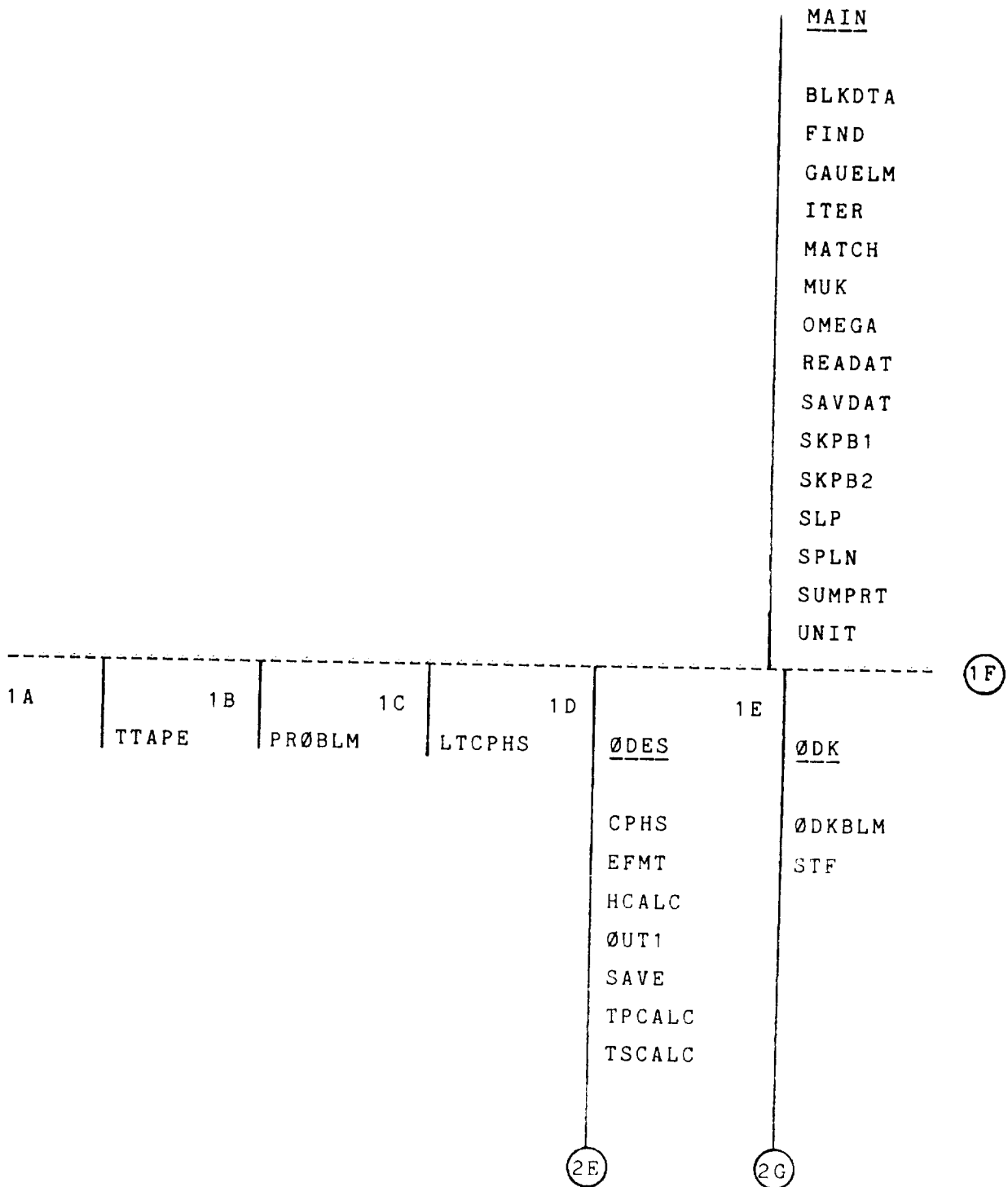
This section contains an over-all description of the structure of the TDK computer program. TDK consists of a master control module (MCM) and five major computational modules, as follows: ODE, ODK, TRAN, MOC, and BLM. Each module is described briefly in Figure 4-1. The computational modules have been combined with the MCM so that they can be run together automatically. The extensive use of internal communication between the modules has eliminated the need for redundant inputs by the user.

A schematic of an overlay structure for TDK is presented in Figure 4-2. This figure should prove useful to programmers who wish to convert TDK to a computer, such as CDC or Univac, on which an overlay structure is mandatory. TDK has been developed for the DEC 11/780 Virtual Address Extension (VAX) computer for which no overlay structure is required.

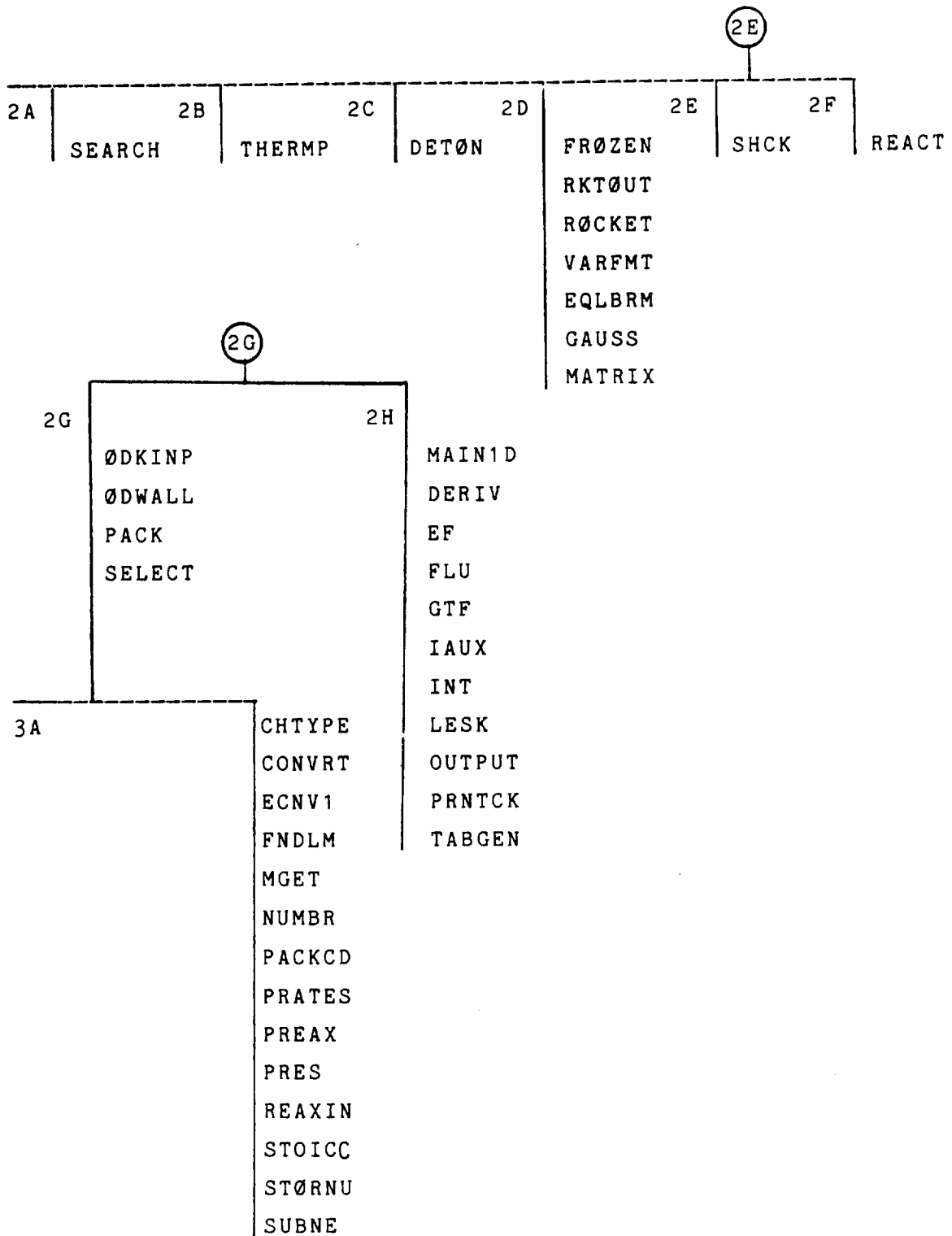
Figure 4-1: BASIC MODULES OF TDK

<u>MODULE</u>	<u>DESCRIPTION</u>
MCM	The Master Control Module is used to control the execution of TDK by selecting the computation modules to be exercised. The MCM is also used to process output files for the purpose of creating printed and plotted output.
ODE	The One-Dimensional Equilibrium module is used to calculate ideal engine performance. Engine performance can also be calculated assuming that the chemical composition is frozen at chamber (stagnation) conditions.
ODK	The One-Dimensional Kinetics module is used to calculate the loss in nozzle performance caused by finite-rate chemistry of the expansion products.
TRANS	The Transonic Flow module is used to calculate two-dimensional flow conditions in the throat region of the nozzle. It is used to obtain an initial data line for the MOC module.
MOC	The Method of Characteristics module is used to calculate the loss in nozzle performance caused by flow divergence, including the effects of chemistry and mixture ratio variation.
BLM	The Boundary Layer Module is used to calculate the loss in nozzle performance due to a viscous boundary layer and its interaction with the nozzle wall. The effects of both drag and heat transfer are included.

FIGURE 4-2: SUGGESTED OVERLAY STRUCTURE TDK, VERSION 4.0  
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1F

1F

TWØD  
TSTDK

1G

2I

TRAN

2J

TDK  
ERRORZ

BANDI  
FCALC  
FINDT  
GETIL  
GETILV  
NEWTL  
PTAB  
SAUER  
TRIM

3C

CHAR  
CUBIC  
WALL

3D

AXISPT  
CHECK  
  
CRIT  
EF2D  
GPF  
GPFKIN  
GPFPG  
INPT  
INSRT  
NESK  
SDERIV  
SINT  
THERM  
WLPT

BLMAIN  
BLEDGE  
BLH  
BLØCKD  
BLPLTS  
BLSEG  
BLTABL  
BLW  
CØEF  
CØEF1  
CUBICB  
DIFF  
EDDY  
INPUTB  
IVPL  
LINI  
OUTPBL  
RBL  
READBL  
SØLV5L  
WRPROF

4A

CNTRL  
DSPT  
PRINT  
SUBIL

4B

ATSHCK  
CKEXIT  
CKSHCK  
CNTRL1  
CNTRL2  
CNTR12  
CNTR13  
CNTR14  
CNTR16  
CNTR21  
CNTR31  
CNTR91

ENCALC  
FTHRST  
GETPT  
INPTR  
INPTRS  
INPTR1  
INPTS  
INTEXT  
ITER1  
ITER2  
ITER3  
MLCK  
MRCK  
MRCK1

PRINTS  
SAVPT  
SCK  
SETID  
SHCKA  
SHCKA1  
SHCKL  
SHCKR  
SHCKW  
SHCKW1  
SHØCK  
STRACE  
SUBILR  
TCALC  
WLCALC

#### 4.1 PROGRAM FILES

The files used by TDK are listed in Table 4-1. For those files referred to by a Fortran variable name, the name is listed. The description of the file includes the name of the labeled common block in which the file name is communicated. Subroutines using the file are also listed.

The type of file is indicated by the following codes:

B	binary
F	formatted
MS	mass storage (saved)
DA	direct access
TMS	temporary mass storage

For Univac machines, write statements to unit 50 must be replaced by PUNCH statements.

Table 4-1: Files Used by TDK

Logical Unit	Fortran Variable Name	Type	Description
5	MUN	F	Data input stream COMMON/NUCM30/
6	-	F	Printed output stream
8	IPUNIT	F,TMS	Initial Data Line file, \$LINE, COMMON/PCHILF, Subroutine CHAR
10	LU	F,TMS	Temporary input, COMMON/NUCM 30/, Subroutines MAIN, SAVDAT,CHAR, LTCPHS, ODES, OKDINP, REACT, REAXIN, TDK, TTAPE
11*	LUBLM	F,TMS,MS	TDK-BLM interface data, COMMON/BLM2/,Subroutines BLKDTA, ODES, PRINT, PRINTS, PTAB, READAT, READBL
12	LUØUT	F,TMS,MS	BLM-TDK interface data, Subroutines BLMAIN, BLW, RBL
13	NUPLT	B,TMS	BLM plots Subroutine BLMAIN
14	NUPRØF	B,TMS	BLM plots Subroutine WRPRØF

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15*	-	B,TMS,MS	TDK restart Subroutines READAT, SAVDAT, MAIN
16	-	DA	Direct access file for variable mixture ratio option (1st pass) Subroutines FINDT, GETILV, GETIL
17	-	DA	Direct access file for shock option (1st pass) Subroutines GETPT, SAVPT
18	-	DA	Direct access file for shock option (2nd pass) Subroutine CNTR91
19	-	DA	Same as 16, (2nd pass)
20	IRRED	B,TMS	Scratch data, COMMON/NTAPE/, Subroutines BLKDTA, ØDKINP
21	KREX	B,TMS	Initial line data, COMMON/NTAPE/, Subroutines BLKDTA, CHAR, GETIL, GETILV, ØDKINP, PACK, SUBIL, TRAN, TSTDK
23	JTABLE	B,TMS	TDE unit, COMMON/NTAPE1/, Subroutines BLKDTA, ØDES, OUTPUT, TDK, TRAN
25	JANAF	F,TMS,MS	Thermodynamic data, COMMON/CUTIL/, Subroutines MAIN, TTAPE, ØDK, PACK, SEARCH



26	KREAX	B,TMS	Scratch data, COMMON/CUTIL/, Subroutines MAIN, ODKINP, REAXIN
27	KSTF	F,TMS	Scratch data, COMMON/CUTIL/, Subroutines MAIN, PACK, SEARCH
28	IRREAD	B,TMS	Scratch data, COMMON/CUTIL/, Subroutines MAIN, ODKINP, REAXIN
29*	ITSTAB	B,TMS,MS	Transonic data, COMMON/CUTIL/, Subroutines MAIN, GETIL, GETILV, MAIN1D,TWØD
50	-	F,TMS,MS	Boundary layer edge data computed by TDK, TDE, or TDF. Subroutines PRINT, PRINTS, PTAB

\* Files 11, 15, and 29 must be saved if the restart option,  
IRSTRT = 1, is to be used on later runs.

## 4.2 SUBROUTINE AND COMMON BLOCK CROSS-REFERENCES

This section provides tables that contain cross-references for subroutines and common blocks. Referral to these tables, or their equivalent, is usually necessary if the program is to be modified.

Table 4-2 lists in alphanumeric order each TDK subroutine. All modules are included. Opposite each subroutine name are the names of all subroutines that call the subroutine.

Table 4-3 lists in alphanumeric order each TDK common block. Again, all modules are included. Opposite each common block name are the names of all subroutines that contain the common block.

Tables 4-2 and 4-3 do not contain the names of system supplied subroutines, such as SIN, COS, or the I/Ø subroutines.

TABLE 4-2 SUBROUTINE ENTRY POINT CROSS-REFERENCES

SUBROUTINE	REFERRED BY ...			
ATSHCK	CNTR16	CNTR21	CNTR31	CNTR41
AXIS	BLPLTS			
AXISPT	CNTR14	CNTRL	CNTRL1	SHCKA1
BANDI	NEWT			
BLEDGE	BLMAIN			
BLH	MAIN			
BLKDTA				
BLMAIN	MAIN			
BLOCKD				
BLPLTS	BLMAIN			
BLSEG	BLMAIN			
BLTABL	BLEDGE	INPUTB		
BLW	MAIN			
CHAR	TDK			
CHECK	ATSHCK	AXISPT	DSPT	INPT
	INPTR	INPTR1	INPTRS	INPTS
	WLPT			
CHTYPE	PREAX			
CKEXIT	CNTR21	CNTR31	CNTR41	CNTRL1
	CNTRL2			
CKSHCK	CNTRL1			
CNTR12	CNTR91			
CNTR13	CNTR91			
CNTR14	CNTR91			
CNTR16	CNTR91			
CNTR21	CNTR91			
CNTR31	CNTR91			
CNTR41	CNTR91	(SUBROUTINE NOT USED)		
CNTR91	TDK			
CNTRL	TDK			
CNTRL1	CNTR13	CNTR21	CNTR31	CNTR41
CNTRL2	CNTR12	CNTR14	CNTR16	CNTR41
COEF	BLSEG	IVPL		
COEF1	BLSEG			
CONVRT	PACK			
CPHS	EQLBRM	FROZEN	HCALC	OUT1
	ROCKET	SHCK		
CRIT	CHECK	DSPT	SHCKA1	SHCKL
	SHCKR	SHCKW1		
CUBIC	WALL			
CUBICB	BLTABL			
DERIV	IAUX	INT	MAIN1D	
DETON	ODES			
DIFF	BLEDGE			
DSPT	CNTRL			
ECNV1	MGET	PRATES	REAXIN	
EDDY	BLSEG			
EF	DERIV			
EF2D	SDERIV			
EFMT	OUT1			
ENCALC	SHOCK	TCALC		
EQLBRM	DETON	ROCKET	SHCK	THERMP
	TPCALC			
ERRORZ	CHAR	CNTRL	TDK	
FCALC	TRAN			

## SUBROUTINE

## REFERRED BY ...

SUBROUTINE	REFERRED BY ...			
FIND	CHAR	CPHS	ENCALC	GPFPG
	IAUX	MAIN1D	MUK	PACK
	PRES	PTAB	STF	THERM
FINDT	GETIL	GETILV		
FLU	DERIV			
FNDLM	MGET	PRATES	REAXIN	
FROZEN	ROCKET			
FTHRST	CNTR12	CNTR13	CNTR14	CNTR16
	CNTR21	CNTR31	CNTR41	CNTRL2
GAUELM	SKPB1			
GAUSS	EQLBRM			
GETIL	TRAN			
GETILV	TRAN			
GETPT	CNTR12	CNTR13	CNTR14	CNTR16
	CNTR41	INPTRS	INPTS	SUBILR
GPF	ATSHCK	AXISPT	DSPT	INPT
	INPTR	INPTR1	INPTRS	INPTS
	INSRT	SHCKA	SHCKA1	SHCKL
	SHCKR	SHCKW	SHCKW1	SUBIL
	SUBILR	WLPT		
GPFKIN	GPF	SUBIL		
GPFPG	GPF			
GTF	DERIV	MAIN1D		
HCALC	DETON	SAVE	SHCK	
IAUX	INT	MAIN1D		
INPT	CNTRL	CNTRL2		
INPTR	CNTRL1			
INPTR1	CNTR16			
INPTRS	CNTR14			
INPTS	CNTR13			
INPUTB	BLMAIN			
INSRT	CNTRL	CNTRL1	CNTRL2	WLCALC
INT	MAIN1D			
INTEXT	CNTR12	CNTR14	CNTR16	CNTR21
	CNTR31	CNTR41		
ITER	PRINT	PRINTS	TCALC	TRAN
	TSCALC			
ITER1	ENCALC			
ITER2	SHOCK			
ITER3	ATSHCK			
IVPL	BLMAIN			
LESK	IAUX			
LINE	BLPLTS			
LINE	BLEDGE	BLTABL	INPUTB	OUTPBL
LINE	WRPROF			
LTCPHS	MAIN			
MAIN				
MAIN1D	ODK			
MATCH	ODKBLM	ROCKET		
MATRIX	EQLBRM			
MGET	REAXIN			
MLCK	CNTR12	CNTR14	CNTR16	CNTR41
MRCK	CNTR13	CNTR21	CNTR31	CNTR41
MRCK1	CNTRL1			
MUK	ODKBLM	ROCKET		

## SUBROUTINE

## REFERRED BY ...

SUBROUTINE	REFERRED BY ...			
NESK	SINT			
NEWOF	DETON	ROCKET	SHCK	THERMP
NEWT	TRAN			
NUMBER	BLPLTS			
ODES	MAIN			
ODK	MAIN			
ODKBLM	ODK			
ODKINP	ODK			
ODWALL	ODKINP			
OMEGA	ODKBLM	ROCKET		
OUT1	DETON	RKTOUT	SHCK	THERMP
OUT2	DETON	RKTOUT	SHCK	THERMP
OUT3	DETON	RKTOUT	SHCK	THERMP
OUTPBL	BLMAIN	BLSEG		
OUTPUT	INT	MAIN1D	PRNTCK	
PACK	ODK			
PACKCD	REAXIN			
PLOT	BLPLTS			
PLOTS	BLPLTS			
PRATES	REAXIN			
PREAX	REAXIN			
PRES	PACK			
PRINT	CNTRL			
PRINTS	CNTR12	CNTR13	CNTR14	CNTR16
	CNTR21	CNTR31	CNTR41	CNTRL1
	CNTRL2			
PRNTCK	INT	MAIN1D		
PROBLM	MAIN			
PTAB	TRAN			
RBL	BLH	BLW		
REACT	ODES			
READAT	MAIN			
READBL	INPUTB			
REAXIN	ODKINP			
RKTOUT	ROCKET			
ROCKET	ODES			
SAUER	TRAN			
SAVDAT	MAIN			
SAVE	DETON	ROCKET	SHCK	THERMP
SAVPT	CNTR12	CNTR13	CNTR14	CNTR16
	CNTR31	CNTR41	CNTRL1	CNTRL2
	SUBILR	WLCALC		
SCALE	BLPLTS			
SCK	CNTR12	CNTR14		
SDERIV	GPFKIN	SINT		
SEARCH	ODES			
SELECT	ODKINP			
SETID	CNTR12	CNTR13	CNTR14	CNTR16
	CNTR21	CNTR31	CNTR41	CNTRL1
	CNTRL2	SUBILR	WLCALC	
SHCK	ODES			
SHCKA	CNTR12	CNTR14		
SHCKA1	CNTR13			
SHCKL	CNTR13	SHCKW		
SHCKR	CNTR12	CNTR14	CNTR16	

## SUBROUTINE

## REFERRED BY ...

SHCKW	CNTR13			
SHCKW1	CNTR14	CNTR16		
SHOCK	ATSHCK	SHCKA	SHCKA1	SHCKL
	SHCKR	SHCKW	SHCKW1	
SINT	ATSHCK	AXISPT	DSPT	INPT
	INPTR	INPTR1	INPTRS	INPTS
	SHCKA	SHCKA1	SHCKL	SHCKR
	SHCKW1	SUBIL	SUBILR	WLPT
SKPB1	ODWALL	SKPB2	WALL	
SKPB2	ODWALL	WALL		
SLP	PACK	TDK	WALL	
SOLV5	BLSEG	IVPL		
SPLN	CHAR	CNTRL	CPHS	ENCALC
	FLU	GPFPG	IAUX	MAIN1D
	MUK	PACK	PRES	PTAB
	STF	THERM		
STF	CONVRT	DERIV	MAIN1D	ODKBLM
STOICC	CONVRT	PACK		
STORNU	REAXIN			
SUBIL	CNTRL			
SUBILR	CNTR21	CNTR31	CNTR41	
SUBNE	PRES			
SUMPRT	MAIN			
SUMPRT1	SUMPRT			
SYMBOL	BLPLTS			
TABGEN	IAUX	MAIN1D		
TCALC	SHOCK			
TDK	TWOD			
THERM	ENCALC	SDERIV		
THERMP	ODES			
TIMERX	CHAR	CNTRL	MAIN	MAIN1D
	MLCK	MRCK	TRAN	
TPCALC	TSCALC			
TRAN	TWOD			
TRIM	TRAN			
TSCALC	ODES			
TTAPE	MAIN			
TWOD	MAIN			
UNIT	MAIN			
VARFMT	RKTOUT			
WALL	CHAR			
WLCALC	CNTR21	CNTR31	CNTR41	
WLPT	CNTR13	CNTRL	CNTRL2	SHCKW1
	WLCALC			
WRPROF	BLSEG			

TABLE 4-3 COMMON BLOCK CROSS-REFERENCES

Labeled Common -----	Referred by Subroutine -----	Labeled Common -----	Referred by Subroutine -----
A		BLC0	
ABMAPS	REAXIN STORNU PRATES PREAX		BLEDGE BLSEG COEF COEF1 EDDY WRPROF
ABOUND	MAIN TDK FLU	BLC1	
AL	CHAR GPFKIN		IVPL OUTPBL SOLV5 BLSEG COEF COEF1 EDDY WRPROF
ARODE	BLMAIN INPUTB OUTPBL BLEDGE	BLC2	
	MAIN BLKDTA ODES PACK REACT SEARCH DETON OOKINP OUT1 OUTPUT	BLC3	OUTPBL COEF1 EDDY
ARPRNT		BLC6	IVPL SOLV5 BLSEG
AVGS	ODES PROBLM OOKINP	BL1NTP	SOLV5 COEF
BCON	REACT SUMPRT TWOD MAINTD	BLM1	BLOCKD INPUTB BLEDGE
BLC0	BLOCKD INPUTB READBL BLEDGE	BLM2	MAIN PROBLM READAT SAVDAT PRINT PTAB PRINTS
	BLOCKD BLMAIN INPUTB IVPL OUTPBL READBL SOLV5	BLM3	BLKDTA ODES READAT READBL ODKBLM TDK PRINT PTAB PRINTS
			ODES

Labeled Common -----	Referred by Subroutine -----	Labeled Common -----	Referred by Subroutine -----
BLM3	ROCKET	CINT	MAIN1D IAUX INT LESK
BLM4	ODES OUT1	CKSHCK	CHAR
BLMF	ODK PROBLM SUMPRT	CMAXIT	TDK CHAR PRINT PRINTS
BLMPLT	BLOCKD BLMAIN INPUTB BLEGE BLSEG WRPROF	COOTDK	MAIN ODK MAIN1D ODKINP TDK FLU
BLMSPR	BLH BLW SUMPRT BLSEG	COEFFX	SEARCH CPHS
BLPLOT	BLMAIN BLSEG	COM4	MAIN SUMPRT TRAN CHAR
BLTK	BLMAIN OUTPBL	COM6	TRAN GETIL GETILV SAUER
BLTKPR	PROBLM	COMCAS	MAIN BLW ODES PACK READAT SAVDAT SUMPRT CONVRT MAIN1D ODKBLM ODKINP OUTPUT PRES REAXIN SELECT STF STORNU
CCINT	SINT NESK		
CDELHX	MAIN ODES SAVE TWOD MAIN1D		
CDELHY	BLH ODES SAVE TWOD MAIN1D		
CDINTG	SUMPRT SUMPRT1 TRAN		
CINLLN	CHAR		



LABELED COMMON  
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REFERRED BY SUBROUTINE  
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LABELED COMMON  
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REFERRED BY SUBROUTINE  
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COMCAS

SUMPRT1  
TRAN  
CHAR  
CNTRL  
DERIV  
DSPT  
EF  
FCALC  
FLU  
GETIL  
GETILV  
GTF  
IAUX  
INPT  
INT  
ODWALL  
PRATES  
PRINT  
PTAB  
SINT  
SUBIL  
WLPT  
AXISPT  
GPFKIN  
INPTR  
INPTR1  
INPTRS  
INPTS  
NESK  
PRINTS  
SDERIV  
SUBILR  
TCALC  
THERM  
ATSHCK  
EF2D  
ENCALC

COMXP

MAIN  
OES  
SUMPRT  
TRAN

COMY

MAIN  
PACK  
READAT  
SAVDAT  
CONVRT  
MAIN1D  
ODKBLM

COMY

CONSTS

COOLC

CPEES

OOKINP  
OUTPUT  
PRES  
REAXIN  
STF  
TRAN  
CHAR  
DERIV  
EF  
FLU  
GTF  
IAUX  
INT  
SDERIV  
EF2D

MAIN  
LTCPHS  
OES  
SAVE  
SUMPRT  
UNIT  
CONVRT  
EQLBRM  
FROZEN  
MAIN1D  
OOKINP  
OUT1  
OUTPUT  
RKTOUT  
SUMPRT1  
TDK  
TPCALC  
TRAN  
CHAR  
IAUX  
ODWALL  
PRINT  
PTAB  
WALL  
GPFPG  
PRINTS  
ENCALC

BLH  
BLW  
INPUTB  
  
ROCKET  
CPHS

LABELED COMMON  
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REFERRED BY SUBROUTINE  
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LABELED COMMON  
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REFERRED BY SUBROUTINE  
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CPEES

CPRNT

CPUNCH

CSPRXC

CTRBDY

CUTIL

OUT1

MAIN  
PACK  
MAIN1D  
ODKINP  
INT  
ODWALL

PRINT  
PRINTS

MAIN  
PACK  
STOICC  
CONVRT  
REAXIN  
SELECT  
STORNU

AXISPT  
CNTR14  
CNTRL1  
SHCKA  
SHCKA1

MAIN  
ODES  
ODK  
PACK  
REACT  
READAT  
ROCKET  
SAVDAT  
SEARCH  
SPLN  
TTAPE  
TWOD  
CONVRT  
CPHS  
MAIN1D  
MUK  
ODKBLM  
ODKINP  
OUT1  
OUTPUT  
PRES  
REAXIN  
RKTOUT  
SELECT

CUTIL

CWALL

CWALL1

DASTOI

DELHN

DFSAV

DIRACC

STF  
TDK  
TRAN  
CHAR  
CNTRL  
FLU  
GETIL  
GETILV  
IAUX  
PRINT  
SUBIL  
GPFPG  
PRINTS  
SUBILR  
THERM

MAIN  
ODES  
PACK  
READAT  
SAVDAT  
MAIN1D  
ODKINP  
PRES  
CHAR  
FLU  
ODWALL  
PTAB  
WALL

PROBLM  
WALL

PACK  
READAT  
SAVDAT  
DERIV  
EF  
SDERIV  
EF2D

BLH  
ODES

OUTPBL  
SUMPRT  
COEF1  
SUMPRT1

TDK

LABELED COMMON  
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REFERRED BY SUBROUTINE  
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LABELED COMMON  
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REFERRED BY SUBROUTINE  
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DIRACC			
	CNTR91	ERR	
	GETPT		WLPT
DOLOOP	SAVPT		AXISPT
	MAIN		CNTR12
	READAT		CNTR13
	SAVDAT		CNTR14
	MAIN1D		CNTR16
	OOKINP		CNTRL1
	PRNTCK		CNTRL2
	DERIV		GPFPG
	EF		INPTR
	IAUX		INPTR1
	INT		INPTRS
	SDERIV		INPTS
DOUBLE	EF2D		PRINTS
	ODES		SDERIV
	SHCK		SHCKA
	EQLBRM		SHCKA1
	GAUSS		SHCKL
	MATRIX		SHCKR
EDGE	OUT1		SHCKW
			SHCKW1
	BLOCKD		SUBILR
	BLMAIN		WLCALC
	INPUTB	EXTRAP	ATSHCK
	OUTPBL		ENCALC
	BLEDGE	FLAGS	
	BLSEG		PACK
	COEF1		CNTR91
ENDFLG	EDDY		CNTR12
	WRPROF		CNTR13
			CNTR14
	CNTR91		CNTR16
ERR	PRINTS		CNTR21
			CNTR31
	MAIN		CNTR41
	TTAPE	FLOW2D	CNTRL1
	TDK		CNTRL2
	TRAN		
	CHAR		PROBLM
	CNTRL		TRAN
	DSPT		CHAR
	GETIL		CNTRL
	GETILV		FTHRST
	INPT		
	PRINT		MAIN1D
	SUBIL		DERIV
	WALL		FLU
			IAUX

<u>LABELED COMMON</u>	<u>REFERRED BY SUBROUTINE</u>	<u>LABELED COMMON</u>	<u>REFERRED BY SUBROUTINE</u>
GBLK	BLOCKD BLMAIN INPUTB OUTPBL BLEGDE BLSEG COEF1 EDDY WRPROF	HTL	SAVDAT ODKBLM CHAR GPFKIN GPPFG
GEOM	BLW ODES PROBLM READBL SUMPRT ODKINP RKTOUT TRAN CHAR PRINTS	HTOTAL	INPUTB READBL BLEGDE
GEOMN	BLW PROBLM	HTPR	BLW PROBLM
GRD	BLOCKD BLMAIN INPUTB IVPL OUTPBL SOLV5 BLEGDE BLSEG COEF COEF1 EDDY	ICONT	MAIN
HHTCOM	ODES EQLBRM	IDIL	SUBILR
HTABLE	INPUTB BLEGDE	IDNO	PROBLM CNTR91 SETID
HFLX	BLMAIN OUTPBL BLSEG	IHIT	CNTR21 CNTR31 CNTR41 CNTRL1
HTL	ODES PROBLM READAT	INDSEG	BLSEG COEF1
		INDX	MAIN ODES REACT ROCKET SAVE SEARCH SHCK THERMP CPHS DETON EQLBRM FROZEN GAUSS HCALC MATRIX OUT1 RKTOUT TPCALC
		INDXX	ODES REACT

LABELED COMMON

REFERRED BY SUBROUTINE

LABELED COMMON

REFERRED BY SUBROUTINE

INDXX

ROCKET  
SAVE  
SHCK  
THERMP  
CPHS  
DETON  
EQLBRM  
FROZEN  
GAUSS  
HCALC  
MATRIX  
OUT1  
RKTOUT  
TPCALC

KINFO

MAIN  
BLH  
ODES  
PACK  
REACT  
READAT  
ROCKET  
SAVDAT  
SUMPRT  
TWOO  
FROZEN  
MAIN1D  
OOKINP  
OUT1  
OUTPUT  
PRES  
REAXIN  
RKTOUT  
SELECT  
TDK  
TRAN  
CHAR  
GETIL  
GETILV  
PRINT  
PTAB  
PRINTS

INERTS

REAXIN  
SELECT

IOFF

PROBLM  
READBL

IRRC

CHAR  
INPTR

IRSTRT

MAIN  
PROBLM  
READAT  
SUMPRT  
SUMPRT1

LASTM

ISPLN

PROBLM  
SPLN

LKEQKN

CNTR16  
CNTRL2

IUSE

MAIN  
ODES  
ROCKET  
SAVE  
SEARCH  
SHCK  
THERMP  
CPHS  
DETON  
EQLBRM  
FROZEN  
HCALC  
MATRIX  
OUT1  
RKTOUT  
SELECT

LKMELT

ROCKET

LOWTH

MAIN1D  
DERIV

M1

MAIN  
LTCPHS  
READAT  
SAVDAT  
CPHS  
STF  
THERM

READAT  
SAVDAT  
SINT  
GPFKIN  
SDERIV

LABELED COMMON

REFERRED BY SUBROUTINE

LABELED COMMON

REFERRED BY SUBROUTINE

MACHDR

MARKET

MASFLW

MESHC

MESHCH

MESHCHW

DERIV  
FLU

MAIN  
OES  
ODK  
PACK  
PROBLM  
READAT  
ROCKET  
TWO  
CONVRT  
MAINID  
OOKINP  
OUTPUT  
REAXIN  
SELECT  
TDK  
TRAN  
CHAR  
FLU  
PRINT  
GPFP  
PRINTS

MLCK  
MRCK  
MRCK1  
SUBILR

TDK  
CHAR  
CNTRL  
PRINT  
SUBIL  
MLCK  
MRCK  
MRCK1  
PRINTS  
SUBILR

CHAR  
INPT  
INPTR  
SHCKL  
SHCKR

CHAR  
WLPT

MESHCH

MISC

MISCT

MISCH

CHAR  
CNTRL  
PRINT  
WALL  
WLPT  
PRINTS  
ATSHCK

MAIN  
BLKDTA  
OES  
PACK  
REACT  
ROCKET  
SAVE  
SEARCH  
SHCK  
THERMP  
CPHS  
DETON  
EQLBRM  
FROZEN  
HCALC  
MATRIX  
OUT1  
RKTOUT  
TPCALC

BLOCKD  
BLH  
BLMAIN  
INPUTB  
OUTPBL  
READBL  
BLEGE  
BLSEG  
COEF1  
EDDY  
WRPROF

OES  
REACT  
ROCKET  
SAVE  
SHCK  
THERMP  
CPHS  
DETON  
EQLBRM

LABELED COMMON  
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REFERRED BY SUBROUTINE  
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LABELED COMMON  
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REFERRED BY SUBROUTINE  
-----

MISCX

MOLWTS

MUST

NAMBC

NAME

FROZEN  
HCALC  
MATRIX  
RKTOUT

ROCKET  
SEARCH  
OUT1

DERIV  
FLU

TRAN  
FCALC  
SAUER

SUMPRT  
SUMPRT1  
TDK  
CHAR  
CNTR91  
CNTRL  
DSPT  
INPT  
PRINT  
SUBIL  
CNTR12  
CNTR13  
CNTR14  
CNTR16  
CNTR21  
CNTR31  
CNTR41  
CNTRL1  
CNTRL2  
FTHRST  
INPTR  
INPTR1  
INPTRS  
INPTS  
MLCK  
MRCK  
MRCK1  
PRINTS  
SHCKA1  
SHCKL  
SHCKR  
SHCKW1  
SUBILR  
WLCALC

NAMEP

NAMEQ

TDK  
CHAR  
CNTRL  
DSPT  
INPT  
CNTR12  
CNTR13  
CNTR14  
CNTR16  
CNTR21  
CNTR31  
CNTR41  
CNTRL1  
CNTRL2  
GPFPG  
INPTR  
INPTR1  
INPTRS  
INPTS  
MLCK  
MRCK  
MRCK1  
SHCKA  
SHCKA1  
SHCKL  
SHCKR  
SHCKW1  
WLCALC  
CKSHCK  
ENCALC

TDK  
CHAR  
CNTR91  
CNTRL  
DSPT  
INPT  
INSRT  
PRINT  
SINT  
SUBIL  
WLPT  
AXISPT  
CHECK  
CNTR12  
CNTR13  
CNTR14  
CNTR16  
CNTR21

LABELED COMMON  
.....

NAMEQ

NAMEQB

NAMES

REFERRED BY SUBROUTINE  
.....

CNTR31  
CNTR41  
CNTRL1  
CNTRL2  
GPFKIN  
GPFPG  
INPTR  
INPTR1  
INPTRS  
INPTS  
MLCK  
MRCK  
PRINTS  
SHCKA  
SHCKA1  
SHCKL  
SHCKR  
SHCKW  
SHCKW1  
SHOCK  
SUBILR  
WLCALC  
ATSHCK  
CKSHCK

CNTR12  
CNTR13  
CNTR14  
CNTR16  
CNTR21  
CNTR31  
CNTR41  
CNTRL1  
PRINTS  
SHCKA  
SHCKA1  
SHCKL  
SHCKR  
SHCKW  
SHCKW1  
SHOCK  
ATSHCK

MAIN  
TRAN  
CHAR  
GETIL  
GETILV  
SUBIL  
SUBILR

LABELED COMMON  
.....

NAMEV

NAMEW

NAMIN

NC01

REFERRED BY SUBROUTINE  
.....

TRAN  
FCALC  
GETIL  
GETILV

MAIN  
ODKINP  
TRAN  
CHAR  
CNTRL  
PRINT  
WALL  
WLPT  
CNTR12  
CNTR14  
CNTR16  
CNTR21  
CNTR31  
CNTR41  
CNTRL1  
CNTRL2  
INTEXT  
PRINTS  
SHCKW  
WLCALC  
ATSHCK  
CKEXIT

MAIN  
BLH  
PROBLM  
TWO  
MAIN1D  
ODKINP  
TDK  
TRAN  
CHAR  
FCALC  
PRINT  
GPFPG  
PRINTS

CNTRL  
ODWALL  
PRINT  
WALL  
CNTR21  
CNTR31  
CNTRL1



Labeled Common	Referred by Subroutine	Labeled Common	Referred by Subroutine
NC01		NUCOM2	ODES ODK PACK PROBLM ROCKET THOO ODKINP OUTPUT TDK TRAN CHAR DSPT GPF INPT ODWALL PRINT PTAB SUBIL WLPT AXISPT GPFPG INPTR INPTR1 INPTRS INPTS PRINTS SHCKA SHCKA1 SHCKL SHCKR SHCKW1 ATSHCK ENCALC
NDEBUG	MLCK MRCK PRINTS		
NEWPR1	TRAN FCALC		
NODK	BLW ODKINP		
NOINST	ODK ODKINP		
NRXDIR	CNTRL1 INPTR		
NTAPE	PACK CONVRT REAXIN PRATES		
	BLKDTA PACK ODKINP TRAN CHAR GETIL GETILV SUBIL SUBILR		
NTAPE1	BLKDTA ODES OUTPUT TDK TRAN	NUCOM3	MAIN ODES PROBLM READAT SAVDAT PRINT PTAB PRINTS
NUCM30	MAIN INPUTB LTCPHS ODES PROBLM REACT SHCK TTAPE ODKINP REAXIN TRAN CHAR	NUCOM4	BLKDTA PROBLM OUT1 OUTPUT RKTOUT CHAR

LABELED COMMON  
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REFERRED BY SUBROUTINE  
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LABELED COMMON  
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REFERRED BY SUBROUTINE  
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NUCOM4

PRINT  
PRINTS

ODKCOM

MAIN  
ODES  
ODK  
PACK  
READAT  
ROCKET  
SAVDAT  
CONVRT  
MAIN1D  
ODKBLM  
ODKINP  
OUT1  
OUTPUT  
PRES  
PRNTCK  
REAXIN  
RKTOUT  
SELECT  
CHAR  
DERIV  
EF  
FLU  
IAUX  
INT  
PRINT  
PTAB  
SINT  
PRINTS  
SDERIV  
EF2D

NUCOM5

MAIN  
ODES  
TDK  
TRAN  
CHAR

NUCOM6

MAIN  
TRAN  
PRINT  
CNTR21  
CNTR31  
CNTR41  
PRINTS

NUCOM7

MAIN  
ODES  
ODKINP  
OUT1  
TRAN  
CHAR

NUCOM8

ODES  
CHAR

NUCOMN

ODES  
ROCKET  
OUT1

NUT

TDK  
GETIL

ODKRX

OAE

ODES  
PROBLM  
ODKINP  
TRAN

ODEOUT

ROCKET  
OUT1

ODKSP

ODERG

ODES  
ROCKET  
OUT1

ODESAV

TWOD  
MAIN1D  
OUT1  
RKTOUT

MAIN  
PACK  
READAT  
SAVDAT  
CONVRT  
TWOD  
CONVRT  
MAIN1D  
ODKBLM

LABELED COMMON  
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REFERRED BY SUBROUTINE  
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LABELED COMMON  
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REFERRED BY SUBROUTINE  
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OOKSP

OOKINP  
OUTPUT  
REAXIN  
STF  
CHAR  
DERIV  
EF  
FLU  
GTF  
IAUX  
PRINT  
SUBIL  
GPFKIN  
GPFPG  
PRINTS  
SDERIV  
SUBILR  
THERM  
EF2D  
ENCALC

PCTBL

PTAB

PERF

MAIN  
ODES  
ROCKET  
SHCK  
DETON  
EQLBRM  
FROZEN  
OUT1  
RKTOUT  
TPCALC

PERFX

ODES  
ROCKET  
SHCK  
DETON  
EQLBRM  
FROZEN  
OUT1  
RKTOUT

OPTION

INPUTB  
PROBLM  
SUMPRT

PEXIT

SUMPRT  
SUMPRT1  
CNTR91  
CNTRL

OUPT

BLKDTA  
SHCK  
THERMP  
DETON  
FROZEN  
OUT1  
RKTOUT  
VARFMT  
EFMT

PLUMEC

SUMPRT  
TWOD  
CHAR  
CNTRL  
PRINT  
CNTR21  
CNTR31  
CNTR41  
PRINTS

PATHL

READAT  
SAVDAT  
CNTRL  
SINT  
SUBIL  
SDERIV  
SUBILR

POINTS

MAIN  
ODES  
ROCKET  
SHCK  
THERMP  
DETON  
EQLBRM  
FROZEN  
HCALC  
MATRIX  
OUT1  
RKTOUT  
TPCALC

PCHILF

CHAR

PCTBL

READAT  
SAVDAT  
SUMPRT  
OUT1  
TRAN

LABELED COMMON  
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REFERRED BY SUBROUTINE  
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LABELED COMMON  
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REFERRED BY SUBROUTINE  
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POINTS

POINTX

PPPXX

PRES

PRFGAS

CHAR

ODES  
ROCKET  
SHCK  
THERMP  
DETON  
EQLBRM  
FROZEN  
HCALC  
MATRIX  
RKTOUT

CHAR  
CNTRL  
SUBILR

BLMAIN  
INPUTB  
BLEdge  
COEF  
COEF1  
EDDY

MAIN  
PROBLM  
SUMPRT  
TWOD  
TDK  
CHAR  
DSPT  
GPF  
INPT  
PRINT  
SINT  
WLPT  
AXISPT  
INPTR  
INPTR1  
INPTRS  
INPTS  
PRINTS  
SHCKA  
SHCKA1  
SHCKL  
SHCKR  
SHCKW1  
ATSHCK  
ENCALC

PRNTRX

PTABLE

PTSAVE

PUNCHC

RATES

RDCARD

RDIREX

REL POT

REPEAT

BLPLTS

MAIN10  
ODKINP  
PRES  
FLU  
IAUX

MAIN  
ODES

PROBLM  
PRINT  
PTAB  
PRINTS

ODKINP  
REAXIN  
PRATES

MAIN

MAIN  
ODES  
PACK  
SEARCH  
STOICC  
CONVRT  
REAXIN  
SELECT  
PRATES

BLW  
PROBLM  
SUMPRT  
SUMPRT1

MAIN  
ODES  
PROBLM  
READAT  
ODKINP  
TDK  
CHAR  
CNTR91  
GETIL  
GETILV  
PRINT  
PTAB

LABELED COMMON  
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REFERRED BY SUBROUTINE  
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LABELED COMMON  
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REFERRED BY SUBROUTINE  
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REPEAT		SHOCKC	
RLMNR	PRINTS		PROBLM
	BLMAIN		SUMPRT
RVACOM	COEF1		TDK
	MAIN1D	SKIP	TRAN
	ODKINP		CHAR
SAVODE	OUTPUT	SPECES	CNTRL1
	INT		INPTR
SAVPRI	MAIN		ODES
	ODES		ROCKET
SCLFTR	SUMPRT		SAVE
	PRINTS		SEARCH
SCRJT1	INPUTB		SHCK
	READBL		THERMP
SHCK1	BLEDGE		CPHS
	ODES		DETON
	PROBLM		EQLBRM
	SUMPRT	SPECEX	FROZEN
	CHAR		HCALC
	CNTR91		MATRIX
	WLPT		OUT1
	CNTR41		RKTOUT
SHCK2	CNTRL1		ODES
	PRINTS		ROCKET
	SUMPRT		SAVE
	CHAR		SHCK
	WLPT		THERMP
	CNTR16		CPHS
	CNTR21		DETON
	CNTR31		EQLBRM
	CNTR41	SPINFO	FROZEN
SHGAMA	PRINTS		HCALC
	MAIN		MATRIX
	ODK		RKTOUT
	PROBLM		ODES
	SUMPRT		PACK
	ODKINP		ROCKET
	TDK		SEARCH
	CHAR		SHCK
	DERIV		SUMPRT
	SINT		CPHS
	SDERIV		EQLBRM
			ODKINP
			OUT1

LABELED COMMON -----	REFERRED BY SUBROUTINE -----	LABELED COMMON -----	REFERRED BY SUBROUTINE -----
SPINFO	RKTOUT SELECT SUMPRT1 PTAB	TBLDT2	MAIN1D OUT1 IAUX PRINT PTAB PRINTS
SSUMS	ROCKET OUT1	TBRSAV	ODKINP REAXIN SELECT
STREAM	ODES SUMPRT TWO MAIN1D TRAN CHAR GETIL GETILV GPFKIN	TDKMAX	TDK CHAR CNTRL DSPT INPT INSRT PRINT SUBIL WLPT AXISPT CNTR12 CNTR13 CNTR14 CNTR16 CNTR21 CNTR31 CNTR41 CNTRL1 CNTRL2 FTHRST GETPT GPFKIN GPFPG INPTR INPTR1 INPTRS INPTS INTEXT PRINTS SAVPT SHCKA SHCKA1 SHCKL SHCKR SHCKW SHCKW1 SUBILR WLCALC ATSHCK
TABL	BLOCKD INPUTB OUTPBL READBL BLEDDG COEF1 WRPROF		
TABS	BLMAIN OUTPBL BLSEG		
TBLDT1	MAIN ODES PROBLM READAT SAVDAT MAIN1D ODKBLM ODKINP TRAN GETIL GETILV IAUX PRINT PTAB PRINTS		
TBLDT2	MAIN ODES READAT SAVDAT		

LABELED COMMON

REFERRED BY SUBROUTINE

LABELED COMMON

REFERRED BY SUBROUTINE

TEMP	BLSEG EDDY	WALL	BLOCKD BLMAIN INPUTB OUTPUTB SOLVS BLEDGE BLSEG COEF COEF1 EDDY
TEGEC	ODES		
THISPT	ROCKET		
THMO	BLOCKD BLMAIN INPUTB IVPL OUTPUTB READBL BLEDGE BLSEG COEF1 EDDY	WALLTM	BLOCKD INPUTB BLEDGE
THRST	FTHRST	WTYPE	BLW PROBLM SUMPRT SUMPRT1
TOTSC	MAIN READAT SAVDAT MAIN1D TRAN FCALC GETIL GETILV IAUX	XTNDED	BLOCKD BLMAIN INPUTB READBL BLEDGE
TSTABL	MAIN READAT SAVDAT TWO MAIN1D GETIL GETILV IAUX	YSAVE	BLSEG WRPROF
TTDK	ODK OUTPUT	ZDEBUG	READAT SAVDAT STF DERIV THERM
TW1	INPUTB	ZLAST	SUMPRT TDK CNTRL PRINT CNTRL1 CNTRL2 PRINTS
TWOPHZ	PACK CONVRT MAIN1D ODKINP OUTPUT	ZTRAN	MAIN READAT SAVDAT TWO MAIN1D TRAN GETIL GETILV IAUX INT

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## 5. PROGRAM SUBROUTINES

This section contains descriptions of the TDK subroutines. TDK is organized into 6 modules, as follows: MCM, ØDE, ØDK, TRANS, MØC, and BLM. The subroutines descriptions are presented by modules, i.e., the MCM subroutines are given in Section 5-1, the ØDE subroutines are given in Section 5-2, etc. At the present time, complete descriptions are not available for all of the MØC subroutines.

## 5.1 MCM SUBROUTINES

The Master Control Module is used to control the execution of TDK by selecting the computation modules to be exercised. The MCM is also used to process output files for the purpose of creating printed and plotted output. The MCM consists of the following subroutines:

MAIN	SAVDAT
BLKDTA	SKPB1
FIND	SKPB2
GAUELM	SLP
ITER	SPLN
LTCPHS	SUMPRT
MATCH	TTAPE
MUK	UNIT
ØMEGA	
PRØBLM	
READAT	

MAIN provides the entry point to TDK and is the master subroutine for the entire program.

### 5.1.1 PROGRAM MAIN

This is the main program for TDK and as such provides communication between modules, defines the upper level labeled common blocks, and initializes certain logical control variables. MAIN calls the thermodynamic tape generation subroutine, TTAPE, as required. Subroutine PRØBLM is called to read the \$DATA namlist and determine the sequence of modules to be executed. Subroutines ØDE and ØDK are called to perform equilibrium/frozen and one dimensional kinetic calculations. Subroutine TWØD is called to perform transonic and two dimensional method of characteristics calculations. Subroutine BLMAIN is called to perform the boundary layer calculations. Subroutine BLW is called to calculate the displaced nozzle wall. Subroutine BLH is called to calculate the increase in propellant enthalpy contributed by the regenerative cooling circuits. The ØDE, ØDK, TRANS, and MOC calculations are then repeated if the repeat option has been specified.

5.1.2 SUBROUTINE BLKDTA

BLKDTA contains atomic data stored in ATØM(l,j) and many of the variables used with the variable format, FMT. The ATØM variables are defined in appendix B, Reference 3. The format variables are stored in the common labeled ØUPT and are described here.

A variable format was used so that one format, FMT, could be used in the final output with changes in the number of decimal places according to the sizes of the numbers. The format is used to print a label and from 1 to 13 associated numbers. The labels contain 14 alphanumeric characters stored in four words and printed with 3A4,A2. The numbers are all printed in a field of 9. FMT is initially set in BLKDTA as follows:

FMT	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)
	(1H	,3A4	,A2,	F9.	0,	F9.	0,	F9.	0,	F9.	0,
FMT	(12)	(13)	(14)	(15)	(16)	(17)	(18)	(19)	(20)	(21)	
	F9.	0,	F9.	0,	F9.	0,	F9.	0,	F9.	0,	
FMT	(22)	(23)	(24)	(25)	(26)	(27)	(28)	(29)	(30)		
	F9.	0,	F9.	0,	F9.	0,	F9.	0	)		

where the spaces are stored as blanks.

Some variables set in BLKDTA to modify FMT are as follows:

Variable:	F0	F1	F2	F3	F4	F5	FB	FMT13	FMT9X	FMT19
Storage:	0,	1,	2,	3,	4,	5,		13,	9X,	19,

The following is a list of variables used as labels and printed with 3A4, A2 in FMT:

Variable	Stored label
FP	P, ATM
FT	T, DEG K
FH	H, CAL G
FS	S, CAL/(G) (K)
FM	M, MOL WT
FV	(DLV/DLP) T
FD	(DLV/DLT) P
FC	CP, CAL/(G) (K)
FG	GAMMA (S)
FL	SON VEL, M/SEC
FRI	PC/P
FCI	CF
FN	MACH NUMBER
FR	CSTAR, FT/SEC
F1	ISP, LB-SEC/LB
FA	IVAC, LB-SEC/LB
FA1, FA2	AE/AT

### 5.1.3 SUBROUTINE FIND

This subroutine locates the index, I, in a table such that  $X(I) \leq X \leq X(I+1)$ .

5.1.4 Subroutine GAUELM(A,B,X,N,M,NDIM,MDIM,LDIM,EPS,KERR)

This subroutine solve a linear system of equations using Gaussian elimination with row interchange. The equation is put in matrix form as:

$$A X = B$$

where A,B and X are matrices of proper dimensions.

Calling Sequence

A,B,X	Matrices coefficients
N,M	Dimensions used: A(N,N), X(N,M), B(N,M)
NDIM	Maximum row dimension of A
MDIM	Maximum row dimension of B
LDIM	Maximum row dimension of X
EPS	Lower bound for the absolute value of the pivot
KERR	Error indicator, nonzero means error

### 5.1.5 SUBROUTINE ITER (F1, X1, XNEW, NØØ)

The purpose of this subroutine is to find the root or zero of the algebraic equation

$$f(X) = 0$$

using the method of secant or false position. In particular this subroutine is designed to take advantage of the fact that the secant method will always find the root of the above equation if the root has been spanned.

#### Calling Sequence:

- F1 is the value of the dependent variable, f, corresponding to the value of X1.  
X1 is the value of the independent variable, X, which corresponds to F1.  
XNEW is the predicted or new value of the independent variable  
NØØ is a flag such that  
    NØØ = -1 the first time ITER is called.  
    NØØ = +1 upon subsequence calls.

#### Restrictions:

The user is expected to check for convergence as there are no internal checks made in ITER.

#### Method:

Subroutine ITER utilizes the secant method predictor formula

$$X_{i+1} = X_i - f_i \cdot (X_i - X_{i-1}) / (f_i - f_{i-1})$$

where the subscript i refers to the current value of X and f

except for the first iteration in which the value of X is perturbed only slightly. When the root has been spanned the subroutine saves 2 back value of f and X in order that the root may always be straddled and thus found. The linkage to the subroutine is set up so that if bounds on the root are known, then the value of XNEW may be disregarded and bounded values may be used for the first two guesses. This type of linkage necessitates that the value of X1 must be set equal to XNEW or the bounded value of X. In order to speed up convergence, if the error within the bounded domain of the dependent variable exceeds a ratio of 10, then the new value of X is set equal to one half of the range.

#### 5.1.6 SUBROUTINE LTCPHS

This subroutine processes the low temperature  $C_p$ , H, S Thermodynamic Data extension input as described in detail in Section 6.1.

#### 5.1.7 SUBROUTINE MATCH

This subroutine is called by RØCKET to supply subroutine MUK with a vector of internal sequence numbers which point to the appropriate Lennard-Jones parameters used by MUK to calculate transport properties. The input to MATCH is the species name (from the SUB array) and the output corresponds to the index numbers in the table in the MUK write up.



5.1.8 Subroutine MUK (CP, XW, T, C, IT, N, XM, XMT, TK, PR)

This routine calculates the viscosity, thermal conductivity and Prandtl number for a gas composed of a mixture of species.

CALLING SEQUENCE:

CP	is an array of N specific heats of the species (ft <sup>2</sup> /sec <sup>2</sup> °R)	(INPUT)
XW	is an array of N molecular weights of the species (slug/slug mole)	(INPUT)
T	is the temperature of the gas (°R)	(INPUT)
C	is an array of N mass fractions of the species	(INPUT)
IT	is an array of N indices of the species into a table of collision diameter (σ) and energy of attraction (ε/k)	(INPUT)
N	is the number of species in the gas	(INPUT)
XM	is an array of N viscosities of the species, (lb·sec/ft <sup>2</sup> )	(OUTPUT)
XMT	is the total viscosity of the gas, (lb·sec/ft <sup>2</sup> )	(OUTPUT)
TK	is the thermal conductivity of the gas, (ft·lb/ft <sup>2</sup> sec (°R/ft))	(OUTPUT)
PR	is the Prandtl number of the gas,	(OUTPUT)

Method:

$$C_p = \sum_{i=1}^N C_i C_{p_i} \quad \text{Specific Heat}$$

$$M_w = \frac{1}{\sum_{i=1}^N \frac{C_i}{M_{w_i}}} \quad \text{Molecular Weight}$$

$$X_1 = C_1 \cdot \frac{M_w}{M_{w_1}}$$

$$T_1^* = \frac{T/1.8}{(\epsilon/k)_1}$$

$$\Omega_1 = \text{table } (T_1^*)$$

table of  $\Omega$  vs  $T^*$

$$\sigma_1 = \text{table } (i)$$

table of  $\sigma$  and  $\epsilon/k$   
vs. individual  
species

$$\mu_1 = \frac{4.15822 \times 10^{-8} \sqrt{M_{w_1} T}}{\sigma_1^2 \Omega_1}$$

$$\phi_{1j} = \frac{1}{2^{3/2}} \left( 1 + \frac{M_{w_1}}{M_{w_j}} \right)^{-1/2} \left[ 1 + \left( \frac{\mu_1}{\mu_j} \right)^{1/2} \left( \frac{M_{w_j}}{M_{w_1}} \right)^{1/4} \right]^2$$

$$\mu = \sum_{i=1}^N \left[ \mu_1 \left( 1 + \sum_{\substack{j=1 \\ j \neq 1}}^N \phi_{1j} \frac{X_j}{X_1} \right)^{-1} \right]$$

viscosity of the gas

$$K_1 = \frac{\mu_1 R}{M_{w_1}} \left( .45 + 1.32 \frac{C_{p_1}}{(R/M_{w_1})} \right)$$

$$K = \left[ \sum_{i=1}^N K_1 \left( 1 + 1.065 \sum_{\substack{j=1 \\ j \neq 1}}^N \phi_{1j} \frac{X_j}{X_1} \right)^{-1} \right]$$

thermal conductivity

$$P_r = \frac{C_p \mu}{K}$$

Prandtl number

Equations for  $K_1$  and  $\mu_1$  are from Reference 14. The values of the collision integral are from Table 2 of Appendix B in Reference 15. The relations used to calculate  $\mu$  and  $K$  of the mixture are from References 15 and 16, respectively.

Also from Reference 14 are the values of the collision diameters,  $\sigma$ , and energy of attraction,  $\epsilon/k$ .

Table 5-1 correlates the chemical name of the species to the internal number assigned to it by the subroutine. Also included is the key-punch name assigned to the species, since lower-case letters and subscripts are non-standard features in most computer configurations.

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Ref.14. Svehla, R. H. , "Estimated Viscosities and Thermal Conductivities of Gases at High Temperatures", NASA TR R-132, 1962.

Ref.15. Bird, R. B., Stewart, W.E., Lightfoot, E.N., Transport Phenomena, John Wiley & Sons. Inc. New York, 1960.

Ref.16. Mason, E. A., and Saxena, S. C., Physics of Fluids, Volume 1, No. 5, pp. 361-369, 1958.

Table 5-1: SPECIES NAMES AND IDENTIFIERS

Species Number	Chemical Name	Key Punch Name
1	Al	AL
2	AlCl	ALCL
3	AlCl <sub>3</sub>	ALCL3
4	AlF	ALF
5	AlF <sub>3</sub>	ALF3
6	AlN	ALN
7	AlO	ALO
8	AlS	ALS
9	Al <sub>2</sub>	AL2
10	Air	AIR
11	Ar	AR
12	AsH <sub>3</sub>	ASH3
13	B	B
14	BBr <sub>3</sub>	BBR3
15	BCl	BCL
16	BCl <sub>2</sub>	BCL2
17	BCl <sub>3</sub>	BCL3
18	BF	BF
19	BF <sub>2</sub>	BF2
20	BF <sub>3</sub>	BF3
21	BI <sub>3</sub>	BI3
22	BO	BO
23	B(OCH <sub>3</sub> ) <sub>3</sub>	B(OCH3)3
24	B <sub>2</sub>	B2
25	B <sub>2</sub> H <sub>6</sub>	B2H6
26	B <sub>2</sub> O <sub>3</sub>	B2O3
27	Be	BE
28	BeBr <sub>2</sub>	BEBR2
29	BeCl	BECL
30	BeCl <sub>2</sub>	BECL2
31	BeF	BEF
32	BeF <sub>2</sub>	BEF2
33	BeI <sub>2</sub>	BEI2
34	Be <sub>2</sub>	BE2

Species Number	Chemical Name	Key Punch Name
35	Br	BR
36	BrF	BRF
37	BrF <sub>3</sub>	BRF3
38	BrO	BRO
39	Br <sub>2</sub>	BR2
40	C	C
41	CBrF <sub>3</sub>	CBRF3
42	CBr <sub>4</sub>	CBR4
43	CCl	CCL
44	CClF <sub>3</sub>	CCLF3
45	CCl <sub>2</sub>	CCL2
46	CCl <sub>2</sub> F <sub>2</sub>	CCL2F2
47	CCl <sub>3</sub>	CCL3
48	CCl <sub>3</sub> F	CCL3F
49	CCL <sub>4</sub>	CCL4
40	CF	CF
51	CF <sub>2</sub>	CF2
52	CF <sub>3</sub>	CF3
53	CF <sub>4</sub>	CF4
54	CH	CH
55	CHBrClF	CHBRCLF
56	CHBrCl <sub>2</sub>	CHBRCL2
57	CHBr <sub>3</sub>	CHBR3
58	CHClF <sub>2</sub>	CHCLF2
59	CHCl <sub>3</sub>	CHCL3
60	CHF <sub>3</sub>	CHF3
61	CH <sub>2</sub> BrCl	CH2BRCL
62	CH <sub>2</sub> ClF	CH2CLF
63	CH <sub>2</sub> Cl <sub>2</sub>	CH2CL2
64	CH <sub>2</sub> F <sub>2</sub>	CH2F2
65	CH <sub>2</sub> I <sub>2</sub>	CH2I2
66	CH <sub>3</sub> Br	CH3BR
67	CH <sub>3</sub> Cl	CH3CL

Species Number	Chemical Name	Key Punch Name
68	CH <sub>3</sub> F	CH3F
69	CH <sub>3</sub> I	CH3I
70	CH <sub>3</sub> OH	CH3OH
71	CH <sub>4</sub>	CH4
72	CN	CN
73	CO	CO
74	COS	COS
75	CO <sub>2</sub>	CO2
76	CP	CP
77	CS	CS
78	CS <sub>2</sub>	CS2
79	C <sub>2</sub>	C2
80	C <sub>2</sub> H <sub>2</sub>	C2H2
81	C <sub>2</sub> H <sub>4</sub>	C2H4
82	C <sub>2</sub> H <sub>6</sub>	C2H6
83	C <sub>2</sub> H <sub>5</sub> Cl	C2H5CL
84	C <sub>2</sub> H <sub>5</sub> OH	C2H5OH
85	C <sub>2</sub> N <sub>2</sub>	C2N2
86	CH <sub>3</sub> OCH <sub>3</sub>	CH3OCH3
87	CH <sub>2</sub> CHCH <sub>3</sub>	CH2CHCH3
88	CH <sub>3</sub> CCH	CH3CCH
89	cyclo-C <sub>3</sub> H <sub>6</sub>	CYCLO-C3H6
90	C <sub>3</sub> H <sub>8</sub>	C3H8
91	n-C <sub>3</sub> H <sub>7</sub> OH	N-C3H7OH
92	CH <sub>3</sub> COCH <sub>3</sub>	CH3COCH3
93	CH <sub>3</sub> COOCH <sub>3</sub>	CH3COOCH3
94	n-C <sub>4</sub> H <sub>10</sub>	N-C4H10
95	iso-C <sub>4</sub> H <sub>10</sub>	ISO-C4H10
96	C <sub>2</sub> H <sub>5</sub> OC <sub>2</sub> H <sub>5</sub>	C2H5OC2H5
97	CH <sub>3</sub> COOC <sub>2</sub> H <sub>5</sub>	CH3COOC2H5
98	n-C <sub>5</sub> H <sub>12</sub>	N-C5H12
99	C(CH <sub>3</sub> ) <sub>4</sub>	C(CH3)4
100	C <sub>6</sub> H <sub>6</sub>	C6H6

Species Number	Chemical Name	Key Punch Name
101	$C_6H_{12}$	C6H12
102	n- $C_6H_{14}$	N-C6H14
103	Cd	CD
104	Cl	CL
105	ClCN	CLCN
106	ClF	CLF
107	$ClF_3$	CLF3
108	ClO	CLO
109	$Cl_2$	CL2
110	F	F
111	FCN	FCN
112	$F_2$	F2
113	H	H
114	HBr	HBR
115	HCN	HCN
116	HCl	HCL
117	HF	HF
118	HI	HI
119	HS	HS
120	$H_2$	H2
121	$H_2O$	H2O
122	$H_2O_2$	H2O2
123	$H_2S$	H2S
124	He	HE
125	Hg	HG
126	$HgBr_2$	HGBR2
127	$HgCl_2$	HGCL2
128	$HgI_2$	HGI2
129	I	I
130	ICl	ICL
131	$I_2$	I2
132	Kr	KR
133	Li	LI
134	LiBr	LIBR

Species Number	Chemical Name	Key Punch Name
135	LiCN	LICN
136	LiCl	LICL
137	LiF	LIF
138	LiI	LII
139	LiO	LIO
140	Li <sub>2</sub>	LI2
141	Li <sub>2</sub> O	LI2O
142	Mg	MG
143	MgCl	MGCL
144	MgCl <sub>2</sub>	MGCL2
145	MgF	MGF
146	MgF <sub>2</sub>	MGF2
147	Mg <sub>2</sub>	MG2
148	N	N
149	NF <sub>3</sub>	NF3
150	NH	NH
151	NH <sub>3</sub>	NH3
152	NO	NO
153	NOCl	NOCL
154	N <sub>2</sub>	N2
155	N <sub>2</sub> O	N2O
156	Na	NA
157	NaBr	NABR
158	NaCN	NACN
159	NaCl	NACL
160	NaF	NAF
161	NaI	NAI
162	NaO	NAO
163	NaOH	NAOH
164	Na <sub>2</sub>	NA2
165	Na <sub>2</sub> O	NA2O
166	Ne	NE
167	O	O
168	OF	OF



Species Number	Chemical Name	Key Punch Name
169	OF <sub>2</sub>	OF2
170	OH	OH
171	O <sub>2</sub>	O2
172	P	P
173	PCl	PCL
174	PCl <sub>3</sub>	PCL3
175	PF	PF
176	PF <sub>3</sub>	PF3
177	PH <sub>3</sub>	PH3
178	PN	PN
179	PO	PO
180	PS	PS
181	P <sub>2</sub>	P2
182	P <sub>4</sub>	P4
183	S	S
184	SF <sub>6</sub>	SF6
185	SO	SO
186	SO <sub>2</sub>	SO2
187	S <sub>2</sub>	S2
188	S <sub>2</sub> F <sub>2</sub>	S2F2
189	SI	SI
190	SiCl	SiCL
191	SiCl <sub>4</sub>	SiCL4
192	SIF	SIF
193	SIFCl <sub>3</sub>	SIFCL3
194	SIF <sub>2</sub> Cl <sub>2</sub>	SIF2CL2
195	SIF <sub>3</sub> Cl	SIF3CL
196	SIF <sub>4</sub>	SIF4
197	SiH <sub>4</sub>	SIH4
198	SIO	SIO
199	SiO <sub>2</sub>	SIO2
200	SIS	SIS
201	Si <sub>2</sub>	SI2
202	SnBr <sub>2</sub>	SNBR2
203	SnCl <sub>4</sub>	SNCL4
204	UF <sub>6</sub>	UF6
205	Xe	XE
206	Zn	ZN

### 5.1.9 Subroutine OMEGA

This subroutine calculates the exponent,  $\omega$ , used in the viscosity-temperature relationship

$$\mu = \mu_{\text{ref}} \left( \frac{T}{T_{\text{ref}}} \right)^{\omega}$$

using the method of least squares. That is, it calculates the value of  $\omega$  which gives the smallest sum of the errors squared. This form of the viscosity-temperature relationship was selected since the BLM module requires viscosity data in this manner.

In order to supply the maximum amount of accuracy and also to minimize the variation in data due to the selection of an exit area ratio, it was decided to match the throat value of viscosity exactly and select an  $\omega$  which would provide the best fit for viscosity at the chamber and exit of the motor.

The form of the error,  $E$ , was taken to be

$$E = \ln \mu / \mu^* - \omega \ln T / T^*$$

Squaring the errors, differentiating with respect to  $\omega$ , and setting the results equal to zero, yields the following value for  $\omega$

$$\omega = (\ln T_c / T^* \ln \mu_c / \mu^* + \ln T_e / T^* \ln \mu_e / \mu^*) / (\ln T_c / T^*)^2 + (\ln T_e / T^*)^2$$

where

$T$  = temperature

$\mu$  = viscosity

$e$  = refers to the exit plane

$c$  = refers to the chamber

$*$  = refers to the throat plane

#### 5.1.10 SUBROUTINE PRØBLEM

Subroutine PRØBLEM sets those default values that are concerned with the computational options of the program, such as the module execution flags (ØDE, ØDK, TDK, BLM, TDE, IRPEAT, and IRSTRT). The \$DATA namelist is read (see Section 6.). Flags controlling the sequence of module execution are set as determined by the options requested through the \$DATA input. Nozzle geometry parameters are placed into the GEOM array for communication to the various modules.

#### 5.1.11 SUBROUTINE READAT(NTAPE)

Subroutine READAT is called by Program MAIN to read data written by subroutine SAVDAT on unit NTAPE (=15) for the purpose of restarting the ODE and ODK modules.

#### 5.1.12 SUBROUTINE SAVDAT (NTAPE)

Subroutine SAVDAT is called by Program MAIN to write data on unit NTAPE (=15) to be used later for restarting the ODE and ODK modules. This data is read later by subroutine READAT.

5.1.13 Subroutine SKPB1(XA, YA, XE, YE, THA, THR, C1, D1, E1)

This subroutine computes the coefficients for the skewed parabola defined by two points and the tangent at one of these points and the axis angle. The equation of a skewed-parabola is

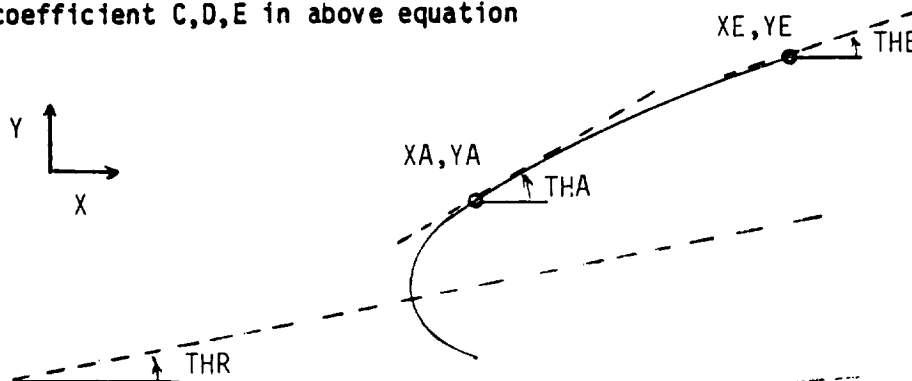
$$(Y - \tan(\text{Tr}) X)^2 + C X + D Y + E = 0$$

where Tr is the axis angle.

The subroutine solves for the coefficient C, D and E by using the condition on the two points and their tangents. The resulting equations form a linear system of 3 equations in 3 unknowns which is solved by Gaussian elimination with improvement correction using subroutine GAUELM.

Calling sequence:

XA, YA      coordinates of attachment point  
 XE, YE      coordinates of nozzle exit lip  
 THA        attachment angle  
 THR        axis angle, Tr  
 C1, D1, E1    coefficient C, D, E in above equation



5.1.14 Subroutine SKPB2(XA, YA, XE, YE, THA, THE, B1, C1, D1, E1)

This subroutine computes the equation for a skewed parabola defined by two points and their tangents. The equation for a skewed parabola is

$$(B X+Y)^2 + C X + D Y + E = 0$$

Subroutine SKPB1 and the secant method are used to solve for the axis angle that gives rise to the given exit lip angle.

Calling sequence:

XA, YA	coordinate of attachment point
XE, YE	coordinate of exit lip point
THA	attachment angle
THE	exit lip angle
B1, C1, D1, E1	coefficients B, C, D and E in above equation

### 5.1.15 SUBROUTINE SLP (X, Y, N, MFLAG, YP, W1, W2, W3, IFLAG)

The purpose of this subroutine is to supply derivatives for a tabulated function. The end point derivatives may be specified or are calculated internally by parabolic interpolation. Interior point derivatives may be found by a cubic spline fit procedure.

#### Calling Sequence:

- X** is a table of independent variables,  $x_1$
- Y** is a table of the dependent variables,  $y_1$
- N** is the number of entries in each of the tables X, Y, and YP.  
 $l = 1, \dots, N$
- MFLAG** this entry is a flag,  $m$ , such that
- $m > 0$  implies  $x$  is equally spaced
  - $m < 0$  implies  $x$  is not equally spaced
  - $|m| = 1$   $y'$  will be continuous
  - $|m| = 2$   $y'$  and  $y''$  will be continuous
- YP** is a table of the derivative,  $y'_1$
- W1** working storage of length N
- W2** working storage of length N
- W3** working storage of length N
- IFLAG** this entry is a flag,  $l$ , such that
- $l = 0$  implies value for YP(1) and YP(N) will be calculated internally by parabolic differencing
  - $l = 1$  implies values for YP(1) and YP(N) will be input

#### Method

The cubic spline fit procedure utilizes the interpolation formula given below:

$$\begin{aligned}y &= A(x - x_0)^3 + B(x - x_0)^2 + C(x - x_0) + D \\y' &= 3A(x - x_0)^2 + 2B(x - x_0) + C \\y'' &= 6A(x - x_0) + 2B\end{aligned}$$

The piecewise cubic fit to a tabular function by the above relations will yield a discontinuity in the second derivative  $y''$ , between adjacent fits of:

$$y''_{1_{01}} - y''_{1_{12}} = \frac{1}{h_{01}} \left( 2y'_0 + 4y'_1 - 6 \frac{k_{01}}{h_{01}} \right) - \frac{1}{h_{12}} \left( 6 \frac{k_{12}}{h_{12}} - 4y'_1 - 2y'_2 \right)$$

where

$$h_{01} = x_1 - x_0$$

$$h_{12} = x_2 - x_1$$

$$k_{01} = y_1 - y_0$$

$$k_{12} = y_2 - y_1$$

The method consists of setting the left-hand side of the above relation equal to zero so that the second derivative is continuous across juncture points. As applied to a tabular function, the above procedure results in a set of linear simultaneous equations (tri-diagonal) to be solved for the  $y'_1$ , provided that values for  $y'$  at the end points are known.

### 5.1.16 SUBROUTINE SPLN

Performs either cubic or linear interpolation between two given points.

Cubic interpolation for a function and its first two derivatives is performed as described below:

Given function values  $y_n$  and  $y_{n+1}$  and first derivative values  $y'_n$  and  $y'_{n+1}$  at  $x_n$  and  $x_{n+1}$ , this subroutine evaluates  $y(x)$ ,  $y'(x)$ , and  $y''(x)$  for  $x_n \leq x < x_{n+1}$  using:

$$y = A(x - x_n)^3 + B(x - x_n)^2 + C(x - x_n) + D$$

$$y' = y'_n + \frac{x - x_n}{x_{n+1} - x_n} \cdot [y'_{n+1} - y'_n]$$

$$y'' = (y'_{n+1} - y'_n) / h$$

where:

$$A = \frac{1}{h^3} \cdot [(y'_{n+1} + y'_n)h - 2k]$$

$$B = -\frac{1}{h^2} \cdot [(y'_{n+1} + 2y'_n)h - 3k]$$

$$C = y'_n$$

$$D = y_n$$

$$h = x_{n+1} - x_n$$

$$k = y_{n+1} - y_n$$

Linear interpolation for a function and its first two derivatives is performed as described below:

$$y = y_n + \frac{x - x_n}{x_{n+1} - x_n} \cdot [y_{n+1} - y_n]$$

$$y' = \frac{y_{n+1} - y_n}{x_{n+1} - x_n}$$

$$y'' = 0.0$$



#### 5.1.17 SUBROUTINE SUMPRT

This subroutine is called by Program MAIN to write the "TDK PERFORMANCE SUMMARY" output that is printed after the execution of the MOC and/or BLM modules. An example of this output together with a detailed description is given in Section 7 of this report, Input and Output for Example Cases.

#### 5.1.18 SUBROUTINE TTAPE

When a THERMO directive card is read by the main program this subroutine is called to generate a master Thermodynamic Data tape (Logical Unit 25). The input Thermodynamic Data is in curve fit form and is identical to that required for the ODE computer program described in NASA SP-273, Reference 3. The format for this curve fit data is described in the User's Manual, Section 6.1.

#### 5.1.19 SUBROUTINE UNIT

This subroutine is called by Program MAIN and is used to establish a consistent set of physical constants and conversion factors for the engineering units that are used throughout the program. The values are stored in COMMON/CONSTS/C000(25). The values used have been taken from the back cover of Zucrow and Hoffman, Reference 10.

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ODE MODULE SUBROUTINES

The one-Dimensional Equilibrium module is used to calculate ideal engine performance. Engine performance can also be calculated assuming that the chemical composition is frozen at the chamber (stagnation) conditions. Gas mixture properties, including transport properties, are also calculated by the ODE module to be used by the TDE, BLM and other options of the program. The ODE module is a modified version of the chemical Equilibrium Compositions (CEC) program that is described in Reference 3. Reference 3 should be referred to for a more complete description of this program. The ODE module consists of the following subroutines:

ODES	REACT
CPHS	RKTOUT
DETON	RCKET
EFMT	SAVE
EQLBRM	SEARCH
FRZEN	SHCK
GAUSS	THERMP
HCALC	TPCALC
MATRIX	TSCALC
OUT1	VARFMT

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### 5.2.1 SUBROUTINE ØDES

This is the main program for ØDE and corresponds to the Main Program described in Reference 3. Generally, the routine performs the following functions:

1. Reads code cards THERMØ, REACTANTS, ØMIT, INSERT, and NAMELISTS and directs flow of program accordingly.
2. Stores THERMØ data on tape.
3. Calls subroutine REACT to read and process REACTANTS cards.
4. Reads ØMIT and INSERT cards and stores species names.
5. Initializes variables in namelist \$ØDE.
6. Reads and writes namelist \$ØDE.
7. Converts assigned densities, if any, (RHO(i) in \$ØDE) to specific volumes:  $VLM(i) = 1/RHO(i)$ .
8. Stores the number of pressures or volumes in NP.
9. Stores values of o/f in ØXF array. If o/f values have not been input directly, they are calculated as follows:

Values	Code	o/f calculation in main program
Oxidant to fuel weight ratio, o/f	ØF = .TRUE.	$ØXF(i) = o/f$
Fuel to air weight ratio, f/a	FA = .TRUE.	$ØXF(i) = 1/(f/a)$
Percent fuel, %F	FPCT = .TRUE.	$ØXF(i) = (100 - \%F) / (\%F)$
Equivalence ratio, r	ERATIO = .TRUE.	$ØXF(i) = \frac{-rV^{-(2)} - V^{+(2)}}{rV^{-(1)} + V^{+(1)}}$
If above values not specified	default to	$ØXF(i) = \frac{WP(1)}{WP(2)} = 1.0$

10. Makes necessary adjustments to consider charge balance if IØNS = .TRUE.. This is done by adding 1 to NLM and E to LLMT array.
11. Calls SEARCH to pull required THERMØ data from tape and to store the data in core.
12. Sets initial estimates for compositions. These estimates are set with each \$ØDE read. They are used only for the first point in the lists of variables in namelist (e.g., the first o/f and the first T and P in a TP problem). All succeeding points use results from a previous point for estimates.

For the first point the program assigns an estimate of 0.1 for  $n$ , the total number of kilogram-moles per kilogram. The initial estimate of number of moles of each gaseous species per kilogram of mixture  $n_j$  is set equal to  $0.1/m$  where  $m$  is the total number of gaseous species. Condensed species are assigned zero moles.

13. Sets IUSE(j) positive for condensed species listed on INSERT cards (see IUSE array).
14. Calls THERMP if TP, HP, SP, TV, UV, or SV is true.
15. Calls DETØN if DETN is true.
16. Calls SHCK if SHØCK is true.
17. Calls RØCKET is RKT is true.

### 5.2.2 SUBROUTINE CPHS

This subroutine evaluates the thermodynamic functions  $\frac{C_p^\circ}{R}$ ,  $\frac{H_T^\circ}{RT}$ ,  $\frac{S_T^\circ}{R}$  from the curve fit coefficients. Two sets of coefficients are used for two adjacent temperature intervals. The functions evaluated are presented below:

$$\begin{aligned}\frac{C_p^\circ}{R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \frac{H_T^\circ}{RT} &= a_1 + \frac{a_2 T}{2} + \frac{a_3 T^2}{3} + \frac{a_4 T^3}{4} + \frac{a_5 T^4}{5} + \frac{a_6}{T} \\ \frac{S_T^\circ}{R} &= a_1 \ln T + a_2 T + \frac{a_3 T^2}{2} + \frac{a_4 T^3}{3} + \frac{a_5 T^4}{4} + a_7 \\ \frac{G_T^\circ}{RT} &= \frac{H_T^\circ}{RT} - \frac{S_T^\circ}{R}\end{aligned}$$

When the temperature falls below the lower limit of the curve fit coefficients, the above thermodynamic functions are obtained via linear interpolation from the input for subroutine LTCPHS.

### 5.2.3 SUBROUTINE DETØN

This subroutine does the calculations required to obtain Chapman-Jouget detonation properties as described in the section CHAPMAN-JOUGET DETONATIONS of Reference 3. The calculation involves a Newton-Raphson iteration to determine detonation conditions in addition to the iteration for determining equilibrium compositions.

### 5.2.4 SUBROUTINE EFMT

Subroutine EFMT (E-format) writes statements in a special exponent form. This form is similar to the standard FORTRAN E-format, but the letter E and some of the spaces have been removed for compactness. It is used to write density and mole fractions with the TRACE option.

### 5.2.5 SUBROUTINE EQLBRM

EQLBRM is the control routine for the equilibrium module which calculates equilibrium compositions and thermodynamic properties for a particular point. A free-energy minimization technique is used. The program permits calculations such as (1) chemical equilibrium for assigned thermodynamic states (T,P), (H,P), (S,P), (T,V), (U,V), or (S,V), (2) theoretical rocket performance for both equilibrium and frozen compositions during expansion, (3) incident and reflected shock properties, and (4) Chapman-Jouguet detonation properties. The program considers condensed species as well as gaseous species. A detailed description of the equations and computer program for computations involving chemical equilibria in complex systems is given in Reference 3. Figures 4(a) through 4(c) of Reference 3 gives a complete flow diagram for this subroutine.

The equilibrium compositions are obtained by a Newton-Raphson iteration. The iteration equations are those of the modified Huff method.<sup>18</sup> These equations are presented as Table 5-2. The corrections to the estimates that are obtained from this set of iteration equations are unaffected by the choice of components and are only affected by the current estimates. These equations make no distinction between components and constituents, and thus any species can be dropped from the calculation. The iteration equations give corrections to the moles of each condensed species and the variables A and T directly. The corrections to the moles of gaseous species are obtained from the following equation:

$$\Delta \ln n_i = -\mathcal{F}_i + \sum_{k=1}^L a_{ki} \Delta \ln u_k + \frac{v_i}{R} \Delta \ln T \quad (i = 1, 2, \dots, m)$$

It is sometimes disadvantageous to apply the entire correction called for by the iteration equations. Consequently an empirical convergence parameter  $\lambda$  ( $0 < \lambda \leq 1$ ) is used to control the size of the corrections. A numerical value for  $\lambda$  is determined at each iteration. Methods for evaluating  $\lambda$  are discussed later under Evaluation of Convergence Parameter  $\lambda$ . New estimates are obtained from the following equations:

$$\begin{aligned} \ln n_i^{(j+1)} &= \ln n_i^{(j)} + \lambda \Delta \ln n_i \quad (i = 1, 2, \dots, m) \\ n_i^{(j+1)} &= n_i^{(j)} + \lambda \Delta n_i \quad (i = m+1, m+2, \dots, n) \end{aligned}$$

TABLE 5-2. - ITERATION EQUATIONS TO DETERMINE EQUILIBRIUM COMPOSITIONS  
FOR EITHER ASSIGNED PRESSURE AND TEMPERATURE, ASSIGNED  
PRESSURE AND ENTHALPY, OR ASSIGNED PRESSURE AND ENTROPY

$\Delta \ln u_1$	$\Delta \ln u_2$	$\Delta \ln u_3$	$\Delta n_1$	$\Delta n_2$	$-\Delta \ln A$	$\Delta \ln T$	Constant
$r_{11}$	$r_{12}$	$r_{13}$	$a_{1,n-1}$	$a_{1,n}$	$\sum_{k=1}^m a_{1,k} n_k$	$\sum_{k=1}^m a_{1,k} \ln n_k$	$A \Delta b_1 + \sum_{k=1}^m a_{1,k} n_k \phi_k$
$r_{21}$	$r_{22}$	$r_{23}$	$a_{2,n-1}$	$a_{2,n}$	$\sum_{k=1}^m a_{2,k} n_k$	$\sum_{k=1}^m a_{2,k} \ln n_k$	$A \Delta b_2 + \sum_{k=1}^m a_{2,k} n_k \phi_k$
$r_{31}$	$r_{32}$	$r_{33}$	$a_{3,n-1}$	$a_{3,n}$	$\sum_{k=1}^m a_{3,k} n_k$	$\sum_{k=1}^m a_{3,k} \ln n_k$	$A \Delta b_3 + \sum_{k=1}^m a_{3,k} n_k \phi_k$
...	...	...	...	...	...	...	...
...	...	...	...	...	...	...	...
$a_{1,n-1}$	$a_{2,n-1}$	$a_{3,n-1}$	0	0	0	$\ln n_{n-1}$	$\phi_{n-1}$
$a_{1,n}$	$a_{2,n}$	$a_{3,n}$	0	0	0	$\ln n_n$	$\phi_n$
$\sum_{k=1}^m a_{1,k} n_k$	$\sum_{k=1}^m a_{2,k} n_k$	$\sum_{k=1}^m a_{3,k} n_k$	0	0	0	$\sum_{k=1}^m \ln n_k$	$\sum_{k=1}^m \phi_k n_k + \Delta P$
$\sum_{k=1}^m a_{1,k} \ln n_k$	$\sum_{k=1}^m a_{2,k} \ln n_k$	$\sum_{k=1}^m a_{3,k} \ln n_k$	$\ln n_{n-1}$	$\ln n_n$	$\sum_{k=1}^m \ln n_k$	$\sum_{k=1}^m \ln n_k + \sum_{k=1}^m \ln n_k \phi_k$	$A \Delta h + \sum_{k=1}^m \ln n_k \phi_k$
$\sum_{k=1}^m a_{1,k} \phi_k n_k$	$\sum_{k=1}^m a_{2,k} \phi_k n_k$	$\sum_{k=1}^m a_{3,k} \phi_k n_k$	$\ln n_{n-1}$	$\ln n_n$	$\sum_{k=1}^m \ln n_k$	$\sum_{k=1}^m \ln n_k + \sum_{k=1}^m \ln n_k \phi_k$	$A \Delta j + \Delta P + \sum_{k=1}^m \ln n_k \phi_k$

Iteration for assigned pressure and temperature  
Iteration for assigned pressure and enthalpy  
Iteration for assigned pressure and entropy

\* This column not used for assigned pressure and temperature.



$$\ln A^{(j+1)} = \ln A^{(j)} + \lambda \Delta \ln A$$

$$\ln T^{(j+1)} = \ln T^{(j)} + \lambda \Delta \ln T$$

The indices  $j$  and  $j+1$  signify the estimates for the  $j^{\text{th}}$  and  $(j+1)^{\text{st}}$  iterations. When the iteration has converged, the moles of gaseous species  $n_i$  will be numerically equal to the partial pressures  $p_i$  ( $i = 1, 2, \dots, m$ ).

After the equilibrium compositions have been determined, the three independent first derivatives  $c_p$ ,  $(\partial \ln Mw / \partial \ln T)_p$ , and  $(\partial \ln Mw / \partial \ln P)_T$  can be evaluated by a procedure analogous to that described in reference 19. The calculation of  $c_p$  and  $(\partial \ln Mw / \partial \ln T)_p$  requires the derivatives  $(\partial \ln n_i / \partial \ln T)_p$  ( $i = 1, 2, \dots, m$ ),  $(\partial n_i / \partial \ln T)_p$  ( $i = m+1, m+2, \dots, n$ ), and  $(\partial \ln A / \partial \ln T)_p$ . Following the procedure of reference 19 for the elimination of linear combination terms, the set of equations in Table 5-2 is obtained for the derivatives  $(\partial \ln u_i / \partial \ln T)_p$  ( $i = 1, 2, \dots, l$ ),  $(\partial n_i / \partial \ln T)_p$  ( $i = m+1, m+2, \dots, n$ ), and  $(\partial \ln A / \partial \ln T)_p$ . The  $(\partial \ln n_i / \partial \ln T)_p$  are related to these by

$$\left( \frac{\partial \ln n_i}{\partial \ln T} \right)_p = \sum_{k=1}^l a_{ki} \left( \frac{\partial \ln u_k}{\partial \ln T} \right)_p + \alpha_i \quad (i = 1, 2, \dots, m)$$

Writing the equation for evaluating the specific heat and substituting the above equation gives

$$c_p = \frac{R}{A} \left[ \sum_{k=1}^l \sum_{i=1}^m a_{ki} \alpha_i n_i \left( \frac{\partial \ln u_k}{\partial \ln T} \right)_p + \sum_{i=m+1}^n \alpha_i \left( \frac{\partial n_i}{\partial \ln T} \right)_p + \sum_{i=1}^m \alpha_i n_i \left( \frac{-\partial \ln A}{\partial \ln T} \right)_p + \sum_{i=1}^m \mathcal{E}_i n_i + \sum_{i=1}^m \alpha_i \alpha_i n_i \right]$$

TABLE 5-3 - EQUATIONS FOR EVALUATING DERIVATIVES WITH RESPECT TO  
TO LOGARITHM OF TEMPERATURE AT CONSTANT PRESSURE

$\left(\frac{\partial \ln u_1}{\partial \ln T}\right)_P$	$\left(\frac{\partial \ln u_2}{\partial \ln T}\right)_P$	$\left(\frac{\partial \ln u_3}{\partial \ln T}\right)_P$	...	$\left(\frac{\partial \ln u_{n-1}}{\partial \ln T}\right)_P$	$\left(\frac{\partial \ln u_n}{\partial \ln T}\right)_P$	$-\left(\frac{\partial \ln A}{\partial \ln T}\right)_P$	Constant
$r_{11}$	$r_{12}$	$r_{13}$	...	$a_{1,n-1}$	$a_{1,n}$	$\sum_{k=1}^n a_{1,k} n_k$	$-\sum_{k=1}^m a_{1,k} H_k n_k$
$r_{21}$	$r_{22}$	$r_{23}$	...	$a_{2,n-1}$	$a_{2,n}$	$\sum_{k=1}^n a_{2,k} n_k$	$-\sum_{k=1}^m a_{2,k} H_k n_k$
$r_{31}$	$r_{32}$	$r_{33}$	...	$a_{3,n-1}$	$a_{3,n}$	$\sum_{k=1}^n a_{3,k} n_k$	$-\sum_{k=1}^m a_{3,k} H_k n_k$
...	...	...	...	...	...	...	...
...	...	...	...	...	...	...	...
$a_{1,n-1}$	$a_{2,n-1}$	$a_{3,n-1}$	...	0	0	0	$-H_{n-1}$
$a_{1,n}$	$a_{2,n}$	$a_{3,n}$	...	0	0	0	$-H_n$
$\sum_{k=1}^m a_{1,k} n_k$	$\sum_{k=1}^m a_{2,k} n_k$	$\sum_{k=1}^m a_{3,k} n_k$	...	0	0	0	$-\sum_{k=1}^m H_k n_k$

The solution of the equations in Table 5-3 also gives one of the molecular weight derivatives by means of the relation

$$\left( \frac{\partial \ln Mw}{\partial \ln T} \right)_P = \left( \frac{\partial \ln A}{\partial \ln T} \right)_P$$

The derivative  $(\partial \ln M / \partial \ln P)_T$  can be calculated from

$$\left( \frac{\partial \ln Mw}{\partial \ln P} \right)_T = \frac{P}{\sum_{k=1}^l \sum_{i=1}^m \left( a_{ki}^{n_i} \frac{\partial \ln u_k}{\partial \ln A} \right)_T} - 1$$

where the required partial derivatives are obtained by a solution of the equations of Table 5-4 of this report. It should be noted that the matrix elements of Tables 5-3 and 5-4 are identical with the corresponding elements of Table 5-2 except for the sign of the last column in Table 5-3. The isentropic exponent,  $\gamma$ , used in the calculations of the velocity of sound is

$$\gamma \equiv \left( \frac{\partial \ln P}{\partial \ln \rho} \right)_s = \frac{1}{\left[ 1 + \left( \frac{\partial \ln Mw}{\partial \ln P} \right)_T \right] - \frac{R}{c_p Mw} \left[ 1 - \left( \frac{\partial \ln Mw}{\partial \ln T} \right)_P \right]^2}$$

Convergence in an iterative calculation involves two numerical problems: (1) how to assure numerical convergence, and (2) to determine at what stage the iteration should be terminated. Both of these are discussed in the following sections.

#### Evaluation of Convergence Parameter $\lambda$

When poor estimates are used in a Newton-Raphson iteration, the iteration equations will invariably give corrections that are too large. If these corrections were to be used directly, they could produce a nonconvergent iteration. This type of situation normally occurs in the early stages of a calculation.

TABLE 5-4. - EQUATIONS FOR EVALUATING DERIVATIVES WITH RESPECT TO LOGARITHM OF A AT CONSTANT TEMPERATURE

$\left(\frac{\partial \ln u_1}{\partial \ln A}\right)_T$	$\left(\frac{\partial \ln u_2}{\partial \ln A}\right)_T$	$\left(\frac{\partial \ln u_3}{\partial \ln A}\right)_T$	...	...	$\left(\frac{\partial \ln u_{n-1}}{\partial \ln A}\right)_T$	$\left(\frac{\partial \ln u_n}{\partial \ln A}\right)_T$	Constant
$r_{11}$	$r_{12}$	$r_{13}$	...	...	$a_{1,n-1}$	$a_{1,n}$	$\sum_{k=1}^n a_{1,k} u_k$
$r_{21}$	$r_{22}$	$r_{23}$	...	...	$a_{2,n-1}$	$a_{2,n}$	$\sum_{k=1}^n a_{2,k} u_k$
$r_{31}$	$r_{32}$	$r_{33}$	...	...	$a_{3,n-1}$	$a_{3,n}$	$\sum_{k=1}^n a_{3,k} u_k$
...	...	...	...	...	...	...	...
...	...	...	...	...	...	...	...
$a_{1,n-1}$	$a_{2,n-1}$	$a_{3,n-1}$	...	...	0	0	0
$a_{1,n}$	$a_{2,n}$	$a_{3,n}$	...	...	0	0	0

At later stages of the iteration when the problem seems to be converging satisfactorily, the iteration sometimes attempts to make large increases in the partial pressures of species that are present in trace amounts. In both of these cases it is essential to place some restriction on the size of the correction. This is accomplished by introducing a convergence parameter  $\lambda$ .

The numerical value of the convergence parameter  $\lambda$  is determined on the basis of two empirical rules, which experience has shown to be satisfactory. For the variables  $T$ ,  $A$ , and  $n_j$  for those gaseous species for which  $\ln(n_j/P_0) > -18.5$  and for which  $\Delta \ln n_j > 0$ , a number  $\lambda$  is defined as

$$\lambda_1 = \frac{2}{\max(|\Delta \ln T|, |\Delta \ln A|, \Delta \ln n_j)} \quad (j = 1, 2, \dots, m)$$

This limits the change in  $T$  and  $A$  and the increase in  $n_j$ , for those gaseous species whose gas phase mole fraction exceeds  $10^{-8}$ , to a factor  $e^2 = 7.3891$ . For those gaseous species for which  $\ln(n_j/P_0) \leq -18.5$  and  $\Delta \ln n_j > 0$ , a number  $\lambda_2$  is defined as

$$\lambda_2 = \min \left( \frac{\ln P_0 - 9.212 - \ln n_j}{\Delta \ln n_j} \right) \quad (j = 1, 2, \dots, m)$$

This prevents a gaseous species with a mole fraction less than  $10^{-8}$  from increasing its partial pressure so that its gas phase mole fraction would exceed  $10^{-4}$ . The parameter  $\lambda$  to be used is defined in terms of  $\lambda_1$  and  $\lambda_2$  as

$$\lambda = \min(1, \lambda_1, \lambda_2)$$

## Criteria for Convergence

Equilibrium compositions. - It is assumed that the iteration has converged to the correct composition when

$$\frac{n_j}{\sum_{k=1}^n n_k} |\Delta \ln n_j| < 0.5 \times 10^{-5} \quad (j = 1, 2, \dots, m)$$

and

$$\frac{|\Delta n_j|}{\sum_{k=1}^n n_k} < 0.5 \times 10^{-5} \quad (j = m + 1, m + 2, \dots, n)$$

This has the effect of insuring accuracy to five places in composition when it is expressed as mole fractions.

### 5.2.6 SUBROUTINE FRØZEN

Subroutine FRØZEN is called from subroutine RØCKET to calculate the temperature and thermodynamic properties for the following assigned conditions:

1. Composition frozen at combustion conditions.
2. An assigned exit pressure.
3. An assigned entropy equal to the entropy at combustion conditions.

The iteration procedure used for obtaining the exit temperature is discussed in the section Procedure for Obtaining Frozen Rocket Performance (p.40, Reference 3.)

For a mixture of fixed composition, entropy, and pressure, the temperature is calculated by a Newton-Raphson iteration. The correction to the current estimate for temperature is obtained from

$$\Delta \ln T = \frac{s_f - s_f^0}{\sum_{i=1}^n c_{p_i} x_i}$$

The improved estimate for temperature is then obtained by means of

$$\ln T^{(j+1)} = \ln T^{(j)} - \Delta \ln T$$

For frozen composition, the three independent first partial derivatives are:

$$c_p = R \frac{\sum_{i=1}^n c_{p_i} x_i}{\sum_{i=1}^m x_i}$$

and

$$\left( \frac{\partial \ln Mw}{\partial \ln T} \right)_P = 0$$

and

$$\left( \frac{\partial \ln Mw}{\partial \ln P} \right)_T = 0$$

The isentropic exponent  $\gamma$  is

$$\gamma = \frac{c_p Mw_c}{c_p Mw_c - R}$$

The throat conditions are evaluated with the aid of a secondary Newton-Raphson iteration using the equation

$$\left(\frac{P_c}{P}\right)_{k+1} = \frac{\left(\frac{P_c}{P}\right)_k}{1 + \frac{2Mw(h_c - h_k^*)}{(\gamma + 1) RT}}$$

where  $(P_c/P)_k$  is the  $k^{\text{th}}$  estimate for pressure ratio at the throat and  $h_k^*$  is the value of  $h^*$  for the pressure corresponding to this pressure ratio and an entropy equal to the combustion entropy. The initial estimate for  $P_c/P$  and  $T$  at the throat is described below.

An excellent estimate of the throat pressure ratio for both equilibrium and frozen compositions is

$$P_c/P = \left(\frac{\gamma_c + 1}{2}\right)^{\frac{\gamma_c}{\gamma_c - 1}}$$

This relation usually gives a throat pressure ratio, which is correct to three places. The throat temperature is estimated from the equation

$$T = \frac{2}{1 + \gamma_c} T_c$$

The throat conditions for a rocket nozzle are assumed to be satisfied if

$$\left| \frac{h_c - h^*}{h_c - h} \right| \leq 0.4 \times 10^{-4}$$

This condition in effect makes certain that the Mach number will satisfy the condition that

$$M = 1 \pm 0.2 \times 10^{-4}$$



### 5.2.7 SUBROUTINE GAUSS

Subroutine GAUSS is used to solve the set of simultaneous linear iteration equations constructed by subroutine MATRIX. The solution is effected by performing a Gauss reduction using a modified pivot technique. In this modified pivot technique only rows are interchanged. The row to be used for the elimination of a variable is selected on the basis that the largest of its elements, after division by the leading element, must be smaller than the largest element of the other rows after division by their leading elements.

The solution vector is stored in X(k). In the event of a singularity, IMAT (which is equal to the number of rows) is set equal to IMAT - 1. IMAT is tested later in subroutine EQLBRM.

### 5.2.8 SUBROUTINE HCALC

The purpose of HCALC is to calculate thermodynamic properties for reactants under certain circumstances. HCALC is called from entry NEWØF of SAVE and DETØN.

HCALC is called from NEWØF when CALCH is set true. CALCH is set true in the main program when zeros have been punched in card columns 37 and 38 on one or more REACTANTS cards. The zeros are a code indicating that the enthalpy (or internal energy for UV problems) for the reactant should be calculated from the THERMØ data at the temperature punched on the card. This temperature has been stored in the RTEMP array. CPHS is called to calculate the enthalpy. The value is sorted in the ENTH array and printed in the final tables.

The properties calculated in subroutine HCALC, their FORTRAN symbols, and the conditions for which they are used are as follows:

Property	FORTTRAN symbol	Equation	
$H(k)T$	HPP(k)	(192)	SHØCK problem. DETN problem with T schedule HP, RKT, or DETN problem if 00 in cc 37 and 38
$h_o/R$	HSUB0	(193)	SHØCK problem. DETN problem with T schedule HP, RKT, or DETN problem if 00 in cc 37 and 38
$u(k)T$	HPP(k)	(194)	UV problem if 00 in cc 37 and 38
$u'_o/R$	HSUB0	(195)	UV problem if 00 in cc 37 and 38
$M_o$	AM1	(197)	SHØCK or DETN problem
$m_i$	EN(j)	(205)	SHØCK problem
$\tau_o$	CPRI	(206)	SHØCK problem
$d_o$	S0	(207)	SHØCK problem

The quantity  $m_i$  was deliberately subscripted differently from EN(j) to allow for the fact that the same compound may have a different index as a reactant than as a reaction species. Thus, for example,  $O_2$  (g) might be the third reactant read in from REACTANTS cards and also the tenth species read in by SEARCH. In this case  $m_3$  would be stored in EN(10).

### 5.2.9 SUBROUTINE MATRIX

This subroutine sets up the matrices corresponding to tables I through IV of Reference 3. The assigned thermodynamic state being set up (tables I and II) is specified by the following codes:

Assigned thermodynamic state	Codes
TP	TP = .TRUE. VOL = .FALSE. CONVG = .FALSE.
HP	HP = .TRUE. VOL = .FALSE. CONVG = .FALSE.
SP	SP = .TRUE. VOL = .FALSE. CONVG = .FALSE.
TV	TP = .TRUE. VOL = .TRUE. CONVG = .FALSE.
UV	HP = .TRUE. VOL = .TRUE. CONVG = .FALSE.
SV	SP = .TRUE. VOL = .TRUE. CONVG = .FALSE.

After convergence of any of the previous six problems, setup of the derivative matrices (tables III and IV) is specified by the following codes:

Derivative	Codes
DLVTP	CONVG = .TRUE. LOGV = .FALSE.
DLVPT	CONVG = .TRUE. LOGV = .FALSE.

#### 5.2.10 SUBROUTINE ØUT1

This subroutine, together with entries ØUT2 and ØUT3, writes statements common to all problems. ØUT1 writes statements giving the data on REACTANTS and on o/f, percent fuel, equivalence ratio, and density.

Entry ØUT2. - This entry writes the statements for printing values of pressure, temperature, density, enthalpy, entropy, molecular weight,  $(\partial \ln V / \partial \ln P)_T$  (if equilibrium),  $(\partial \ln V / \partial \ln T)_P$  (if equilibrium), heat capacity,  $\gamma_S$ , and sonic velocity. These variables and corresponding labels are printed with a variable format described in BLKDTA.

Entry ØUT3. - Entry ØUT3 writes statements giving the equilibrium mole fractions of reaction species.

#### 5.2.11 SUBROUTINE REACT

The purpose of subroutine REACT is to read and process the data on the REACTANTS cards. The subroutine is called from the main program after a REACTANTS code card has been read. The data on these cards are described in the REACTANTS Cards section (p. 62) of Reference 3. References to page numbers and equations given below also pertain to Reference 3.

The reactants may be divided into two groups according to card column 72 on the REACTANTS cards. The two groups are oxidants (O in cc 72) and fuels (cc 72  $\neq$  O). We generally keypunch F in card column 72 for fuels even though this is not necessary. The contents of card column 72 are read into FØX. Depending on the contents of FØX, program variables relating to oxidants or fuels are subscripted 1 for oxidants and 2 for fuels.

The FORTRAN symbols for the properties read from the REACTANTS cards and their associated properties (discussed in INPUT CALCULATIONS, p. 55 of Reference 3) are as follows:

Property	FORTTRAN symbol
$a_{ij}^{(k)}$	ANLM(j, m) <sup>a</sup>
$W_j^{(k)}$	PECWT(j) (if no M in cc 53)
$N_j^{(k)}$	PECWT(j) (if M in cc 53)
$(H_T^O)^{(k)}$	ENTH(j) (if not UV problem and 00 not in cc 37 and 38)
$(U_T^O)^{(k)}$	ENTH(j) (if UV problem and 00 not in cc 37 and 38)
$\rho_j^{(k)}$	DENS(j)

<sup>a</sup>Each of the j REACTANTS cards contains from 1 to 5 stoichiometric coefficients read (indicated by subscript m) into ANUM(j, m) and their corresponding chemical symbols read into NAME(j, m). In relating an ANUM(j, m) with  $a_{ij}^{(k)}$ , the index i associated with a particular chemical element is determined from the chemical symbol in NAME(j, m).

If there are several oxidants their properties are combined by subroutine REACT into properties of a total oxidant using the relative proportion of each oxidant given on the REACTANTS cards. Similarly, if there are several fuels, their properties are combined into properties of a total fuel. The total oxidant and total fuel properties discussed in INPUT CALCULATIONS<sup>3</sup> and their associated FORTRAN symbols are as follows:

Property	FORTTRAN symbol	Equation
$b_i^{(k)}$	BOP(i, k)	(187)
$M_j^{(k)}$	RMW(j)	(190)
$H_T^{(k)}$	HPP(k) (if not UV problem and 00 not in cc 37 and 38)	(192)
$U_T^{(k)}$	HPP(k) (if UV problem and 00 not in cc 37 and 38)	(194)
$M^{(k)}$	AM(k)	(196)
$\rho^{(k)}$	RH(k)	(198)
$V^+(k)$	VPLS(k)	(200)
$V^-(k)$	VMIN(k)	(201)
$W_j^{(k)} / \sum_{j=1}^{NREAC} W_j^{(k)}$	PECWT(j)	

If any of the  $\rho_j^{(k)}$  are zero then  $RH(1) = RH(2) = 0$ .

These total oxidant and total fuel properties are subsequently combined into total reactant properties by using the values of oxidant-fuel mixture ratios obtained from the main program. This is done in NEWØF, an entry in SAVE.

Other common variables set by REACT are LLMT, NAME, ANUM, ENTH, FAZ, RTEMP, FOX, DENS, RMW, MØLES, NLM, NEWR, and NREAC.

A provision is made for eliminating a second tape search when two consecutive sets of REACTANTS cards contain the same elements. This is done by saving the element symbols (LLMT( $l$ )) in LLMTS( $l$ ), the kilogram-atoms per kilogram (BOP( $l, k$ )) in SBOP( $l, k$ ), and the number of elements (NLM) in NLS.

Atomic weights  $M_i$  used in equation (190)<sup>3</sup> are stored in ATØM(2,  $i$ ). The corresponding chemical symbols are stored in ATØM(1,  $i$ ). The oxidation states of the chemical elements  $V_i^+$  or  $V_i^-$  used in equations (200) and (201)<sup>3</sup> are stored in ATØM(3,  $i$ ). The ATØM array is stored by BLKØTA.

## 5.2.12 SUBROUTINE RKTØUT

This subroutine calculates various rocket performance parameters from previously calculated thermodynamic properties.

It is also the control program for writing rocket performance output. It contains the WRITE statements that apply specifically to rocket parameters and it calls subroutine ØUT1 and entries ØUT2 and ØUT3 for the WRITE statements common to all problems. The rocket parameters are printed with the variable format, FMT, described in BLKDTA.

The following formulas used in computing the various performance parameters were derived from the one-dimensional forms of continuity, energy, and momentum equations and the following assumptions: zero velocity in the combustion chamber, perfect gas law, complete combustion, homogeneous mixing, adiabatic combustion, and isentropic expansion. (The units used were  $h = \text{cal/gm}$ ,  $T = ^\circ\text{K}$ ,  $P = \text{lb force/sq in.}$ ,  $A = \text{sq in.}$ ,  $w = \text{lb mass/sec}$ , and  $g_c = 32.174 \text{ (lb mass/lb force) (ft/sec}^2\text{).}$ )

Specific impulse with ambient and exit pressures equal, (lb force) (sec)/lb mass:

$$I = 294.98 \sqrt{\frac{h_c - h}{1000}}$$

Specific impulse in vacuum (ambient pressure zero), (lb force) (sec)/lb mass:

$$I_{\text{vac}} = I + P \frac{A}{w}$$

Characteristic velocity, ft/sec:

$$c^* = g_c P_c \left( \frac{A}{w} \right)_t = 32.174 P_c \left( \frac{A}{w} \right)_t$$

Coefficient of thrust:

$$C_F = \frac{g_c I}{c^*} = 32.174 \frac{I}{c^*}$$

Mach number:

$$M = \frac{U}{U_s} = \frac{I}{\sqrt{\frac{86.4579 \gamma T}{Mw}}}$$

### 5.2.13 SUBROUTINE RØCKET

This subroutine is the control program for the RKT problem (rocket performance calculations discussed in section RØCKET PERFORMANCE).<sup>3</sup> A flow diagram for this subroutine is given in Figure 5 of Reference <sup>3</sup>. Subroutine RØCKET obtains the required thermodynamic properties for equilibrium performance by calling subroutine EQLBRM. For frozen performance, subroutine RØCKET calls subroutine FRØZEN to obtain the required thermodynamic properties. Rocket performance parameters are then obtained by calling subroutine RKTØUT. In addition to calling RKTØUT and FRØZEN, and in addition to using controls common to all problems (discussed in section MODULAR FORM OF THE PROGRAM, p. 75, Reference 3) subroutine RØCKET also does the following:

1. It reads and processes the input data in RKTINP namelist.
2. It calculates estimates for throat pressure ratios.
3. It calculates estimates for pressure ratios corresponding to assigned area ratios (if any).

5.2. 14 SUBROUTINE SAVE

This subroutine has several functions, all of which are concerned with saving some information from a completed calculation for subsequent use in later calculations. The primary purpose is to save computer time by having good initial estimates for compositions.

These estimates for the next point, NPT, come from either the point just completed, ISV, or some other previous point. The flow of the routine is directed by ISV as follows:

1. ISV positive. Transfer compositions for point just completed for use as initial estimates for next point (transfer EN(j, ISV) to EN(j, NPT)).

2. ISV negative. Save values of ENLN(j) for gases and EN(j) for condensed in SLN(j), ENN in ENSAVE, ENNL in ENLSAV, IQ1 in IQSAVE, JSØL in JSØLS, JLIQ in JLIQS, and NLM in LL1. (These values are saved because they are to be used as initial estimates for some future point and they may be overwritten in the meantime.) Make ISV positive and transfer EN(j, ISV) to EN(j, NPT).

3. ISV zero. Use the data previously saved (as discussed in 2.) as initial estimates for current point. Restore IUSE codes and inclusion or exclusion of "E" as an element for IØNS option.

Entry NEWØF. - NEWØF combines the properties of total oxidant and total fuel calculated in subroutine REACT with an o/f value to give properties for the total reactant. NEWØF is called for each mixture assigned in the MIX array in \$ØDE namelist. It is called from either THERMP, RØCKET, SHCK, or DETON. The calculated properties and corresponding FORTRAN symbols are as follows:

Property	FORTTRAN symbol	Equation
$b_i^o$	B0(i)	(191)
$h_o/R$	HSUB0 (if not UV problem)	(193)
$u_o'/R$	HSUB0 (if UV problem)	(195)
$\rho_o$	RHØP	(139)
r	EQRAT	(204)

Subroutine HCALC is called by Entry NEWØF to calculate the enthalpies for each reactant that has zeros keypunched in card columns 37 and 38 in its REACTANTS card.

Values of HPP(2), HPP(1), HSUB0, BOP(i,2), BOP(i,1), and B0(i) are printed out.



## 5.2.15 SUBROUTINE SEARCH

This subroutine selects the Thermodynamic Data to be used in the problem. A scan is made of the master Thermodynamic Data tape and those species that are consistent with the chemical system under consideration are selected. As the thermodynamic data are being selected, the subroutine also compiles a set of formula numbers,  $a_{ij}$ , from the formulas of the reaction products. A short Thermodynamic Data file is also generated for use in subsequent calculations (multizone).

A check is made near the beginning of the routine to prevent THERMØ data from exceeding their storage allotments. These variables are all in labeled common SPECIES and are currently dimensioned for 150 species. However, this dimension may be reduced to save storage.

SEARCH is called from the main program when the logical variable NEWR is true. NEWR is set true in REACT to indicate a new chemical system. REACT also stores chemical element symbols for the current chemical system in the LLMT array. SEARCH stores THERMØ data in core for each species whose elements are included in the LLMT array (unless the species name was listed on an ØMIT card).

The THERMØ data are stored in common variables TLØW, TMID, THIGH, SUB, A, CØEF, and TEMP. SEARCH writes out the names and dates of species whose data are stored in core.

SEARCH initializes the IUSE array. IUSE(j) for gaseous species are set equal to zero. IUSE(j) for condensed species are set equal to negative integers. For the chemical system under consideration, the first possible condensed species is set equal to -1, the second to -2, and so on, with one exception. In the event there are two or more condensed phases of the same species, each phase is given the same negative integer. Thus, if IUSE(j) for  $B_2O_3(l)$  is set equal to -4, for example, IUSE(j) for  $B_2O_3(s)$  will also be set equal to -4. A description of the IUSE array is given below.

The various condensed phases of a species are expected to be adjacent in the THERMØ data as they are read from tape. These phases must be either in increasing or decreasing order according to their temperature intervals.

NS contains the total number of species stored in core. NC contains the total number of condensed species (counting each condensed phase of a species as a separate species).

EQLBRM. For condensed species, the sign is adjusted as species are included or excluded in the current iteration.

For the IONS option, IUSE(j) values for ionic species are set to -10000 when the mole fractions of all ionic species are less than  $10^{-8}$ .

IUSE array. - Each value in the IUSE array is associated with a species. These values of IUSE serve two purposes:

1. They indicate which species are to be included in the current iteration (IUSE(j) < 0 for excluded species and IUSE(j) ≥ 0 for included species).

2. They indicate multiple phases of the same species if absolute values of IUSE(j) are equal.

The IUSE(j) are initialized in subroutine SEARCH and the main program as follows:

1. IUSE(j) = 0 for all gaseous species.
2. IUSE(j) = n for all condensed species whose names have been listed on INSERT cards. The number n indicates the species was the n<sup>th</sup> condensed species whose THERMØ data were read from tape.
3. IUSE(j) = -n for all condensed species not listed on INSERT cards where n is defined in 2.

These initial values of IUSE(j) may be adjusted later in subroutine

#### 5.2.16 SUBROUTINE SHCK

Subroutine SHCK is the application module for the SHOCK problems. It calculates the shock parameters discussed in the section "INCIDENT AND REFLECTED SHOCKS". It reads and processes the input data in SHKINP namelist. Depending on which options are specified, it calculates incident shock conditions based on compositions frozen at initial conditions and/or based on equilibrium compositions after shock. It also calculates, based on specified options, frozen and/or equilibrium reflected shock conditions relative to equilibrium and/or frozen incident shock conditions.

#### 5.2.17 SUBROUTINE THERMP

This subroutine is the application module for TP, HP, SP, TV, UV, and SV problems. Common variables which must be set according to the assigned thermodynamic states are given in the section Application Modules (p. 76) of Reference 3.

For these problems, the variables TP, HP, SP, S0, and VOL are set or read in subroutine ODES. HSUB0 is set either in SAVE (entry NEWOF) or HCALC. The general flow of the routine is given in figure 3 of Reference 3.

Indices run from 1 to NP both for assigned pressures P and assigned volumes (V in ODE and VL in THERMP). Indices run from 1 to NT for assigned temperature T. NP and NT are set in the subroutine ODES.

#### 5.2.18 SUBROUTINE TPCALC

This subroutine is used to obtain equilibrium values of  $C_p$ ,  $\gamma$ ,  $R$ , and  $h$  from given values of  $T$  and  $P$ . Subroutine EQLBRM is called to obtain the solutions.

#### 5.2.19 SUBROUTINE TSCALC

This subroutine finds equilibrium solutions from given values of  $T$  and  $S$ . The method used is to call subroutine TPCALC to find equilibrium solutions from given values of  $T$  and  $P$ , then the  $P$  value is adjusted until the input value of  $S$  is matched. Iteration on  $P$  is done using subroutine ITER (secant method). Subroutine TSCALC is used to construct the gas properties tables used by the BLM which are discussed in Section 2.6.3.

#### 5.2.20 SUBROUTINE VARFMT

Subroutine VARFMT (variable format) adjusts the number of decimal places printed in F-format in the variable format. FMT, according to the size of the number. It is used for  $P_c/P_e$ ,  $P$ , and  $A_e/A_t$ . Variable format is described in BLKDTA.

### 5.3 ODK MODULE SUBROUTINES

The One-Dimensional Kinetics (ODK) module is used to calculate the loss in nozzle performance caused by finite-rate chemistry of the expansion products. The method of analysis used is described in Section 2.1 and 2.2. Since the ordinary differential equations that are solved can be extremely stiff, a stable integration method is required. The integration method is described in Section 3.1.

The ODK module consists of the following subroutines:

ODK	ODKINP
CHTYPE	ODWALL
CONVRT	OUTPUT
DERIV	PACK
ECNV1	PACKCD
EF	PRATES
FLU	PREAX
FNDLM	PRES
GTF	PRNTCK
IAUX	REAXIN
INT	SELECT
LESK	STF
MAIN1D	STØICC
MGET	STORNU
NUMBR	SUBNE
ODKBLM	TABGEN

### 5.3.1 SUBROUTINE ODK

This subroutine acts as the driver for the one dimensional kinetic expansion calculation (ODK). It calls subroutine ODKINP to read the \$ODK input. Subroutine PACK is then called to prepare master tables for the chemical species and reactions to be used. Then subroutine MAIN1D is called which is the main program for the ODK module.

### 5.3.2 SUBROUTINE CHTYPE (KRD, ITY, NC)

Given the array KRD containing in each entry one character, left justified, this subroutine stores an interger code into the corresponding entry of array ITY. NC is the number of characters (consecutive entries) in KRD which are to be processed. The character-code table is as follows.

Character	Code
=	-4
*	-3
+	-2
0	0
1	1
2	2
3	3
4	4
5	5
6	6
7	7
8	8
9	9
all others	-1

### 5.3.3 SUBROUTINE CONVRT

This subroutine converts input data from the externally input units to internally used computation units. In order to conserve computation time during the kinetic expansion, parameters such as molecular weights, are included in these conversions. Barred values are input quantities.

- a) Reaction rate ratio input for reactions requiring third body terms  
units: unitless

internal units: (lbs-mass/lb-mole)<sup>-1</sup>

$$\text{formula: } XMM_{j,i} = \overline{XMM}_{j,i} / Mw_i$$

- b) Pre-exponential reaction rate parameter

input units: cm, °K, g-mole, sec

internal units: ft<sup>3</sup>, °R, lb-mole, sec

$$a_j = \frac{\overline{a}_j \cdot (.0160183)^{\lambda_j} \cdot 1.8^{\overline{n}_j}}{\prod_{i=1}^n Mw_i^{\nu'_{ij}}}$$

Where  $\lambda$  depends on the order of the reaction, i.e. where  $\lambda = (\Sigma \nu) - 1$  for binary exchange and  $\Sigma \nu$  for third body recombination. Also:

$$.0160183 = \frac{3.53147 \cdot 10^{-5} \text{ ft}^3}{1 \text{ cm}^3} \cdot \frac{1 \text{ g-mass}}{2.20462 \cdot 10^{-3} \text{ lbs-mass}}$$

- c) Exponential Term:

input units: kcal/mole

internal units: °R

$$\text{formula: } b_j = \overline{b}_j \cdot 905.770$$

$$\text{where } 905.770 = \frac{1000 \text{ cal}}{1 \text{ kcal}} \cdot \frac{1}{1.98726 \text{ cal/mole} \cdot \text{°K}} \cdot \frac{1.8 \text{°R}}{1.0 \text{°K}}$$

d) Equilibrium Constant Multiplicative Factor:

Input units: not input

Internal units: (lbs-mass) - °R/ft<sup>3</sup>

formula:

$$DATEF(J) = \frac{\prod_{i=1}^{\text{products}} M w_i}{\prod_{i=1}^{\text{reactants}} M w_i} \quad (0.73034)^{-(v'-v)}$$

where

$$\text{i.e. } .73034 = 49,721.011 \cdot \frac{\text{ft-poundals}}{(\text{lbs-mole}) \cdot \text{°R}} \cdot \frac{1 \text{ atmos}}{68,059.59 \text{ poundals/ft}^2}$$

$$.73034 = (RJG)/(144 \text{ g } 14.69)$$

e) Pressure:

input units: PSIA

internal units: poundals/ft<sup>2</sup>

formula:  $P = \bar{P} \cdot 4633.056$

where

$$4633.056 = \frac{144 \text{ in}^2}{1 \text{ ft}^2} \cdot 32.174 \frac{\text{ft}}{\text{sec}^2}$$

f) The initial reference enthalpy is computed using

$$H_{\text{Ref}} = \sum_{i=1}^N c_i h_i + \frac{v^2}{2}$$

Subroutine CONVRT has been modified to calculate the total amount of condensed phase present at the kinetic expansion initial conditions.



5.3.4 SUBROUTINE DERIV

This subroutine computes the total derivatives  $f_i$  and the partial derivatives  $\beta_{ij}$  described in the analysis presented in Section 3

The implicit integration method used to integrate the differential equations governing the chemical system, i. e.

$$y_i' = f_i(x, y_1, \dots, y_{NSP+3}) \quad i=1, \dots, NSP+3$$

where the variables

$$y_i \quad i=1, \dots, NSP+3$$

are  $V, \rho, T, C_i \quad i=1, \dots, NSP$

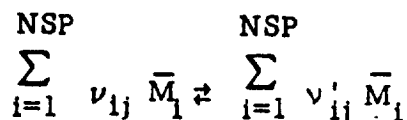
respectively, requires evaluation of the Jacobian of the system, i. e.

$$\beta_{ij} = \frac{\partial f_i}{\partial y_j} \quad \begin{array}{l} i=1, \dots, NSP+3 \\ j=1, \dots, NSP+3 \end{array}$$

Subroutine DERIV computes only certain of the  $\beta_{ij}$  (those taken with respect to  $C_i$ ) and the others are computed in subroutine FLU.

Also calculated by DERIV are the reaction rates,  $k_j$ , and the net production rates,  $X_j$ .

The generalized chemical reaction which is handled by this subroutine is defined by:



where  $\bar{M}_i$  represents the  $i^{\text{th}}$  chemical species.

The reverse reaction rate constant is defined by the equation:

$$k_j \quad SK(j) \quad = a_j \cdot T^{-n_j} \cdot \exp(-b_j/T)$$

The net production rate for a reaction is given by:

$$X_j \quad X(j) \quad = \left[ K_j \cdot \prod_{i=1}^{NSP} C_i^{\nu_{ij}} - \rho \lambda_j \cdot \prod_{i=1}^{NSP} C_i^{\nu'_{ij}} \right] \cdot k_j \cdot M_j \rho^{(\sum \nu_{ij})-1}$$

where:  $\lambda_j$  depends on the order of the reaction\*

with  $M_j = \sum_{i=1}^{NSP} XMM_{j,i} \cdot C_i$  for reactions requiring a third body

and  $M_j = 1$  for all other reactions

where  $XMM_{ji} \equiv m_{ji}/Mw_i$ ,  $m_{ji} = a_{ij}/a_{kj}$

The net individual species production rate is given by the equation:

$$\frac{dC_1}{dx} \text{ FN(I)} = \bar{K}_1 \cdot \sum_{j=1}^l \psi_{1j} \cdot X_j$$

where:

$$\bar{K}_1 = (Mw_1 \cdot \rho \cdot r^*)/V$$

$$\psi_{1j} \equiv v'_{1j} - v_{1j}$$

The partial derivatives of the net species production rate with respect to: the chemical species; the gas velocity; the gas density; and the gas temperature are:

$$\beta(C_k, C_1) \text{ ET(I, K)} = \bar{K}_1 \cdot \sum_{j=1}^l \psi_{1j} \frac{\partial X_j}{\partial C_1} \quad \begin{array}{l} i = 1, \dots, \text{NSP} \\ k = 1, \dots, \text{NSP} \end{array}$$

$$\beta(C_1, V) \text{ PHI(I, 1)} = -\frac{1}{V} \frac{dC_1}{dx} \quad i = 1, \dots, \text{NSP}$$

$$\beta(C_1, \rho) \text{ PHI(I, 2)} = \frac{1}{\rho} \cdot \frac{dC_1}{dx} + \bar{K}_1 \cdot \sum_{j=1}^m \psi_{1j} \frac{\partial X_j}{\partial \rho} \quad i = 1, \dots, \text{NSP}$$

$$\beta(C_1, T) \text{ PHI(I, 3)} = \bar{K}_1 \cdot \sum_{j=1}^l \psi_{1j} \frac{\partial X_j}{\partial T} \quad i = 1, \dots, \text{NSP}$$

\*  $\lambda_j = \sum_{i=1}^{NSP} (v'_{ij} - v_{ij})$  so that  $\lambda_j = 0$  for binary exchange,  $\lambda_j = 1$  for most dissociation recombination reactions.

The subscript notation used above is:

- i = Species subscript
- j = Reaction subscript
- l = Total number of chemical reactions
- m = Number of reactions requiring third body terms
- NSP = Total number of gaseous species

Subroutine DERIV calls subroutine FLU to calculate the derivatives and partial derivatives of V, P, and T. In the event of solidification, this routine also recalculates the condensed phase species derivatives and their partial derivatives and recalls subroutine FLU to recalculate the flow derivatives.

### 5.3.5 SUBROUTINE ECV1

This subroutine translates a BCD string of characters into one floating point numeric value. E, I, and F formats are permitted with the result always a floating point number. It is called by subroutine REAXIN to decode numeric fields in the species and reactions cards. The subroutine is coded entirely in FORTRAN. A BCD string of blanks will result in a floating point zero returned value.

5.3.6 SUBROUTINE EF

This subroutine computes equilibrium constants,  $K_j$ .

$$K_j \quad EK(J) = \frac{DATEF(J)}{T^{\lambda_j}} \cdot \exp \left[ - \sum_{i=1}^n Ft_i \cdot \nu_{ij} + \sum_{i=1}^n Ft_i \cdot \nu'_{ij} \right]$$

also computed are

$$\frac{dK_j}{dT} \quad DKT(J) = \left[ \frac{- \sum_{i=1}^n \frac{Ht_i}{R_i} \cdot \nu_{ij} + \sum_{i=1}^n \frac{Ht_i}{R_i} \cdot \nu'_{ij}}{T} - \lambda_j \right] \cdot \frac{K_j}{T}$$

where:  $Ft_i$  = species free energy at the current temperature

$Ht_i$  = species enthalpy at the current temperature

$DATEF(J)$  = is defined in subroutine  $CØNVRT$

### 5.3.7 SUBROUTINE FLU

This subroutine computes the total derivatives  $f_i$  and the partial derivatives  $\alpha_i$  and  $\beta_{ij}$  for the fluid dynamic equations. While the flow is subsonic, pressure defined fluid dynamic equations are used. When the flow becomes supersonic, area defined fluid dynamic equations are used. The summation terms, energy exchange term B, the diabatic heat addition term A, the Mach number, and all the partial derivatives of these terms are computed. For a subsonic integration the pressure and its derivatives are obtained from the subsonic pressure table. For a supersonic integration the area ratio and its derivatives are computed from the input geometric constraints.

The calculations logically fall into three types: a) Those done for all integrations; b) Those done only for subsonic integration; c) Those done only for supersonic integration. The following will adhere as closely as possible to a sequential description of the computations.

The operators  $\Phi(i, l)$ ,  $l = 1, 2, 3$  are defined as

$$\Phi(i, 1) = \beta(C_i, V)$$

$$\Phi(i, 2) = \beta(C_i, \rho)$$

$$\Phi(i, 3) = \beta(C_i, T)$$

The total derivatives,  $f_i = \frac{dC_i}{dx}$ , for  $i = 1, \dots, n$  are computed as

$$f_i = \frac{\omega_i r^*}{\rho V}$$

where  $n$  is the total number of species, NSP.

For an ODTDK problem, tables of  $C_p$ ,  $R$ ,  $AA$ ,  $BB$ , as functions of temperature are written on logical unit JANAF.

Computation of the Summation Terms and their derivatives:

First Summation

$$S1 \quad S1 = \frac{1}{R} \cdot \sum_{i=1}^n \frac{dC_i}{dx} \cdot R_i$$

$$\frac{\partial S1}{\partial V} \quad DS1V = \frac{1}{R} \cdot \sum_{i=1}^n \phi_{(1,1)} \cdot R_i$$

$$\frac{\partial S1}{\partial \rho} \quad DS1R\emptyset = \frac{1}{R} \cdot \sum_{i=1}^n \phi_{(1,2)} \cdot R_i$$

$$\frac{\partial S1}{\partial T} \quad DS1T = \frac{1}{R} \cdot \sum_{i=1}^n \phi_{(1,3)} \cdot R_i$$

$$\frac{\partial S1}{\partial C_i} \quad DS1C(I) = \frac{1}{R} \cdot \left[ \sum_{j=1}^n \beta(C_j, C_i) \cdot R_j - S1 \cdot R_i \right] \quad i = 1, \dots, n$$

Second Summation

$$S2 \quad S2 = \frac{1}{R \cdot T} \cdot \sum_{i=1}^n \frac{dC_i}{dx} \cdot h_i$$

$$\frac{\partial S2}{\partial V} \quad DS2V = \frac{1}{R \cdot T} \cdot \sum_{i=1}^n \phi_{(1,1)} \cdot h_i$$

$$\frac{\partial S2}{\partial \rho} \quad DS2R\emptyset = \frac{1}{R \cdot T} \cdot \sum_{i=1}^n \phi_{(1,2)} \cdot h_i$$

$$\frac{\partial S2}{\partial T} \quad DS2T = \frac{1}{R \cdot T} \cdot \sum_{i=1}^n \left[ \phi_{(1,3)} \cdot h_i + \frac{dC_i}{dx} \cdot Cp_i \right] - \frac{S2}{T}$$

$$\frac{\partial S2}{\partial C_i} \quad DS2C(I) = \frac{1}{R} \cdot \left[ \sum_{j=1}^n \frac{\beta(C_j, C_i) \cdot h_j}{T} - S2 \cdot R_i \right] \quad i = 1, \dots, n$$

\*  $R_i$  is the gas constant/molecular wt. of species i

Computation of the Energy Exchange Term B and Its Derivatives:

$$\begin{aligned}
 B \quad BB &= \frac{\gamma-1}{\gamma} \cdot S_2 \\
 \frac{\partial B}{\partial V} \quad DBBV &= \frac{\gamma-1}{\gamma} \cdot \frac{\partial S_2}{\partial V} \\
 \frac{\partial B}{\partial \rho} \quad DBBR\emptyset &= \frac{\gamma-1}{\gamma} \cdot \frac{\partial S_2}{\partial \rho} \\
 \frac{\partial B}{\partial T} \quad DBBT &= \frac{\gamma-1}{\gamma} \cdot \frac{\partial S_2}{\partial T} + \frac{S_2}{\gamma^2} \cdot \frac{\partial \gamma}{\partial T} \\
 \frac{\partial B}{\partial C_1} \quad DBBC(I) &= \frac{\gamma-1}{\gamma} \cdot \frac{\partial S_2}{\partial C_1} + \frac{S_2}{\gamma^2} \cdot \frac{\partial \gamma}{\partial C_1} \quad i = 1, \dots, n
 \end{aligned}$$

Computation of the Diabatic Heat Addition Term A and Its Derivatives:

$$\begin{aligned}
 A \quad AA &= S_1 - B \\
 \frac{\partial A}{\partial V} \quad DAAV &= \frac{\partial S_1}{\partial V} - \frac{\partial B}{\partial V} \\
 \frac{\partial A}{\partial \rho} \quad DAAR\emptyset &= \frac{\partial S_1}{\partial \rho} - \frac{\partial B}{\partial \rho} \\
 \frac{\partial A}{\partial T} \quad DAAT &= \frac{\partial S_1}{\partial T} - \frac{\partial B}{\partial T} \\
 \frac{\partial A}{\partial C_1} \quad DAAC(I) &= \frac{\partial S_1}{\partial C_1} - \frac{\partial B}{\partial C_1} \quad i = 1, \dots, n
 \end{aligned}$$



Computation of the Mach number and its derivatives:

$$M^2 \quad XM2 \quad = \quad \frac{V^2}{\gamma \cdot R \cdot T}$$

$$\frac{\partial M^2}{\partial V} \quad DM2V \quad = \quad \frac{2 \cdot M^2}{V}$$

$$\frac{\partial M^2}{\partial T} \quad DM2T \quad = \quad - \frac{M^2}{T} - \frac{M^2}{\gamma} \cdot \frac{\partial \gamma}{\partial T}$$

$$\frac{\partial M^2}{\partial C_l} \quad DM2C(l) \quad = \quad - M^2 \cdot \left[ \frac{\partial \gamma}{\partial C_l} \cdot \frac{1}{\gamma} + \frac{R_l}{R} \right] \quad l = 1, \dots, n$$

For the subsonic portion of the nozzle, pressure defined fluid dynamic equations are used. The pressure, and its first and second derivatives are computed via interpolation in the pressure table generated by subroutine PRES. The Subsonic Gas Velocity derivatives are computed:

$$\frac{dV}{dx} \quad FNX(1) \quad = \quad - \frac{1}{\rho \cdot V} \cdot \frac{dP}{dx}$$

$$\frac{\partial [FNX(1)]}{\partial x} \quad AL(1) \quad = \quad - \frac{1}{\rho \cdot V} \cdot \frac{d^2 P}{dx^2}$$

$$\beta(V, V) \quad BETA(1, 1) \quad = \quad - \frac{1}{V} \cdot \frac{dV}{dx}$$

$$\beta(V, \rho) \quad BETA(1, 2) \quad = \quad - \frac{1}{\rho} \cdot \frac{dV}{dx}$$

The Subsonic Gas Density derivatives are computed:

$$\frac{d\rho}{dx} \quad FNX(2) \quad = \quad \rho \cdot \left[ \frac{dP}{dx} \cdot \frac{1}{\gamma \cdot P} - A \right]$$

$$\frac{\partial [FNX(2)]}{\partial x} \quad AL(2) \quad = \quad \frac{\rho}{\gamma \cdot P} \cdot \left[ \frac{d^2 P}{dx^2} - \left( \frac{dP}{dx} \right)^2 \cdot \frac{1}{P} \right]$$

$$\beta(\rho, V) \quad \text{BETA}(2, 1) = - \rho \cdot \frac{\partial A}{\partial V}$$

$$\beta(\rho, \rho) \quad \text{BETA}(2, 2) = - \frac{1}{\rho} \cdot \frac{d\rho}{dx} - \rho \cdot \frac{\partial A}{\partial \rho}$$

$$\beta(\rho, T) \quad \text{BETA}(2, 3) = - \rho \cdot \frac{\partial A}{\partial T} - \frac{\rho}{P \cdot \gamma^2} \cdot \frac{\partial \gamma}{\partial T} \cdot \frac{dP}{dx}$$

$$\beta(\rho, C_i) \quad \text{BETA}(2, 1+3) = - \frac{\rho}{\gamma^2 P} \cdot \frac{\partial \gamma}{\partial C_i} \cdot \frac{dP}{dx} - \rho \cdot \frac{\partial A}{\partial C_i} \quad i = 1, \dots, n$$

The Subsonic Gas Temperature derivatives are computed:

$$\frac{dT}{dx} \quad \text{FNX}(3) = T \cdot \left[ \frac{\gamma-1}{\gamma} \cdot \frac{1}{P} \cdot \frac{dP}{dx} - B \right]$$

$$\frac{\partial [\text{FNX}(3)]}{\partial x} \quad \text{AL}(3) = \frac{\gamma-1}{\gamma} \cdot \frac{T}{P} \cdot \left[ \frac{d^2 P}{dx^2} - \left( \frac{dP}{dx} \right)^2 \cdot \frac{1}{P} \right]$$

$$\beta(T, V) \quad \text{BETA}(3, 1) = - T \cdot \frac{\partial B}{\partial V}$$

$$\beta(T, \rho) \quad \text{BETA}(3, 2) = - T \cdot \frac{\partial B}{\partial \rho}$$

$$\beta(T, T) \quad \text{BETA}(3, 3) = \frac{1}{T} \cdot \frac{dT}{dx} + T \cdot \frac{1}{\gamma^2 \cdot P} \cdot \frac{dP}{dx} \cdot \frac{\partial \gamma}{\partial T} - T \cdot \frac{\partial B}{\partial T}$$

$$\beta(T, C_i) \quad \text{BETA}(3, 1+3) = T \cdot \left[ \frac{1}{\gamma^2 \cdot P} \cdot \frac{dP}{dx} \cdot \frac{\partial \gamma}{\partial C_i} - \frac{\partial B}{\partial C_i} \right] \quad i = 1, \dots, n$$

For the supersonic portion of the nozzle, area defined fluid dynamic equations are used. The area ratio, and its derivatives are computed according to the input geometric constraints.

Area ratio and its derivatives:

- 1) On the circular arc of radius  $R_d$  (input item RWTD) defining the downstream throat region,  $X \leq X_{\text{tangent}}$

$$a = \left[ 1 + R_d - \left( R_d^2 - x^2 \right)^{1/2} \right]^2$$

$$\frac{da}{dx} = \frac{2x}{\left( R_d^2 - x^2 \right)^{1/2}} \cdot \left[ 1 + R_d - \left( R_d^2 - x^2 \right)^{1/2} \right]$$

$$\frac{d^2a}{dx^2} = \left[ \frac{2}{\left( R_d^2 - x^2 \right)^{1/2}} + \frac{2x^2}{\left( R_d^2 - x^2 \right)^{3/2}} \right] \cdot \left[ 1 + R_d - \left( R_d^2 - x^2 \right)^{1/2} \right] + \frac{2x^2}{R_d^2 - x^2}$$

- 2) For a conical nozzle and  $X > X_{\text{tangent}}$

$$a = \left[ r_t + \left( x - x_t \right) \tan \theta_t \right]^2$$

$$\frac{da}{dx} = 2 \left[ r_t + \left( x - x_t \right) \tan \theta_t \right] \cdot \tan \theta_t$$

$$\frac{d^2a}{dx^2} = 2 \tan^2 \theta_t$$

3) For a contoured nozzle and  $X > X_{\text{tangent}}$

$$a = Y^2$$

$$\frac{da}{dx} = 2 \cdot Y \cdot \frac{dY}{dx}$$

$$\frac{d^2a}{dx^2} = 2 \cdot \left[ Y \frac{d^2Y}{dx^2} + \left( \frac{dY}{dx} \right)^2 \right]$$

where  $Y$ ,  $dY/dx$ ,  $d^2Y/dx^2$  are computed via interpolation in the table of derivatives of the input wall table generated in Subroutine SLP.

The Supersonic Gas Velocity derivatives are computed:

$$\frac{dV}{dx} \quad \text{FNX(1)} = \frac{V}{M^2-1} \cdot \left[ \frac{1}{a} \frac{da}{dx} - A \right]$$

$$\frac{\partial[\text{FNX(1)}]}{\partial x} \quad \text{AL(1)} = \frac{V}{M^2-1} \cdot \frac{1}{a} \cdot \left[ \frac{d^2a}{dx^2} - \frac{1}{a} \cdot \left( \frac{da}{dx} \right)^2 \right]$$

$$\begin{aligned} \beta(V, V) \quad \text{BETA(1,1)} &= \frac{1}{V} \cdot \frac{dV}{dx} - \frac{1}{M^2-1} \cdot \frac{dV}{dx} \cdot \frac{\partial M^2}{\partial V} \\ &\quad - \frac{V}{M^2-1} \cdot \frac{\partial A}{\partial V} \end{aligned}$$

$$\beta(V, \rho) \quad \text{BETA(1,2)} = - \frac{V}{M^2-1} \cdot \frac{\partial A}{\partial \rho}$$

$$\beta(V, T) \quad \text{BETA(1,3)} = - \frac{1}{M^2-1} \cdot \frac{dV}{dx} \cdot \frac{\partial M^2}{\partial T} - \frac{V}{M^2-1} \cdot \frac{\partial A}{\partial T}$$

$$\beta(V, C_i) \quad \text{BETA(1,1+3)} = - \frac{1}{M^2-1} \cdot \frac{dV}{dx} \cdot \frac{\partial M^2}{\partial C_i} - \frac{V}{M^2-1} \cdot \frac{\partial A}{\partial C_i} \quad i=1, \dots, n$$

The Supersonic Gas Density derivatives are computed:

$$\begin{aligned} \frac{d\rho}{dx} \quad \text{FNX(2)} &= -\rho \cdot \left[ \frac{M^2}{M^2-1} \cdot \left( \frac{1}{a} \cdot \frac{da}{dx} - A \right) + A \right] \\ \frac{\partial[\text{FNX(2)}]}{\partial x} \quad \text{AL(2)} &= -\rho \cdot \frac{M^2}{M^2-1} \cdot \frac{1}{a} \cdot \left[ \frac{d^2a}{dx^2} - \frac{1}{a} \left( \frac{da}{dx} \right)^2 \right] \\ \beta(\rho, V) \quad \text{BETA(2,1)} &= \rho \cdot \left[ \frac{1}{(M^2-1)^2} \cdot \left( \frac{1}{a} \frac{da}{dx} - A \right) \cdot \frac{\partial M^2}{\partial V} + \frac{1}{M^2-1} \cdot \frac{\partial A}{\partial V} \right] \\ \beta(\rho, \rho) \quad \text{BETA(2,2)} &= \frac{1}{\rho} \cdot \frac{d\rho}{dx} + \frac{\rho}{M^2-1} \cdot \frac{\partial A}{\partial \rho} \\ \beta(\rho, T) \quad \text{BETA(2,3)} &= \rho \cdot \left[ \frac{1}{(M^2-1)^2} \cdot \left( \frac{1}{a} \frac{da}{dx} - A \right) \cdot \frac{\partial M^2}{\partial T} + \frac{1}{M^2-1} \cdot \frac{\partial A}{\partial T} \right] \\ \beta(\rho, C_1) \quad \text{BETA(2,1+3)} &= \rho \cdot \left[ \frac{1}{(M^2-1)^2} \cdot \left( \frac{1}{a} \frac{da}{dx} - A \right) \cdot \frac{\partial M^2}{\partial C_1} + \frac{1}{M^2-1} \cdot \frac{\partial A}{\partial C_1} \right] \\ & \quad \quad \quad i = 1, \dots, n \end{aligned}$$

The Supersonic Gas Temperature derivatives are computed:

$$\begin{aligned} \frac{dT}{dx} \quad \text{FNX(3)} &= -T \cdot \left[ (\gamma-1) \cdot \frac{M^2}{M^2-1} \cdot \left( \frac{1}{a} \frac{da}{dx} - A \right) + B \right] \\ \frac{\partial[\text{FNX(3)}]}{\partial x} \quad \text{AL(3)} &= -T \cdot \frac{M^2}{M^2-1} \cdot \frac{\gamma-1}{a} \cdot \left[ \frac{d^2a}{dx^2} - \frac{1}{a} \cdot \left( \frac{da}{dx} \right)^2 \right] \\ \beta(T, V) \quad \text{BETA(3,1)} &= T \cdot \left[ \frac{\gamma-1}{(M^2-1)^2} \cdot \left( \frac{1}{a} \frac{da}{dx} - A \right) \cdot \frac{\partial M^2}{\partial V} + \gamma-1 \cdot \frac{M^2}{M^2-1} \cdot \frac{\partial A}{\partial V} - \frac{\partial B}{\partial V} \right] \\ \beta(T, \rho) \quad \text{BETA(3,2)} &= T \cdot \left[ \gamma-1 \cdot \frac{M^2}{M^2-1} \cdot \frac{\partial A}{\partial \rho} - \frac{\partial B}{\partial \rho} \right] \end{aligned}$$

$$\beta(T, T) \quad \text{BETA}(3,3) = \frac{1}{T} \cdot \frac{dT}{dx} + T \cdot \left[ \frac{\gamma-1}{(M^2-1)^2} \left( \frac{1}{a} \frac{da}{dx} - A \right) \frac{\partial M^2}{\partial T} \right. \\ \left. + \gamma-1 \cdot \frac{M^2}{M^2-1} \cdot \frac{\partial A}{\partial T} - \frac{\partial B}{\partial T} \right. \\ \left. - \frac{M^2}{(M^2-1)} \cdot \left( \frac{1}{a} \frac{da}{dx} - A \right) \frac{\partial \gamma}{\partial T} \right]$$

$$\beta(T, C_l) \quad \text{BETA}(3,1+3) = T \cdot \left[ \frac{\gamma-1}{(M^2-1)^2} \left( \frac{1}{a} \frac{da}{dx} - A \right) \frac{\partial M^2}{\partial C_l} + \gamma-1 \cdot \frac{M^2}{M^2-1} \cdot \frac{\partial A}{\partial C_l} \right. \\ \left. - \frac{\partial B}{\partial C_l} - \frac{M^2}{M^2-1} \cdot \left( \frac{1}{a} \frac{da}{dx} - A \right) \frac{\partial \gamma}{\partial C_l} \right]$$

$$l = 1, \dots, n$$

5.3.8 SUBROUTINE FNDLM (IC, NS, IP, IDLM)

Given a card image stored 80A1 in the IC array, this subroutine searches left to right, starting with character number NS, until a match is found to the input character IDLM. The character number is returned in IP. If no match is found, a -1 is returned in IP. This subroutine is used by subroutines MGET, PRATES, and REAXIN to locate field delimiters.

### 5.3.9 SUBROUTINE GTF

This subroutine computes the effective gas constant, gaseous heat capacity,  $\gamma$ ,  $\partial\gamma/\partial T$ ,  $\partial\gamma/\partial C_1$  from the following formulae:

$$R = \sum_{i=1}^{NSP} C_i \cdot R_i$$

$$C_p = \sum_{i=1}^{NSP} C_i \cdot C_{p_i}$$

$$\gamma = \frac{C_p}{C_p - R}$$

$$\frac{\partial\gamma}{\partial T} = - \frac{\gamma \cdot (\gamma - 1)}{C_p} \cdot \sum_{i=1}^{NSP} C_i \cdot \frac{\partial C_{p_i}}{\partial T}$$

$$\frac{\partial\gamma}{\partial C_1} = \gamma \cdot (\gamma - 1) \cdot \left[ \frac{R_1}{R} - \frac{C_{p_1}}{C_p} \right] \quad i = 1, \dots, n$$

For condensed phases,  $R_i=0$ , to account for the assumption that the particles exert no pressure on the gas.



5.3.10 SUBROUTINE IAUX (HL, H, QK, RK, JK)

This subroutine performs implicit integration according to the method discussed in Section 3. The increments for the chemical species concentrations and the fluid dynamic variables at the forward point are calculated by solving the appropriate implicit finite difference formulas. Subroutine IAUX also performs explicit integration, using a modified Euler method, when the gas temperature falls below an input value.

The calling sequence parameters are:

- HL - last integration step size
- H - current integration step size
- QK - last increments for variables
- RK - computed increments for variables
- JK -
  - 1 initial 3 steps
  - 2 general step
  - 3 special step
  - 4 restart step

The total derivatives,  $f_{i,n}$ , and partial derivatives,  $\beta_{i,j,n}$  at the back point are calculated in subroutines DERIV and FLU.

The special step calculation is used at print stations, in halving the step size if required, or for integrating to specific calculation stations. If the special step calculation is used to determine the properties at a print station, the calculation is resumed using the general step calculation and the previous step size.

After each integration step, subroutine IAUX obtains the derivatives at the then current axial position.

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For implicit integration the equations used are:

### Initial Step and Restart

$$k_{i,1} = \left[ f_{i,0} + \alpha_{i,0} h + \sum_{j=1}^N \beta_{i,j,0} k_{j,1} \right] \cdot h$$

### General Step

$$k_{i,n+1} = \frac{1}{3} \left[ k_{i,n} + 2 \cdot \left( f_{i,n} + \alpha_{i,n} h + \sum_{j=1}^N \beta_{i,j,n} k_{j,n+1} \right) \cdot h \right]$$

### Special Step

$$k_{i,n+1} = \frac{h_{n+1}^2}{(2h_{n+1} + h_n) \cdot h_n} \left[ k_{i,n} + \left[ f_{i,n} + \alpha_{i,n} h_{n+1} + \sum_{j=1}^N \beta_{i,j,n} k_{j,n+1} \right] \cdot \frac{h_n}{h_{n+1}} (h_{n+1} + h_n) \right]$$

For explicit integration the above equations are used deleting the partial derivative terms  $\alpha$  and  $\beta$ .

If the TDK problem directive was selected, gas tables for the Transonic Analysis Subprogram are written on logical unit ITSTAB.

If the option to generate input tables for the Turbulent Boundary Layer Nozzle Analysis Computer Program was selected, tables of  $M$ ,  $P/P_c$ ,  $T/T_c$ ,  $C_p$ ,  $V$ ,  $\rho$  are tabulated using subroutine TABGEN.

### 5.3.11 SUBROUTINE INT

Provides control for the implicit integration procedure, determines the proper set of nonhomogeneous equations to solve, and, after each integration step, computes the next integration step size according to the following relations:

$$h_{n+2} = 2h_{n+1}, \quad \left| \frac{k_{i,n+1} - 2k_{i,n} + k_{i,n-1}}{3y_{\max}} \right| < \frac{\delta}{\text{MAX} \cdot 20}$$

$$h_{n+2} = \frac{1}{2}h_{n+1}, \quad \left| \frac{k_{i,n+1} - 2k_{i,n} + k_{i,n-1}}{3y_{\max}} \right| > \delta$$

$$h_{n+2} = h_{n+1}, \quad \frac{\delta}{20} \leq \left| \frac{k_{i,n+1} - 2k_{i,n} + k_{i,n-1}}{3y_{\max}} \right| \leq \delta$$

where

$$y_{\max} = \max [ |y_{i,n}|, 10^{-5} ] \quad ; i = 1, 2, \dots, \text{NSP}+3$$

On option, (JF=1) only the fluid dynamic variables are used in determining the next integration step size.

If the step size is halved for the fourth step, the integration is restarted using one-half the original step size.

The correspondence between equation number and physical property is:

<u>Equation Number</u>	<u>Property</u>
1	Velocity of Gas
2	Density of Gas
3	Temperature of Gas
4 NSP+3	Gaseous species mass fraction (1...NSP) correspondence to (4...NSP + 3)

When the flow is supersonic, continuity is used to control the integration step size to insure that:

$$\left| \frac{(\rho VA)_{N+1} - (\rho VA)_N}{(\rho VA)_{N+1}} \right| < \text{C\O NDEL}$$

where C\O NDEL is an input relative criterion with a default value  $10^{-5}$ .

### 5.3.12 SUBROUTINE LESK (Y)

**This subroutine is a single precision linear equation solver which is used to perform the matrix inversions required by subroutine IAUX. Gaussian elimination is used with row interchange taking place to position maximum pivot elements after the rows are initially scaled.**

SUBROUTINE MAIN1D

This subroutine provides the overall logic control for the one-dimensional kinetic expansion. The following functions are controlled:

- 1) Variable initialization
- 2) Option to start the kinetic expansion from equilibrium throat conditions
- 3) Controls of the integration to hit specific area ratios, the nozzle throat point, the nozzle tangent point, and the requested end point
- 4) Controls of the switch from the subsonic pressure defined equations to the supersonic area defined equations when  $(M^2 \geq 1.02)$
- 5) Controls the switch from implicit to explicit integration.

For the normal mode of operation of the program, this subroutine locates the throat in the following manner:

The gaseous mass flow per unit area  $(\rho v)$  is calculated and stored as a function of nozzle axial location for the present and past integration step. When

$$(\rho v)_{n+1} < (\rho v)_n$$

where  $n$  refers to the  $n^{\text{th}}$  integration step, the throat location is calculated from:

$$X^* = X_n + \frac{(X_n - X_{n-1})^2 \cdot [(\rho v)_{n+1} - (\rho v)_n] + (X_{n+1} - X_n)^2 \cdot [(\rho v)_n - (\rho v)_{n-1}]}{2 \cdot [(X_{n+1} - X_n) \cdot [(\rho v)_n - (\rho v)_{n-1}] - (X_n - X_{n-1}) \cdot [(\rho v)_{n+1} - (\rho v)_n]]}$$

and the  $n+1^{\text{th}}$  integration step is repeated using a step size of  $X^* - X_n$  to determine the throat conditions.

To prevent the location of a false throat due to roughness of an input pressure table, ten integration steps are required before the throat will be sought.

Through the downstream throat radius of curvature the step size is controlled so as to be less than or equal to  $RWTD * \sin(\text{THETA}) / 25.0$ ,

Subroutine MAIN1D also contains the logic to control the integration through solidification of multiple condensed liquid phases if they are present. This logic allows the integration procedure to hit the beginning and ending of solidification exactly and to turn on the solidification equations in subroutine DERIV via the flag IFMELT in COMMON/LKMELT/.

#### 5.3.14 SUBROUTINE MGET

This subroutine is used to decode the M's in the 3rd body reactions. It uses subroutine FNDLM to locate the field delimiter, and subroutine ECV1 to translate the M value from a character to a floating point number.

#### 5.3.15 SUBROUTINE NUMBR

This FORTRAN subroutine converts a one character BCD number to an integer number.

#### 5.3.16 SUBROUTINE ODKBLM

If BLM is to be run following the execution of a Two-Dimensional Frozen (TDF=1.) calculation, then subroutine ODK calls ODKBLM to obtain the required gas properties. These consist of gas viscosity, Prandtl number, and total enthalpy; followed by tables of  $C_{pg}$ ,  $Y$ ,  $h$ , and  $R$  vs temperature. All of the above properties are written on unit LUBLM. The properties correspond to a) the chamber equilibrium species compositions expanded in a frozen state, or b) the input species compositions expanded in a frozen state.

5.3.17 SUBROUTINE ØDKINP

This subroutine provides the input processing for the kinetic expansion calculation. It performs the following functions:

- 1) Variable initialization to nominal values
- 2) Calls subroutine REAXIN to input the reactions cards and species cards if necessary
- 3) For an ØDE-ØDK problem, calls subroutine SELECT to select those species to be considered for the kinetic expansion calculation
- 4) Reads \$ØDK namelist input data
- 5) Converts nozzle geometric parameters from input units: inches, degrees; to internal computational units: feet, radians
- 6) Computes nozzle tangent coordinates using:

$$r_t = 1 + R_d (1 - \cos \theta)$$

$$x_t = R_d \sin \theta$$

- 7) For conical nozzles, computes the axial coordinate for the exit station from the following relation:

$$x_{\text{exit}} = \frac{\sqrt{\epsilon} - r_t + x_t \cdot \tan \theta}{\tan \theta} \quad x_{\text{exit}} \geq x_t$$

$$x_{\text{exit}} = \left\{ R_d^2 - (1 + R_d - \sqrt{\epsilon})^2 \right\}^{\frac{1}{2}} \quad x_{\text{exit}} < x_t$$

- 8) For conical nozzles, the internal axial print stations are computed using:

$$X_j = \frac{\sqrt{\text{ARPRNT}(j)} - r_t + x_t \cdot \tan \theta}{\tan \theta} \quad X_j \geq X_t$$

$$X_j = \left\{ R_d^2 - \left[ 1 + R_d - (\text{ARPRNT}(j))^{\frac{1}{2}} \right]^2 \right\}^{\frac{1}{2}} \quad X_j < X_t$$



- 9) The sum of input or selected species concentrations is checked for unity ( $\pm$  XMFTST, where XMFTST is an input number), and then normalized.
- 10) If the input parameter RZNØRM is input, the input contoured nozzle table is normalized by RZNØRM.

In addition to the above, the following are done in the ØDKINP routine.

- a) If the nozzle geometry has been input via the \$DATA namelist, ØDKINP stores the variables from this input into the correct locations and performs the appropriate unit conversions.
- b) Accepts the parabolic and circular arc options (IWALL=2 and 3) from the \$DATA namelist. This is done by computing the nozzle wall points and derivatives at 20 equally spaced points and substituting them into the tables used in the contoured wall input option.
- c) Accepts as input the quantities needed to calculate the zero particle lag flow equations.

5.3.18 SUBROUTINE ODWALL

This subroutine is called by subroutine ODKINP for the purpose of calculating the nozzle wall contour and setting print stations for ODK when the following wall options are used:

IWALL = 2	parabola,
IWALL = 3	circular arc,
IWALL = 6	skewed parabola

### 5.3.19 SUBROUTINE OUTPUT

This subroutine provides conversion from internal computational units to output engineering units and the calculation of performance parameters. The following output parameters are computed by this subroutine:

The pressure (in PSIA) is computed from:

$$P_{(\text{PSIA})} = P/4633.056$$

The gaseous species mole fractions are computed from:

$$C_{i,m} = \frac{R_i}{R} \cdot C_i$$

The gas molecular weight is computed from:

$$\text{Mw} = 49721.011/R$$

The percentage mass fraction change is computed from:

$$\% \Delta (\text{Mass Fraction}) = 100.0 \cdot \left(1.0 - \sum_{i=1}^n C_i\right)$$

The gas heat capacity is computed from:

$$C_{p_g} (\text{BTU/LB-}^\circ\text{R}) = 3.9969 \cdot 10^{-5} \cdot C_{p_g}$$

The gas enthalpy is computed from:

$$H_g (\text{BTU/LB}) = 3.9969 \cdot 10^{-5} \cdot \sum_{i=1}^n C_i \cdot h_i$$

At the throat, the characteristic exhaust velocity (ft/sec) is computed from:

$$C^* = \frac{P_c}{\rho^* \cdot V^*}$$

The vacuum specific impulse is computed from:

$$ISP_{VAC} = \frac{V + P/P_c \epsilon c^*}{g}, g = 32.174$$

The vacuum thrust coefficient is computed from:

$$C_{F_{VAC}} = \frac{I_{sp_{vac}} g}{C^*}$$

The percentage enthalpy change is computed from:

$$\% \Delta H_T = \frac{100 \cdot (HREF_c - HREF)}{V^2/2}$$

where

$$HREF = \sum_{i=1}^{NSP} C_i \cdot h_i + V^2/2$$

$HREF_c$  is HREF evaluated at the initial condition for the  $\emptyset DK$  integration (i.e. at the initial contraction ratio, ECRAT).

In addition the actual molecular weight of the mixture of gases and condensed phases is also printed out.

### 5.3.20 SUBROUTINE PACK

On the basis of those species currently being considered, this subroutine packs species and reaction information from the master tables into those control sections utilized by the one-dimensional kinetic expansion subprogram.

The following is a sequential description of the packing procedures:

- 1) Thermodynamic data for the species being considered is read into core storage.
- 2) The chemical species' molecular weights are computed
- 3) The symbolic reactions are checked for mass balance.
- 4) For a contoured nozzle the slope at each input wall point is computed using subroutine SLP. The wall coordinates, and each computed slope are printed for each input wall point and the print stations are set to the input axial coordinates.

In addition to the above, the PACK routine processes condensed phases by setting  $R_i=0$  for those species and storing pointers for up to 10 condensed phase species (5 pairs). This routine also calculates the print positions for specified area ratios when the contoured (spline) wall option is selected.

### 5.3.21 SUBROUTINE PACKCD (KRD, IPK, KNT)

This subroutine packs down a card image stored 80A1 in the KRD array by removing blanks. The packed card image is returned in the IPK array. The number of non blank characters found is returned in KNT.

### 5.3.22 SUBROUTINE PRATES

This subroutine processes the input reaction rate constant data to determine the form of the reaction rate. Three types of reactions are allowed, as shown in Table 5-5.

Table 5-5: EXPRESSIONS FOR THE REACTION RATE CONSTANTS, k

Reaction Expression	Input*	Comments
$k = P_1 T^{-P_2} e^{-P_3 * 1000/RT}$ <p>as above</p>	$A = P_1, N = P_2, B = P_3$ KF or KR = P <sub>1</sub> , P <sub>2</sub> , P <sub>3</sub>	Arrhenius form
$k = e^{(P_1 + P_2/T^{1/3} + P_3/T^{2/3})}$	KF or KR = *P <sub>1</sub> , P <sub>2</sub> , P <sub>3</sub>	Landau-Teller form
$\log_{10} k = P_1 + P_2 T$	KF or KR = % P <sub>1</sub> , P <sub>2</sub>	Log 10 form

\* P<sub>1</sub>, P<sub>2</sub>, and P<sub>3</sub> are numbers written with E or F format

### 5.3.23 SUBROUTINE PREAX

This subroutine processes the chemical reaction as determined by subroutine PRATES. It returns the stoichiometric coefficients and the corresponding species names.

### 5.3.24 SUBROUTINE PRES

This subroutine is used (when JPFLAG = 1) to compute the derivatives of an input pressure table.

This subroutine is also used (when JPFLAG = 0) to generate a pressure table through use of an average expansion coefficient, Ne. The generated table extends from the initial contraction ratio through the nozzle attachment point plus one normalized throat radius.

#### Input Pressure Table Derivative Computation (JPFLAG = 1)

If a pressure table of NTB entries is input, the table of first derivatives is computed using:

$$\left. \frac{dP}{dx} \right|_{x_1} = 0$$

$$\left. \frac{dP}{dx} \right|_{x_n} = \frac{P(x_{n+1}) - P(x_{n-1})}{x_{(n+1)} - x_{(n-1)}} \quad , \quad 1 < n < NTB$$

$$\left. \frac{dP}{dx} \right|_{x_{NTB}} = \frac{P(x_n) - P(x_{n-1})}{x_{(n)} - x_{(n-1)}} \quad , \quad n = NTB$$

The pressure at the initial axial position is obtained by interpolation using subroutine SPLN.

Internally Computed Pressure Table Computation (JPFLAG = 0)

An average equilibrium pressure expansion coefficient from the chamber to the throat,  $N_e$ , is computed by iteration using subroutine SUBNE. The initial value for  $N_e^{(1)}$  is 1.2.

The approximate equilibrium contraction ratio at the initial axial position is computed from:

$$a_c = \left[ \frac{N_e - 1}{2} \cdot \frac{\left[ \frac{2}{N_e + 1} \right]^{\frac{N_e + 1}{N_e - 1}}}{\left( \frac{P_i}{P_c} \right)^{\frac{2}{N_e}} \cdot \left[ 1 - \left( \frac{P_i}{P_c} \right)^{\frac{N_e - 1}{N_e}} \right]} \right]^{\frac{1}{2}}$$

where  $P_i$  = pressure at the initial axial position  
 $P_c$  = equilibrium chamber pressure

A check is then made to determine the compatibility between the nozzle geometry and the requested contraction ratio.

If

$$\sqrt{a_c} < 1 + [R_u + R_i] \cdot [1 - \cos \theta_1],$$

the circular arcs  $R_u$  and  $R_i$  overlap and the following error message is printed:

INLET GEOMETRY INCOMPATIBLE WITH INITIAL CONDITIONS

The program will proceed to the next case.



Tables for pressure and its derivatives are constructed as functions of area ratio,  $a$ , and expansion coefficient,  $N_e$ . Formula used for the  $j + 1$  iteration for pressure is:

$$\frac{P^{(j+1)}}{P_c} = \frac{P^{(j)}}{P_c} + 2 \left\{ \frac{N_e - 1}{N_e} \cdot \left[ 1 - \left( \frac{P^{(j)}}{P_c} \right)^{\frac{N_e - 1}{N_e}} \right]^{-1} \right. \\ \left. \left( \frac{P^{(j)}}{P_c} \right)^{-\frac{1}{N_e}} - \frac{2}{N_e} \cdot \left( \frac{P^{(j)}}{P_c} \right)^{-1} \right\}^{-1} \\ \cdot \left\{ \left[ \frac{N_e - 1}{2} \cdot \frac{[2/(N_e + 1)]^{(N_e + 1)/(N_e - 1)}}{\left( \frac{P^{(j)}}{P_c} \right)^{2/N_e} \cdot \left[ 1 - \left( \frac{P^{(j)}}{P_c} \right)^{(N_e - 1)/N_e} \right]} \right]^{-1/2} \cdot a^{-1} \right\}$$

for  $j = 1$

$$\left. \frac{P^{(1)}}{P_c} \right|_{x_{n+1}} = \left. \frac{P}{P_c} \right|_{x_n} + \left. \frac{d(P/P_c)}{dx} \right|_{x_n} (x_{n+1} - x_n)$$

where  $n$  refers to the  $n^{\text{th}}$  table entry.

The pressure derivative formula used is:

$$\frac{d(P/P_c)}{dx} = \left[ \frac{N_e - 1}{N_e} \left( \frac{P}{P_c} \right)^{-\frac{1}{N_e}} \left[ 1 - \left( \frac{P}{P_c} \right)^{\frac{N_e - 1}{N_e}} \right]^{-1} - \frac{2}{N_e} \left( \frac{P}{P_c} \right)^{-1} \right]^{-1} \cdot \frac{2}{a} \frac{da}{dx}$$

Next, tables for pressure and its derivatives are constructed by the program. Table entries are at increments of

$-x_1/75$  for  $x_1 < x < 0$

$(R_d \sin \theta) / 25$  for  $0 < x < R_d \sin \theta$

and

$1/25$  for  $R_d \sin \theta < x < R_d \sin \theta + 1$

where the initial nozzle axial position,  $x_1$ , is computed from:

$$x_1 = - \left[ (R_u + R_i) \cdot \sin \theta_i + \frac{\sqrt{a_c} - 1 - (R_u + R_i) \cdot (1 - \cos \theta_i)}{\tan \theta_i} \right]$$

See Figure 5-1 below:

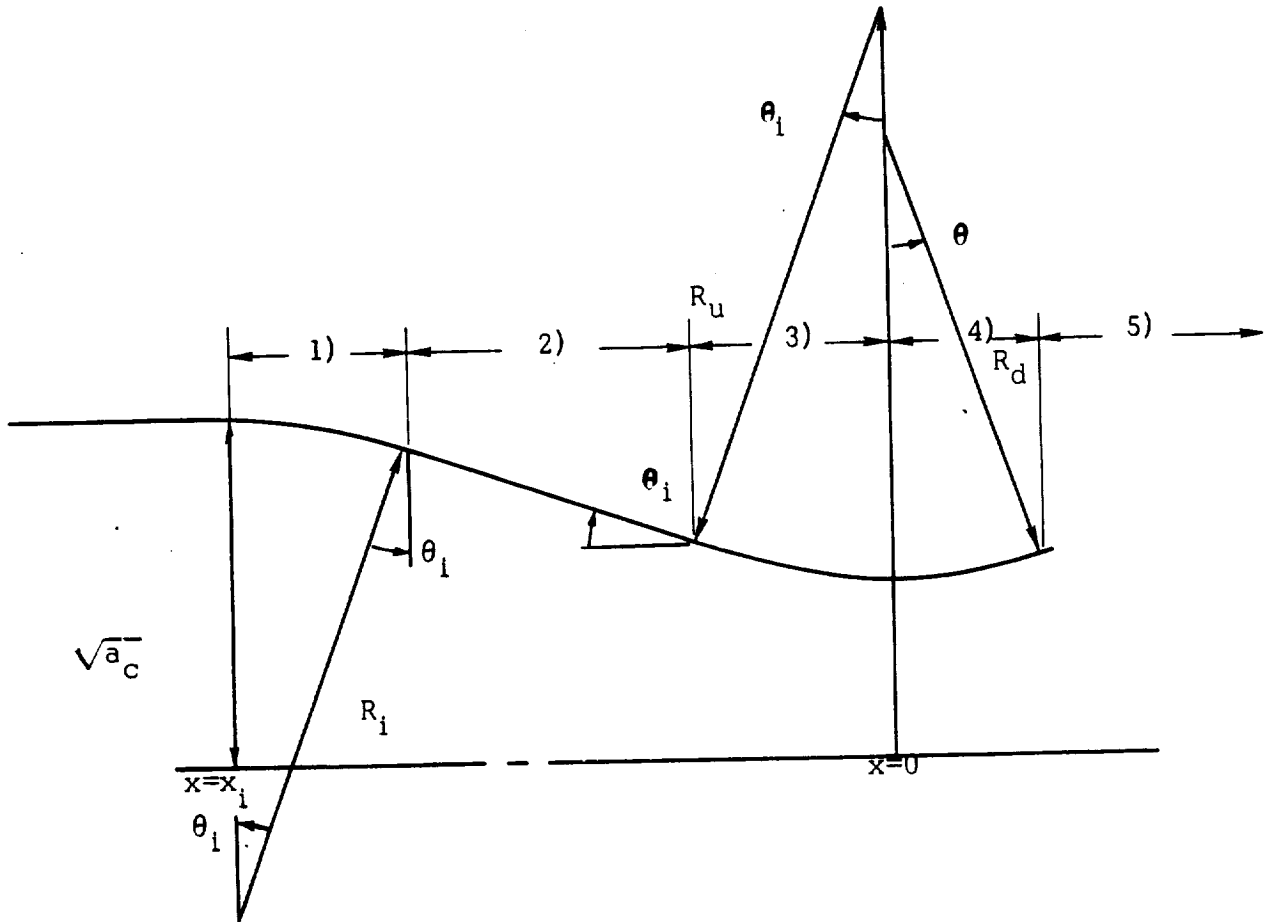


Figure 5-1 NOZZLE GEOMETRY

Area ratio and its derivative and  $(a \text{ and } \frac{da}{dx})$  are found by the five formulae below:

$$1) \quad x < x_i + R_i \sin \theta_i$$

$$a = \left[ \sqrt{a_c} - R_i \left( 1 - \sqrt{1 - \frac{(x-x_i)^2}{R_i^2}} \right) \right]^2$$

$$\frac{da}{dx} = \frac{-2(x-x_i)}{[R_i^2 - (x-x_i)^2]^{1/2}} \cdot \sqrt{a}$$

$$2) \quad x_i + R_i \sin \theta_i < x < -R_u \sin \theta_i$$

$$a = \left[ \sqrt{a_c} - R_i (1 - \cos \theta_i) - (x-x_i - R_i \sin \theta_i) \tan \theta_i \right]^2$$

$$\frac{da}{dx} = -2 \cdot \sqrt{a} \cdot \tan \theta_i$$

$$3) \quad -R_u \cdot \sin \theta_i < x < 0$$

$$a = \left[ 1 + R_u \left( 1 - \sqrt{1 - \frac{x^2}{R_u^2}} \right) \right]^2$$

$$\frac{da}{dx} = \frac{2x}{[R_u^2 - x^2]^{1/2}} \cdot \sqrt{a}$$

$$4) \quad 0 < x < R_d \cdot \sin \theta$$

$$a = \left[ 1 + R_d \left( 1 - \sqrt{1 - \frac{x^2}{R_d^2}} \right) \right]^2$$

$$\frac{da}{dx} = \frac{2x}{[R_d^2 - x^2]^{1/2}} \cdot \sqrt{a}$$

$$5) R_d \cdot \sin \theta < x \leq R_d \cdot \sin \theta + 1$$

for cone

$$a = \left[ r_t + (x - x_t) \cdot \tan \theta \right]^2$$

$$\frac{da}{dx} = 2 \cdot a \cdot \tan \theta$$

for contour

$$a = Y^2$$

$$\frac{da}{dx} = 2 \cdot Y \cdot \frac{dY}{dx}$$

Three special points are included in the pressure table. These are a point at  $x = x_1$  such that

$$\frac{P}{P_c} = \frac{P_i}{P_c}$$

$$\frac{d(P/P_c)}{dx} = 0$$

and two points at  $x = 0$  such that

$$\frac{P}{P_c} = \left( \frac{P^*}{P_c} \right) \text{ equilibrium}$$

$$\frac{d(P/P_c)}{dx} = - \frac{N_e}{\sqrt{R^*}} \cdot \left[ \frac{2}{N_e + 1} \right]$$

$$\frac{3N_e - 1}{2(N_e - 1)}$$

with  $R^* = R_u$  and  $R^* = R_d$ , respectively.

The following items are input directly to the computer program as described in Section 6 and shown in Figure 6-1, left to right.

$R_i$		RI
$R_u$		RWTU
$\theta_i$		THETA I
$\theta$		THETA
$R_d$		RWTD

### 5.3.25 SUBROUTINE PRNTCK

For the ODK option to print starting at step ND1, printing every ND3<sup>rd</sup> step up to step ND2, this subroutine checks whether or not the current step should be printed. If it is to be printed this subroutine calls subroutine OUTPUT.

### 5.3.26 SUBROUTINE REAXIN

This subroutine processes SPECIES, REACTIØNS, and THIRD BØDY REAX RATE RATIOØS input cards. Reference may be made to Section 6.5 for a complete description of input requirements. A table of all species appearing in the input reaction set is generated for further processing by subroutine SELECT if required.

### 5.3.27 SUBROUTINE SELECT

This subroutine provides the interface logic required to select the minimum species list required for the kinetic expansion calculations. The subroutine is only used for the ØDE-ØDK interface. The list of all species appearing in the input reaction set is matched against the list of species considered for the equilibrium calculation. All species which appear in both a reaction and the equilibrium calculation list are selected for the kinetic expansion calculation. If a species appears in the reaction set but has not been considered for the equilibrium calculation, the program prints an error message and terminates the current case.

If the INERTS directive was specified those species specified under that directive will be added to the list for the kinetic expansion calculation along with the other species selected.

If the INERTS directive was not specified, all those species, considered for the equilibrium calculation, whose mole fractions are greater than or equal to an input selection criterion will also be selected for the kinetic expansion calculation. Species selected in this way will be listed as inert species on the program output since they do not enter into chemical reaction.

This subroutine also selects pairs of condensed phases if either of the phases passes one of the above selection criteria.

#### 5.3.28 SUBROUTINE STF

This subroutine evaluates the thermodynamic functions  $C_{p,T}^{\circ}/R$ ,  $H_T^{\circ}/RT$ ,  $S_T^{\circ}/R$ , from curve fit coefficients. The subroutine uses the same procedure as subroutine CPHS. The additional functions  $d(C_{p,T}^{\circ})/dt$  and free energy,  $G_T^{\circ}/RT$ , are also computed. The calculated functions are then converted to the internal computational units for use by the kinetic expansion calculations. Also, low temperature thermodynamic data from tables are used when required if the LTCPHS directive was specified in the program input.

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### 5.3.29 SUBROUTINE STOICC

For each reaction this subroutine constructs two vectors of stoichiometric coefficients, one for reactants and one for products. Up to 10 reactants and 10 products may be considered for each reaction. The total number of entries in the resultant linear reaction table is 600, i.e., the sum of all stoichiometric coefficients can not exceed 600.

### 5.3.30 SUBROUTINE STORNU

The purpose of this subroutine is to store the stoichiometric coefficients into the ITABLE arrays in COMMON/CSP RXC/. The coefficients will be positive for reactant species and negative for product species.



5.3.31 SUBROUTINE SUBNE

Calculates the average equilibrium pressure expansion coefficient from the chamber to the throat by iteration from the following formula (Newton's method):

$$N_e^{(n+1)} = N_e^{(n)} + \frac{\left(\frac{2}{N_e^{(n)}+1}\right) \frac{N_e^{(n)}}{N_e^{(n)}-1} - \frac{P_e^*}{P_c}}{\left(\frac{2}{N_e^{(n)}+1}\right) \frac{N_e^{(n)}}{N_e^{(n)}-1} \left(\frac{1}{N_e^{(n)}-1}\right) \left[ \frac{1}{N_e^{(n)}-1} \ln \left(\frac{2}{N_e^{(n)}+1}\right) + \frac{N_e^{(n)}}{N_e^{(n)}+1} \right]}$$

where  $N_e^{(1)} = 1.2$ .

$P_e^*$  is the equilibrium throat pressure

$P_c$  is the equilibrium chamber pressure

This subroutine is used by subroutine PRES.

5.3.32

SUBROUTINE TABGEN (IFLAG, LTABLE,XTAB,YTAB,LUSED, X, Y,  
IERRØR, NY)

This subroutine records a tabular function (X,Y(NY)) in tables of fixed length. The first and last event will always be tabulated and the table will either contain all of the values specified or will be at least half full. Once the number of events exceed the table length, the table will be repacked by the deletion of every other table entry and tabulation will proceed choosing every  $2^N$ th event (N=0, 1, 2. . . etc., where N is the number of times the table must be repacked). The table spacing will be a power of two except for the last event which will always be tabulated.

The calling sequence parameters are:

- IFLAG - denotes type of entry to subroutine
  - = - 1 first entry
  - = 0 normal entry
  - = + 1 last entry
- LTABLE - length of tables available for tabulation
- XTAB - table for tabulation of the variable X
- YTAB - table for tabulation of the variable
- LUSED - number of table entries currently used (output)
- X - the variable X
- Y - the variable Y
- IERRØR - error flag
- NY - number of Y variables to be tabulated

Note: One Dimensional Mach Number Tabulation Procedure

At the initial axial position, X and Mach number are recorded. TABGEN is then used with LTABLE=50 (assuring 25 saved values). The last recorded values are the end values for the transonic tables.

#### 5.4 TRANS MODULE SUBROUTINES

The transonic flow module (TRANS) calculates the two-dimensional flow conditions in the throat region of the nozzle. It is used to obtain an initial data line for the MOC module. The analysis is based on a modification to the method of Sauer<sup>8</sup>. A detailed derivation and description of the method used is given in Reference 9. An abbreviated description of the method is presented in Section 2.4. Section 2.4 described how the method has been adapted to treat flows with variable mixture ratio.

The TRANS module consists of the following subroutines:

TRAN	GETILV
BANDI	NEWT
FCALC	PTAB
FINDT	SAUER
GETIL	TRIM

5.4.1 SUBROUTINE TRAN

This subroutine is the controlling program for the transonic calculations, and is used to construct an initial data line for the method of characteristics calculations. Subroutine TRAN reads the Namelist \$TRANS input as described in section 6. The calculations given below are performed by this subroutine. The method of analysis used is described in detail in reference

Transonic Calculations

From data supplied by the ODK subprogram expansion coefficients,  $\bar{\gamma}_n$ , are computed for each of N zones as

$$\bar{\gamma}_n = \frac{\ln(P_2/P_1)_n}{\ln(\rho_2/\rho_1)_n} \quad n = 1, \dots, N$$

The nomenclature for numbering zones and the slipline locations dividing the zones is given in Figure 5.2.

Slipline locations,  $Y_n$ , are calculated (using subroutine TRIM) as

$$\begin{bmatrix} (1 + A_1 K_1) & & & -1 \\ & -A_2 K_2 & & \\ & & (1 + A_2 K_2) & \\ & & & \ddots \\ & & & & -A_{N-1} K_{N-1} & (1 + A_{N-1} K_{N-1}) \end{bmatrix} \begin{bmatrix} Y_1^2 \\ Y_2^2 \\ \cdot \\ \cdot \\ \cdot \\ Y_{N-1}^2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 1 \end{bmatrix}$$

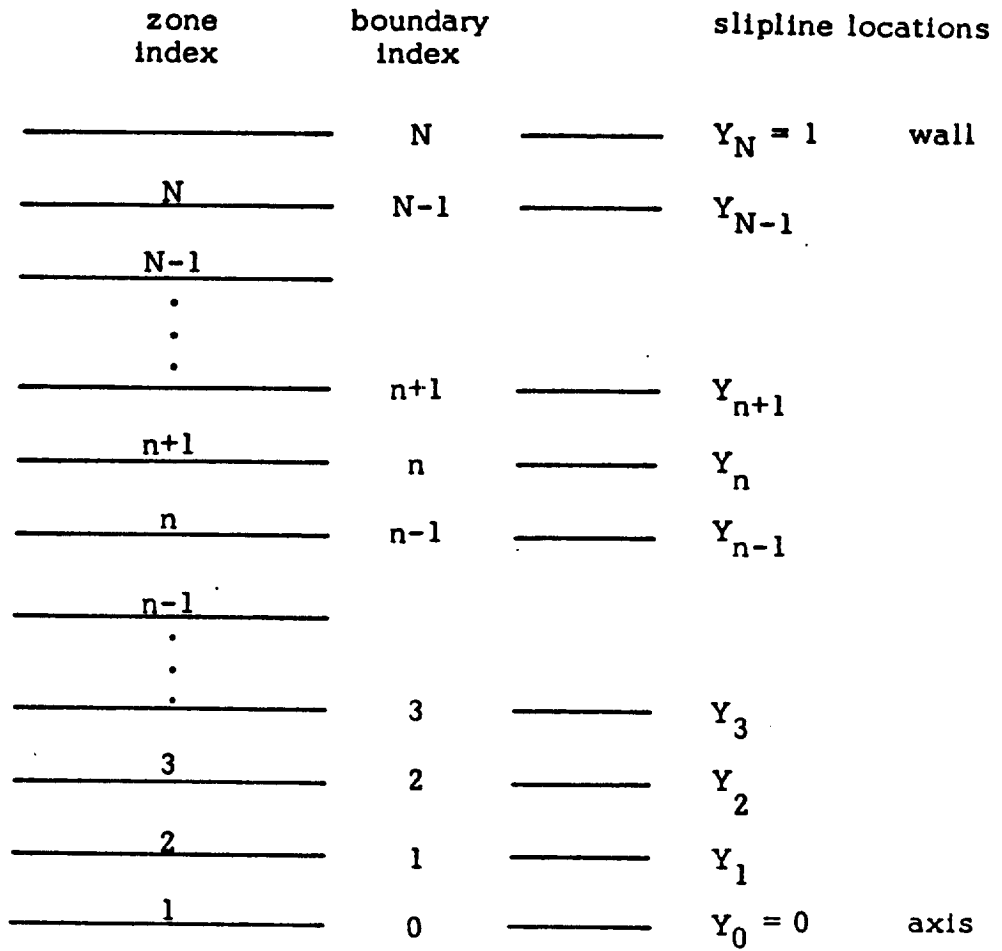


Figure 5-2: Nomenclature for the Numbering of Zones

where

$$A_n = \frac{\rho_n^* a_n^*}{\rho_{n+1}^* a_{n+1}^*}$$

$$K_n = \frac{\dot{m}_{n+1}}{\dot{m}_n}$$

$n = 1, 2, \dots, N-1$

The sonic conditions  $\rho_n^*$  and  $a_n^*$  are provided by the ODK subprogram and the partial mass flow rates,  $\dot{m}_n$ , are input.

Newton's method (subroutines NEWT and BANDI) is used to calculate the transonic coefficients  $B_{0_n}$ ,  $B_{1_n}$ ,  $C_{1_n}$ , and  $C_{2_n}$ . Subroutine FCALC evaluates the boundary conditions which must be satisfied.

#### Distribution of Initial Line Points

Subroutine TRAN next calculates the location of points on the initial data line used to start the method of characteristics calculations. First the radial position coordinates,  $r_i$ , are computed. A sinusoidal distribution of the following form is used:

$$r_i = \left\{ r_w \sin \left( \frac{1}{N} \frac{\pi}{2} \right) \right\}^{\epsilon_1} \quad i = 0, 1, 2, \dots, N$$

where

- N is the number of points on the initial line before editing.
- $\epsilon_1$  is an exponent used for modifying the distribution function. Ordinarily a value of 1.2 is used.
- $r_w$  is the radial coordinate at which the initial data line intersects the wall.

The values computed for  $r_i$  are then edited to prevent locating points too close to sliplines, or too close to the wall. Some of the editing procedures can be controlled by input, as described in Section 6.6.

The axial coordinate positions,  $z_i$ , are then computed. First, a value of  $z_{axis}$  is found such that the Mach number at  $r = 0, z = z_{axis}$  is the same as at the point  $r_w, z_w$ . The values of  $z_i$  are located on a parabola as follows:

$$z_i = z_w + \left( (r_w - r_i) / r_w \right)^2 * (z_{axis} - z_w)$$

where  $z_{axis}$  is located on the axis half way between the sonic point and the point with a pressure equal to the pressure at the wall at  $r=0$ .

With  $r_i$  and  $z_i$  determined the transonic analysis is used to obtain corresponding values of pressure and flow angle. Using pressure as an independent variable, the flow tables computed by ODK (ODE if the TDE option used) are searched and values of  $\rho$ ,  $V$ ,  $T$ , and chemical species concentrations are obtained by interpolation. Subroutine GETIL is called for this purpose when one or more zones of constant mixture ratio are used, and subroutine GETILV is called when a variable mixture ratio is used.

Once constructed, the initial data line is integrated to obtain the nozzle flow coefficient  $C_D$ , where

$$C_D = \dot{m}_{2D} / \dot{m}_{1D}$$

and the result is printed.

Subroutine PTAB is called to write a table of boundary layer edge conditions for the results obtained up to the initial data line. This file is written on unit LUBLM and is continued later by subroutine PRINT as further values are computed using the MOC. If edge conditions for BLIMP-J are to be prepared, they are written on unit 50.



5.4.2 SUBROUTINE BANDI (A, NBW, NEQ, NMAX, B, X, INEW, KERR)

Purpose

BANDI solves a set of linear equations  $Ax = b$  where A is a nonsymmetric band matrix.

Restrictions

The matrix A is destroyed.

Usage

Calling sequence:

CALL BANDI (A, NBW, NEQ, NMAX, B, X, INEW, KERR)

where

A is a matrix of at least NEQ rows and NBW columns (see below) which initially contains the elements of the band matrix, stored as follows:

To solve a system of the form

$$\begin{array}{rcl}
 a_{11}x_1 + a_{12}x_2 & & = b_1 \\
 a_{21}x_1 + a_{22}x_2 + a_{23}x_3 & & = b_2 \\
 & a_{32}x_2 + a_{33}x_3 + a_{34}x_4 & = b_3 \\
 & & a_{43}x_3 + a_{44}x_4 + a_{45}x_5 & = b_4 \\
 & & & a_{54}x_4 + a_{55}x_5 & = b_5
 \end{array}$$

To transform an original (N by M) MATRIX A(I, J) into a packed (N by NBW) BANDED MATRIX AB (I, J), the following transformation applies.

$$AB(I, JB) = A(I, J)$$

where  $JB = \left(\frac{NBW}{2} + 1\right) - (I - J)$

and  $NBW = \text{BAND WIDTH}$

	$A_{1,1}$	$A_{1,2}$	$A_{1,3}$
$A_{1,j}$	0.0	$a_{11}$	$a_{12}$
$A_{2,j}$	$a_{21}$	$a_{22}$	$a_{23}$
$A_{3,j}$	$a_{32}$	$a_{33}$	$a_{34}$
$A_{4,j}$	$a_{43}$	$a_{44}$	$a_{45}$
$A_{5,j}$	$a_{54}$	$a_{55}$	0.0

- NBW** is the width of the band (odd).
- NEQ** is the number of equations in the system.
- NMAX** is the maximum number of rows for which A has been dimensioned.
- B** is the right-hand vector for the system.
- X** is the solution vector returned by BANDI.
- INEW** is a flag, set = 0 unless the coefficient matrix A is unchanged from a previous call to BANDI, in which case set INEW = 1.
- KERR** is an error flag returned by BANDI:  
 = 0 if no error;  
 = 1 if any diagonal element becomes zero during triangularization of A.

### Method

BANDI finds the solution vector X by single-pass Gaussian elimination. If INEW = 0, the coefficient matrix A is upper-triangularized by forward substitution. Backward substitution then yields the solution X. If INEW = 1, BANDI assumes that the coefficient matrix A has already been reduced on a previous entry and that only the right-hand vector B has changed. Therefore, the forward substitution is bypassed.

### Programming Information

Note that the matrix A is upper-triangularized by BANDI, destroying the original band matrix coefficients. For very large or ill-conditioned systems, one may increase the accuracy of the solution as follows:

- 1) Save the original band matrix coefficients from A in a similar matrix AP.
- 2) Call BANDI with INEW = 0 to obtain a solution  $x_0$  of  $Ax = b$ .
- 3) Calculate  $b_n = Ax_n$  using the coefficients saved in AP. (A subroutine BMMULT exists to do this.)
- 4) Calculate a new right-hand vector  $e_n = b - b_n$ .
- 5) Call BANDI with INEW = 1 to solve the system  $A\delta x_n = e_n$ .
- 6) Set  $x_{n+1} = x_n + \delta_n$ .
- 7) Repeat steps 3-6 until the desired convergence is attained.

### Error Return

If, during triangularization of the matrix, any diagonal element becomes zero, an appropriate message is printed and KERR is set to unity before returning to the calling program.

### 5.4.3 SUBROUTINE FCALC

The purpose of this subroutine is the evaluation of boundary condition functions required to be zero by the transonic analysis. Subroutine FCALC is called by subroutine NEWT in which Newton's Method is used to find the zeros.

Input:

$Y_n$  slipline heights  $n = 1, \dots, N - 1$

$\gamma_n$  specific heat ratio for each zone  $n = 1, \dots, N$

$B_{0_n}, B_{1_n}, C_{1_n}, C_{2_n}$  estimates for the constant coefficients sought by NEWT to satisfy the boundary conditions  $n = 1, \dots, N$

$N$  total number of zones

Output:

The values of the following functions are computed and output. If the boundary conditions are correctly satisfied, each of these ( $F_{1_n}, F_{2_n}, F_{3_n}, F_{4_n}$ ) are zero.

At the sliplines,  $n = 1, \dots, N - 1$

linear term  $v_n = v_{n+1}$  (i.e. match on streamline angle, 1st order);

$$F_{1_n} = \left[ \frac{1}{2} (\gamma_n + 1) B_{1_n}^2 Y_n + C_{1_n} Y_n^{-1} \right] - \left[ \frac{1}{2} (\gamma_{n+1} + 1) B_{1_{n+1}}^2 Y_n + C_{1_{n+1}} Y_n^{-1} \right]$$

constant term  $v_n = v_{n+1}$ ;

$$F_{2_n} = \left[ \frac{1}{16} (\gamma_n + 1)^2 B_{1_n}^3 Y_n^3 + \frac{1}{2} (\gamma_n + 1) B_{1_n} C_{1_n} Y_n \left( \ln Y_n - \frac{1}{2} \right) \right. \\ \left. + \frac{1}{2} (\gamma_n + 1) B_{1_n} B_{0_n} Y_n + C_{2_n} Y_n^{-1} \right] \\ - \left[ \frac{1}{16} (\gamma_{n+1} + 1)^2 B_{1_{n+1}}^3 Y_n^3 + \frac{1}{2} (\gamma_{n+1} + 1) B_{1_{n+1}} C_{1_{n+1}} Y_n \left( \ln Y_n - \frac{1}{2} \right) \right. \\ \left. + \frac{1}{2} (\gamma_{n+1} + 1) B_{1_{n+1}} B_{0_{n+1}} Y_n + C_{2_{n+1}} Y_n^{-1} \right]$$

linear term  $P_n = P_{n+1}$  ;

$$F_{3_n} = \gamma_n B_{1_n} P_n^* - \gamma_{n+1} B_{1_{n+1}} P_{n+1}^*$$

constant term  $P_n = P_{n+1}$  ;

$$F_{4_n} = \left\{ \gamma_n \left[ \frac{1}{4} (\gamma_n + 1) B_{1_n}^2 Y_n^2 + C_{1_n} \ln Y_n + B_{0_n} \right] - 1 \right\} P_n^* \\ - \left\{ \gamma_{n+1} \left[ \frac{1}{4} (\gamma_{n+1} + 1) B_{1_{n+1}}^2 Y_n^2 + C_{1_{n+1}} \ln Y_n + B_{0_{n+1}} \right] - 1 \right\} P_{n+1}^*$$

At the wall ,  $n = N$

linear term  $v_N(1, z) = z$  ;

$$F_{1_N} = \frac{1}{R} - \left[ \frac{1}{2} (\gamma_N + 1) B_{1_N}^2 + C_{1_N} \right]$$

constant term  $v_N(1, z) = z$  ;

$$F_{2_N} = \left[ \frac{1}{16} (\gamma_N + 1)^2 B_{1_N}^3 - \frac{1}{4} (\gamma_N + 1) B_{1_N} C_{1_N} \right. \\ \left. + \frac{1}{2} (\gamma_N + 1) B_{1_N} B_{0_N} + C_{2_N} \right]$$

Since at the axis  $v_1(0, z) = 0$  it is required that  $C_{1_1} = C_{2_1} = 0$ .

#### 5.4.4 SUBROUTINE FINDT

This subroutine is called by subroutine GETILV to read unit 16, which is a direct access file containing flow properties computed by ODK. Values are found from the file as a function of the input pressure, and values at the pressure are obtained from these by linear interpolation.

#### 5.4.5 SUBROUTINE GETIL (IZ, IP, PPSI)

If one or more zones of constant mixture ratio are to be used, then this subroutine generates the initial data entries for the MOC module. The values are obtained using subroutine SPLIN for interpolation in the gas tables generated by the One Dimensional Kinetic module. The values obtained are  $\rho$ ,  $V$ ,  $T$ , and the chemical species concentrations. The values used for interpolation are read from unit KSTF1.

#### 5.4.6 SUBROUTINE GETILV

If variable mixture ratio is to be used, then this subroutine generates initial data line entries for the MOC module. Values are obtained as a function of pressure using subroutine FINDT. The method described in Section 2.4.4 is used to obtain values at each initial data line point.

#### 5.4.7 SUBROUTINE

NEWT(M, F, MF, N, VAR, NVAR, FCALC, WF, PERTV, EPS1, MAXIT, NUMIT, BIN, AB, NBW, KERR)

Given a set of  $n$  functions in  $n$  unknown variables where each function is coupled as below:

$$\begin{aligned} f_i(X_j) & & i = 1, \dots, n \\ & & j = i-k, \dots, i+k \\ & & \text{and } 1 \leq j \leq n \end{aligned}$$

this routine will attempt by Newton's method to find values

$$X_1, X_2, \dots, X_n$$

such that

$$\sum_{i=1}^n f_i^2(X_j) = 0.$$

#### Method

Newton's method is used to iterate for a solution vector. The matrix of partial derivatives,  $J$ , required by the method is generated automatically by the subroutine. This matrix will be banded of width  $2k+1$ . The matrix inversion is performed by subroutine BANDI. In the event Newton's method yields a vector which is farther from a solution in a least squares sense than the previous estimate, the increment vector is halved. Newton's algorithm for the  $(k+1)^{\text{th}}$  iterant is:

$$X^{(k+1)} = X^{(k)} - J^{(k)^{-1}} f^{(k)}.$$

#### Restrictions

The user must supply initial values for the solution vector and also a subroutine to evaluate the functions. The subroutine must communicate with NEWT through COMMON statements. Subroutine BANDI is required.

## Usage

Call NEWT(M, F, MF, N, VAR, NVAR, FCALC, WF, PERTV, EPS1, MAXIT, NUMIT, NUMIT, BIN, AB, NBW, KERR)

### Index to Calling Sequence:

Input: M, MF, N, VAR, NVAR, WF, PERTV, EPS1, MAXIT, NBW  
Output: VAR, F, NUMIT, KERR  
Working: BIN, AB

### Explanation of Calling Sequence:

- 1) M is the length of the array containing the n functions.
- 2) F is the array containing the n function values evaluated by FCALC.
- 3) MF is an array of M control words:  
if MF(I)=0, include F(I)  
if MF(I)=1, exclude F(I)
- 4) N is the length of the array containing the n variables.
- 5) VAR is the array containing the n variables,  $x_i \quad i = 1, \dots, n$
- 6) NVAR is an array of N control words:  
if NVAR(J)=0, include VAR(J)  
if NVAR(J)=1, exclude VAR(J)
- 7) FCALC is a name for the subroutine which calculates the functions, F(I). A program which calls NEWT must have an EXTERNAL statement containing this name.
- 8) WF is an array of n weighting factors. These are used in conjunction with EPS1 to determine whether a solution has been reached.

$$\omega_i = WF(I)$$

- 9) PERTV is a perturbation factor used in calculating the partial derivatives required by Newton's method. If  $PERTV = \epsilon$ , then:

$$\frac{\partial F}{\partial x} = \frac{F(x + \delta) - F(x)}{\delta}, \text{ where } \delta = \max(|\epsilon x|, \epsilon * 10^{-3})$$



- 10) EPS1 is an error bound used to determine whether a solution has been reached. If  $\epsilon_1 = \text{EPS1}$ , then a solution is claimed when

$$\sum_{i=1}^n (\omega_i F_i)^2 \leq \epsilon_1$$

- 11) MAXIT is the maximum number of iterations allowed.
- 12) NUMIT is the number of iterations required for solution.
- 13) BIN is an array required by LESK and must be at least of dimension  $N + 1$ .
- 14) AB is a two-dimensional array containing the augmented matrix of subroutine LESK and must be at least of dimension  $AB(M, N+1)$ .
- 15) NBW band width =  $2k+1$ , see subroutine BANDI.
- 16) KERR error indicator, see subroutine BANDI.

#### 5.4.8 SUBROUTINE PTAB (PØNED)

This subroutine is used to write a table of boundary layer edge conditions for the results obtained up to the initial data line for the MOC. Unit LUBLM is used for passing this data to BLM. If edge conditions for BLIMP-J are to be prepared, they are written on unit 50 (i.e., IPTAB = 1 in \$ODE, see Section 6.4.3.2.).

The following procedure is followed to make the one-dimensional throat coincident with the axisymmetric throat.

- 1) The pressure,  $P_{1D}$ , at the axisymmetric throat ( $r=1, x=0$ ) must be given (PØNED in the calling sequence above).
- 2) The axial position,  $x^*$ , in the one-dimensional gas tables corresponding to the above pressure is obtained by interpolation. The points downstream of this axial position are deleted.
- 3) The table of axial positions (saved in the one-dimensional calculations - TABGEN) is reCOORDINATED to fit smoothly with the axisymmetric geometry using:

$$x' = x_1 + (x - x_1) \left( \frac{-x_1}{x^* - x_1} \right)$$

where

- $x'$  = reCOORDINATED axial position
- $x$  = tabulated axial position
- $x_1$  = initial axial position
- $x^*$  = axial position from 2) above

- 4) The radial coordinate, corresponding to each re-coordinated axial coordinate, is computed using the input geometric constraints. Reference may be made to Figure 6-1 for a description of the inlet and throat geometry.
- 5) The axial and radial coordinates and the fluid properties are punched. The punched cards may be input directly to the boundary layer computer program.

#### 5.4.9 SUBROUTINE SAUER (R, X, Y, G, N, I, PPS, THETA)

The purpose of this subroutine is to compute fluid dynamic properties in the transonic region of a rocket nozzle. The method used is based on the analysis of Sauer and is applicable to the situation where the flow is assumed divided into N zones (i.e. striated), each of which is characterized by a constant expansion coefficient,  $\gamma_n$ . The analysis has been further modified so as to extend its range of applicability to nozzles with small ( $R/r^* \geq .5$ ) radius of curvature in the throat section.

Given position coordinates  $(r, x)$ , this subroutine returns the fluid dynamic properties  $(P/P^*, \theta)$ .

#### Calling Sequence

##### Input;

R	radial position coordinate, r
X	axial position coordinate, x
Y	vector $Y_n$ ; $n = 1 \dots N$ containing the zone boundary coordinates
G	vector $\gamma_n$ ; $n = 1, \dots, N$ containing the zone expansion coefficients
N	total number of zones

##### Output

I	zone number, n, corresponding to r
PPS	$P/P^*$ at $(r, x)$
THETA	$\theta$ at $(r, x)$ , the gas streamline angle in radian

#### Method

$$R' = R + \frac{\gamma}{4}$$

$$X = \left(\frac{R}{R'}\right)^{1/2} x$$

If only one zone is specified ( $N = 1$ ), then

$$u' = \frac{1}{4} (\gamma + 1) B_1^2 r^2 + B_0 + B_1 X$$

$$v' = \frac{1}{16} (\gamma + 1)^2 B_1^3 r^3 + \frac{1}{2} (\gamma + 1) B_1 B_0 r + \frac{1}{2} (\gamma + 1) B_1^2 r x$$

where

$$B_1^2 = \frac{2}{(\gamma + 1)} \frac{1}{R'}$$

$$B_0 = -\frac{1}{4} \frac{1}{R'}$$

If more than one zone is specified ( $N \geq 2$ ), then

$$u' = \frac{1}{4} (\gamma + 1) B_1^2 r^2 + C_1 \ln r + B_0 + B_1 X$$

$$v' = \frac{1}{16} (\gamma + 1)^2 B_1^3 r^3 + \frac{1}{2} (\gamma + 1) B_1 C_1 r (\ln r - \frac{1}{2}) \\ + \frac{1}{2} (\gamma + 1) B_1 B_0 r + C_2 r + \left[ \frac{1}{2} (\gamma + 1) B_1^2 r + C_1/r \right] x$$

where the coefficients  $B_0, B_1, C_1, C_2$  are input through COMMON/NAMBC/ and the  $n^{\text{th}}$  value is selected, corresponding to the  $n^{\text{th}}$  zone. The zone,  $n$ , is determined such that

$$Y_{n+1} \geq r \geq Y_n$$

For all  $N$

$$u = 1 + u'$$

$$v = v'$$

$$P/P^* = 1 - \gamma_n u'$$

$$\theta = \arctan (v/u)$$

### 5.4.10 SUBROUTINE TRIM (A, X, B, N, NN)

This subroutine solves the system

$$\bar{A}\bar{X} = \bar{b}$$

for  $\bar{X}$  where  $\bar{A}$  is tridiagonal, i. e.;

$$\text{all } a_{ij} = 0 \text{ if } i > j+1 \text{ or } i < j-1.$$

The method used is Gaussian elimination.

#### Calling Sequence

- A Is the input coefficient matrix and must be dimensioned at least A(N, 3). The elements  $a_{ij}$  must be input as

$$\begin{bmatrix} - & A(1,2) & A(1,3) \\ A(2,1) & A(2,2) & A(2,3) \\ A(3,1) & A(3,2) & A(3,3) \\ & \cdot & \\ & \cdot & \\ & \cdot & \\ & \cdot & \\ A(N,1) & A(N,2) & - \end{bmatrix} = \begin{bmatrix} - & a_{11} & a_{12} \\ a_{21} & a_{22} & a_{23} \\ a_{32} & a_{33} & a_{34} \\ & \cdot & \\ & \cdot & \\ & \cdot & \\ & \cdot & \\ a_{n,n-1} & a_{nn} & - \end{bmatrix}$$

The contents of A will be destroyed by TRIM.

- X Is the output solution vector  $\bar{X}$  and must be dimensioned at least X(N).
- B Is the input vector  $\bar{b}$  and must be dimensioned at least B(N). The contents of B will be destroyed by TRIM.
- N Is the order of the system.  $N \geq 2$  is required.
- NN Is the dimension of A (NN, 3), X(NN), and B(NN) in the calling program.

## 5.5 MOC MODULE SUBROUTINES

The Method of Characteristics (MOC) module is used to calculate the loss in nozzle performance caused by flow divergence, including the effects of chemistry and mixture ratio variation. The effect of shock waves can also be calculated. Obtaining an accurate nozzle performance prediction usually requires a closely spaced characteristics mesh. In order to allow both shock waves and a fine mesh, random access files are used for storing and retrieving mesh point information.

The TDK module consists of the following subroutines:

TDK	INSRT
ATSHCK	INTEXT
AXISPT	ITER1
CHAR	ITER2
CHECK	ITER3
CKEXIT	MLCK
CKSHCK	MRCK
CNTRL	MRCK1
CNTRL1	NESK
CNTRL2	PRINT
CNTR12	PRINTS
CNTR13	SAVPT
CNTR14	SCK
CNTR16	SDERIV
CNTR21	SETID
CNTR31	SHCKA
CNTR91	SHCKA1
CRIT	SHCKL
CUBIC	SHCKR
DSPT	SHCKW
EF2D	SHCKW1
ENCALC	SHØCK
ERRØRZ	SINT
FTHRST	SUBIL
GETPT	SUBILR
GPF	TCALC
GPFKIN	THERM
GPFPG	TSTDK
INPT	TWØD
INPTR	WALL
INPTRS	WLCALC
INPTR1	WLPT
INPTS	



### 5.5.1 SUBROUTINE TDK

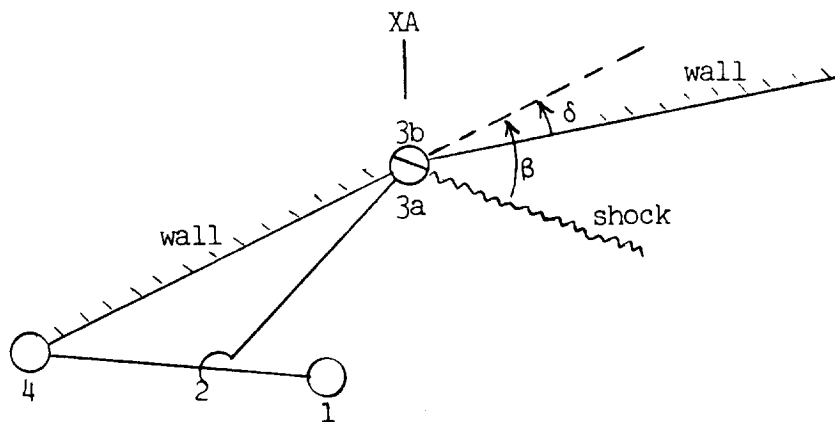
This subroutine is called by subroutine MAIN and is the driver for the MOC module. It performs the functions described below.

First, the MOC mesh point arrays P, PP, Q, Q3A, and Q4A, are initialized to zero. If the TDE option is to be executed, then the equilibrium gas properties tables described in Section 2.5.2 are converted to the system of units used internally by the MOC module and are stored for its use. Subroutine CHAR is then called to read the \$MOC Namelist input, and perform all calculations that are preliminary to the MOC construction.

If the MOC construction is to ignore shocks (SHOCK=0 IN \$MOC), then subroutine CNTRL is called, otherwise subroutine CNTRL91 is called.

## 5.5.2 SUBROUTINE ATSHCK

This subroutine calculates an attached shock point at axial position  $XA$  on the nozzle wall. Properties on the upstream side of the shock are calculated at point 3a. Values used in the calculation of point 3a are from the known points 4 and 1. Properties on the downstream side of the shock are then calculated at point 3b. Point 3b is found by solving the shock relations given the upstream conditions at point 3a and a streamline deflection angle equal to the change in wall angle at position  $XA$ .



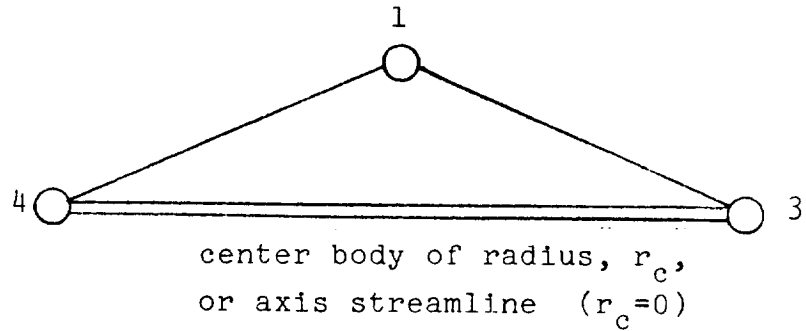
The procedure consists of 4 steps, as follows:

- 1) Locate point 2 on the RRC 4-1 such that the LRC from point 2 reaches the wall at  $XA$ .
- 2) Using point 2 and point 4, calculate values at point 3a.
- 3) Iterate step 1 and 2 until the point 3a properties converge.
- 4) Find the shock angle,  $\beta_3$ , corresponding to the upstream conditions at point 3a and a streamline deflection angle equal to the change in wall angle at position  $XA$ .

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5.5.3 SUBROUTINE AXISPT

This subroutine calculates an axis point (or point on a center body of radius,  $r_c$ ) using the known points 4 and 1.



Points 1 and 4 are known points and point 3 is the unknown point to be computed. At point 3:

$$r_3 = r_c$$

and

$$\theta_3 = 0.$$

Initial estimates for values at point 3 are:

$$A_3 = A_4, \beta_3 = \beta_4, \alpha_3 = \alpha_4, \gamma_3 = \gamma_4$$

and

$$G_3 = G_1$$

$$A_3 G_3 H_3 = A_1 G_1 H_1$$

$$G_3 H_3 = G_1 H_1$$

The axial location of point 3 is calculated from

$$x_3 = x_1 + \frac{r_c - r_1}{\tan 1/2(\theta_1 - \alpha_1 - \alpha_3)}$$

The flow properties at point 3 are calculated from

$$P_3 = P_1 + \frac{P_3 + P_1}{2} \left\{ \frac{1}{2} [-A_1 G_1 H_1 - A_3 G_3 H_3 + (G_1 H_1 + G_3 H_3) \frac{\sin \theta}{r_1}] (x_3 - x_1) - \frac{1}{2} (G_1 + G_3) \theta_1 \right\}$$

$$\rho_3 = \rho_4 \left[ \frac{P_3}{P_4} \right]^{\frac{1}{2} \left[ \frac{1}{\gamma_4} + \frac{1}{\gamma_3} \right]} \exp \left\{ - \frac{1}{2} [A_4 + A_3] [x_3 - x_4] \right\}$$

$$T_3 = T_4 \left[ \frac{P_3}{P_4} \right]^{\frac{1}{2} \left[ \frac{1}{\gamma_4} + \frac{1}{\gamma_3} \right]} \exp \left\{ - \frac{1}{2} (B_4 + B_3) (x_3 - x_4) \right\}$$

For the 1st iteration (all iterations if constant  $\gamma$  option):

$$V_3 = \left\{ V_4^2 - 4 (P_3 - P_4) / (\rho_3 + \rho_4) \right\}^{\frac{1}{2}}, \text{ Bernoulli Equation}$$

For subsequent iterations (calculated in GPFKIN or GPFPG):

$$V_3 = \left\{ 2(H_t - \sum c_i h_i) \right\}^{\frac{1}{2}}, \text{ Energy Equation}$$

The above equations are iterated ( $i=1, \dots$ ) until  $x_3$ ,  $P_3$ ,  $\rho_3$ ,  $T_3$ , and  $V_3$  converge to the required accuracy.

Throughout the method of characteristics computations the variables used are equivalenced to entries in dimensioned arrays. This equivalency of variables is always in the same order as prescribed in Table 5-6. This equivalencing occurs for the I subscript in the following arrays: P(I,J), PP(I,J), PS(I), PSS(I), Q(I,J), Q3A(I), and Q4A(I).

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TABLE 5-6 EQUIVALENCE TABLE FOR MOC VARIABLES

I	Variable	Units
P(1,J)	P, pressure	lb f/ft <sup>2</sup>
2	ρ, density	lb m/ft <sup>3</sup>
3	θ, streamline angle	radians
4	V, velocity	ft/sec
5	r, radial coordinate	
6	x, axial	° R
7	T, temperature	
8	A, term computed in subroutine GPF	
9	B, " " " " "	
10	C, " " " " "	
11	D, " " " " "	
12	Stream function (0 at axis, 1 at wall)	
13	F, term computed in subroutine GPF	
14	G, " " " " "	
15	H, " " " " "	
16	α, " " " " "	
17	γ, " " " " "	
18	dividing streamline flag	
19	zone number	
20	point ID no. in direct access file	
21	β, shock angle	
22	point type (axis, interior, etc.)	
23	Mach no.	
24	ID no. of previous streamline pt.	
25	ID no. of previous pt. on the char.	
26	ID no. of next pt. on the char.	
27	ID no. of pt. on the other side of shock	
28-30	not used currently	
31	c <sub>1</sub> , mass fraction of species 1	
.	.	
.	.	
.	.	
60	c <sub>60</sub> , mass fraction of species 60	

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#### 5.5.5 SUBROUTINE CHECK (NØ)

This subroutine compares current and previous values of the flow variables  $P_3$ ,  $\rho_3$ ,  $\theta_3$ ,  $V_3$ ,  $r_3$ ,  $x_3$ , and  $T_3$  for relative convergence by calling subroutine CRIT. As soon as a variable is encountered failing the test, the variables are updated one iteration and the program returns with the convergence flag set as failed ( $NØ = 1$ ). If convergence is achieved the variables are updated one iteration and the subroutine returns with the convergence flag set as passed ( $NØ = 0$ ).

#### 5.5.6 Subroutine CKEXIT (P, EFLAG)

This subroutine checks if a point, P, is outside the nozzle by comparing the axial location, Z, against the nozzle length, ZEXIT.

If  $Z \geq ZEXIT * 1.03$ , then set  $EFLAG = 2$ .

If  $ZEXIT * 1.03 > Z \leq ZEXIT$ , then set  $EFLAG = 1$ .

#### 5.6.7 Subroutine CKSHCK (SFLAG)

This subroutine checks for a crossing of right-running characteristics, which determines the start point of a right-running shock wave. The shock flag, SFLAG, is set to 1 when a crossing has occurred, or will occur at the next point.



### 5.5.8 SUBROUTINE CNTRL

The purpose of this subroutine is to control the construction of the finite difference mesh for the method of characteristics solution of the supersonic nozzle flow when the LRC method is used (SHOCK=0 in \$MOC). Left running characteristics and fluid streamlines are constructed starting at the nozzle throat point ( $r = 1, x = 0$ ). These left running characteristics extend from the initial data line or nozzle axis to the wall. The mesh points are calculated by subroutines INPT, AXISPT, WLPT and DSPT under control of this subroutine.

Additional points are inserted in the mesh by subroutine CNTRL by property averaging using subroutine INSRT. The circumstances which cause point insertion are listed below. In each case a point is inserted along the initial line or the previous streamline and the calculation of point 3 is repeated:

- 1) If subroutine INPT or DSPT find point 1 to fall beyond the nozzle wall.
- 2) If subroutine INPT finds point 1 to fall above a dividing streamline point.
- 3) If subroutine INPT or DSPT find

$$|\theta_1 - \theta_4| > \Delta\theta_{tw}, \text{ input item DTWI}$$

- 4) If a wall point on the circular arc immediately downstream of the throat is calculated such that

$$|\theta_3 - \theta_4| > \Delta\theta_{wc}, \text{ input item DWCI}$$

or if a wall point between the circular arc and the nozzle exit point is calculated such that

$$|\theta_3 - \theta_4| > \Delta\theta_w, \text{ input item DWI}$$

- 5) When iterating to locate the end of the nozzle wall. (Input tolerance of EPW).
- 6) If subroutine AXISPT, INPST, DSPT, or WLPT locate point 3 such that its distance from point 4 is greater than input item DS times the square root of the Mach number.

At the end of each completed characteristic surface the mesh points are examined and points discarded as described below. Only interior points (ID=2) are to be discarded.

For  $n = 2$  to  $n = \text{IPPW}-1$ , (i.e., from the initial line or axis to the wall) discard point  $n$  if

$$|\theta_{n-1} - \theta_n| + |\theta_{n+1} - \theta_n| < \epsilon_\theta^2$$

and

$$(r_{n-1} - r_n)^2 + (z_{n-1} - z_n)^2 < \epsilon_s^2$$

where  $\epsilon_\theta$  and  $\epsilon_s$  are the input quantities ETHI and ES.

Whenever a mesh point calculation or insertion is completed successfully, the output subroutine, PRINT, is called so that the point may be printed.

Subroutine CNTRL also integrates the wall pressure by trapezoidal rule to determine the axial component of force existing between adjacent wall points,

$$\Delta F = 2\pi r_*^2 \int_{r_4}^{r_3} p r dr = \frac{\pi}{2} (p_3 - p_4) (r_3^2 - r_4^2) r_*^2$$

Total thrust is item found by

$$F_t = F + 2\pi r_*^2 \int_1^r p r dr$$

where  $F$  is the thrust across the initial line as calculated by subroutine CHAR.

## DETAILED DISCUSSION OF CNTRL

Detailed documentation for subroutine CNTRL of the TDK computer program is presented on the following pages. It is intended that this documentation be read in conjunction with the FORTRAN listing of subroutine CNTRL.

The CNTRL subroutine calculates flow field points using point calculation subroutines and constructs the method of characteristics point mesh. The points are calculated in the Q array. The left running characteristic (LRC) under construction is stored in the P array, and the previous characteristic is stored in the PP array. In these two dimensional arrays (i.e., Q, P, and PP) the column number is the point number and the row number is the flow field property number. The flow field properties storage is defined in Table 5-6, subroutine CHAR, and is the same for all three arrays. For dividing streamline points, two arrays are required for Points 3 and 4. Storage for these extra points are provided in Q.

Besides the point calculation subroutines (AXISPT, DSPT, INPT, and WLPT), subroutines ERRORZ, INSRT, PRINT, SPLN, SUBIL, and TIMERX, are the only other subroutines called directly from CNTRL.

The CNTRL subroutine is divided into areas 1 through 9. A description of the programming of each of these areas is presented below. Presented in Table 5-7 are definitions for the variables used by subroutine CNTRL. FORTRAN variables which are input to the program have not been included in Table 5-7. These variables are described in Section 6.7.1.

#### Area 1:

In this area of CNTRL constants are initialized and the Point 3 arrays are zeroed. Other variables needed by CNTRL are initialized in subroutine CHAR. Subroutine SUBIL is called and the first initial line point is brought in and stored in PP(i, 1). The point is also placed in the Point 1 working storage and printed. The same procedure is followed for the second initial line point; this time storing the point in P(i, 1). A check is made to see if an error was detected by subroutine PRINT. The point counters IP for the P array and IPP for the PP array are set to one.

#### Area 2:

This area defines the general procedure for initial line point set up. The initial line point counter, MS, is incremented and IP and IPP are initialized to one. Initial line point number MS is brought in and stored in P(i, 1). It is also placed in Point 1 and printed. If a dividing streamline point calculation is indicated (i.e., PS [JFLAG] not zero), the point is also stored into the next point in PP.

#### Area 3:

The counters IPP and IP are incremented and the print subroutine is called with ID as set by the point subroutine just completed (see subroutine PRINT for the definitions of ID). If too many points have been calculated along the LRC (i.e., IP < IPMX) the error flag is set to 7 and CNTRL is exited. Otherwise, the values just calculated in Q(i, 3) are stored in the LRC array and Q(i, 3) is cleared. If the Point 3 is a single point (interior point), this part of the logic is

complete. Otherwise, Q3A(1) is placed in Point 3 and Area 3 is repeated.

### Area 3.5

If the exit plane option has been requested (EXITPL = true), no check is made on the end of wall flag (EØW2) that otherwise is used to stop the calculation. The EØW2 flag is set when the end of the wall has been reached within a tolerance of EPW (nominally .01).

If the exit plane calculation has been requested, as soon as the nozzle calculation is complete (i.e., EØW2 set to one) the wall is artificially extended a distance DELWX in the axial direction. The slope used for this extension is that of the last two points in the wall table. The flag EXITCK is used to assure that this is only done once. The point just calculated is written on unit ITSTAB to be used later as the first exit plane point. The statement "BEGIN EXIT PLANE CALCULATION" is printed.

If the exit plane option has been requested and the programming described in the above paragraph has been executed, the last entry in the insert table, IT(LAST), is checked. If the insertion process is complete and the last two points calculated fall on either side of the exit plane, values at the exit plane are found by interpolation and written on unit ITSTAB for later use. If the point just written out is an axis point, or if the first point on the LRC is beyond the exit plane, the program goes to statement 1700 to write out the exit plane summary and to terminate the calculation. Otherwise the program proceeds to Area 4.

If the exit plane calculation is in progress and the LRC has already crossed the exit plane successfully, checks are made to

see if NCHEPE, NPTEPE, and P(6, IP) are within their minimum values. If so, Area 4 is entered at the beginning, otherwise it is entered at 1610 and a special check is made.

#### Area 4:

If Area 4 is entered at the beginning, a check is made to see if the point just used on the previous LRC was the last point (IPPW) on the LRC. If not, the program goes to Area 7. Otherwise, starting at 1610 NCHEPE is checked as follows; if EXITCK is true, and the point just calculated is not beyond the exit plane, and NCHEPE exceeds its maximum value, transfer is made to Area 9 and the error message "EXIT PLANE OPTION REQUIRES LARGER NCHMXE, NPTMXE" is printed. If no error was found, the program sets IPPW = IP and checks to see if the insertion table is empty. If so, the program transfers to Area 7.

If the insert table is not empty, it is necessary to restart the LRC calculation at the last point entered in the table. The reason for this is as follows. Whenever it is necessary to insert a point along a streamline, the inserted point will start a new LRC. It is then necessary to complete this new LRC and then come back to the point of insertion and complete the LRC that was being computed when the insertion occurred. This procedure is carried out in Area 4 by mapping point numbers IT(LAST) through IP of the P array into the PP array. IP is then set to IT(LAST)-1 and IPP is set to IT(LAST)+1 so that the LRC calculation can start from the point of last insertion. This point is then removed from the IT table by setting LAST = LAST-1. The program then goes to Area 7.

#### Area 5:

Area 5 is entered when a LRC has been completed. This means that the insertion table has been emptied. Next, the PP

array is updated by transferring into it the values in the P array. If the LRC just completed is in the nozzle, the LRC surface is integrated from the axis (or initial line) to the wall using the trapezoidal rule method to obtain the mass flow rate. The integral to each point is stored in the array XMASSF. Tests are made on the input variable MASSFL and print out of the mass flow is done accordingly. Next, an adjustment is made to the pressure so that mass flow is conserved. The density is recalculated from the perfect gas law. At the end of Area 5 the edit logic using  $\epsilon_0$  and  $\epsilon_s$  is carried out as discussed earlier. The characteristic number, LRC, is then updated and the program transfers to Area 2 if the next LRC starts from the initial line, and to Area 6 if the next LRC starts from the axis.

#### Area 6:

Area 6 is entered when it has been determined that an axis point is to be calculated. The point counters (IP and IPP) and the insert counters (CS) are initialized and Points 1 and 4 are set up. The axis point subroutine is called and return is made with either the axis point calculated or the INSERT flag set. If an insert is requested or if Point 3 is found to be farther than a distance DS downstream from Point 4, a new Point 1 is inserted half way between the old Point 1 and Point 4. Inserts are counted and an error is detected if more than the maximum are required.

If the axis point has been successfully calculated and an insert was required, then subroutine PRINT is called to print the inserted point. Transfer is then made to Area 3.

#### Area 7:

Area 7 is entered for the purpose of performing a wall point calculation. If the point to be calculated is not a wall point the program goes to Area 8. If a wall point is to be calculated

checks are made concerning the exit plane option. If the exit plane option is in effect, the point to be calculated is either on an LRC which: (1) ends upstream of the nozzle exit plane (EXITCK false), or (2) is one of the NCHMXE LRC's ending on the nozzle wall extension, or (3) is a LRC farther downstream which is ended as soon as a point is calculated with an axial coordinate greater than XEXTEN. In the first two cases the wall point calculation proceeds normally as described in the next paragraph. In the third case the program goes to Area 9 and constructs an end point for the LRC so that it can be finished without a wall point, and then goes to Area 4. However, if the point just calculated is beyond XEXTEN then it is not necessary to go to Area 9 and the program goes directly to Area 4.

The wall point calculation logic is as described in Area 6 for an axis point with the exceptions noted below. The Point 2 is set up rather than Point 1. After a wall point is calculated, the streamline angle is checked to be sure it has not turned more than  $\Delta\theta_w$ . The axial pressure component is integrated to determine the thrust increment for the wall differential just completed (see the equations discussed earlier). If a point was inserted on the previous streamline, it is entered into the insert table. When the wall point procedure is completed the program goes to Area 3.

#### Area 8:

Area 8 is entered for the purpose of performing an interior point or a dividing streamline double point calculation. The point calculation logic is as follows. A check is made to determine if the point to be calculated is a interior point or a dividing streamline point. Points 2 and 4 are set up accordingly and the appropriate point calculation subroutine is called (INPT or DSPT). If it is necessary to insert a point, the insert procedure is the same in both cases and is also the



same as used for a wall point calculation as previously described. These three point calculations are set up differently, but use the same code for the insert procedures.

#### Area 9:

This area of the subroutine contains the error termination procedure, the nozzle exit plane summary print procedure, two error messages, and the end point procedure for the exit plane option.

The error termination procedure begins by calling the error subroutine, ERRØRZ, giving it the number of the error statement to be printed. Subroutine PRINT is then called so as to print the last point calculated. If exit plane points have been saved, these also are printed. Subroutine CNTRL is then exited.

The nozzle exit plane summary print procedure is as follows. A title is printed, then each exit plane point is read from unit ITSTAB and printed using subroutine PRINT. Subroutine CNTRL is then exited.

The two error messages printed in Area 9 relate to the exit plane option. When this option was added to the program, these messages were placed here rather than in subroutine ERRØRZ.

The end point procedure for the exit plane option found at the end of Area 9 is that described in Area 7.

TABLE 5-7

DEFINITIONS FOR FORTRAN VARIABLES USED BY SUBROUTINE CNTRL†

Variables beginning with I through N are typed as integer. All others are typed as real unless noted as logical. No other types are used. Assumed values are listed in parentheses.

<u>Variable</u>	<u>Definition</u>
ARATIO	Area ratio of wall point
CS	Insertion counter
CSMAX	Maximum allowed number of insertions (20.)
DELWX	Length of nozzle extension for exit plane option (10.)
DS2	DS * DS; where DS is input
EOW1	Flag set in WLPT when the end of nozzle wall is detected
EOW2	Flag set in WLPT when iterations to reach end of wall point are complete
ES2	ES * ES; where ES is input
EXITCK	Logical variable set true for the exit plane option as soon as the end of the nozzle is reached
EXITPL	Logical input variable. Input true if the exit plane option is desired (.FALSE.)
ID	Point type input to subroutine PRINT
IERR	Error flag, set to error number

† The following input variables are used by subroutine CNTRL: DS, DTWI, DWWI, EPW, ES, ETHI, IMAX, and IMAXF. These variables are discussed in Section 6.7.1

TABLE 5-7

DEFINITIONS FOR FORTRAN VARIABLES USED BY SUBROUTINE CNTRL

(Continued)

Variable	Definition
IMX	Number of variables for a point
INSERT	Insert flag. A non-zero value asks CNTRL to insert a point
IP	Point counter for the LRC under construction
IPMX	Maximum number of points allowed on a LRC (151)
IPP	Point counter for the last LRC finished
IPPS	Value of IPP for Point 4
IPPW	The largest IPP value, that of the wall point
IT (20)	Insertion table where the point numbers are stored for insertions requiring LRC completion
ITSTAB	Unit on which exit plane points are stored until printed (29)
JFLAG	Index for flag in the point arrays identifying dividing streamline double points
LAST	Number of last entry into IT array
LASTMX	Maximum number of LRC generating insertions for the original LRC (20)
LRC	Number of LRC
MASSFL	Input variable controlling the mass flow print out (1)
MS	Initial line point counter
MW	Wall point counter
N	Statement number for ASSIGNED GO TO controlling the point calculations
NCHEPE	For exit plane option, LRC counter in the wall extension region

TABLE 5-7

DEFINITIONS FOR FORTRAN VARIABLES USED BY SUBROUTINE CNTRL

(Continued)

Variable	Definition
NCHMXE	For exit plane option, number of LRC's to be calculated on the wall extension (6)
NEXITP	Exit plane point counter
NPTEPE	For exit plane option, LRC counter in the region beyond the wall extension
NPTMXE	For exit plane option, maximum number of LRC's allowed in the region beyond the wall extension (10)
P(70,275)	Array in which LRC is constructed
PP(70,275)	Array containing LRC just completed
PS(70)	Working storage for initial line point
PW(1208)	Array containing wall point coordinates
Q(70,5)	Working storage for point calculations, column number is the point number
Q3A(70)	Working storage for Point 3A of dividing streamline double point
Q4A(70)	Working storage for Point 4A of dividing streamline double point
REXIT	Radial coordinate at end of nozzle wall
XEXIT	Axial coordinate at end of nozzle wall
XEXTEN	For exit plane option, length of nozzle extension reached after LRC number NCHMXE
XMASSF(275)	Array containing integrated mass flow rate of each LRC point

#### 5.5.9 Subroutine CNTRL1

Given a right-running characteristic (RRC) stored in the PP(-,-) array, and the starting point of the next RRC stored in P(-,IP), this subroutine computes a RRC emanating from P(-,IP). The RRC is traced until it reaches the axis, or goes outside the nozzle.

#### 5.5.10 Subroutine CNTRL2

This subroutine performs the same function as subroutine CNTRL1, but applies to a left-running characteristic (LRC). Here, the calculation is carried out until the LRC reaches the wall.

#### 5.5.11 Subroutine CNTR12

This is a control subroutine for the shock calculation. It is called after an induced right-running shock has been detected. Its function is to compute a right-running shock point, followed by the construction of a LRC to the wall. The procedure is repeated until the end of nozzle is reached, or the shock wave reflects off the center line. At this point control is returned to CNTR91 and CNTR13 is called.

#### 5.5.12 Subroutine CNTR13

This is a control subroutine for the shock calculation. Its function is to compute a left-running shock point, followed by the construction of a RRC from the shock point to the axis. The procedure is repeated until the end of the nozzle is reached, or the shock wave reflects off the wall. At this point control is returned to CNTR91 and CNTR14 is called.

#### 5.5.13 Subroutine CNTR14

This is a control subroutine for the shock calculation. Its function is to compute a right-running shock point, followed by the construction of a LRC from the shock point to the wall. The procedure is repeated until the end of the nozzle is reached, or the shock wave reflects off the axis. CNTR14 is similar in function to CNTR12, but it is designed for multiple reflections, while CNTR12 is designed to start the induced shock calculation.

#### 5.5.14 Subroutine CNTR16

This is a control subroutine for the shock calculation. Its function is to compute a second attached shock wave. The construction is as follows. First, the flow field is computed assuming the second shock wave is negligible. When the end of the nozzle is reached, then subroutine CNTR16 is called. By using existing information an attached shock is calculated at the wall location having axial coordinate XB. Next, a right-running shock wave is constructed from XB. A LRC is traced from each shock point to the nozzle wall using subroutine CNTR12. The calculations stop when the wall end point is reached.

#### 5.5.15 Subroutine CNTR21

This is a control subroutine for the shock calculation. Its function is to compute right-running characteristics beginning at the bottom of the initial data line. Successive RRC's are constructed starting at the initial data line and ending at the axis or exit plane. Once the wall is reached, successive RRC's are constructed starting at the wall and ending at the axis or exit plane. The procedure is repeated until the nozzle end point is reached. However, if an induced right-running shock is detected, then control is returned to CNTR91 and subroutine CNTR12 is called.

#### 5.5.16 Subroutine CNTR31

This is the control subroutine for the attached shock wave calculation. First, it computes right-running characteristics beginning at the bottom of the initial data line. Successive RRC's are constructed starting at the initial data line and ending at the axis or exit plane. Once the wall is reached, successive RRC's are constructed starting at the wall and ending at the axis or exit plane. The procedure is repeated until position XA is reached on the wall. Control is then returned to CNTR91 and subroutine CNTR14 is called.

#### 5.5.17 Subroutine CNTR91

This is the master control subroutine for the shock calculations. It calls subroutine CNTR12, CNTR13, CNTR14, CNTR16, CNTR21, and CNTR31 as required to compute the flow field from the initial line to the end of the nozzle.

5.5.18 | SUBROUTINE CRIT (XN, XM, NØ)

The purpose of this subroutine is to compare two values for absolute or relative convergence and return an indicator stating if convergence has been achieved.

Calling Sequence:

XN             $x_n$  , input

XM             $x_m$  , input

NØ            indicator, output

NØ = 0    implies convergence

NØ = 1    implies no convergence

where:

if  $|x_m - x_n| < \epsilon_1$             then NØ = 0 , return

if  $|x_n| = 0$                         then NØ = 1 , return

if  $|x_m - x_n| / |x_n| < \epsilon_2$         then NØ = 0 , return

otherwise                            NØ = 1 , return

$$\epsilon_1 = \epsilon_2 = 5 \cdot 10^{-5}$$



5.5.19 SUBROUTINE CUBIC (X, Y, YP, N, ARG, YARG)

The purpose of this subroutine is to perform cubic interpolation for a tabulated function whose derivatives are known.

Calling Sequence:

X	is a table of the independent variable, $x_i$ , such that $x_{i+1} \geq x_i$
Y	is a table of the dependent variable, $y_i = y(x_i)$
YP	is a table of the derivatives of the dependent variable $y_i' = y'(x_i)$
N	is the number of entries in each of the above tables; $i = 1, \dots, N$
ARG	is the argument, $x$ , for which interpolation is requested
YARG	is the result, $y = y(x)$

Restrictions:

The calling program must define arrays for the dummy variables X, Y, and YP. These arrays must be at least of lengths  $N + 1$ ,  $N$ , and  $N$  respectively. The subroutine will save its last used table position number in  $X(N + 1)$ .

If  $x < x_1$  the program returns  $y = y_1$

If  $x > x_N$  the program returns  $y = y_N$

Method:

Given :  $x_0 \leq x < x_1$

so that  $y_0, y_0', y_1$ , and  $y_1'$  are known. The cubic interpolation formula given below is used to determine  $y$

$$y = A(x - x_0)^3 + B(x - x_0)^2 + C(x - x_0) + D$$

where

$$A = \frac{1}{h^3} \left[ (y_1' + y_0') h - 2k \right]$$

$$B = \frac{-1}{h^2} \left[ (y_1' + 2y_0') h - 3k \right]$$

$$C = y_0'$$

$$D = y_0$$

and

$$h = x_1 - x_0$$

$$k = y_1 - y_0$$

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## 5.6 BLM SUBROUTINES

The Boundary Layer Module (BLM) is used to calculate the loss in nozzle performance due to a viscous boundary layer and its interaction with the nozzle wall. The effects of both drag and heat transfer are included. The method used is described in Section 2.6.

The BLM consists of the following subroutines:

BLMAIN	DIFF
BLEDGE	EDDY
BLH	INPUTB
BLØCKD	IVPL
BLPLTS	LINI
BLSEG	ØUTPBL
BLTABL	RBL
BLW	READBL
CØEF	SØLV5
CØEF1	WRPROF
CUBICB	

The BLM is entered through subroutine BLMAIN. The boundary layer is divided into segments consisting of equally spaced grid lines. The control subroutine for analyzing a segment is subroutine BLSEG. There can be as many as 101 grid lines per segment, and as many as 10 segments. Many of the variables used in the BLM analysis are stored in arrays. The most important array variables are listed in Table 5-8.

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TABLE 5-8: ARRAYS USED BY THE BLM

Variable (with dimension)	Common /Name/	Contents
A (101)	/GRD/	$(\eta_j - \eta_{j-1})/2$ , grid spacing
ALFA (101)	/AL/	$\alpha_e$ , angle of b.l. to nozzle center line
ALMDA (101)	/EDGE/	$\lambda_e$ , mean free path at edge
B (101,2)	/BLC1/	b, see equation 2.6-12
BC (101)	/BLC1/	$(\rho\mu/\rho_e\mu_e)$ , see equation 2.6-12
C (101,2)	/BLC1/	$(\rho_e/\rho)$ , see equation 2.6-12
CII (101)	/MISCT/	$I_1$ , integral, see equation 2.6-21
CK (101)	/BLC2/	$\gamma$ versus T, gas property table
CKE (101)	/EDGE/	$\gamma_e$ versus $T_e$
CNUE (101)	/EDGE/	$(\mu_e/\rho_e)$
CP (101)	/BLC2/	$C_p$ versus T, gas property Table
CPE (101)	/EDGE/	$C_{p_e}$ versus $T_e$
CQ (101)	/WALL/	$(\rho v)_w$ versus $T_w$
D (101,2)	/BLC1/	d, see equation 2.6-12
E (101,2)	/BLC1/	e, see equation 2.6-12
HHE (101)	/EDGE/	$H_e$ , total enthalpy at edge
HSE (101)	/EDGE/	$h_e^*$ , static enthalpy at edge
HSW (101)	/WALL/	$h_w^*$ , static enthalpy at wall
PE (101)	/EDGE/	$P_e$ , pressure at edge
P1 (101)	/PRES/	$m_1$ , see equation 2.6-13
P2 (101)	/PRES/	$m_2$ , see equation 2.6-13
P3 (101)	/PRES/	$m_3$ , see equation 2.6-14
RINØ (201)	/BCØN/	$r_o$ , radial coordinate of b.l., input
RKK (101)	/BLC2/	k versus T, gas property table

RHØE	(101)	/EDGE/	$\rho_e$ , density at edge
RMU	(101)	/BLC1/	$\mu$ versus T, gas property table
RMUE	(101)	/EDGE/	$\mu_e$ , viscosity at edge
RR	(101)	/BLC2/	$R_g$ versus T, gas property table
RX	(101)	/EDGE/	$R_\xi$ , local Reynold No., $U_e \xi / \nu_e$
RO	(101)	/GRD/	$(r_o/L)^k$ , local radius of body revolution (L=1)
S	(201)	/GBLK/	x, surface distance, equally spaced
SØ	(201)	/GBLK/	x, surface distance, input
T	(101)	/BLC2/	T, temperature for gas property tables
TE	(101)	/EDGE/	$T_e$ , temperature at edge
TVCT	(101)	/MISCT/	$(1-t)^{2k}$ where $t = y \cos\phi / r_o$ , transverse curvature
TW	(101)	/WALL/	$T_w$ , temperature at wall
U	(101,2)	/BLC1/	$f' = U/U_e$
UE	(101)	/EDGE/	U, velocity at edge
V	(101,2)	/BLC1/	$f''$ , shear parameter
WW	(101)	/WALL/	$g'_w$ , dimensionless total enthalpy gradient at wall
X	(101)	/GRD/	$\xi$ , see XØ
XINØ	(201)	/BCØN/	X, axial coordinate, input
XØ	(101)	/GBLK/	$\xi$ , transformed surface distance, see equation 2.6-6a
Y	(101)	/MISCT/	$\eta = y/y$

### 5.6.1 SUBROUTINE BLMAIN

This is the main program for the BLM. The functions performed by this routine are described below.

Input data is read by calling subroutine INPUTB. INPUTB also prepares tables and initializes variables and indexes required for subsequent calculations. Next, subroutine IVPL is called, and initial velocity and temperature profiles are computed on a finite difference grid.

The boundary layer is divided into segments with as many as 101 grid lines per segment. For each segment, 1 through NSEG, the following events occur. First, subroutine BLEdge is called to prepare tables of variables that describe conditions at the wall and at the inviscid edge of the boundary layer. Next, subroutine BLSEG controls the computation of the boundary layer. It computes the growth of the boundary layer from the beginning to the end of each segment, i.e., up to 101 grid lines.

Subroutine BLMAIN prints out text heading the numerical output of the program.

At the end of the print out for each segment, BLMAIN prints the following quantities which are evaluated at the last point on the segment:

Mean Free Path

$$\lambda = 1.26 \ v^{1/2} / (gRT) \quad (\text{ft})$$

Total Integrated Wall Heat Flux

$$Q_w = \int \dot{q}_w \ d A \quad (\text{BTU/sec})$$

At the end of the print out for the last segment, the following additional quantities (evaluated at the last point) are printed:  
Knudsen No. based on  $\delta^*$

$$Kn_{\delta}^* = \lambda / \delta^*$$

Nozzle Mass Flow

$$\dot{m}_{2D} \quad (\text{lbm/sec})$$

Boundary Layer Specific Impulse Loss

$$\Delta I_{sp, BL} = \Delta F_{BL} / \dot{m}_{2D} \quad (\text{sec})$$

### 5.6.2 SUBROUTINE BLEDGE (ISEG)

This subroutine constructs the boundary conditions for segment number ISEG of the boundary layer. Tables containing the boundary layer coordinates  $XIN\emptyset$ ,  $RIN\emptyset$ ,  $S\emptyset$ , AND  $X\emptyset$  (see Table 5-8 ) are input. The beginning and ending axial coordinates for the segment,  $XSEG(ISEG)$  and  $XSEG(ISEG+1)$ , and the number of subdivisions to be used,  $NISPS(ISEG)$ , are also input (see Section 6.8-3). Using this information, tables that are equally spaced in boundary layer length are prepared. These tables are (see Table 5-8 ):

$X, S, RO, XI, TE, UE, PE, TW, CQ, CPE, CKE, HSE, HSW, ALFA.$

The above tables are then printed under the heading "BOUNDARY CONDITIONS (IHFLAG = I1 )".

### 5.6.3 SUBROUTINE BLH

This subroutine is used to calculate the propellant enthalpy picked up by the regenerative cooling circuits. The method used is described in Section 6.8.4, Regenerative Cooling Heat Transfer. It consists of integrating the wall heat flux over the surface area covered by the regen cooling circuits and dividing the results by the engine mass flow rate. The wall heat flux is calculated by subroutine OUTPBL. The integrated heat flux is read from the BLM linkage file (unit 12) using subroutine RBL. As many as three circuits are allowed. The subroutine prints out the results of the calculations under the label "PROPELLANT ENTHALPY FROM THE COOLING CIRCUITS".



#### 5.6.4 Block Data BLØCKD

This subprogram initializes the variables listed below:

- NXT - total number of x-stations, set for 101
- NTR - location of transition, set for 3
- ETAE - transformed boundary-layer thickness for first station, set for 8. The boundary-layer thickness for other stations is computed internally.
- VGP - variable grid parameter set for 1.14.
- RUMI - reference viscosity set for  $0.250 \times 10^{-4} \text{ lb}_m/\text{ft-sec}^*$
- TI - reference temperature for viscosity, set for  $1500^\circ\text{R}$ .
- ØMEGA - exponent in the density-viscosity relationship set for 0.76
- PR - molecular Prandtl number, Pr, set for 0.72
- ITYPE - through this flag the flow type is specified as follows:  
a nozzle (ITYPE=1), and external axisymmetric body (ITYPE=2), or a two-dimensional external flow in which flow starts as a stagnation point flow (ITYPE=3). Set for 1.
- CQ - mass transfer parameter, set for 0. It is equal to  $(\rho v)_w$  and has units of  $\text{lb}_m/\text{ft}^2\text{-sec}$
- IHFLAG - this flag indicates whether the wall temperature is input (IHFLAG=0) or wall heat flux (IHFLAG=1). Set for 1.
- NTAB - in the computer program  $C_p$ ,  $Y$ ,  $k$ ,  $R$  are specified as functions of  $T(=T_0)$  and form a "fluid-property table". NTAB refers to the number of  $T_0$  values in this table. It is set here as 3, maximum being 101.

\* The assumed values of RUMI, TI, ØMEGA, PR, CPO and CKO are for air.

- TO - values of temperature for the table.
- CPO - specific heat at constant pressure, Set  $\text{ft}^2/\text{sec}^{\circ}\text{R}$ . for 101 \* 6006.
- CKO - ratio of specific heat at constant pressure to specific heat at constant volume, dimensionless. Set for 101 \* 1.4.
- IPRNT - the flag that controls the print output. Set for 0.

IPRNT=0 corresponds to short print and

IPRNT=1 corresponds to long print

Short print consists of the boundary-layer parameters such as  $\delta^*$ ,  $\theta$ ,  $H$ ,  $c_f$ ,  $R_{\delta^*}$ ,  $R_{\theta}$ ,  $R_s$ ,  $c_H$ ,  $\Delta F$ , and  $\Delta I_{sp}$ .

Long print includes short print plus the velocity and temperature profiles. These are defined in Subroutine  $\emptyset\text{UTPBL}$ .

- QF - This is the factor that converts input values of heat flux (TQW(1) entries when IHFLAG=1) from the input units of  $\text{BTU}/\text{in}^2\text{sec}$ . to the internal program units of  $\text{lbm}/\text{sec}^3$ .  
 $QF = 3.605259 * 10^6$ ,  
 i.e. ;  
 $\dot{q}_w (\text{lbm}/\text{sec}^3) = 144 \text{ Jg} (\text{BTU}/\text{in}^2\text{-sec})$ .

#### 5.6.5 SUBROUTINE BLPLTS

This subroutine performs all the plotting for the BLM module. Data written by the BLM on data files is read and plots are made for requested items. Plot capabilities include displacement thickness, momentum thickness and wall temperature versus axial station. Also available are temperature and velocity profiles through the boundary layer at selected area ratios. Inputs for using the BLM plotting are described in Section 6.8.5.

### 5.6.6 SUBROUTINE BLSEG

The over-all logic of the boundary layer computations is controlled by this subroutine. A flow chart of the logic is presented in Figure 5-3. The nozzle is divided into segments, and subroutine BLSEG computes the growth of the boundary layer from the beginning to the end of the segment when called by subroutine BLMAIN. There are 100 grid lines in a segment, and these are counted using the FORTRAN variable NX. Each grid line is iterated until the solution converges. Iterations are counted using FORTRAN variable IT.

Subroutine BLSEG checks the convergence of the iterations by using the wall shear parameter  $f_w''$  as a convergence criterion. For laminar flows, calculations are considered converged when

$$f_w'' < 10^{-4}$$

If  $f_w''$  becomes negative during the iterations, calculations are stopped. For turbulent flows a relative convergence criterion is used, as follows:

$$\frac{f_w''}{f_w'' + .5 f_w''} < .02$$

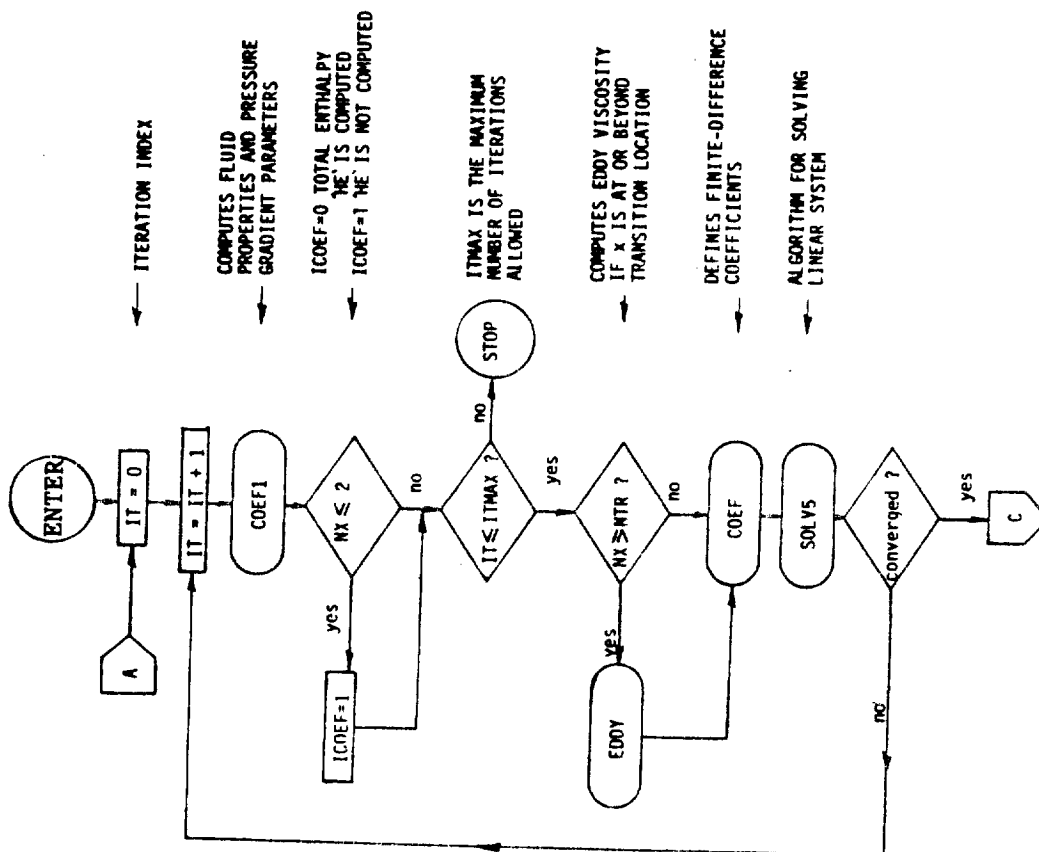
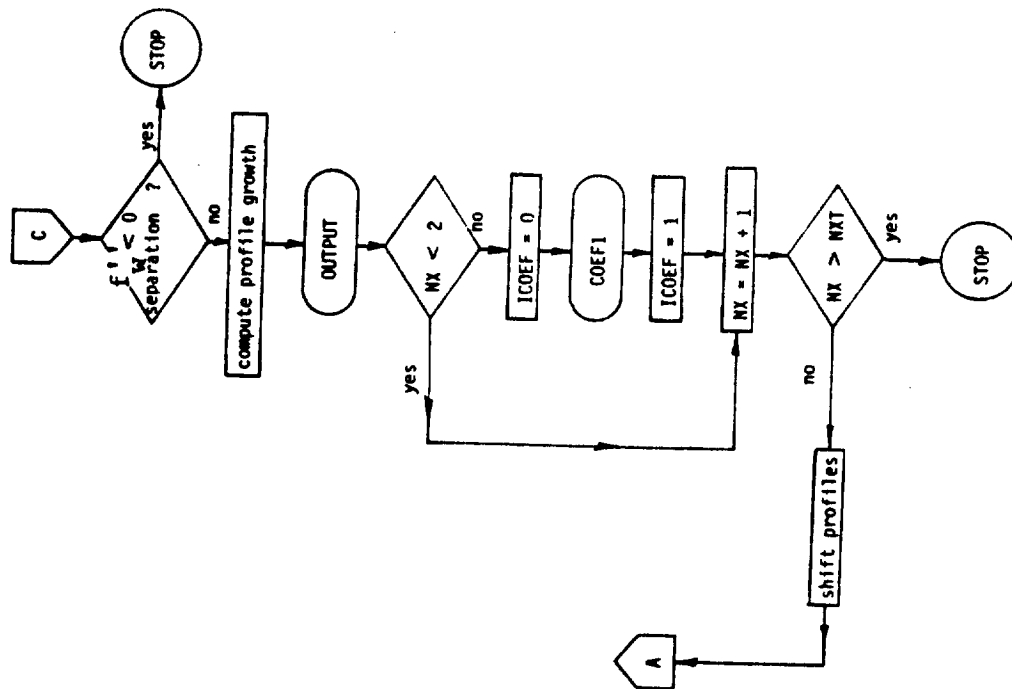


Figure 5-3: Flow Diagram for Subroutine BLSEG of BLM

5.6.7 SUBROUTINE BLTABL (INTERP, NTAB, XTAB, YTAB, XOUT, YOUT)

The purpose of this subroutine is to generate a table

$$y_i \text{ vs. } x_i$$

from a given table of

$$\bar{y}_j \text{ vs. } \bar{x}_j$$

Method:

Given  $\bar{y}_j, \bar{x}_j$   $j=1,2,\dots,NJ$

and  $x_i$   $i=1,2,\dots,NI$

This subroutine interpolates to find

$$y_i \quad i=1,2,\dots,NI$$

One of these following interpolation methods can be selected: linear, linear log, or cubic.

Calling Sequence:

INTERP    Interpolation method; input  
          = 1 for linear, using subroutine LINI  
          = 2 for linear log, using subroutine LINI  
          = 3 for cubic, using subroutine CUBICB

NTAB      NJ, number of entries input for XTAB and YTAB

XTAB       $\bar{x}_j$  input

YTAB       $\bar{y}_j$ , input versus  $\bar{x}_j$

NOUT      NI, number of entries input for XOUT

XOUT       $x_i$ , input

YOUT       $y_i$ , output versus  $x_i$

#### 5.6.8 SUBROUTINE BLW

This subroutine uses results obtained from the BLM analysis for the boundary layer displacement thickness,  $\delta^*$ , to obtain a displaced wall contour. The wall is either displaced inwards (when given the real wall), or outwards (when designing the real wall), a distance  $\delta^*$  normal to the original contour. The nozzle throat radius is also corrected by  $-\delta^*$  or  $+\delta^*$ , respectively. The results of these calculations are printed.

The values of  $\delta^*$  vs X that are required for the above calculations are obtained from unit 12 using subroutine RBL.

#### 5.6.9 SUBROUTINE CØEF

This subroutine contains the coefficients of the linearized momentum and energy equations written in a form described in Chapter 8 of Reference 13.

---

Ref. 13. Bradshaw, P., Cebeci, T., and Whitelaw, J.H.,  
Engineering Calculation Methods for Turbulent Flows.  
Academic Press, London, 1981.

### 5.6.10 SUBROUTINE CØEF1

This subroutine calculates the fluid properties and the pressure-gradient parameters used in the momentum and energy equations.

For most applications boundary-layer calculations are carried out based on the assumption that the external flow is isentropic and that the total enthalpy  $H_e$  is constant. This assumption is not used here.  $H_e$  is allowed to vary along the nozzle length. The following procedure is used for this purpose:

The static enthalpy,  $h^*$ , is computed from

$$h^* = \int_{T_o}^{T_e} C_p(T) dT + h^*(T_o)$$

and stored together with  $C_p$ (CPO),  $\gamma$ (CKO),  $k$ (RKKO),  $R$ (RRO) all expressed as functions of  $T(TO)$  thus forming a "fluid property table." This table is used to interpolate fluid properties across the layer.

The boundary-layer equations require that at two adjacent  $x$ -stations the total edge enthalpy  $H_e$  must be constant. To provide for variation in  $H$ , local similarity ideas are used.



For two adjacent x-stations, 1 and 2, an average  $H_e$  is defined as:

$$H_e = 1/2[H_e^* (1) + H_e^* (2)] \quad (1)$$

Then with an initial dimensionless total enthalpy ratio  $g$  known from the boundary-layer solutions, static enthalpy,  $h_j$ , is computed from.

$$h_j = g_j H_e - \frac{u_e^2 (f_j')^2}{2} \quad (2)$$

Once  $h_j$  is known, then using the "fluid property table", values for  $C_{pj}$ ,  $T_j$ ,  $\gamma_j$ ,  $R_j$  and  $k_j$  are found by interpolation, and  $\mu_j$  is found from

$$\mu_j = \mu_r \left( \frac{T_j}{T_r} \right)^\omega$$

The edge values of density  $\rho_e$ ,  $\mu_e$ ,  $\nu_e (= \mu_e / \rho_e)$  and  $R_x (u_e x / \nu_e)$  are then computed. Edge values corresponding to  $j = J$  and  $\rho_e$  are computed from

$$\rho_e = \frac{p_e}{T_J R_J}$$

Next, the coefficients  $c$ ,  $b$ ,  $e$ ,  $d$  and the pressure gradient parameters  $m_1, m_2, m_3$  appearing in the momentum and energy equations are computed.

Finally, wall conditions are computed depending on whether the wall temperature or heat flux are specified. When the wall temperature is given the dimensionless total enthalpy ratio at the wall, which serves as a boundary condition, is computed as:

$$g_w = \frac{h_w^*}{H_e}$$

In the case of specified heat flux  $q_w$ , the dimensionless total enthalpy gradient,  $g_w'$ , is computed as

$$q_w' = - \frac{\xi}{\sqrt{R\xi}} \left(\frac{L}{r_0}\right)^k \frac{\rho_e}{\rho_w} \frac{C_{p_w}}{k_w H_e} \dot{q}_w(\xi)$$

Here the units of each term are as follows:

$$\rho = \frac{\text{lb}_m}{\text{ft}^3} \qquad H_e = \left(\frac{\text{ft}}{\text{sec}}\right)^2$$

$$C_p = \frac{\text{ft}^2}{\text{sec}^2 R} \qquad \xi = \text{ft}$$

At the convergence of the solutions for a given x-station, this subroutine is also used to account for the nonconstant nature of the total edge enthalpy. To explain this point, let us assume that we have done all that is described in COEF1, and that we can solve the equations at the specified x-station. Since the equations are nonlinear, solutions are iterated until a convergence criterion is met and then subroutine OUTPBL is called to print the desired quantities from that station. Before we increment the value of x and shift the profiles to perform calculations at the next x-station, we call COEF1 to compute a new value of  $H_e$  from Equation (1) and recompute static enthalpy variation from Equation (2) and redefine all the fluid properties and pressure gradient parameters at that x-station for the calculations to be done at the next x-station.

#### 5.6.11 SUBROUTINE CUBICB

Subroutine CUBICB is used for interpolation in a table with unequally spaced points. It uses a third-order polynomial to interpolate the data between four points.

#### 5.6.12 SUBROUTINE DIFF

Subroutine DIFF is used to determine the derivative at each point in an input table.

#### 5.6.13 SUBROUTINE EDDY

This subroutine contains the formulas used in the Cebeci-Smith eddy-viscosity model. The eddy-viscosity model is described in Section 2.6.2.

#### 5.6.14 SUBROUTINE INPUTB

This subroutine reads input data defining the problem to be solved by the Boundary Layer Module. Data calculated by the MOC module is read by calling subroutine READBL.

Next, user input data is read from unit 5 for the \$BLM Namelist data set. These input-items are described in Section 6.8 of this report.

This subroutine also calculates the surface distance from the input  $(r_o/c)$  and  $(x/c)$  values for NXIN-stations. The printed surface distance is dimensional and is expressed in feet.

The input NXIN-stations are then redistributed in order to have 101 x-stations uniformly distributed, except for the first five stations which are generated non-uniformly. The input values of  $u_e(x)$ ,  $p_e(x)$ ,  $T_e(x)$ ,  $(pv)_w$ ,  $(x/c)$ ,  $(y/c)$  are then interpolated for the new x-stations to be used in the boundary-layer calculations. In this subroutine, a total enthalpy,  $H_e^*(x)$ , is computed for each x-station by using the interpolated values of  $T$ , and  $u$  and the equation

$$H_e^*(x) = h_e + \frac{u_e^2}{2}$$

This subroutine prints out part of the input geometry which consists of

$X, r_0, s, u_e, P_e$

#### 5.6.15 SUBROUTINE IVPL

Since the boundary-layer equations are nonlinear, before they are solved at the stagnation point, they need initial velocity and temperature profiles. This subroutine provides the necessary data to start the calculations.

5.6.16 Subroutine LINI (X, Y, N, ARG, YARG, NSAVE)

The purpose of this subroutine is to linearly interpolate from tables of values and to save its place in the table.

Calling Sequence:

X is a table of the independent variables,  $x_i$   
Y is a table of the dependent variables,  $y_i$   
N is the number of entries in each table  
ARG is the argument for the X table  
YARG is the result of the interpolation  
NSAVE is a cell in which the table index is saved.

Restrictions:

If the argument exceeds the table of independent variables, the result is set equal to the appropriate table limit of the dependent variable.

### 5.6.17 SUBROUTINE ØUTPBL

Through the flag IPRNT discussed in Subroutine BLOCKD, this subroutine prints out the velocity and temperature profiles and the boundary-layer parameters  $\delta^*$ ,  $\theta$ ,  $H$ ,  $c_f$ ,  $R_{\delta^*}$ ,  $R_s$ ,  $C_H$  as well as the thrust decrement  $\Delta F$  due to the boundary layer.

They are defined by the following formulas:

Displacement thickness,  $\delta^*(\text{DELS})$ , in ft.

$$\delta^* = \int_0^{\infty} \left(1 - \frac{\rho u}{\rho_e u_e}\right) dy$$

Momentum thickness  $\theta$  (THETA), in ft.

$$\theta = \int_0^{\infty} \frac{\rho u}{\rho_e u_e} \left(1 - \frac{u}{u_e}\right) dy$$

Shape Factor,  $h$ , dimensionless

$$h = \delta^* / \theta$$

Local skin-friction coefficient,  $c_f(\text{CF})$ , dimensionless

$$c_f = \frac{\tau_w}{1/2 \rho_e u_e^2}$$

Reynolds number based on displacement thickness,  $R_{\delta^*}$

$$R_{\delta^*} = \frac{u_e \delta^*}{\nu_e}, \quad \nu_e = \mu_e / \rho_e$$

Reynolds number based on surface distance,  $R_s$

$$R_s = \frac{u_e s}{\nu_e}$$

Stanton number,  $C_H(CH)$ , dimensionless

$$C_H = \frac{\dot{q}_w}{\rho_e u_e (H_w - H_e)}$$

Thrust decrement  $\Delta F$ , in  $lb_f$

$$\Delta F = 2\pi r_o \theta \rho_e u_e^2 \cos\phi - 2\pi r_o \delta^* \cos\phi (P_e - P_a)$$

Here  $X$  and  $r_o$  correspond to the nozzle coordinates,  $s$  to the surface distance; all expressed in feet. The units of velocity  $u$  and pressure  $p_e$  are ft/sec and  $lb_f/ft^2$ , respectively.

In addition, this subroutine prints out the interpolated values of input geometry referred to as "edge conditions". It consists of  $X$ ,  $r_o$ ,  $s$ ,  $u_e$  and  $p_e$ .

#### 5.6.18 SUBROUTINE RBL (X, FX, IDX)

This subroutine reads the BLM linkage file (unit 12) and locates  $X_i$  and  $X_{i+1}$  such that

$$X_i \leq X \leq X_{i+1}$$

The value  $FX$  is then found by linear interpolation

$$FX = FX_i + (X - X_i) (FX_{i+1} - FX_i) / (X_{i+1} - X_i)$$

where  $FX$  is the variable number  $IDX$  stored on the file.



5.6.19 SUBROUTINE READBL

The purpose of this subroutine is to transfer data from the ODE and MOC modules to the BLM module.

If ODE has been run, values defining viscosity, Prandtl number, and edge total enthalpy are mapped for use by the BLM. The ODE linkage data is then read from unit LUBLM for use by BLM. The data file is checked for possible errors, and if detected, one of the following warning or error messages will be printed:

"NO LINKAGE FOUND, EXPECT MANUAL INPUT"

OR

"DATA FROM xxxxx MODULE OUT OF ORDER IN MODULE BLM. CARD  
xxxxx HAS SEQUENCE NO. xxxxx"

\*\*\*\*\*

OR

"INCORRECT CARD TYPE IN DATA FROM TDK FOUND BY READBL. EDG  
OR GPT EXPECTED xxxx FOUND AT SEQUENCE NO. xxxxx"

\*\*\*\*\*

OR

"INCORRECT CARD TYPE IN DATA FROM TDK FOUND BY READBL. END  
EXPECTED, xxxx, FOUND AT SEQ. NO. xxxxx"

\*\*\*\*\*

The last three errors above terminate program execution immediately after printing.

If no errors are encountered, the items read by subroutine READBL will include the nozzle mass flow rate, nozzle wall coordinates and associated edge temperature, pressure, and velocity data, and also the gas property tables.

If ODE was not run, the following message is printed:

"BLM MODULE COULD NOT FIND DATA FROM TD2P MODULE -- WILL  
ASSUME DATA TO BE READ IN \$BLM"

\*\*\*\*\*

5.6.20 SUBROUTINE SØLV5

This subroutine solves the matrix equation for which coefficients were computed by subroutine CØEF. One call to SØLV5 yields one pass through the elimination procedure. This procedure consists of a forward sweep, followed by a backward sweep of the system. The elimination scheme is specialized to treat this particular matrix equation.

5.6.21 SUBROUTINE WRPRØF

This subroutine interpolates between two wall stations and writes temperature and velocity profile data at selected area ratios onto a data file for post plotting. Area ratios are selected by input into the APROF array in the \$BLM namelist, see Section 6.8.5.

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6.0 PROGRAM USER'S MANUAL.

Description of the Computer Program Input.

The TDK computer program consists of five modules, ODE, ODK, TRANS, MOC, and BLM. All of these modules are required to perform a complete two dimensional non-equilibrium nozzle performance calculation with a boundary layer. Various options exist in the program, however, which exercise the above modules alone, in part, or in combination.

Data is read by the program sequentially in the order required for the execution of the modules. This order is as follows:

- Thermodynamic data,
- Data common to the modules,
- ODE module inputs,
- ODK module inputs,
- TRANS module inputs,
- MOC module inputs, and
- BLM module inputs.

A more detailed description of these input data sets is presented in Table 6-1. The documentation in which each of the data sets is completely described is also indicated in Table 6-1.

Of the data sets listed in Table 6-1, only the \$DATA data set is required for every computer run. Input of the other data sets is required only if the options they contain are to be used. For example, input of the thermodynamic data is not required if an existing thermodynamic data file is to be used.

Table 6-1. Input Data Set Description

<u>Card Input</u>	<u>Section No.,</u>	<u>Description</u>
THERMO	6.1,	thermodynamic data cards, see Tables 6-2 and 6-3
.		
END		
LOW T CPHS	6.1.1,	extension of thermodynamic data to temperatures below 300°K, see Table 6-5
.		
END LOW T CPHS		
TITLE	6.2,	one or more title cards
DATA	6.3,	data directive card
\$DATA	6.3,	data <u>namelist for module selection</u> , and geometry
\$END		
REACTANTS	6.4,	reactants directive card
.	6.4.1,	reactants cards, see Tables 2-6 and 2-7
.	6.4.1,	blank card required to end reactants cards
OMIT	6.4.2,	cards to omit species
INSERT	6.4.2,	cards to insert species
NAMELISTS	6.4.3,	ØDE directive card
\$ODE	6.4.3,	ØDE namelist
SPECIES	6.5.1,	species cards for ØDK
.		
REACTIONS	6.5.2,	reaction cards for ØDK
.		
LAST REAX		
INERTS	6.5.2.6,	inerts cards for ØDK. (to inert those species that are not named in reactions)
.		
.		

<u>Card Input</u>	<u>Section No.,</u>	<u>Description</u>
THIRD BODY . .	6.5.2.7,	reaction rate ratios for third bodies
LAST CARD		
\$ODK \$END	6.5.3	ODK module namelist
\$TRANS \$END	6.6	TRANS module namelist
\$MOC \$END	6.7	MOC module namelist
\$BLM \$END	6.8	BLM module namelist

Table 6-1 can be used as a guide when preparing input for given problem. It lists the data sets in the order in which they must appear in the data deck, and also shows the special cards which must appear in each set (first card, last card, etc.) if the program is to function properly. The table is basically self-explanatory when used together with the detailed input descriptions which follow.

Certain special options to the computer program are described separately in Section 6.9.

An input data card listing for a sample case is presented in Section 7, followed by the corresponding computer output. In preparing input to the computer program it is useful to review this input card listing.

Successive cases can be run using the computer program but complete data should be input for each case.

## 6.1 Thermodynamic Data.

Ordinarily, a thermodynamic data file is available for use with the program, and is assigned to logical unit 25. The input described here can be used to generate a thermodynamic data file if one is not available.

This data set is identical to the THERMO DATA described in Appendix D of NASA SP-273 (i.e. Reference 3).

Using this data set, thermodynamic data curve fit coefficients may be read from cards. The curve fit coefficients are generated by the PAC computer program described in NASA TN D-4097 (i.e. Reference 20).

The thermodynamic data (i.e.  $C_{pT}^0$ , etc.) are expressed as functions of temperature using 5 least squares curve fit coefficient ( $a_{1-5}$ ) and two integration constants ( $a_{6-7}$ ) as follows:

$$\frac{C_{pT}^0}{R} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$\frac{H_T^0}{RT} = a_1 + \frac{a_2T}{2} + \frac{a_3T^2}{3} + \frac{a_4T^3}{4} + \frac{a_5T^4}{5} + \frac{a_6}{T}$$

$$\frac{S_T^0}{R} = a_1 \ln T + a_2T + \frac{a_3T^2}{2} + \frac{a_4T^3}{3} + \frac{a_5T^4}{4} + a_7$$

For each species, two sets of coefficients ( $a_{1-7}$  and  $a'_{1-7}$ ) are specified for two adjacent temperature intervals, lower and upper respectively. For the data available in Reference 3 the lower temperature interval is 300° to 1000°K and the upper temperature interval is 1000°K to 5000°K.

---

Ref. 20. McBride, B.J., and Gordon, S., "Fortran IV Program for Calculation of Thermodynamic Data", NASA TN-D-4097, Aug. 1967.



The input format required for this thermodynamic data is defined in Table 6-2. Data cards for the species AR, H, H<sub>2</sub>, H<sub>2</sub>O, N<sub>2</sub>, O, OH, and O<sub>2</sub> are listed in Table 6-3 as examples. Thermodynamic data coefficients for many chemical species are supplied with the computer program. A list of these species is presented in Table 6-4. (For temperature range below 300° K see Section 6.1.1)

#### Data Tape Generation and Usage:

A computer run using thermodynamic data card input will generate a data tape on logical unit JANAF. This tape may then be saved and used at a later time. The program writes the THERMO data card images on unit JANAF as read but with two minor exceptions. The THERMO code card and the card numbers in card column 80 are omitted.

If thermodynamic data cards are not input, the program assumes the thermodynamic data is on logical unit JANAF. Logical unit JANAF is currently assigned a value of 25.

TABLE 6-2      FORMAT FOR THERMODYNAMIC DATA CARDS

Card order	Contents	Format	Card column
1	THERMO	3A4	1 to 6
2	Temperature ranges for 2 sets of coefficients: lowest T, common T, and highest T	3F10.3	1 to 30
3	Species name	3A4	1 to 12
	Date	2A3	19 to 24
	Atomic symbols and formula	4(A2, F3.0)	25 to 44
	Phase of species (S, L, or G for solid, liquid, or gas, respectively)	A1	45
	Temperature range	2F10.3	46 to 65
4	Integer 1	I15	80
	Coefficients $a_i'$ ( $i = 1$ to 5) in equations (6-1) to (6-3) <sup>1</sup> (for upper temperature interval)	5(E15.8)	1 to 75
5	Integer 2	I5	80
	Coefficients in equations (6-1) to 6-3) ( $a_6'$ , $a_7'$ for upper temperature interval and $a_1$ , $a_2$ , and $a_3$ for lower)	5(E15.6)	1 to 75
6	Integer 3	I5	80
	Coefficients in equations (6-1) to (6-3) ( $a_4$ , $a_5$ , $a_6$ , $a_7$ for lower temperature interval)	4(E15.8)	1 to 60
(a)	Integer 4	I20	80
(a)	Repeat cards numbered 1 to 4 in cc 80 for each species		
(Final card)	END (Indicates end of thermodynamic data)	3A4	1 to 3

<sup>a</sup>Gaseous species and condensed species with only one condensed phase can be in any order. However, the sets for two or more condensed phases of the same species must be adjacent. If there are more than two condensed phases of a species their sets must be either in increasing or decreasing order according to their temperature intervals.

TABLE 6-3. THERMO DATA CARDS FOR AN O<sub>2</sub>/H<sub>2</sub> PROPELLANT  
(SPECIES AR, H, H<sub>2</sub>, H<sub>2</sub>O, N<sub>2</sub>, O, OH, AND O<sub>2</sub>)

```

THERMO
  300.000  1000.000  5000.000
AR      L 5/66AR 1.00 0.00 0.00 0.G   300.000  5000.000
.25000000E 01 0.      0.      0.      0.      0.
-.74537502E 03 .43660006E 01 .25000000E 01 0.      0.
0.      0.      -.74537498E 03 .43660006E 01
H      J 6/74H 1.      0.      0.      0.G   300.000  5000.000
.24999996E+01 .70881143E-09 -.38728927E-12 .85096613E-16 -.65768080E-20
.25474390E+05 -.45989618E+00 .25000002E+01 -.19925608E-08 .54929899E-11
-.64292197E-14 .26794037E-17 .25474390E+05 -.45989941E+00
H2     J 3/61H 2.0 0.0 0.0 0.G   300.000  5000.000
.31001901E+01 .51119464E-03 .52644210E-07 -.34909973E-10 .36945345E-14
-.87738042E+03 -.19629421E+01 .30574451E+01 .26765200E-02 -.58099162E-05
.55210391E-08 -.18122739E-11 -.98890474E+03 -.22997056E+01
H2O    J 3/61H 2.0 1.00 0.00 0.G   300.000  5000.000
.27167633E+01 .29451374E-02 -.80224374E-06 .10226682E-09 -.48472145E-14
-.29905826E+05 .66305671E+01 .40701275E+01 -.11084499E-02 .41521180E-05
-.29637404E-08 .80702103E-12 -.30279722E+05 -.32270046E+00
N2     J 9/65N 2.0 0.0 0.0 0.G   300.000  5000.000
.28963194E+01 .15154866E-02 -.57235277E-06 .99807393E-10 -.65223555E-14
-.90586184E+03 .61615148E+01 .36748261E+01 -.12081500E-02 .23240102E-05
-.63217559E-09 -.22577253E-12 -.10611588E+04 .23580424E+01
O      J 6/74O 1.      0.      0.      0.G   300.000  5000.000
.25352638E+01 -.14371898E-04 -.11360139E-07 .66005131E-11 -.61181626E-15
.29230265E+05 .49575621E+01 .29558662E+01 -.17061536E-02 .25925154E-05
-.17837980E-08 .45709012E-12 .29143654E+05 .29243614E+01
OH     J12/700 1.H 1.0 0.0 0.G   300.000  5000.000
.29131230E+01 .95418248E-03 -.19084325E-06 .12730795E-10 .24803941E-15
.39647060E+04 .54288735E+01 .38365518E+01 -.10702014E-02 .94849757E-06
.20843575E-09 -.23384265E-12 .36715807E+04 .49805456E+00
O2     J 9/65O 2.0 0.0 0.0 0.G   300.000  5000.000
.36219535E+01 .73618264E-03 -.19652228E-06 .36201558E-10 -.28945627E-14
-.12019825E+04 .36150960E+01 .36255985E+01 -.18782184E-02 .70554544E-05
-.67635137E-08 .21555993E-11 -.10475226E+04 .43052778E+01
END

```

Table 6-4. SPECIES WITH THERMODYNAMIC DATA PROVIDED.

E	AL2O2	BE	CH2O2	C4
AL	AL2O2+	BE+	CH3	C4H8O4
AL+	AR	BEBO2	CH3CL	N-C4H10
AL-	AR+	BEBR	CH2OH	I-C4H10
ALBO2	B	BEBR2	CH3O	C4N2
ALBR	B+	BECL	CH4	C5
ALBR3	B-	BECL+	CH3OH	C6H5
ALC	BCL	BECLF	CN	C6H6
ALCL	BCL+	BECLF2	CN+	CA
ALCL+	BCLF	BEF	CN-	CA+
ALCLF	BCL2	BEF2	CN2	CABR
ALCLF+	BCL2+	BEH	CNN	CABR2
ALCLF2	BCL2-	BEH+	CO	CACL
ALCL2	BCL3	BEI	COCL	CACL2
ALCL2+	BF	BEI2	COCLF	CAF
ALCL2-	BF2	BEN	COCL2	CAF2
ALCL2F	BF2+	BEO	COF	CAI
ALCL3	BF2-	BEOH	COF2	CAI2
ALF	BF3	BEOH+	COS	CAO
ALF+	BH	BEO2H2	CO2	CAOH
ALF2	BHF2	BES	CO2-	CAOH+
ALF2+	BH2	BE2O	CP	CAO2H2
ALF2-	BH3	BE2OF2	CS	CAS
ALF2O	BN	BE2O2	CS2	CA2
ALF2O-	BO	BE3O3	C2	CL
ALF3	BOCL	BE4O4	C2-	CL+
ALF4-	BOF	BI	C2CL2	CL-
ALH	BOF2	BIS	C2F2	CLCN
ALI	BO2	BR	C2F4	CLF
ALI3	BO2-	BR2	C2H	CLF3
ALN	BS	C	C2HF	CLO
ALO	B2	C+	C2H2	CLO2
ALO+	B2O	C-	C2H4	CL2
ALO-	B2O2	CCL	C2H4O2	CL2O
ALOCL	B2O3	CCL2	C2H4O4	CR
ALOF	B3O3CL3	CCL2F2	C2H5	CRN
ALOH	B3O3F3	CCL3	C2H6	CRO
ALOH+	B3O3H3	CCL3F	CH3N2CH3	CRO2
ALOH-	BA	CCL4	C2H5OH	CRO3
ALO2	BABR	CF	CH3OCH3	CS
ALO2-	BABR2	CF+	C2N	CS+
ALO2H	BACL	CF2	C2N2	CSCL
ALS	BACL2	CF2+	C2O	CSF
AL2	BAF	CF3	C3	CSO
AL2BR6	BAF+	CF3+	C3H6O	CSOH
AL2CL6	BAF2	CF4	N-C3H7	CSOH+
AL2F6	BAOH	CH	I-C3H7	CS2
AL2I6	BAOH+	CH+	C3H8	CS2CL2
AL2O	BAO2H2	CH2	1-C3H7OH	CS2F2
AL2O+	BAS	CH2O	C3O2	CS2O

Table 6-4. (cont.)

CS2O2H2	HBS+	KO	MGN	NAH
CS2SO4	HBR	KO-	MGO	NAI
CU	HCN	KOH	MGOH	NAO
CU+	HCO	KOH+	MGOH+	NAO-
CUCL	HCO+	K2	MGO2H2	NAOH
CUF	HCP	K2C2N2	MGS	NAOH+
CUF2	HCL	K2CL2	MG2	NA2
CUO	HD	K2F2	MG2F4	NA2C2N2
CU2	HD+	K2O2H2	N	NA2CL2
CU3CL3	HD-	K2SO4	N+	NA2F2
D	HDO	KR	N-	NA2O
D+	HF	LI	NCO	NA2O2H2
D-	HI	LI+	ND	NA2SO4
DCL	HNCO	LIALF4	ND2	NB
DF	HNO	LIBO2	ND3	NBO
DOCL	HNO2	LICL	NF	NBO2
D2	HNO3	LIF	NF2	NE
D2+	HOCL	LIFO	NF3	NE+
D2-	HOF	LIF2-	NH	NI
D2O	HO2	LIH	NH2	NICL
D2S	HSO3F	LIN	NH3	NICL2
F	H2	LIO	NO	NIO
F-	H2+	LIO-	NO+	NIS
FCN	H2-	LIOH	NOCL	O
FO	H2F2	LIOH+	NOF	O+
FO2	H2N2	LION	NOF3	O-
F2	H2O	LI2	NO2	OD
F2O	H2O2	LI2CL2	NO2-	OH
FS2F	H2S	LI2F2	NO2CL	OH+
FE	H2SO4	LI2O	NO2F	OH-
FE+	H3B3O6	LI2O2	NO3	O2
FE-	H3F3	LI2O2H2	N2	O2+
FEC5O5	H4F4	LI2SO4	N2+	O2-
FECL	H5F5	LI3CL3	N2-	O3
FECL2	H6F6	LI3F3	N2D2	P
FECL3	H7F7	MG	N2H4	P+
FEO	HE	MG+	N2O	PCL3
FEO2H2	HE+	MGBR	N2O+	PF
FES	HG	MGBR2	N2O4	PF+
FE2CL4	HGBR2	MGCL	N2O5	PF-
FE2CL6	I	MGCL+	N3	PF2
H	I2	MGCLF	NA	PF2+
H+	K	MGCL2	NA+	PF2-
H-	K+	MGF	NAALF4	PF3
HALO	KBO2	MGF+	NABO2	PF5
HBO	KCN	MGF2	NABR	PH
HBO+	KCL	MGF2+	NACN	PH3
HBO-	KF	MGH	NACL	PN
HBO2	KF2-	MGI	NAF	PO
HBS	KH	MGI2	NAF2-	PO2

Table 6-4. (cont.)

PS	SOF2	SI2	ALCL3 (L)	BI (L)
P2	SO2	SI2C	ALF3 (A)	BI2S3 (S)
P4	SO2CLF	SI2N	ALF3 (B)	BR2 (L)
P4O6	SO2CL2	SI3	ALF3 (L)	C (GR)
P4O10	SO2F2	SR	ALI3 (S)	CA (A)
PB	SO3	SRBR	ALI3 (L)	CA (B)
PBBR	S2	SRCL	ALN (S)	CA (L)
PBBR2	S2CL	SRCL2	AL2O3 (A)	CABR2 (S)
PBBR4	S2CL2	SRF	AL2O3 (L)	CABR2 (L)
PBCL	S2F2	SRF+	AL2SIO5 (AN)	CACO3 (CAL)
PBCL+	S2O	SRF2	AL6SI2O13 (S)	CACL2 (S)
PBCL2	S8	SRI2	B (S)	CACL2 (L)
PBCL2+	SI	SRO	B (L)	CAF2 (A)
PBCL4	SI+	SROH	BN (S)	CAF2 (B)
PBF	SIBR	SROH+	B2O3 (L)	CAF2 (L)
PBF2	SIBR2	SRO2H2	B3O3H3 (C)	CAO (S)
PBF4	SIBR3	SRS	BA (A)	CAO (L)
PBI	SIBR4	TA	BA (B)	CAO2H2 (S)
PBI2	SIC	TAO	BA (C)	CAS (S)
PBI4	SIC2	TAO2	BA (L)	CASO4 (S)
PBO	SIC4H12	TI	BABR2 (S)	CR (S)
PBS	SICL	TI+	BABR2 (L)	CR (L)
PB2	SICL2	TI-	BACL2 (A)	CRN (S)
S	SICL3	TICL	BACL2 (B)	CR2N (S)
S+	SICL4	TICL2	BACL2 (L)	CR2O3 (S)
S-	SIF	TICL3	BAF2 (AB)	CR2O3 (L)
SCL	SIF2	TICL4	BAF2 (C)	CS (S)
SCL2	SIF3	TIO	BAF2 (L)	CS (L)
SCL2+	SIF4	TIOCL	BAO (S)	CSCL (A)
SD	SIH	TIOCL2	BAO (L)	CSCL (B)
SF	SIH+	TIO2	BAO2H2 (S)	CSCL (L)
SF+	SIHBR3	V	BAO2H2 (L)	CSF (S)
SF-	SIHCL3	VCL4	BAS (S)	CSF (L)
SF2	SIHF3	VN	BE (S)	CSOH (A)
SF2+	SIHI3	VO	BE (L)	CSOH (C)
SF2-	SIH2BR2	VO2	BEAL2O4 (S)	CSOH (L)
SF3	SIH2CL2	XE	BEAL2O4 (L)	CS2SO4 (II)
SF3+	SIH2F2	XE+	BEBR2 (S)	CS2SO4 (I)
SF3-	SIH2I2	ZN	BECL2 (S)	CS2SO4 (L)
SF4	SIH3BR	ZN+	BECL2 (L)	CU (S)
SF4+	SIH3CL	ZN-	BEF2 (LQZ)	CU (L)
SF4-	SIH3F	ZR	BEF2 (HQZ)	CUF (S)
SF5	SIH3I	ZRN	BEF2 (L)	CUF2 (S)
SF5+	SIH4	ZRO	BEI2 (S)	CUF2 (L)
SF5-	SII	ZRO2	BEI2 (L)	CUO (S)
SF6	SII2	AL (S)	BEO (A)	CUO2H2 (S)
SF6-	SIN	AL (L)	BEO (L)	CUSO4 (S)
SH	SIO	ALBR3 (S)	BEO2H2 (B)	CU2O (S)
SN	SIO2	ALBR3 (L)	BES (S)	CU2O (L)
SO	SIS	ALCL3 (S)	BI (S)	CU2O5S (S)

Table 6-4. (cont.)

FE (A)	K2S (1)	MGTI2O5 (S)	NB2O5 (L)	SRCL2 (L)
FE (C)	K2S (2)	MGTI2O5 (L)	NI (A)	SRF2 (S)
FE (D)	K2S (3)	MG2SIO4 (S)	NI (B)	SRF2 (L)
FE (L)	K2S (L)	MG2SIO4 (L)	NI (L)	SRO (S)
FEC5O5 (L)	K2SO4 (A)	MG2TIO4 (S)	NIS (B)	SRO (L)
FECL2 (S)	K2SO4 (B)	MG2TIO4 (L)	NIS (A)	SRO2H2 (S)
FECL2 (L)	K2SO4 (L)	VN (S)	NIS (L)	SRO2H2 (L)
FECL3 (S)	LI (S)	NA (S)	NIS2 (S)	SRS (S)
FECL3 (L)	LI (L)	NA (L)	NIS2 (L)	TA (S)
FEO (S)	LIALO2 (S)	NAALO2 (A)	NI3S2 (1)	TA (L)
FEO (L)	LIALO2 (L)	NAALO2 (B)	NI3S2 (2)	TAC (S)
FEO2H2 (S)	LICL (S)	NABR (S)	NI3S2 (L)	TAC (L)
FEO3H3 (S)	LICL (L)	NABR (L)	NI3S4 (S)	TA2O5 (S)
FES (A)	LIF (S)	NACN (S)	P (V)	TA2O5 (L)
FES (B)	LIF (L)	NACN (L)	P4O10 (S)	TI (A)
FES (C)	LIH (S)	NACL (S)	PB (S)	TI (B)
FES (L)	LIH (L)	NACL (L)	PB (L)	TI (L)
FESO4 (S)	LIOH (S)	NAF (S)	PBBR2 (S)	TIC (S)
FES2 (S)	LIOH (L)	NAF (L)	PBBR2 (L)	TIC (L)
FE2O3 (S)	LI2O (S)	NAI (S)	PBCL2 (S)	TICL2 (S)
FE2S3O12 (S)	LI2O (L)	NAI (L)	PBCL2 (L)	TICL3 (S)
FE3O4 (S)	LI2SO4 (A)	NAOH (A)	PBF2 (A)	TICL4 (L)
H2O (S)	LI2SO4 (B)	NAOH (L)	PBF2 (B)	TIN (S)
H2O (L)	LI2SO4 (L)	NAO2 (S)	PBF2 (L)	TIN (L)
H2SO4 (L)	LI3N (S)	NA2CO3 (1)	PBI2 (S)	TIO (A)
HG (L)	MG (S)	NA2CO3 (2)	PBI2 (L)	TIO (B)
HGBR2 (S)	MG (L)	NA2CO3 (L)	PBO (RD)	TIO (L)
HGBR2 (L)	MGAL2O4 (S)	NA2O (C)	PBO (YW)	TIO2 (RU)
HGO (S)	MGAL2O4 (L)	NA2O (A)	PBO (L)	TIO2 (L)
I2 (S)	MGBR2 (S)	NA2O (L)	PBO2 (S)	TI2O3 (1)
I2 (L)	MGBR2 (L)	NA2O2 (A)	PBS (S)	TI2O3 (2)
K (S)	MGCO3 (S)	NA2O2 (B)	PBS (L)	TI2O3 (L)
K (L)	MGCL2 (S)	NA2S (1)	PB3O4 (S)	TI3O5 (A)
KCN (S)	MGCL2 (L)	NA2S (2)	S (S)	TI3O5 (B)
KCN (L)	MGF2 (S)	NA2S (L)	S (L)	TI3O5 (L)
KCL (S)	MGF2 (L)	NA2SO4 (IV)	SCL2 (L)	TI4O7 (S)
KCL (L)	MGI2 (S)	NA2SO4 (I)	S2CL2 (L)	TI4O7 (L)
KF (S)	MGI2 (L)	NA2SO4 (L)	SI (S)	V (S)
KF (L)	MGO (S)	NA3ALF6 (A)	SI (L)	V (L)
KHF2 (A)	MGO (L)	NA3ALF6 (B)	SIC (B)	VCL2 (S)
KHF2 (B)	MGO2H2 (S)	NA3ALF6 (L)	SIO2 (LQZ)	VCL3 (S)
KHF2 (L)	MGS (S)	NA5AL3F14 (S)	SIO2 (HQZ)	VCL4 (L)
KOH (A)	MGSO4 (S)	NA5AL3F14 (L)	SIO2 (HCR)	VO (S)
KOH (B)	MGSO4 (L)	NB (S)	SIO2 (L)	VO (L)
KOH (L)	MGSIO3 (CL)	NB (L)	SI2N2O (S)	V2O3 (S)
KO2 (S)	MGSIO3 (RE)	NBO (S)	SI3N4 (A)	V2O3 (L)
K2CO3 (S)	MGSIO3 (PR)	NBO (L)	SR (S)	V2O4 (1)
K2CO3 (L)	MGSIO3 (L)	NBO2 (S)	SR (L)	V2O4 (2)
K2O (S)	MGTIO3 (S)	NBO2 (L)	SRCL2 (1)	V2O4 (L)
K2O2 (S)	MGTIO3 (L)	NB2O5 (S)	SRCL2 (2)	V2O5 (S)

Table 6-4. (cont.)

V2O5 (L)  
ZN(S)  
ZN(L)  
ZNSO4 (A)  
ZNSO4 (AP)  
ZNSO4 (B)  
ZR(A)  
ZR(B)  
ZR(L)  
ZRN(S)  
ZRN(L)  
ZRO2 (A)  
ZRO2 (B)  
ZRO2 (L)



### 6.1.1 THERMODYNAMIC DATA BELOW 300°K.

If the temperature at any point computed by ODE, ODK, or TDK is found to be below the Thermodynamic Data lower temperature limit,  $T_l$ , the polynomial curve fit data (see Section 6.1) will be extrapolated to obtain values for the thermodynamic data. The extrapolated data can be inaccurate. The LOW T CPHS data set can be used to input low temperature data for those species for which extrapolation of the JANNAF data is not accurate. Only  $C_p$  vs.  $T$  is input. Enthalpy and entropy are obtained by integrating  $C_p$  vs.  $T$  within the computer program.

The lower temperature limit,  $T_l$ , in the Thermodynamic Data supplied with the program is 300°K. Thermodynamic Data below the temperature,  $T_l$ , may be input by data cards as described under "Input Specifications for Low Temperature Thermodynamic Data".

An example of this input is given in Table 6-5 which shows a card listing extending the Thermodynamic Data for the 18 chemical species given in Appendix A. Data in Table 6-5 is taken directly from the JANAF tables. The source references for these data are as follows:

Ref. 21: CO, CO<sub>2</sub>, CL<sub>2</sub>, F, HCL, H<sub>2</sub>O, and NO.

Ref. 22: CL.

Ref. 23: CLF, F<sub>2</sub>, F, HF, H<sub>2</sub>, N, N<sub>2</sub>, O, OH, and O<sub>2</sub>.

Ref. 21: Stull, D.R., Prophet, H., et al., JANAF Thermochemical Tables, Second Edition, NSRDS-NBS 37, National Standard Reference Data Series, National Bureau of Standards, June 1971.

Ref. 22: JANAF Thermochemical Tables, 1974 Supplement, J. Phys. Chem. Ref. Data 3,311 (1974).

Ref. 23: JANAF Thermochemical Tables, 1982 Supplement, J. Phys. Chem. Ref. Data 11,695 (1982).



Table 6-5. Low Temperature Thermodynamic Data Input

col. 1 11 21 45

LOW T CPHS			
CO		2	
100.	6.956		1
200.	6.957		2
CO2		2	
100.	6.981		1
200.	7.734		2
CL		2	
100.	4.968		1
200.	5.038		2
CLF		2	
100.	6.961		1
200.	7.200		2
CL2		2	
100.	7.001		1
200.	7.576		2
F		2	
100.	5.068		1
200.	5.403		2
F2		2	
100.	6.958		1
200.	7.095		2
H		2	
100.	4.968		1
200.	4.968		2
HCL		2	
100.	6.959		1
200.	6.961		2
HF		2	
100.	6.962		1
200.	6.962		2
H2		2	
100.	6.729		1
200.	6.560		2
H2O		2	
100.	7.961		1
200.	7.969		2
N		2	
100.	4.968		1
200.	4.968		2
NO		2	
100.	7.721		1
200.	7.721		2
N2		2	
100.	6.956		1
200.	6.957		2
O		2	
100.	5.665		1
200.	5.433		2
OH		2	
100.	7.798		1
200.	7.356		2
O2		2	
100.	6.956		1
200.	6.961		2
END LOW T CPHS			

## 6.2 Title Cards

This input permits labeling of runs with alphanumeric information. As many title cards as desired may be input in sequence. Card format is as follows:

col 1-5	col 6-77
TITLE	any alphanumeric information

The last card that is input will be used as a printed title for the output summary table, and a title for the linkage file to BLIMP (see Section 6.4.3.2, IPTAB).

It is not necessary to input title cards.

### 6.3 DATA Directive and \$DATA Namelist Input.

The DATA directive and the \$DATA Namelist input set described below must always be input. It is required for all problems since it contains the input that controls which calculation modules are to be executed.

The first input item must be a single card, called the DATA directive card. The format of this card is as follows: the letters DATA must be punched in columns 1 through 4. The DATA card is used to inform the program that the \$DATA namelist input is to follow.

The card following the DATA card must contain the name \$DATA, and all cards in the namelist input set must start in column 2 or greater. Since Namelist input is card interpretive, items can be input in any order. The last card in the set must contain \$END.

Users unfamiliar with Namelist input are referred to their FORTRAN reference manual.

<u>Item</u>	<u>Description</u>	<u>Units</u>	<u>Assumed Value(s)</u>
DATA	DATA directive card		-
\$DATA	Namelist name, read in Subroutine PRØBLM		-

### 6.3.1 Specification of Modules to be Executed.

If a module is to be executed, it is necessary to indicate the fact by input of a module flag as described below. For example, if a problem requires that the  $\emptyset$ DE module be run, it is necessary to input  $\emptyset$ DE = 1. Only certain combinations of modules are allowed. These are described in Table 6-6. The module flags are:

<u>Item</u>		<u>Description</u>	<u>Units</u>	<u>Assumed Value(s)</u>
$\emptyset$ DE	=	Set $\emptyset$ DE = 1 if the ODE module is to be executed.	none	0.
$\emptyset$ DK	=	Set $\emptyset$ DK = 1 if the ODK module is to be executed.	none	0.
TDE	=	Set TDE = 1 if the TDE option of the MOC module is to be executed	none	0.
TDK	=	Set TDK = 1 if the TDK option of the MOC module is to be executed	none	0.
TDF	=	Set TDF = 1 if the TDF option of the MOC is to be executed	none	0.
TTDK	=	Set TTDK=1 to run the TDK option with tables supplied by ODK replacing the TDK kinetic calculations. See Section 2.5.3.	none	0.
BLM	=	Set BLM = 1 if the BLM option of the MOC module is to be executed	none	0.
PFGOPT	=	Set PFGOPT = 1 if the constant properties option of the MOC module is to be executed. See Section 6.9.1 for input instructions.	none	0.

Table 6-6: Usage of the Module Flags

<u>Input</u>	<u>Mode of Execution</u>
ØDE=1,	ØDE is run alone. Options other than the rocket (RKT=T) option are allowed. See Section 6.4.3 and Reference 3.
ØDE=1, ØDK=1,	ØDE is run. ØDK is run with ØDE providing start conditions. See Section 6.5.1.
ØDK=1,	ØDK is run alone with initial conditions supplied by the user. See Sections 6.5.1 and 6.5.1.1, and 6.5.3.6.
ØDE=1, ØDK=1, TDK=1,	ØDE is run. ØDK is run with ØDE providing start conditions. TDK is run with ØDK and TRANS providing MØC initial data line conditions. The number of ØDE and ØDK runs will be equal to NZØNES.
ØDE=1, ØDK=1, TDK=1, BLM=1,	As above with a BLM run added.
ØDE=1, ØDK=1, TDK=1, BLM=1, IRPEAT=1,	As above with ØDE, ØDK, and TDK repeated using the BLM results. See Section 6.8.4. This option is for including the BLM results with regen cooling.
ØDE=1, ØDK=1, TDK=1, BLM=1, IRPEAT=2,	As above except that the ØDE and ØDK runs are not repeated because there is no heat input correction due to regen cooling.
ØDE=1, ØDK=1, TTDK=1, BLM=1 IRPEAT=1 or 2	As above except that TDK will use tables computed by ØDK and not compute its own reacting chemistry.
TDE=1,	ØDE will be run for NZØNES. TDE is run with ØDE chemical equilibrium gas properties, and with TRANS providing MØC initial data line conditions.
TDE=1, BLM=1,	As above with BLM.
TDE=1, BLM=1, IRPEAT=1 or 2,	As above with TDE repeated.

Table 6-6: Usage of the Module Flags (continued)

<u>Input</u>	<u>Mode of Execution</u>
ODE=1, ODK=1, TDF=1,	ODE is run. ODK is run with ODE providing start conditions. However, the ODK run will have a frozen chemical composition. TDK will also be run with a frozen composition.
ODE=1, ODK=1, TDF=1, BLM=1,	As above with BLM.
ODE=1, ODK=1, TDF=1, BLM=1, IRPEAT=1 or 2,	As above with TDF repeated.
BLM=1,	BLM is run alone. This option requires a large amount of input that is provided automatically when BLM is run after TDE, TDK or TDF.
PFGOPT=1,	The TRANS and MOC modules are run with constant gas properties. See Section 6.9.1.

6.3.2 Inputs for Control for the Program.

<u>Item</u>	<u>Description</u>	<u>Units</u>	<u>Assumed Value(s)</u>
IRPEAT =	<p>Set IRPEAT = 1 or 2 to request that a TDK (or TDE) calculation be automatically repeated after the BLM module has been used to calculate a displaced nozzle wall.</p> <p>If IRPEAT = 1, the ODE and ODK module executions will be repeated with adjusted enthalpies for regen cooling, see Section 6.8.4.</p> <p>If IRPEAT = 2, the ODE and ODK module executions will not be repeated. The system enthalpy will be unchanged.</p>	none	0
IRSTRT =	<p>The program allows for a limited restart capability. If the MOC module has been run successfully and units 11, 15, (23 if TDE), and 29 have been saved, then the run can be continued by inputting</p> <p style="text-align: center;">IRSTRT = 2,</p> <p>This will restart the program after the MOC calculation and before the BLM calculation. The restart handles all options involving BLM.</p>	none	



<u>Item</u>	<u>Description</u>	<u>Units</u>	<u>Assumed Value(s)</u>
NZONES =	Number of zones N, to be used in the analysis. The ØDE and ØDK modules will be executed N times. Zone 1 represents the flow adjacent to the nozzle axis, and Zone N represents flow adjacent to the nozzle wall.	none	1
SI =	If SI=0, English units are to be used for input and output. If SI=1, SI units are to be used for input and output. The SI units required for input are shown in parenthesis.	none	0
IØFF =	When BLM is run with the MOC module, values defining the boundary layer edge conditions; $x_e$ , $y_e$ , $U_e$ , $T_e$ , and $P_e$ are automatically calculated and stored in the XINØ, RINØ, UEØ, TEØ, and PEØ arrays. If IØFF is not input, then these values are stored starting with the first entry in each array. If IØFF is input then these values are stored starting in the IØFF + 1 entry of each array. Values must then be input into entries 1 through IØFF. The boundary layer calculations will start at position XINØ(1) of these arrays using the \$BLM input. This input allows the user to account for the development of the boundary layer in the nozzle chamber, upstream of ECRAT. IØFF < 100. If IØFF is input, do not input NXINØ \$BLM.		0
BLMF =	This flag controls the choice of gas properties and edge properties to be used by the BLM. (See Section 2.6.3, etc.) If TDK has been run, then for BLMF=F, equilibrium (ØDE) properties will be used. If TDK has been run, then for BLMF=T, frozen (ØDF) properties will be used. For TDE, equilibrium properties will always be used. For TDF, frozen properties will always be used.	none	F

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### 6.3.3 Specification of nozzle geometry.

To eliminate redundancy, all geometry inputs that are common throughout the modules are input here. Note that the center of the nozzle geometry coordinate system is at the centerline at the throat plane, and that all coordinates are normalized by the nozzle throat radius,  $r_t$ . Hence, axial positions upstream of the throat are always negative numbers. In the figures describing the geometry, positive angles are shown as counter-clockwise, and negative angles are shown as clockwise.

Geometric area ratios at which  $\phi_{DE}$  and  $\phi_{DK}$  print out is to be made are specified using the input arrays ASUB(1) and ASUP(1).

The nozzle geometry is defined in Figure 6-1. The  $\phi_{DK}$  calculations start at the downstream end of the combustion chamber with a subsonic area ratio of ECRAT, as shown. The circular arcs RI and RWTU cannot overlap. Thus, it is necessary that ECRAT, RI, RWTU, and THETA1 be input such that

$$\sqrt{\text{ECRAT}} > 1 + (\text{RI} + \text{RWTU}) (1 - \cos \text{THETA1}).$$

If this condition is not met, subroutine PRES of  $\phi_{DK}$  will print the terminal error message:

INLET GEOMETRY INCOMPATIBLE WITH INITIAL CONDITIONS.

In addition, the transonic analysis requires that a value of  $\text{RWTU} \geq .5$  be input.

The wall geometry downstream of the nozzle throat can be specified using any one of several options. All of these geometries begin with a circular arc of radius RWTU which extends from the throat point through an angle of THETA. Geometries that can be input to both the  $\phi_{DK}$  and MOC modules are described in Section 6.3.3.1.

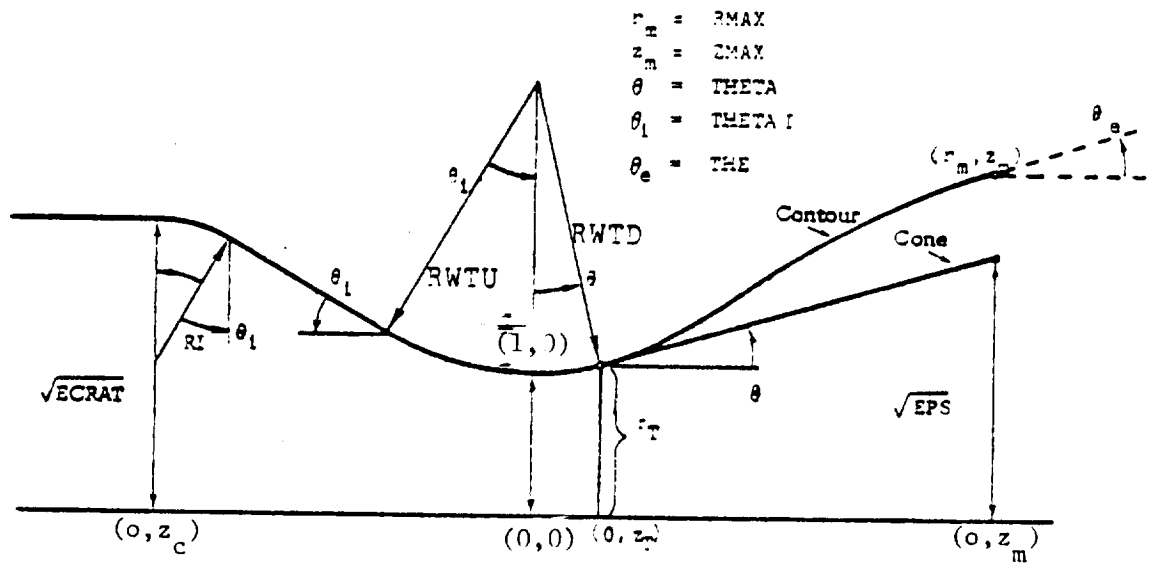


Figure 6-1: Nozzle Geometry, all coordinate values are normalized by  $RSI = r_c$ .

<u>Item</u>	<u>Description</u>	<u>Units</u>	<u>Assumed Value(s)</u>
RSI	= Nozzle throat radius, $r_t$	in, (meters)	0.
ASUB(1)	= Subsonic area ratios at which information will be printed.	none	0.
NASUB	= Number of entries in the ASUB array < 50. Entries must be monotonic decreasing in value.	none	0.
ASUP(1)	= Supersonic area ratios at which information will be printed. Entries must be monotonic increasing in value.	none	0.
NASUP	= Number of entries in the ASUP array < 50.	none	0.
ECRAT	= Nozzle inlet contraction ratio for use in $\emptyset$ DE and $\emptyset$ DK calculations.	none	0.
RI	= Normalized inlet wall radius.	none*	0.
THETA1	= Nozzle inlet angle.	degrees	0.
RWTU	= Upstream normalized wall throat radius RWTU > .5 is required.	none*	0.
IITYPE	= Type of nozzle wall to be input. IITYPE = 0, if the real wall contour is input. IITYPE = 1, if the potential flow wall contour is input. If IRPEAT = 1 or 2, then the nozzle wall will be displaced by $+\delta^*$ as calculated by BLM when the TDK (or TDE) calculations are repeated. This displacement is $-\delta^*$ for the real wall (IITYPE = 0), or $+\delta^*$ for the potential flow wall (IITYPE = 1).	none	0.

---

\* Normalized by the throat radius,  $r_t$

6.3.3.1 Exhaust Nozzle Geometry Specification, for ØDK and the MØC Modules.

<u>Item</u>		<u>Description</u>	<u>Units</u>	<u>Assumed Value(s)</u>
IWALL	=	option flag for specifying the downstream wall.	none	0
	=	1 cone option (input RWTD, THETA, and EPS)		
	=	2 parabolic nozzle contour option (input RWTD, THETA, RMAX, ZMAX)		
	=	3 circular arc nozzle contour option (input as for IWALL=2)		
	=	4 nozzle contour (spline) option (input RWTD, THETA, THE, RS, ZS, NWS)		
	=	5 cone with specified end point. (input RWTD, RMAX, and ZMAX)		
	=	6 skewed parabola option. (input RWTD, THETA, RMAX, ZMAX, THE)		

The items required for the various IWALL options are:

RWTD	=	downstream wall throat radius of curvature ratio**	none*	0.
THETA	=	nozzle attachment angle		
THE	=	nozzle exit angle (input if IWALL=4, or 6)	deg.	0.
EPS	=	nozzle expansion ratio (input if IWALL=1 only)	deg.	0.
RMAX	=	normalized radius at the nozzle exit plane (input if IWALL=2 or 3)	none*	0.
ZMAX	=	normalized axial position at the nozzle exit plane (input if IWALL = 2 or 3)	none*	0.

\* Normalized by the throat radius  $r_t$

\*\* If a corner expansion (i.e. Prandtl-Meyer fan) is desired, a value of RWTD = .05 is recommended. Experience has shown that values smaller than this give the same result but are computationally less efficient.

<u>Item</u>	<u>Description</u>	<u>Units</u>	<u>Assumed Value(s)</u>
RS(2)	= table of normalized wall radii downstream of the nozzle tangency point (input if IWALL=4). The input tables RS and ZS start with the second entry because the first entry is calculated automatically by the program, i.e., $RS(1)=r_T$ and $ZS(1)=z_T$ in Figure 6-1. The wall angle at this position is also calculated so that the spline contour will be properly joined to the nozzle throat contour.	none <sup>+</sup>	0.
ZS(2)	= table of normalized axial position downstream of the nozzle tangency point (input if IWALL=4).	none <sup>+</sup>	0.
NSW	= total number of entries in the RS, ZS tables. Includes the first entry. $NWS \leq 50$ (input if IWALL=4).	none	0
RZNØRM	= optional normalizing factor for the RS, ZS, RIN, ZIN tables. For example, if RS, ZS, and RIN, ZIN were input as dimensional numbers, RZNØRM would be the throat radius in those units.	none	1.

+ See the input variable RZNØRM.

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## 6.4 ØDE INPUT DATA (ALL PROBLEMS SPECIFYING ØDE)

The ØDE Input data described here is exactly as defined in NASA SP-273, Reference 3, except namelists input \$INPT2 and \$RKINP have been combined into a single list named \$ØDE. Any type of equilibrium calculation available with the computer program described in Reference 3 can thus be computed using the \$ØDE input data\*. In this document, however, only the RKT option of namelist is described. The RKT option differs from that of Reference 3 for problem types other than single zone ØDE.

The ØDE input data consists of the following input groups:

1. REACTANTS directive card, followed by up to 15 data cards, followed by a blank card, specifying reactants.
2. ØMIT and INSERT directives to omit or insert species for equilibrium/frozen calculations.
3. NAMELISTS directive card followed by input namelist \$ØDE specifying input case data.

### 6.4.1 REACTANTS CARDS

This set of cards is required for all ØDE problems. The first card in the set contains the word REACTANTS punched in card columns 1 to 9. The last card in the set is blank. In between the first and last cards may be any number of cards up to a maximum of 15, one for each reactant species being considered. The cards for each reactant must give the chemical formula and the relative amount of the reactant. For some problems, enthalpy values are required. The format and contents of the cards are summarized in Table 6-7. A list of some REACTANTS cards is given in Table 6-8

Relative amounts of reactants. - The relative amounts of reactants may be specified in several ways. They may be specified in terms of moles, mole fraction, or mole percent (by keypunching M in card column 53) or in terms of weight, weight fraction, or weight percent (blank in column 53).

Relative amounts of total fuel to total oxidants can also be input. For this situation, each reactant must be specified as a fuel or an oxidizer by keypunching an F or O, respectively, in column 72 of the REACTANTS card. The amounts

\*These options include TP, HP, SP, TV, UV, or SV problems, Chapman-Jouguet detonation problems, and incident or reflected shock problems.

TABLE 6-7 REACTANTS CARDS

Order	Contents	Format	Card columns
First	REACTANTS	3A4	1 to 9
Any	One card for each reactant species (maximum 15). Each card contains:		
	(1) Atomic symbols and formula numbers (maximum 5 sets) <sup>a</sup>	5(A2. F7. 5)	1 to 45
	(2) Relative weight <sup>b</sup> or number of moles	F7. 5	46 to 52
	(3) Blank if (2) is relative weight or M if (2) is number of moles	A1	53
	(4) Enthalpy or internal energy <sup>a</sup> , cal mole	F9. 5	54 to 62
	(5) State: S, L, or G for solid, liquid or gas, respectively	A1	63
	(6) Temperature associated with enthalpy in (4), °K	F8. 5	64 to 71
	(7) F if fuel or O if oxidant	A1	72
	(8) Density in g cm <sup>3</sup> (optional)	F8. 5	73 to 80
Last	Blank		

<sup>a</sup>Program will calculate the enthalpy or internal energy (4) for species in the THERMO data at the temperature (6) if zeros are punched in card columns 37 and 38. (See section Reactant enthalpy for additional information.)

<sup>b</sup>Relative weight of fuel in total fuels or oxidant in total oxidants. All reactants must be given either all in relative weights or all in number of moles.



TABLE 6-8 LISTING OF SAMPLE REACTANTS CARDS

REACTANTS					
H 2.					
N	.7808810 .209795AR.004662	100.	0.	G298.15	F
		100.	-7.202164	G298.15	O

REACTANTS					
N 1.	H 4.	CL1.	O 4.		
C 1.	H	1.869550 .031256S .008415	72.06	-70730.	S298.15 F
AL1.			18.58	-2999.082L	L298.15 F
MG1.	O 1.		9.00	*C.0	S298.15 F
H 2.	O 1.		.20	-143700.	S298.15 F
			.16	-68317.4	L298.15 F

REACTANTS					
H 2.					
O 2.		00	100.	0.	G298.15 F
		00	100.0	0.0	G298.15 O

REACTANTS					
N 2.	H 8.	C 2.			
N 2.	H 4.		50.0	12734.8	L298.15 F .786
F 2.			50.0	12050.	L298.15 F 1.002
			100.	-3030.892L	85.24 O 1.54

REACTANTS					
L11.					
F 2.			100.	0.	S298.15 F
			100.	-3030.892L	85.24 O 1.54

REACTANTS					
N 2.	H 4.				
BE1.			80.	12100.	L298.15 F 1.003
H 2.	O 2.		20.	0.0	S298.15 F 1.85
			100.	-44880.	L298.15 O 1.407

\*Listed above are six examples. Each example must end with a blank card.

given on the REACTANTS cards are relative to total fuel or total oxidant rather than total reactant.

There are four options in the \$ØDE namelist for indicating relative amounts of total fuel to total oxidant as follows:

1. Oxidant to fuel weight ratio (ØF is true)
2. Equivalence ratio (ERATIO is true)
3. Fuel percent by weight (FPCT is true)
4. Fuel to air or fuel to oxidant weight ratio (FA is true)

For each option, except ØDE with NZØNES=1, the values are given in the ØFSKED array of \$ØDE (described in Section 6.4.3). For ØDE with NZØNES=1, the MDX array is used as described in Reference 3.

Reactant enthalpy. Assigned values for the total reactant are calculated automatically by the program from the enthalpies of the individual reactants. Values for the individual reactants are either keypunched on the REACTANTS cards or calculated from the THERMØ data as follows:

Enthalpies are taken from the REACTANTS cards unless zeros are punched in card columns 37 and 38. For each REACTANTS card with the "00" code, an enthalpy will be calculated for the species from the THERMØ data for the temperature given in card columns 64 to 71.

When the program is calculating the individual reactant enthalpy for values from the THERMØ data, the following two conditions are required:

1. The reactant must also be one of the species in the set of THERMØ data. For example,  $\text{NH}_3(\text{g})$  is in the set of THERMØ data but  $\text{NH}_3(\text{l})$  is not. Therefore, if  $\text{NH}_3(\text{g})$  is used as a reactant its enthalpy could be calculated automatically, but that of  $\text{NH}_3(\text{l})$  could not be.
2. The temperature  $T$  must be in the range  $T_{\text{low}}/1.2 \leq T \leq T_{\text{high}} \times 1.2$  where  $T_{\text{low}}$  to  $T_{\text{high}}$  is the temperature range of the THERMØ data.

For cases with  $\text{NZØNES} > 1$  (see Problem card, Section 6.3) it may be desirable to modify the enthalpy of each zone. This can be done by using the DELH input array. For the  $i^{\text{th}}$  zone the  $i^{\text{th}}$  DELH entry will be added to the system

enthalpy as computed by  $\emptyset$ DE from the reactants cards (see above). For example, overall system enthalpy of the propellants in the tank can be input through the reactants cards and the work added or extracted per zone can be input by the DELH entries. An alternate method would be to input zero enthalpy on the Reactants cards and input enthalpy per zone by the DELH entries.

#### 6.4.2 $\emptyset$ MIT and INSERT Cards

$\emptyset$ MIT and INSERT cards are optional. They contain the names of particular species in the library of Thermodynamic Data for the specific purposes discussed below. Each card contains the word  $\emptyset$ MIT (in card columns 1-4) or INSERT (in card columns 1-6) and the names of from 1 to 4 species starting in columns 16, 31, 46, and 61. The names must be exactly the same as they appear in the THERM $\emptyset$  data.

##### 6.4.2.1 $\emptyset$ MIT Cards

These cards list species to be omitted from the THERM $\emptyset$  data. If  $\emptyset$ MIT cards are not used, the program will consider as possible species all those species in the THERM $\emptyset$  data which are consistent with the chemical system being considered. Occasionally it may be desired to specifically omit one or more species from considerations as possible species. This may be accomplished by means of  $\emptyset$ MIT cards.

##### 6.4.2.2 INSERT Cards

These cards contain the names of condensed species only. They have been included as options for two reasons.

The first and more important reason for including the INSERT card option is that, in rare instances, it is impossible to obtain convergence for assigned enthalpy problems (HP or RKT) without the use of an INSERT card. This occurs when, by considering gases only, the temperature becomes extremely low. In these cases, the use of an INSERT card containing the name of the required condensed species can eliminate this kind of convergence difficulty. When this difficulty occurs, the following message is printed by the program: "LOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE BEEN INCLUDED ON AN INSERT CARD".

The second and less important reason is that if one knows that one or several particular condensed species will be present among the final equilibrium compositions for the first assigned point, then a small amount of computer time can be saved by using an INSERT card. Those condensed species whose chemical formulas are included on an INSERT card will be considered by the program during the initial iterations for the first assigned point. If the INSERT card were not used, only gaseous species would be considered during the initial iterations. However, after convergence, the program would automatically insert the appropriate condensed species and reconverge. Therefore, it usually is immaterial whether or not INSERT cards are used. For all other assigned points the inclusion of condensed species is handled automatically by the program.

### 6.4.3 \$ØDE NAMELIST INPUT

The ØDE subprogram contains namelist input sections \$ØDE and \$SHKINP. The Namelist \$ØDE must be preceded by a card with NAMELISTS punched in card columns 1-9.

The \$ØDE Namelist is required if ØDE =1. or TDK =1, in \$DATA as described in section 6.3.

For the ØDE problem type any of nine (9) different equilibrium problems can be solved. These are TP, HP, SP, TV, UV, SV, RKT, DETN, and SHØCK. For the ØDE-ØDK, ØDE-ØDK-TDK, or TDE problem type, only the RKT problem can be solved. In this section only the RKT Input option is discussed. Reference 9 is to be used to prepare input for the other equilibrium problems.

The variables input by the \$ØDE namelist are listed in Table 6-9.

Additional information about some of these variables follows:

Pressure units. - The program assumes the pressure in the P schedule to be in units of atmospheres unless either PSIA = true, or SI = true.

Relative amounts of fuel(s) and oxidizer(s). - These quantities may be specified by assigning 1 to 15 values for either o/f, %F, f/a, or r. If no value is assigned for any of these, the program assumes the relative amounts of fuel(s) and oxidizer(s) to be those specified on the REACTANTS cards. (See discussion in REACTANTS Cards, Section 6.4.1 and Section 5.2.1)

RKT problem. - Only one value for chamber pressure, P, is to be input for cases with NZONES > 1 (see \$DATA input, Section 6.3). The stagnation pressure used for the  $i^{\text{th}}$  zone will be the value input for P multiplied by the  $i^{\text{th}}$  value input in the schedule XP. If not input, all XP entries are assumed equal to one. For TDK type

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problems, zone one is taken about the nozzle axis of symmetry and the last zone is bounded by the nozzle wall. Similarly, the  $i^{\text{th}}$  zone will have a mixture ratio equal to the  $i^{\text{th}}$  entry in the OFSKED schedule.

Print out will be given for the chamber pressure condition (i.e. stagnation) and the throat condition. Print out may be requested at other conditions by use of the PCP schedule and the SUBAR and SUPAR schedules.

The program will calculate both equilibrium and frozen performance unless  $FR\emptyset Z = F$  or  $EQL = F$  are input. If  $FR\emptyset Z = F$ , only equilibrium performance will be calculated. If  $EQL = F$ , only frozen performance will be calculated.

Ordinarily, rocket problems are run by specifying chamber values for P and H. It is possible, however, to run 1 zone cases (N ZONES = 1 in SDATA) by specifying P and T. For example:

```
$ODE  
RKT = 1  
P   = chamber pressure,  
T   = chamber temperature,
```

can be used to set the chamber temperature and run the rocket problem. The resulting chamber enthalpy will be calculated and included in the output.

TABLE 6-9 VARIABLES IN ØDE NAMELIST

Variable	No. of entries	Type	Value before read	Definition and comments
RKT	1	L	False	Rocket problem <sup>a</sup>
P	26	R	0	Assigned pressures: stagnation pressure for rocket problems: values in atm unless PSIA, or SI = .T., (see below)
SI	1	L	False	<sup>a</sup> Values in P array are in N/m <sup>2</sup>
PSIA	1	L	False	<sup>a</sup> Values in P array are in psia units
XP	50	R	1.	Multipliers for the i <sup>th</sup> zone stagnation pressure (zone 1 = inner zone)
ØF	1	L	False	Oxidant to fuel weight ratios are to be input <sup>a</sup>
ERATIO	1	L	False	Equivalence ratios are to be input <sup>a</sup>
FPCT	1	L	False	Percent fuel by weight are to be input <sup>a</sup>
FA	1	L	False	Fuel to air weight ratios are to be input <sup>a</sup>
ØFSKED	50	R	0	For a Rocket problem, and NZØNES ≥ 1, ØFSKED will be used rather than MDX (see Reference 3). Relative amounts of total oxidant to total fuel are input as defined by ØF, ERATIO, FPCT, or FA. For ØDE-ØDK-TDK and TDE problem types these values define the oxidant to fuel ratios for each zone (zone 1 = inner zone)
DELH	50	R	0	Corresponding to each zone this value will be added to the system enthalpy input thru the reactants cards. Units are BTU/# if PSIA=.T., joule/kilogram if SI=.T., otherwise cal/gram.
DELH1	50	R	0	Corresponding to each zone this value will be added to the system enthalpy. These values can be used as a 1st estimate for the heat returned to the main combustion chamber by regen cooling circuits (ØFC input in SBLM). The BLM will recalculate these values and, if IRPEAT =1 in SDATA, rerun the ØDE, ØDK, TDK (or TDE) analysis. Same units as DELH.

<sup>a</sup>If variable is set to be true.

Note: For rocket problems, only one value stagnation pressure can be input. This value multiplied by the i<sup>th</sup> entry of XP will be used for the stagnation pressure of the i<sup>th</sup> zone.

Table 6-9 (cont'd)

Variable	No. of entries	Type	Value before read	Definition and comments
IØNS	1	L	False	Consider ionic species <sup>a</sup>
WFLØW	1	R	0	Input nozzle mass flow option for ØDE-ØDK-TDK or TDE problems. If a value for WFLØW is input an expansion with this mass flow will be computed. The values input for P and XP are used as estimates for computing stagnation pressure for each zone. The program will adjust these stagnation pressures to obtain the desired nozzle mass flow within a tolerance of RELERR. Units are lbs/sec if PSI=.T. otherwise kilograms/sec.
RELERR	1	R	.0005	Relative difference between requested and computed mass flow rate. The program stops if this error is exceeded.
PCP	50	R	0	Compute and print solutions at these values of chamber pressure to pressure ratio (entries must be >1.)
SUBAR	50	R	0	Compute and print solutions at these values of subsonic area ratios (entries must ≠ 1.)
SUPAR	50	R	0	Compute and print solutions at these values of supersonic area ratio (entries must ≠ 1)
ECRAT	1	R	0	Subsonic area ratio to start ØDK calculations with computed equilibrium conditions. The SUBAR input table must include an entry equal to ECRAT.
EQTHST	1	L	False	To start ØDK calculations with computed equilibrium conditions at the nozzle throat. <sup>a</sup>
EQL	1	L	True	Calculate rocket performance assuming equilibrium composition during expansion <sup>b</sup> .
FRØZ	1	L	True	Calculate rocket performance assuming frozen composition during expansion <sup>b</sup> .
LISTSP	1	L	False	List names and dates of all species residing on thermodynamic data used <sup>a</sup> .
KASE	1	I	0	Optional assigned number associated with case.

<sup>a</sup>If variable is set to be true.

<sup>b</sup>Set variable false if these calculations are not desired.



### 6.4.3.1 Variable Mixture Ratio Option

The MOC can be run with a variable mixture ratio option by setting `VARMIX=.TRUE.`, and inputting values into the `STREAM(1)` table as described below.

When the variable mixture ratio option is used, there are no sliplines in the flow. Instead, the flow mixture ratio will vary from the axis ( $\psi=0$ ) to the wall ( $\psi=1$ ) as specified in the tables of `ØFSKED` vs. `STREAM`. Sliplines can not be used when the shock option is invoked (`SHØCK=1` in `$MØC`), because shock-slipline interaction is not provided in the program. Thus, if the shock option is requested and there is variation in mixture ratio from streamline to streamline, then the variable mixture ratio option must be used.

The program will not function properly if the spacing in the mixture ratio table, `ØFSKED(1)`, is too large. The required spacing depends on the chemical system. As a rule each entry in `ØFSKED(1)` must differ no more than 4 or 5% from its adjacent values depending on the stoichiometry of the system. There are no spacing requirements for the `STREAM (1)` table. However, the first entry must be 0 and successive entries must increase monotonically with the last entry equal to 1.

The tables `XP(1)`, `DELH(1)`, and `DELH1(1)` of `$ØDE` can be used, in which case each entry corresponds to entries in `ØFSKED(1)` and `STREAM(1)`.

If `VARMIX=.TRUE.`, the `XM(1)` table of `$ØDK` and `$TRANS` will be computed by the program and need not be input.

<u>Item</u>	<u>Description</u>	<u>Assumed Value(s)</u>
VARMIX=	<p>If VARMIX=.FALSE., do not use variable mixture ratio option.</p> <p>If VARMIX=.TRUE., the variable mixture ratio option is to be used. The following must be input:</p> <p>NZONES in \$DATA,  ØFSKED(1) in \$ØDE and  STREAM(1) in \$ØDE, below.</p>	F
STREAM(1)=	<p>If VARMIX=.TRUE., values must be input here corresponding to the O/F values input in ØFSKED(1).</p> <p>The values input represent <math>(O/F)_i</math> vs <math>\psi_i</math> <math>i=1, \dots, NZONES</math> where <math>\psi_i</math> represents the mass flow between streamline <math>i</math> and the axis, divided by the total mass flow.</p> <p>Thus</p> <p><math>\psi = 0</math> at the axis, and  <math>\psi = 1</math> at the wall.</p> <p>The <math>i</math>th entry of ØFSKED is <math>(O/F)_i</math>.</p> <p>The <math>i</math>th entry of STREAM is <math>\psi_i</math></p> <p><math>0 \leq \psi_i \leq 1</math> <math>i = 1, \dots, NZONES = 50</math></p> <p>and <math>\psi_i &lt; \psi_{i+1}</math></p>	

6.4.3.2 OPTION TO PUNCH TABLES FOR BOUNDARY LAYER PROGRAM INPUT  
 (DOES NOT APPLY TO BLM)

Conditions computed along the nozzle wall can be output as punched cards for input to the BLIMP, TBL, or MABL boundary layer analysis computer programs. These conditions are taken by the boundary layer computer program as being the inviscid flow condition at the edge of the boundary layer. Tables to be punched are:  $x$ ,  $y$ , and  $P/P_c$  (i.e. the nozzle wall coordinates and the ratio of pressure to chamber pressure along the wall). The tables are punched in NAMELIST format readable by BLIMP.

A maximum of 50 entries upstream of the throat are saved and punched. The wall point at the end of every characteristic is punched up to a maximum of 500 total table entries. The user may specify a number by which the punched table will be offset. Thus, the first point may be output with identification 5 by input of  $I\emptyset FF=4$ . The use of  $I\emptyset FF$  enables the user to extend the table by adding points upstream.

If punched cards for input to a boundary layer program are required, the following items must be input as part of the \$ $\emptyset$ DE Namelist input:

<u>Item Name</u>		<u>Description</u>
IPTAB	=	If IPTAB=1, one title card will be punched (this will be the last title card input as described in 6.2) followed by tables of $X$ , $Y$ , and $P/P_c$ along the nozzle wall. These cards are for input to the BLIMP or MABL computer programs. The first point punched will correspond to beginning of the converging section of the nozzle (i.e. at ECRAT; see Figure 6-1, also table 6-9).
$I\emptyset FF$	=	The first point to be punched will be numbered as $I\emptyset FF+1$ .
IPTBL	=	If IPTBL and IPTAB=1, tables of $M$ , $T/T_c$ , $C_p$ , $V$ , and $\rho$ , will also be punched. These additional cards are required for input to the TBL computer program (i.e. the December 21, 1973 version).

If a TDE problem is specified, the following items must also be input when IPTAB=1: RSI, RWTU, THETA1, and RI in \$DATA.

These items define the nozzle geometry from the combustion chamber through the throat as shown in Figure 6-1. For a TDE option it is necessary that IPTBL=0.

## 6.5 ODK INPUT DATA

$\emptyset$ DK input data is required if  $\emptyset$ DK = 1 or TDK = 1 in \$DATA as described in Section 6.3. The ODK input data consists of three data groups as follows:

SPECIES	data group
REACTIONS	data group
\$ $\emptyset$ DK	data group

These data groups are described below in sections 6.5.1, 6.5.2, and 6.5.3, respectively.

### 6.5.1 SPECIES

Species used by the computer program are determined in several possible ways, depending upon the problem type. Methods used to determine chemical species for each problem type are discussed below.

#### $\emptyset$ DK

If  $\emptyset$ DE=0 and  $\emptyset$ DK=1 in \$DATA, then species names and concentrations must be input, see Section 6.5.1.1.

#### $\emptyset$ DE- $\emptyset$ DK

If  $\emptyset$ DE=1 and  $\emptyset$ DK=1 in \$DATA, then the initial start conditions for the kinetic expansion are obtained from an  $\emptyset$ DE equilibrium calculation. The species generated by

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the equilibrium calculation generally contains many more species than the 40 species for which the ØDK subprogram is dimensioned. Therefore a selection process is required to interface the ØDE calculated equilibrium start conditions with the ØDK kinetic expansion calculations. This selection is performed using the following rules:

- Rule 1 If a species appears in a reaction, it is selected for the kinetic calculation.
- Rule 2 If a species is specified using INERTS directive it is selected for the kinetic calculations.
- Rule 3 If any species has a mole fraction greater than an input criterion, it is selected for the kinetic calculation.

Species which are selected but which do not appear in a reaction are treated as Inert and listed as such on the output list of selected species.

ØDE-ØDK-TDK

For problems with ØDE=0 and ØDK=1, species are selected by the above rules. However, for multizone TDK cases it is necessary that each zone have the same species list. Thus the INERTS input (see Section 6.5.2...) must be used to assure the same species are selected for each zone.

6.5.1.1 SPECIES CARD OPTION FOR INPUT OF INITIAL SPECIES CONCENTRATIONS

(APPLIES ONLY IF ØDE=0 AND ØDK=1 IN \$DATA)

This input begins with a single card with SPECIES in columns 1 through 7 and with either MASS FRACTIONS or MOLE FRACTIONS in columns 9 through 22. If the identifier for mass or mole fractions is omitted, mass fractions are assumed. Up to 40 species cards may be input. Only those species specified by input species cards will be considered for an ØDK problem. The order of the input

species cards is independent of the order in which the species appear on the master Thermodynamic Data file.

A chemical species is identified symbolically by 12 alphanumeric characters and must correspond identically with the species name as it appears on the Thermodynamic Data file. A complete list of the current species names are listed in Table 6-4 (condensed species, however, may not be specified in the species list.) The species symbol may not contain the characters \* or =.

<u>Col</u>	<u>Function</u>
1-10	Not used
11-22	Species symbol (left justified)
23-30	Not used
31-60	Value of initial species concentration (if zero must be input as 0.0) free field F or E format
61-80	User Identification if desired

This type of input also requires input of other items that otherwise would be provided by ODE. These other items ( $P_c$ ,  $T_c$ ,  $V_c$ , etc.) are input with the \$ODK data set and are described in Section 6.5.3.6. Example input is given in Table 6-12.

## 6.5.2 THE INPUT OF CHEMICAL REACTIONS

Chemical reactions must be input if  $\text{ODK}=1$  in \$DATA.

Up to 50 reactions with an implied third body and a total 150 reactions may be input to the program. Only one card per reaction, and only one reaction per card is permitted. Cards specifying third body reactions must precede cards specifying all other reactions. Species names appearing in the symbolic reaction set must correspond identically with the species names as they appear in the master Thermodynamic Data (see Table 6-4).

The symbolic reaction set contains directive cards and reaction/data cards in groups as outlined below:

REACTIONS	Directive for start of symbolic reaction input
.	
.	Reactions with implied third body species
END TBR REAX	Directive for end of third body reactions
.	
.	All other reactions
LAST REAX	Directive for end of reactions
INERTS	Specified Inert Species
THIRD BODY REAX RATE RATIOS	Directive for start of third body reaction rate ratios
.	
.	
LAST CARD	Directive for end of REACTIONS input

The content and format of each type of card are defined below:

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### 6.5.2.1 REACTIONS Through LAST REAX

The symbolic reaction input begins with a card containing the word REACTIONS in columns 1 through 9.

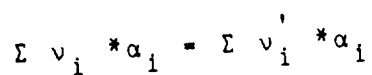
Columns 11 to 23 can be used to specify the nominal direction of the reaction rate data. For example the card

REACTIONS      FORWARD RATES

will cause all reaction rate data to be in the forward (left to right) direction unless otherwise specified. The word REVERSE instead of FORWARD means the rate data is input in the reverse direction. If left out, the nominal rate direction will be the forward direction.

Up to 50 dissociation reactions and a total of 150 reactions may be input following the REACTIONS card. Only one card per reaction and only one reaction per card is permitted. Cards specifying reactions with third bodies must precede cards specifying reactions without third bodies. The content and format of the reaction cards is defined below.

The general form of a reaction is:



where the  $\alpha_i$ 's are species names and the  $v_i$ 's are the stoichiometric coefficients. The left hand side of the above equation represents the reactants and the right hand side the products.

Each species name must correspond identically with the species name as it appears in the Thermodynamic Data File, e.g., see Table 6-4.



The stoichiometric coefficients must be intergers and an \* must separate the stoichiometric coefficient from the species name. If no stoichiometric coefficient is given, the value 1 is assumed. It is also required that

$$\sum v_i \leq 10$$

$$\sum v'_i \leq 10$$

examples:

<u>Reaction</u>		<u>Interpretation</u>	
H+H	= H2	H+H	= H <sub>2</sub>
NA+CL-	= NACL	Na <sup>+</sup> + Cl <sup>-</sup>	= NaCl
B+2+M-2	= BM	B <sup>++</sup> + M <sup>--</sup>	= BM
BE+2+2*ØH-	= BEØHØH	Be <sup>++</sup> + 2ØH <sup>-</sup>	= Be(ØH) <sub>2</sub>

The reaction rates are defined by three numerical values P1, P2, P3 input as E or F format. Three types of reactions can be input, as discussed below.

Arrhenius form

$$\sum v_i \alpha_i = \sum v'_i \alpha_i, \text{ Mn, } A = P1, N = P2, B = P3$$

or

$$\sum v_i \alpha_i = \sum v'_i \alpha_i, \text{ Mn, } KF = P1, P2, P3$$

Input of the above type defines a reaction rate of the form

$$k = P1 * T^{-P2} * e^{-P3 * 1000 / RT}, \text{ R} = 1.987$$

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Landau-Teller form

$$\sum v_i \alpha_i = \sum v_i' \alpha_i, Mn, *KF = P1, P2, P3$$

Input of the above type defines a reaction of the form

$$k = \exp (P1 + P2^{-1/3} + P3^{-2/3}).$$

Log 10 form

$$\sum v_i \alpha_i = \sum v_i' \alpha_i, Mn, \%KF = P1, P2$$

Input of the above type defines a reaction of the form

$$\log_{10} k = P1 + P2*T.$$

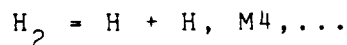
In the above reactions if KF is replaced by KR, then the rate will be for the reverse (right to left) direction.

The Mn's in the above reactions are the third body descriptors for the reaction. These descriptors are optional for dissociation-recombination reactions, but must be left out for exchange reactions. They are used to multiply the reaction rate by a factor that is defined by the descriptor.

The dissociation-recombination reactions with third body terms must precede other types of reactions, and must be followed by the directive starting in column 1:

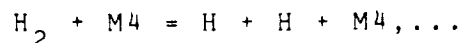
```
Col 1      +  
          END TBR REAX
```

All reactions prior to the above directive will have a third body term added to each side of the reaction; e.g.,



```
END TBR REAX
```

is the same as



where M4 is a generalized third body as specified in Section 6.5.2.3. If no Mn is specified, the generalized third body is assumed to be defined by Mo.

The reaction set is terminated by a card containing LAST REAX in columns 1 to 9.

#### 6.5.2.2 Inert Species Option

Inert species (i.e. species not appearing in reactions) can be included in the input by input of a card with INERTS in columns 1 through 6 followed by a list of inert species names. The species names must each be followed by a comma and each name must be written exactly as in the master Thermodynamic Data. The last comma must be followed by the word END. The species list can continue onto the next card, but a species name cannot overlap onto the next card.

#### 6.5.2.3 Third Body Reaction Rate Ratios

If reaction rate ratios,  $m_{ij}$ , are to be input for the dissociation-recombination reactions, a card with THIRD BODY REAX RATE RATIOS in columns 1 through 27 must be input next. If this card is deleted from the input, the program assumes all  $m_{ij} = 1$ . If this card is included in the input, it must be followed either by a card with ALL EQUAL 1.0 in columns 1 through 13 (which sets all  $m_{ij} = 1$ ) or by cards defining the Mn's as described below.

The Mn's on the reaction cards are used to identify a group of third body efficiencies which pertain to all of the reactions which declare that grouping. The format of the Mn statement is

$$Mn = m_j * \alpha_j, m_k * \alpha_k, \dots, etc$$

where

n = integer between 0 and 100 inclusive  
m<sub>j</sub> = multiplier for the species named  $\alpha_j$   
 $\alpha_j$  = species name  
.  
.  
etc.

If no multiplier is given for an  $\alpha$ , a value of 1.0 is assumed. The user may declare that all of the third body reaction rate ratios for a particular grouping are 1.0 by using the statement

Mn = \*

If no Mn is declared on the reaction card, then M0 is assumed.

Example: (fictitious rates)

REACTIONS FORWARD RATES

H + OH = H2O, A = 7.5E23, N = 2.6, B = 0.0,  
O + H = OH, M2, KF = 4.0 + 18, 1, 0,  
O + O = O2, M2, KF = 1.2E17, 1, 0,  
H<sub>2</sub> = H + H, M3, KR = 6.4E17, 1, 0,  
END TBR REAX

.  
.  
.

LAST REAX

THIRD BODY REAX RATE RATIOS

M0 = .5\*H2, 20.\*H2O,  
M2 = .5\*H2, 5\*H2O ,  
M3 = \*  
LAST CARD

In the above example the first reaction does not declare an Mn, so M0 is used. The second and third reactions share the same third body reaction rate ratios by declaring the same group identifier, M2. The fourth reaction uses the identifier M3 which has all of its third body efficiencies set equal to 1.0.

#### 6.5.2.4 LAST CARD

The reaction input data is terminated by a card containing LAST CARD in columns 1 through 9.

#### 6.5.2.5 Master Reaction Set

A master reaction set is presented in Table 6-10. It contains chemical species and reactions found necessary for C, Cl, F, H, N, and O systems according to the study presented in Appendix A in which the rate data was updated with a literature survey through June 1984. Third body efficiencies are included. For any given chemical system that is to be analyzed, great care must be taken in selecting the appropriate reaction set. Table 6-10 may or may not be sufficient.

Table 6-11 presents a minimal reaction set for Oxygen/Hydrogen systems. The third body efficiencies are included in Table 6-11 and illustrate their usage.

TABLE 6-10 REACTIONS AND RATE DATA FOR C, CL, F, H, N, AND O SYSTEMS  
(SEE APPENDIX A)

REACTIONS	CCLFHNO	SEA, SEPT 12, 1984	K=AT**(-N)*EXP(-10008/RT)
H + H = H2	M1	A = 6.4E17, N = 1.0, B = 0.0, (AR)	BAULCH 72 (A) 30U
H + OH = H2O	M2	A = 8.4E21, N = 2.0, B = 0.0, (AR)	BAULCH 72 (A) 10U
O + O = O2	M3	A = 1.9E13, N = 0.0, B = -1.79, (AR)	BAULCH 76 (A) 10U
N + O = NO	M4	A = 6.4E16, N = 0.5, B = 0.0, (N2)	BAULCH 73 (C) 10U
N + N = N2	M5	A = 3.0E14, N = 0.0, B = 0.0, (AR)	BAULCH 76 (B) 30U
CO + O = CO2	M6	A = 1.0E14, N = 0.0, B = 0.0, (AR)	JENSEN 78 (B) 30U
O + H = OH	M7	A = 3.62E18, N = 1.0, B = 0.0, (AR)	BAULCH 81 (A) 10U
F + F = F2	M8	A = 3.25E8, N = -1., B = -6.38, (AR)	BAULCH 81 (A) 30U
H + F = HF	M9	A = 7.5E12, N = 0.0, B = -35.13, (AR)	BAULCH 81 (A) 10U
CL + CL = CL2	M10	A = 2.23E14, N = 0.0, B = -1.81, (AR)	13/BAULCH 81 5U
H + CL = HCL		A = 2.6E13, N = 0.0, B = -19.9, (AR)	12/BAULCH 81 25U
CL + F = CLF		A = 3.0E16, N = 0.5, B = 0.0, (AVE)	11/CPIA246 25U
END TBR REAX			
O2 + H = O + OH		A = 2.2E14, N = 0.0, B = 16.8,	BAULCH 72 (A) 1.5U
H2 + O = H + OH		A = 1.8E10, N = -1., B = 8.9,	BAULCH 72 (A) 1.5U
H2 + OH = H2O + H		A = 2.2E13, N = 0.0, B = 5.15,	BAULCH 72 (A) 2U
OH + OH = H2O + O		A = 6.3E12, N = 0.0, B = 1.09,	BAULCH 72 (A) 3U
CO + OH = CO2 + H		A = 1.5E7, N = -1.3, B = -.765,	BAULCH 74 (A) 3U
N2 + O = NO + N		A = 7.6E13, N = 0.0, B = 75.5,	BAULCH 73 (C) 3U
O2 + N = NO + O		A = 6.4E9, N = -1.0, B = 6.25,	BAULCH 73 (C) 2U
CO + O = CO2		A = 2.5E6, N = 0.0, B = 3.18,	BAULCH 76 (B) 2U
CO2 + O = CO + O2		A = 1.7E13, N = 0.0, B = 52.7,	BAULCH 76 (B) 3U
F + H2 = HF + H		A = 9.2E13, N = 0.0, B = 1.08,	FOON 75 (A) 30U
H + F2 = HF + F		A = 8.8E13, N = 0.0, B = 2.40,	BAULCH 81 (A) 10U
CL2 + H = HCL + CL		A = 8.6E13, N = 0.0, B = 1.2,	29/BAULCH 81 10U
CL + H2 = HCL + H		A = 1.45E13, N = 0.0, B = 4.4,	31/BAULCH 81 10U
HCL + F = HF + CL		A = 1.9E12, N = -.68, B = .6,	32/CPIA246 25U
CL2 + F = CL + CLF		A = 6.2E12, N = -.68, B = .5,	33/CPIA246 25U
CL + F2 = F + CLF		A = 7.6E12, N = -.68, B = .3,	34/CPIA246 25U
CLF + H = HF + CL		A = 1.8E12, N = -.58, B = 3.2,	35/CPIA246 25U
CLF + H = HCL + F		A = 5.6E12, N = -.68, B = 1.9,	36/CPIA246 25U
CLF + H2 = HCL + HF		A = 1.8E10, N = -.5, B = 46.34,	37/CPIA246 1000U
F2 + HCL = HF + CLF		A = 1.8E10, N = -.5, B = 39.43,	38/CPIA246 1000U
CLF + HCL = HF + CL2		A = 1.8E10, N = -.5, B = 46.03,	39/CPIA246 1000U
F2 + CL2 = CLF + CLF		A = 1.8E10, N = -.5, B = 26.76,	40/CPIA246 1000U
OH + F = HF + O		A = 2.9E12, N = -.68, B = .2,	52/CPIA246 25U
H2O + F = HF + OH		A = 1.4E10, N = -.68, B = .6,	53/CPIA246 25U
CL + OH = HCL + O		A = 5.9E12, N = 0.0, B = 5.72,	BAULCH 81 10U
HCL + OH = H2O + CL		A = 2.25E12, N = 0.0, B = 1.02,	BAULCH 81 10U
LAST REAX			
THIRD BODY REAX RATE RATIOS			
M1 = 1*AR, 1.5*CO, 6.4*CO2, 25*H, 4*H2, 10*H2O, 1*N, 1.5*NO, 1.5*N2, 25*O,			
25*OH, 1.5*O2, 2*HF, 4*F,			
M2 = 1*AR, 3*CO, 4*CO2, 12.5*H, 5*H2, 17*H2O, 1*N, 3*NO, 3*N2, 12.5*O, 12.5*OH,			
6*O2,			
M3 = 1*AR, 4*CO, 8*CO2, 12.5*H, 5*H2, 5*H2O, 10*N, 4*NO, 4*N2, 12.5*O, 12.5*OH,			
11*O2,			
M4 = .8*AR, 1*CO, 3*CO2, 10*H, 2*H2, 7*H2O, 10*N, 1*NO, 1*N2, 10*O, 10*OH, 1*O2,			
M5 = 1*AR, 1*CO, 2*CO2, 10*H, 2*H2, 3*H2O, 10*N, 1*NO, 1*N2, 10*O, 10*OH, 1*O2,			
M6 = 1*AR, 1*CO, 5*CO2, 1*H, 1*H2, 1*H2O, 1*N, 1*NO, 2*N2, 1*O, 1*OH, 25*O2,			
M7 = 1*AR, 4*CO, 5*CO2, 12.5*H, 5*H2, 5*H2O, 1*N, 4*NO, 4*N2, 12.5*O, 12.5*OH,			
5*O2,			
M8 = 1*H2, 2.4*F2, 1*HF, 1*N2, 1*N, 2.4*F, 1*H,			
M9 = 8*H2, 1*F2, 2*HF, 2.8*N2, 1*N, 4*F, 20*H,			
M10 = 1*AR, 1*HCL, 5*CL2, 1*CL,			
LAST CARD			

TABLE 6-11. REACTIONS AND RATE DATA FOR H<sub>2</sub>O SYSTEMS.

REACTIONS	HO	SEA, SEPT 12, 1984	K=AT**(-N)*EXP(-1000B/RT)	
H + H = H <sub>2</sub>		,M1, A = 6.4E17, N = 1.0,	B = 0.0,	(AR) BAULCH 72 (A) 30U
H + OH = H <sub>2</sub> O		,M2, A = 8.4E21, N = 2.0,	B = 0.0,	(AR) BAULCH 72 (A) 10U
O + O = O <sub>2</sub>		,M3, A = 1.9E13, N = 0.0,	B = -1.79,	(AR) BAULCH 76 (A) 10U
O + H = OH		,M7, A = 3.62E18, N = 1.0,	B = 0.0,	(AR) JENSEN 78 (B) 30U
END TBR REAX				
O <sub>2</sub> + H = O + OH		, A = 2.2E14, N = 0.0,	B = 16.8,	BAULCH 72 (A) 1.5U
H <sub>2</sub> + O = H + OH		, A = 1.8E10, N = -1.,	B = 8.9,	BAULCH 72 (A) 1.5U
H <sub>2</sub> + OH = H <sub>2</sub> O + H		, A = 2.2E13, N = 0.0,	B = 5.15,	BAULCH 72 (A) 2U
OH + OH = H <sub>2</sub> O + O		, A = 6.3E12, N = 0.0,	B = 1.09,	BAULCH 72 (A) 3U
LAST REAX				
THIRD BODY REAX RATE RATIOS				
M1=25*H, 4*H <sub>2</sub> , 10*H <sub>2</sub> O, 25*O, 25*OH, 1.5*O <sub>2</sub> ,				
M2=12.5*H, 5*H <sub>2</sub> , 17*H <sub>2</sub> O, 12.5*O, 12.5*OH, 6*O <sub>2</sub> ,				
M3=12.5*H, 5*H <sub>2</sub> , 5*H <sub>2</sub> O, 12.5*O, 12.5*OH, 11*O <sub>2</sub> ,				
M7=12.5*H, 5*H <sub>2</sub> , 5*H <sub>2</sub> O, 12.5*O, 12.5*OH, 5*O <sub>2</sub> ,				
LAST CARD				

### 6.5.3 \$ØDK NAMELIST INPUT.

\$ØDK Namelist input specifies the conditions for the kinetic expansion calculation. The input is read in subroutine ØDKINP and consists of the following groups of data as outlined below:

- 6.5.3.1 Specification of Nozzle Geometry
- 6.5.3.2 Integration Control
- 6.5.3.3 Print Control
- 6.5.3.4 Species Selection and Mass/Mole Fraction Check
- 6.5.3.5 ØDK Problem Input

#### 6.5.3.1 Specification of Nozzle Geometry.

All of the nozzle geometry is to be input using the \$DATA Namelist input, see Section 6.3.3 and Figure 6-1.

An ØDK calculation will be carried out for each mixture ratio input in ØFSKED of \$ØDE whenever ØDK = 1 in \$DATA.

For a TDK problem, it is necessary that the ØDK calculations be run past the nozzle throat. Usually it is not desirable to run the ØDK calculations all the way to the nozzle exit because of the extra computer time and print out that results. However, if this is desired on a TDK problem, it can be requested by input of item EP as described below.

<u>Item</u>		<u>Description</u>	<u>Units</u>	<u>Assumed Value(s)</u>
\$ØDK	=	Namelist, read in subroutine ØDKINP.		
EP	=	If TDK = 1 and a value is input here for EP, then each ODK will be run to expansion ratio EP.	none	0



### 6.5.3.2 INTEGRATION CONTROL

The integration routine controls the step size such that the relative error in the dependent variable increments are less than a prescribed fraction, DEL. Only doubling or halving of the step size is permitted, and on option, either all the variables may be considered (JF=0), or only the fluid dynamic variables (JF=1) may be considered.

When the flow becomes supersonic and the area defined fluid dynamic equations are used, an additional check on continuity is applied in the form

$$\left| \frac{(\rho VA)_{N+1} - (\rho VA)_N}{(\rho VA)_{N+1}} \right| < C\text{ONDEL}$$

where CONDEL is an input relative criterion.

The step size is held between the two input bounds HMIN and HMAX. Fixed step cases may be run by setting input values for HI, HMAX, HMIN all equal.

<u>Item</u>		<u>Description</u>	<u>Units</u>	<u>Assumed Value(s)</u>
HI	=	initial step size	none	.01
HMAX	=	upper bound on step size	none	0.10001
HMIN	=	lower bound on step size	none	.005
DEL	=	fractional incremental error	none	.001

<u>Item</u>		<u>Description</u>	<u>Units</u>	<u>Assumed Value(s)</u>
TEXPLI	=	temperature below which explicit integration will start. Not recommended.	<sup>o</sup> R	0
CØNDEL	=	relative error criterion for continuity check for supersonic flow	none	1x10 <sup>-6</sup>
JF	= 0	all variables considered for step size control	none	0
	= 1	only fluid dynamic variables considered for step size control, i.e., p,u, and T	none	

### 6.5.3.3 PRINT CONTROL

Output from the Kinetic Expansion Calculation consists of complete output for each print station selected. The end point of the nozzle is always printed. Print stations are selected from one of the following options:

<u>Item</u>		<u>Description</u>	<u>Assumed Value(s)</u>
JPRNT	= -2	print throat and <u>input area ratios</u> (see ARPRNT)	-2
	= -1	print at <u>internally set area ratios</u> for conical nozzle.* Print at selected wall contour points for contoured nozzles. For the spline fit option (IWALL=4), print out will occur at each entry in ZS of \$DATA. For other contours (IWALL=2 or 3), print out will occur at 20 equally spaced axial locations along the nozzle.	
	= 0	print at every integration step	
	= +1	print every ND3rd step up to the throat and then nominal area ratios	
	= +2	print every ND3rd step over entire nozzle	

\*For JPRNT = -1 and a conical nozzle (i.e. IWALL = 1), the internally set area ratios are:

ARPRNT(1) = 2,3,4,...,39,40,42,...,58,60,64,...,116,120,128,...,200,210,220,...,400

If JPRNT is +1 or +2, the following must be input:

<u>Item</u>		<u>Description</u>	
ND1	=	first integration step to be selected for print	-
ND2	=	last integration step to be selected for print	-
ND3	=	print every ND3rd step between ND1 and ND2.	-

If JPRNT is -2, the following must be input:

<u>Item</u>		<u>Description</u>	
ARPRNT(1)	=	requested area ratios for print, must be monotonic increasing and greater than 1.0 If no values are input, will use values from ASUP of \$DATA.	-
NJPRNT	=	number of area ratios requested for print $\leq 100$ .	-

An extended print option may be selected as follows:

<u>Item</u>	<u>Value</u>	<u>Description</u>	
IDYSCI	= 0	no extended print requested	0
	= 1	extended print option selected ( <u>not suggested</u> )	

#### 6.5.3.4 SPECIES SELECTION AND MOLE/MASS FRACTION CHECK

In order to interface  $\emptyset$ DE equilibrium calculated start conditions with the kinetic expansion calculations, special consideration must be made for inert species (those not appearing in the reaction set). Inerts may be selected explicitly by use of the INERTS directive or by use of a relative selection criterion.

IF A MULTIZONE TDK PROBLEM IS SPECIFIED INERTS MUST BE SPECIFIED VIA THE INERTS DIRECTIVE. This is required so that the chemistry selected for multizone cases will be compatible.

The INERTS directive is described in Section (6.5.2.2).

The relative selection criterion ( $\emptyset$ DK or 1 Zone TDK problems,) is described below:

<u>Item Name</u>	<u>Function</u>
EPSEL =	all species which do not appear explicitly in the reaction set but whose mole fractions are greater than the input value for EPSEL, will be retained for the kinetic expansion. Species selected under this criterion are treated as inert. The program assumes EPSEL = 1.0E-5, unless input.

In some instances it may be desirable to use input species concentrations which do not sum to unity. Species concentrations, either input or from equilibrium start conditions, are summed and the sum checked as described below.

<u>Item Name</u>	<u>Function</u>
XMFTST =	Input species concentrations are summed and checked versus unity using this input criterion. If $ 1 - \sum \text{species concentrations}  < \text{XMFTST}$ then the test is passed. The species concentrations will then be normalized such that $\sum \text{species concentrations} = 1$ .

The program assumes XMFTST = 1.0E-3, unless input.

If the test is not passed, an error message will be given and the run terminated.

#### 6.5.3.5 Frozen Expansions with the ODK Module

The ODK module can be run using a frozen expansion by input of

SHGAMF = 1,

An example of this option is presented in Table 6-12. Note that the REACTIONS, END TBR REAX, and LAST CARD directives are included in the input, but no chemical reactions are given. This option can be run with ODE, or as in Table 6-12, without ODE. Whenever TDF=1 is input, SHGAMF = 1 is set automatically.

### 6.5.3.6 ODK PROBLEM INPUT

This input is required when  $\emptyset DE=0$ ,  $\emptyset DK=1$  are input in \$DATA.

A kinetic expansion from input arbitrary start conditions is to be computed. In addition to the input items described in section 6.5.3, an  $\emptyset DK$  problem requires input of those items described in Sections 6.5.1.1 and 6.5.2. Input for a hydrazine monopropellant engine is given in Table 6-12 as an example of the ODK problem input.

<u>Item Name</u>		<u>Input Quantity</u>	<u>Units</u>	<u>SI Units</u>
PC	=	chamber pressure	PSIA	N/M <sup>2</sup>
T	=	initial temperature	°R	°K
V	=	initial gas velocity	ft/sec	m/sec
JPFLAG	= 0	pressure table calculated internally	none	none
	= 1	pressure table input		
ECRAT	=	initial contraction ratio	none	none

For JPFLAG = 0 option the following must be input:

<u>Item Name</u>		<u>Input Quantity</u>	<u>Units</u>	<u>SI Units</u>
PI	=	initial pressure	PSIA	N/M <sup>2</sup>
PESTAR	=	throat pressure	PSIA	N/M <sup>2</sup>

For JPFLAG = 1 option the following must be input:

<u>Item Name</u>		<u>Input Quantity</u>	<u>Units</u>
PTB(1)	=	normalized pressure table entries*	none
ZTB(1)	=	normalized pressure table coordinates**	none
NTB	=	number of pressure table entries, ≤ 127	none
Z	=	initial axial position	none

\* normalized to input chamber pressure, PC

\*\* normalized to input throat radius, RSTAR. ZTB represents the streamline path length.

Table 6-12: Input Data For a Hydrazine Monopropellant Engine

```

THERMO
 300.000 1000.000 5000.000
H2      J 3/61H 2.0 0.0 0.0 0.G 300.000 5000.000
.31001901E+01 .51119464E-03 .52644210E-07 -.34909973E-10 .36945345E-14
-.87738042E+03 -.19629421E+01 .30574451E+01 .26765200E-02 -.58099162E-05
.55210391E-08 -.18122739E-11 -.98890474E+03 -.22997056E+01
N2      J 9/65N 2.0 0.0 0.0 0.G 300.000 5000.000
.28963194E+01 .15154866E-02 -.57235277E-06 .99807393E-10 -.65223555E-14
-.90586184E+03 .61615148E+01 .36748261E+01 -.12081500E-02 .23240102E-05
-.63217559E-09 -.22577253E-12 -.10611588E+04 .23580424E+01
NH3     J 9/65N 1H 300 000 0G 300.000 5000.000
0.24165177E 01 0.61871211E-02-0.21785136E-05 0.37599090E-09-0.24448856E-13
-0.64747177E 04 0.77043482E 01 0.35912768E 01 0.49388668E-03 0.83449322E-05
-0.83833385E-08 0.27299092E-11-0.66717143E 04 0.22520966E 01
END
TITLE 5 LB THRUSTER, N2H4 MONOPROPELLANT
DATA
$DATA
ODK      = 1,
RSI      = .0937,
ECRAT    = 29.2,
RI       = .01,
THETA    = 70,
RWIU     = 1.846,
RWID     = 1.846,
IWALL    = 5,
RMAX     = 9.872, ZMAX = 33.404,
$SEND
SPECIES MOLE FRACTIONS
      NH3      .17310
      N2       .30448
      H2       .52242
REACTIONS
END TER REAX
LAST CARD
$ODK
JPRNT    = -2,
EP       = 97.456,
ARPRNT   = 2,5,10,15,20,25,30,40,50,60,70,80,90,97.456,
NUPRNT   = 14,
SHGAMF   = 1,
PSIA     = T,
PC       = 106,
T        = 2030,
V        = 64.76,
PI       = 105.97,
PESTAR   = 57.812,
$SEND

```

6.5.3.7 MASS AVERAGED ØDK ISP

A mass averaged ØDK ISP summary page may be obtained at the end of the ØDK calculations as described below:

<u>Item Name</u>		<u>Description</u>
MAVISP	=1	Specifies mass averaged ISP option
XM(1)	=	Ratio of mass flow rate of each zone (zone 1 = inner zone) to the total mass flow rate.



6.6 \$TRANS NAMELIST INPUT.

When a MOC problem has been specified, the input data set \$TRANS is required for the transonic calculation.

<u>Item</u>	<u>Description</u>	<u>Assumed Value(s)</u>
\$TRANS	= Namelist, read in subroutine TRAN	
XM(1)	= Ratio of mass flow rate of each zone (zone 1 = inner zone) to the total mass flow rate. (need not be input if MAVISP = 1 option specified and XM input in \$ODK).	50*0
ALI	= Number of degrees initial line will be displaced downstream. The program assumes ALI is zero. If ALI is not zero, a symmetric throat is required (RWTU = RWTU).	0
IBUG	= If input is nonzero, intermediate transonic output will be printed.	0

The following input may be used to control the construction of the initial line:

<u>Item</u>	<u>Description</u>	<u>Assumed Value(s)</u>
MP	Number of points to be placed on the initial line. $MP \leq 275$ . A sinusoidal distribution of the following form is used: $r_i = [r_w \sin(\frac{i \pi}{N} \epsilon_1)] \quad i = 0, 1, 2, \dots, N$ where $N = MP$ and $\epsilon_1$ is EXP1 described below. Editing is done to control the spacing, see DRMIN and DRMIN1.	50

<u>Item</u>	<u>Description</u>	<u>Assumed Value(s)</u>
EXP1	= $\epsilon_1$ for sinusoidal distribution.	1.2
DRMIN	= Editing criteria for sinusoidal distribution. The first initial line point below the wall, $r_1$ , will be spaced such that  $r_w - r_1 > \min [DRMIN * RWTD, .025]$ <p>If a value of SHOCK=1 is to be input in \$MOC, then set DRMIN=.001</p>	.01
DRMIN1	= Editing criteria for sinusoidal distribution. Points on the initial line will be spaced such that  $r_n - r_{n-1} > DRMIN1$	$5 * 10^{-4}$
\$END		

6.7 \$MOC NAMELIST INPUT.

This data set contains the input items for the supersonic Method of Characteristics (MOC) module. The items are divided into four types, which are described in the following subsections.

- 6.7.1 Characteristics Mesh Control
- 6.7.2 MOC Check Option
- 6.7.3 Print Control
- 6.7.4 Inputs from DER
- 6.7.5 Exit Plane Option

Often no \$MOC input is necessary since the default values are usually sufficient.

### 6.7.1 Characteristics Mesh Control

<u>Item Name</u>	<u>Input Quantity</u>	<u>Units</u>	<u>Assumed Values</u>
\$MOC	= Namelist name, read by subroutine CHAR.		
DS	= insertions will be made such that successive points along streamlines will not be separated by more than $DS * M^{1/2}$ as described in Subroutine CNTRL.	none	.15
DTWI	= $\Delta\theta_{tw}$ criterion for insertion in subroutines INPT and DSPT as described in Subroutine CNTRL.	degrees	2.
DWCI	= throat wall point insertion control parameter $\Delta\theta_{wc}$ described in Subroutine CNTRL.	degrees	.5
DWWI	= wall point insertion control parameter $\Delta\theta_w$ described in Subroutine CNTRL.	degrees	3.
EPW	= the program will insert such that the wall end point is located within a tolerance EPW.	none	.01
ES	= $\epsilon_s$ for point editing as described in Subroutine CNTRL.	none	.0001

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<u>Item Name</u>	<u>Input Quantity</u>	<u>Units</u>	<u>Assumed Values</u>
ETHI	= $\epsilon_{\theta}$ for point editing as described in Subroutine CNTRL.	degrees	.25
IMAX	= the maximum number of iterations to be allowed while attempting to achieve a relative convergence for the flow variables of $5 \times 10^{-5}$ .	none	10
IMAXF = 1	the program will terminate the case if a printed point requires maximum iterations for convergence.	none	0
or			
IMAXF = 0	the program will continue the case after IMAX iterations per point have occurred.		
STØPIL	= if a value other than zero is input, then the program will construct the initial data line for the MOC and call EXIT at the end of subroutine CHAR. No MOC calculations will be done.	none	0.
TEXPLI	= input temperature below which explicit integration for the species concentrations will be used (not recommended).	$^{\circ}\text{R}$ , $^{\circ}\text{K}$ if SI Units	0.

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### 6.7.2 MOC Shock Option

The shock option can be run for the following problem types:

TDK,  
TDF,  
PFGØPT.

The shock option cannot be run for the following problem types:

TDE,  
TTDK.

There are three methods by which the shocks can be located, as discussed below.

#### a) Induced Shock Option

If the MOC induced shock option is requested (SHØCK=1, ISHCK=2), then the mesh construction begins at the intersection of the initial data line and the flow axis. RRC's are constructed. After the nozzle wall is reached, successive RRC's may cross. If so, a shock is inserted into the flow field at the cross-over point. Next, LRC's are constructed starting at the wall, and the region up to the cross-over point is filled in. The LRC construction then continues with the 1st point on each LRC being a right running shock point. When the axis is reached, the shock is reflected as a left running shock. The program then reverts to a RRC construction scheme and the shock is traced until it reaches the wall. It is then reflected from the wall, and is calculated as a right running shock propagating towards the flow axis. Only one shock will be traced, but multiple reflections are allowed.

b) Attached Shock Option

In the case of an attached shock (ISHCK=3), the mesh construction is the same as for the induced shock up to the requested x-location (XA) of the attached shock. Then, instead of looking for a crossing of RRC's, a shock point is attached to the wall at the XA location. The shock strength is determined by the deflection angle of the wall at the XA location. The shock is then traced just like in the case of an induced shock.

c) Multiple Shock Option

Two shocks can be traced with the multiple shock options (ISHCK=6 or 7). The first shock can be either an induced shock (ISHCK=6) or an attached shock (ISHCK=7), but the second shock must be an attached shock. The x-location of the second attached shock is specified by the variable XB.

The mesh construction for this option is now described. The first shock is calculated as above until the end of the nozzle is reached. Next, the calculation of the second shock and part of the flow field affected by it is repeated. In this construction, the first shock may not go to the center line and the two shocks must not cross over inside the nozzle.

<u>ITEM NAME</u>	<u>INPUT QUANTITY</u>	<u>ASSUMED VALUE</u>
SHOCK=	If SHOCK=0, shocks will be ignored and the MOC flow field will use LRC construction. If SHOCK=1, a shock will be inserted traced as described above.	0

<u>ITEM NAME</u>	<u>INPUT QUANTITY</u>	<u>ASSUMED VALUE</u>
ISHCK=	<p>If ISHCK=2, crossing of RRC's will be ignored for all RRC's that originate at the wall upstream of axial coordinate position XA. If the shock is too strong, it cannot be ignored.</p> <p>If ISHCK=3, an attached shock is started at the XA position.</p> <p>If ISHCK=6, two shocks are traced. The first one is an induced shock as in ISHCK=2 and the second is an attached shock at the axial coordinate position XB.</p> <p>If ISHCK=7, two shocks are traced. The first one is an attached shock as in ISHCK=3 and the second is an attached shock at the axial coordinate position XB.</p>	2
XA=	Axial coordinate position on wall discussed under ISHCK, above.	tangent point at end of throat circular arc.
XB=	Axial coordinate position on wall as discussed under ISHCK=6 or 7 above.	0.



### 6.7.3 Print Control

<u>Item Name</u>	<u>Input Quantity</u>	<u>Units</u>	<u>Assumed Values</u>
N1	= flow parameters will be printed for every N1 <sup>th</sup> interior point along characteristics selected for print	none	1000
N2	= every N2 <sup>th</sup> characteristic will be selected for print	none	1000
NC	= for NC $\neq$ 0 species concentrations (partial densities) will be printed with the flow parameters. If NC=1 the quantities A, B, $\gamma$ , heat capacity (BTU/Lb- <sup>o</sup> R), and enthalpy (ft <sup>2</sup> /sec <sup>2</sup> ) will be appended to the species concentration print.	none	0
MASSFL	= at the completion of each left running characteristic (LRC) the massflow is integrated. If MASSFL = 0 then no mass flow printed MASSFL = 1 then total mass flow and the number of points on the LRC are printed for each LRC MASSFL = 2 then mass flow for each point along LRC is printed MASSFL = 3 Same as MASSFL = 2 with the addition of execution time at the end of each LRC	none	1
NDS	= see Subroutine CHAF for NDS = 1 Dividing Streamline Points will be printed. (Nominal) for NDS = 0 Dividing Streamline Points will be suppressed.	none	1

6.7.4 Inputs from DER, Reference 24.

<u>Item Name</u>		<u>Input Quantity</u>	<u>Units</u>
ØFBAR	=	Overall mixture ratio including condensed phases. For print out only.	none
ETABAR	=	Overall evaporation efficiency, i.e. the ratio of gas flow to total propellant flow at the throat. $I_{sp, total} = I_{sp, gas} * ETABAR$	none
DRPISP	=	Ratio of total condensed phase momentum to the mass flow at the throat. Not used, reserved for future use.	lbf sec/lbm (if SI Units then N sec/kg)

### 6.7.5 Exit Plane Option

On option, the TDK method of characteristics calculation will continue the mesh construction through the exit plane of the nozzle and print a summary of the exit plane properties.(not operational for the shock option.)

<u>Item</u>	<u>Description</u>	<u>Assumed Value(s)</u>
EXITPL	= Exit plane calculation requested if set .TRUE.(not operational for shock option.) For the case when two TDK runs are to be made, i.e., when IRPEAT = 1, or 2 in \$DATA then the exit plane will be computed for the second TDK run, but not for the first TDK run.	.FALSE.

\$END

6.8 Boundary Layer Module (BLM) Input Data, \$BLM

This input data set is required if the BLM is to be executed, i.e., if BLM = 1.0 was input in the \$DATA namelist. Most of the data required by the BLM is communicated automatically by the ODE and/or MOC modules, or is preset as assumed values. Hence, these data items do not necessarily need to be input to the BLM module. However, any value that is read in will override the assumed or communicated value.

The input data items to the BLM module are as follows.

<u>Item</u>	<u>Description</u>	<u>Units</u>	<u>Assumed Value(s)</u>
\$BLM	= Namelist name, read in Subroutine INPUTB		
WDOT2D	= $\dot{w}_{2D}$ , nozzle mass flow. If the MOC module was not executed, a value can be input here so that a boundary layer ISP decrement can be computed.	lb/sec	1.
IPRNT	= If IPRNT = 1, then print the boundary layer profiles at every 5th station.	-	0

6.8.1 BLM Gas Properties

Gas properties that are required by the BLM are  $\gamma$ ,  $C_p$ ,  $R$ , and  $\mu$  versus  $T$ , and a value for the Prandtl number,  $P_r$ , and the total enthalpy,  $h_T$ . Ordinarily these values are supplied automatically by the ODE module. The tables are prepared by ODE using a series of (T,S) equilibrium (or frozen) calculations, where  $T$  varies from  $600^\circ R$  to  $7000^\circ R$  at  $200^\circ R$  increments. The chamber entropy value is used for  $S$ . Values at  $100^\circ R$  are then extrapolated and added to the table. The tables are printed with the BLM output. Constants defining the gas viscosity,  $\mu$ , and the Prandtl number,  $P_r$ , are also prepared by the ODE module.

Values for any or all of the above items can be input and used in place of the values prepared by ODE. If the ODE module has not been run, then all of the items listed below must be input. The assumed values are for air with constant  $C_p$ .

<u>ITEM</u>	<u>DESCRIPTION</u>	<u>UNITS</u>	<u>ASSUMED VALUE(S)</u>
CKO(1) =	Table of ratio of specific heats, none $\gamma$ , versus $T$ .		2*1.4
CPO(1) =	Table of specific heat at constant pressure, $C_p$ , versus $T$	ft/sec-R	2*6006
HS(1) =	Table of static enthalpy, $h$ , versus $T$	ft <sup>2</sup> /sec <sup>2</sup>	-6.01E5, 3.88E6

<u>ITEM</u>	<u>DESCRIPTION</u>	<u>UNITS</u>	<u>VALUE(S)</u>
HTOTAL	= Total enthalpy, $h_T$ , such that $h_T = h(T_{\text{chamber}})$ .	ft <sup>2</sup> /sec <sup>2</sup>	3.85E6
RRO(1)	= Table of gas constant, $R=1546.33/Mw$ vs $T$ .	lb-ft/lbm <sup>o</sup> R	2*53.3
TO(1)	= Temperatures corresponding to the entries in CKO, CPO, RRO, and HS arrays, above.	<sup>o</sup> R	440,7000
NTAB	= number of values entered in the CKO, CPO, and TO arrays. $2 \leq$ $NTAB \leq 101$ .	-	3
RMUI	= Reference viscosity, $\mu_o$ , where lbm/ft-sec. $.605934*10^{-4}$ viscosity is expressed as $\mu = \mu_o (T/T_o)^\omega$		
TI	= reference temperature, $T_o$ , for viscosity. See RMUI, above.	<sup>o</sup> R	6032
OMEGA	= Viscosity exponent, $\omega$ . See RMUI, above.	-	.76
PR	= Molecular Prandtl number, $Pr$ .	-	.72

Note: The above default values for  $\mu_o$ ,  $\omega$ , and  $Pr$  are for air.

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<u>ITEM</u>	<u>DESCRIPTION</u>	<u>UNITS</u>	<u>VALUE(S)</u>
HTOTAL	= Total enthalpy, $h_T$ , such that $h_T = h(T_{\text{chamber}})$ .	ft <sup>2</sup> /sec <sup>2</sup>	3.85E6
RRO(1)	= Table of gas constant, R=1546.33/Mw vs T.	lb-ft/lbm <sup>o</sup> R	2*53.3
TO(1)	= Temperatures corresponding to the entries in CKO, CPO, RRO, and HS arrays, above.	<sup>o</sup> R	440,7000
NTAB	= number of values entered in the CKO, CPO, and TO arrays. $3 \leq$ NTAB $\leq$ 101.	-	3
RMUI	= Reference viscosity, $\mu_o$ , where lbm/ft-sec. $.605934*10^{-4}$ viscosity is expressed as $\mu = \mu_o (T/T_o)^\omega$		
TI	= reference temperature, $T_o$ , for viscosity. See RMUI, above.	<sup>o</sup> R	6032
ØMEGA	= Viscosity exponant, $\omega$ . See RMUI, above.	-	.76
PR	= Molecular Prandtl number, Pr.	-	.72

Note: The above default values for  $\mu_o$ ,  $\omega$ , and Pr are for air.

## 6.8.2 Boundary Layer Edge Conditions

The coordinates for the boundary layer are specified in the RINØ versus XINØ table. Conditions at the inviscid edge are specified in the UEØ, TEØ, and PEØ versus XINØ tables. Conditions at the wall are specified in the TQW and CQW versus XTQW tables. The program will redistribute the input stations (up to 501 total) in order to have 101 x-stations uniformly distributed per segment, except for the first five stations which are generated non-uniformly. The input values of  $y_e, U_e, T_e, P_e, T_w$  (or  $q_w$ ), and  $(\rho V)_w$  are interpolated at the new x-stations and used in the boundary-layer calculations.

Values of RINØ versus XINØ and the conditions at the inviscid edge of the boundary layer will be automatically transmitted from the MOC module if it has been run. Otherwise, they must be input here. See the description of IØFF in \$DATA. Conditions at the wall must always be input here.

<u>Item</u>	<u>Description</u>	<u>Units</u>	<u>Assumed Value(s)</u>
XINØ(1) =	$x_e$ axial coordinate	none	-
RINØ(1) =	$y_e$ , radial coordinate	none	-
UEØ(1) =	$U_e$ , gas velocity at the inviscid edge	ft/sec	-
TEØ(1) =	$T_e$ , gas static temperature at the inviscid edge	$^{\circ}R$	-
PEØ(1) =	$P_e$ , gas pressure at the inviscid edge	psi	-
NXINØ =	number of items in the XINØ, RINØ, UEØ, TEØ, and PEØ tables. $2 \leq NXINØ \leq 501$ Do not input if IØFF was input in \$DATA.	none	-



<u>Item</u>		<u>Description</u>	<u>Units</u>	<u>Assumed Value(s)</u>
XTQW(1)	=	$X_w$ , axial coordinate for the TQW and CQW tables.	none	-1000., 0., 1000.
IHFLAG	=	Flag specifying wall boundary condition input through TQW array.  IHFLAG = 0, for temperature  IHFLAG = 1, for heat flux*	-	1
TQW(1)	=	$T_w$ , wall temperature or $\dot{q}_w$ , wall heat flux, depending in IHFLAG.  For an adiabatic wall, set IHFLAG = 1 and all TQW(1) = 0.  For a non-adiabatic wall with prescribed heat flux, set IHFLAG = 1, and note that for heat flux from the boundary layer to the wall, the TQW(1) entries will be <u>negative</u> .	$^{\circ}R$  or $\frac{BTU}{in^2-sec.}$	5 01*0.
CQW(1)	=	$(\rho V)_w$ , mass transfer parameter at the wall (only useful for suction)	lbm/ft <sup>2</sup> -sec	5 01*0
NTQW	=	Number of axial stations, $X_w$ . Each of the above tables must have this number of entries. $2 \leq NTQW \leq 501$ .	-	3

\* Default values are set for an adiabatic wall, i.e., IHFLAG = 1, and TQW(1) = 501\*0.

### 6.8.3 Integration Step Size Control.

<u>Item</u>	<u>Description</u>	<u>Units</u>	<u>Assumed Value(s)</u>
NSEGS	= Number of Segments, $1 < \text{NSEGS} < 10$ The boundary layer will be divided into segments of equal length unless values are input into XSEG, below.	none	1
NISPS(1)	= Number of Integration Steps per Segment, $\leq 101$ per segment.	none	10*101
XSEG(1)	= Vector containing the axial (x) locations which define the wall segments. The vector is always NSEGS + 1 values long. Default values are:  $\text{XSEG}(i) = z_c + (z_m - z_c) (i-1)/\text{NSEGS} \quad i=1,2,\dots,\text{NSEGS}+1$ where $z_c$ and $z_m$ are the end of the cylindrical combustion chamber, and the end of the nozzle, respectively, as shown in Figure 6-1.  If the boundary layer is to be extended upstream of $z_c$ , the usual procedure is to input  $\text{XSEG}(1) = \text{XIN0}(1)$ and $\text{XIN0}(1)$ through $\text{XIN0}(\text{IOFF})$ , etc., of \$BLM are input by the user as described in \$DATA under input item IOFF.	none	see description
NTR	= Station at which transition to turbulent flow is allowed. The program starts with an assumed boundary layer profile, and then turns on the eddy viscosity terms for turbulent flow at station NTR. For a laminar boundary layer, set NTR large, i.e. $\text{NTR} > \sum \text{NISPS}(I)$ .	none	3

Note: The default value of NSEGS=1 is often too small for reliable results. The user must specify enough segments and integration steps (NISPS) so that reliable results are computed. In general, nozzles with high area ratio and/or low Reynolds number flow will require more integration steps. See example cases in Section 7.

#### 6.8.4 Regenerative Cooling Heat Transfer.

When an engine is cooled using a regenerative device, propellant (usually fuel) is routed around the nozzle so that heat is transmitted from the boundary layer to the coolant. This heat is then returned to the combustion chamber in the form of increased propellant enthalpy. When the nozzle wall temperatures are assumed known (IHFLAG = 0 option), the BLM will calculate the heat flux from the boundary layer to the wall,  $\dot{h}_w$  (BTU/ft<sup>2</sup>-sec). These values can also be input directly (IHFLAG = 1 option). If the coolant circuit extends from position  $x_e$  to position  $x_o$  and operates at an efficiency,  $\eta$ , then the propellant enthalpy entering the chamber will be increased by

$$\Delta H = \frac{1}{\dot{m}_T} \eta \int_{x_o}^{x_e} \dot{h}_w dA \quad (\text{BTU/lbm})$$

where

$\dot{m}_T$  is the total engine mass flow rate

$dA$  is the nozzle surface area differential,  $2\pi r ds$

Using the method outlined above, the BLM will compute increments of propellant enthalpy for up to 3 fuel or oxidizer circuits and print out the resultant enthalpy increments. These can be added to a later computer run by using the DELH1(1) input array. If BLM is to be automatically rerun, then the enthalpy increments will automatically be stored into DELH1(1) for the second pass through ODE, ODK, and TDK. These enthalpy increments can be calculated in two ways. If the enthalpy increase is distributed equally throughout the chamber, then

$$\Delta H_i = \Delta H$$

i.e.

$$\text{DELH1}(1) = \Delta H, \Delta H, \dots \text{ etc.}$$

The second method is to assume that a fuel circuit adds enthalpy only to fuel, and an ox circuit adds enthalpy only to ox. It follows that

for a fuel circuit

$$\Delta H_i = \left( \frac{r+1}{r_i+1} \right) \Delta H$$

and for an ox circuit

$$\Delta H_i = \left( \frac{r+1}{r_i+1} \right) \frac{r_i}{r} \Delta H.$$

where  $r_i$  is the mixture ratio of zone  $i$  and  $r$  is the overall chamber mixture ratio.

For either method, the steady state engine cycle balance can be approximated as follows. First, calculate "adjusted tank enthalpies" for the fuel and for the oxidizer and input these on the reactant cards. These values must approximate the energy content of the propellant entering the main combustion chamber accounting for all energy gains and losses, except heat returned to the main combustion chamber by the regen cooling circuit(s). Estimates for these amounts are to be entered using the DELH1(1) input array. An estimate of zero is usually satisfactory. Corrected estimates will be calculated by BLM and stored in DELH1(1) for a second pass through TDK (or TDE). A second pass using these values will be executed automatically if IRPEAT = 1 was input in the \$DATA namelist.

<u>Item</u>	<u>Description</u>	<u>Assumed Value(s)</u>
XCO(1)	= the Ith entry is the starting position for the Ith cooling circuit*.	3*0
XCE(1)	= the Ith entry is the ending position for the Ith cooling circuit*.	3*0
ETAC(1)	= the Ith entry is the efficiency for the Ith cooling circuit.	3*1
ØFC(1)	= Type of coolant for the cooling circuit: ØFC(I) = 0. if there is no ith circuit ØFC(I) = 1. if the Ith circuit is oxidizer ØFC(I) = 2. if the Ith circuit is fuel $I \leq 3$	3*0
DISTRB(1)	= Flag for method of distributing $\Delta H$ increments  DISTRB(I) = 0. for equal distribution of heat to chamber  DISTRB(I) = 1. for distribution of ox heat to ox in chamber, and fuel heat to fuel in chamber.	3*1.

The Ith entry is for the Ith circuit.

---

\* Normalized by the throat radius,  $r_t$ .

6.8.5 BLM Plotted Output.

The input described below is used to control plotted output from the BLM. The plot options available from BLM are:

- 1) Momentum thickness,  $\theta$ , vs. axial position.
- 2) Displacement thickness,  $\delta^*$ , vs. axial position.
- 3) Wall Temperature,  $T_w$ , vs. axial position.
- 4) Velocity profiles at specified area ratios, or at specified axial locations.
- 5) Temperature profiles at specified area ratios, or at specified axial locations.

Example plots are presented in Figures 6-2 through 6-5 for types 1 through 5, above.

<u>Item</u>	<u>Description</u>	<u>Assumed Value(s)</u>
IPRØF	= If IPRØF = 0, then supersonic area ratios are input in APRØF.  If IPRØF = 1, then axial locations, $x/r_t$ , are input in APRØF	0
APRØF(1)	= Area ratios (or axial locations, see IPRØF) at which velocity ratio and temperature ratio profiles will be plotted. Two frames per area ratio will be plotted: $U/U_{edge}$ vs. $y/y_{edge}$ and $T/T_{edge}$ vs. $y/y_{edge}$ .	20*0
NPRØF	= Number of area ratios (or axial locations) requested in APRØF. $NPRØF \leq 20$ .	0
KDTPLT	= If KDTPLT = 1, then displacement thickness, $\delta^*$ , vs. axial location, x, will be plotted.	0
KMTPLT	= If KMTPLT = 1, then momentum thickness, $\theta$ , vs. axial location, x, will be plotted.	0
KTWPLT	= If KTWPLT = 1, then wall temperature, $T_w$ , vs. axial location will be plotted.	0

\$END

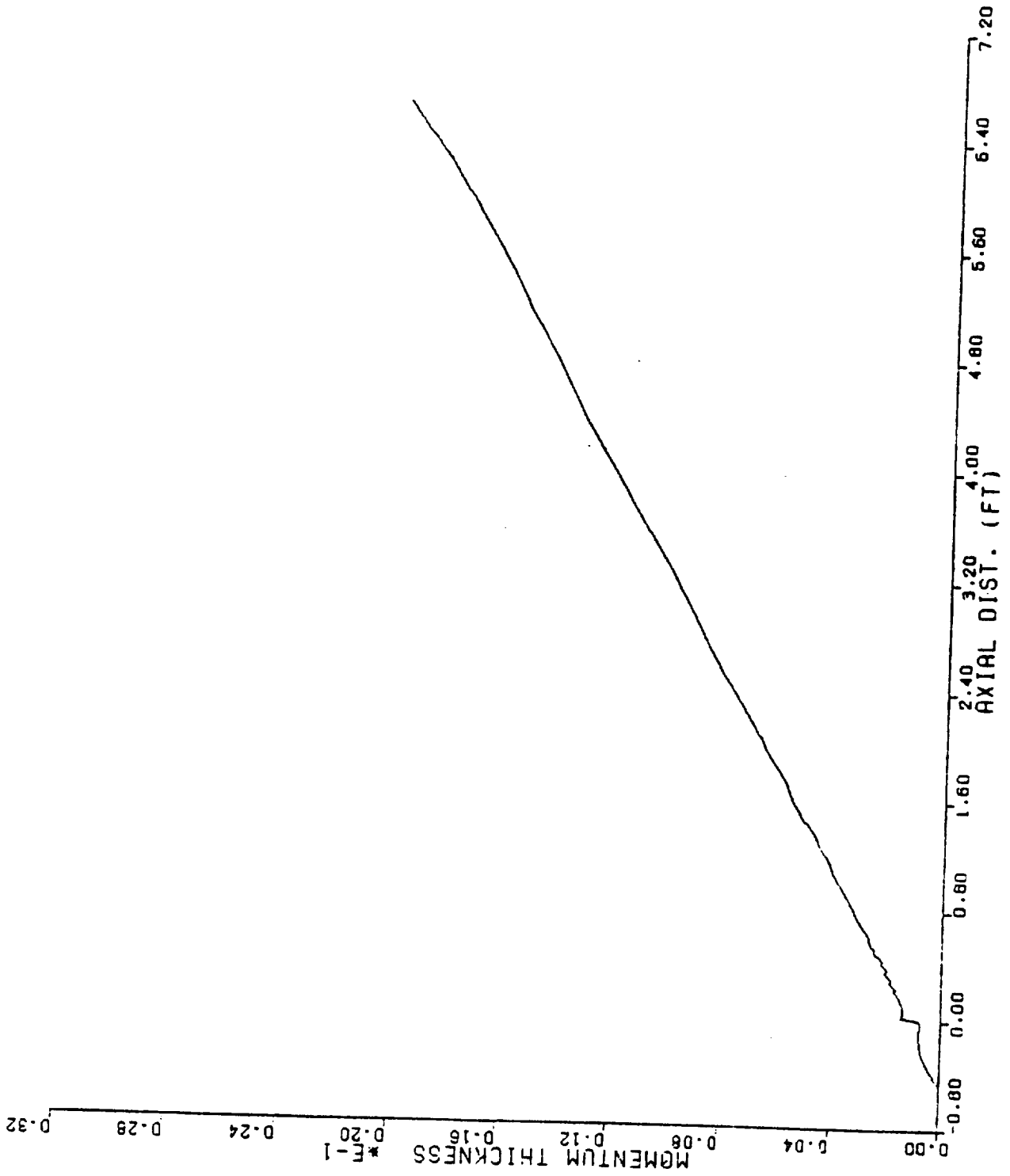


Figure 6-2: Boundary Layer Momentum Thickness vs Axial Position (See Section 7.3)

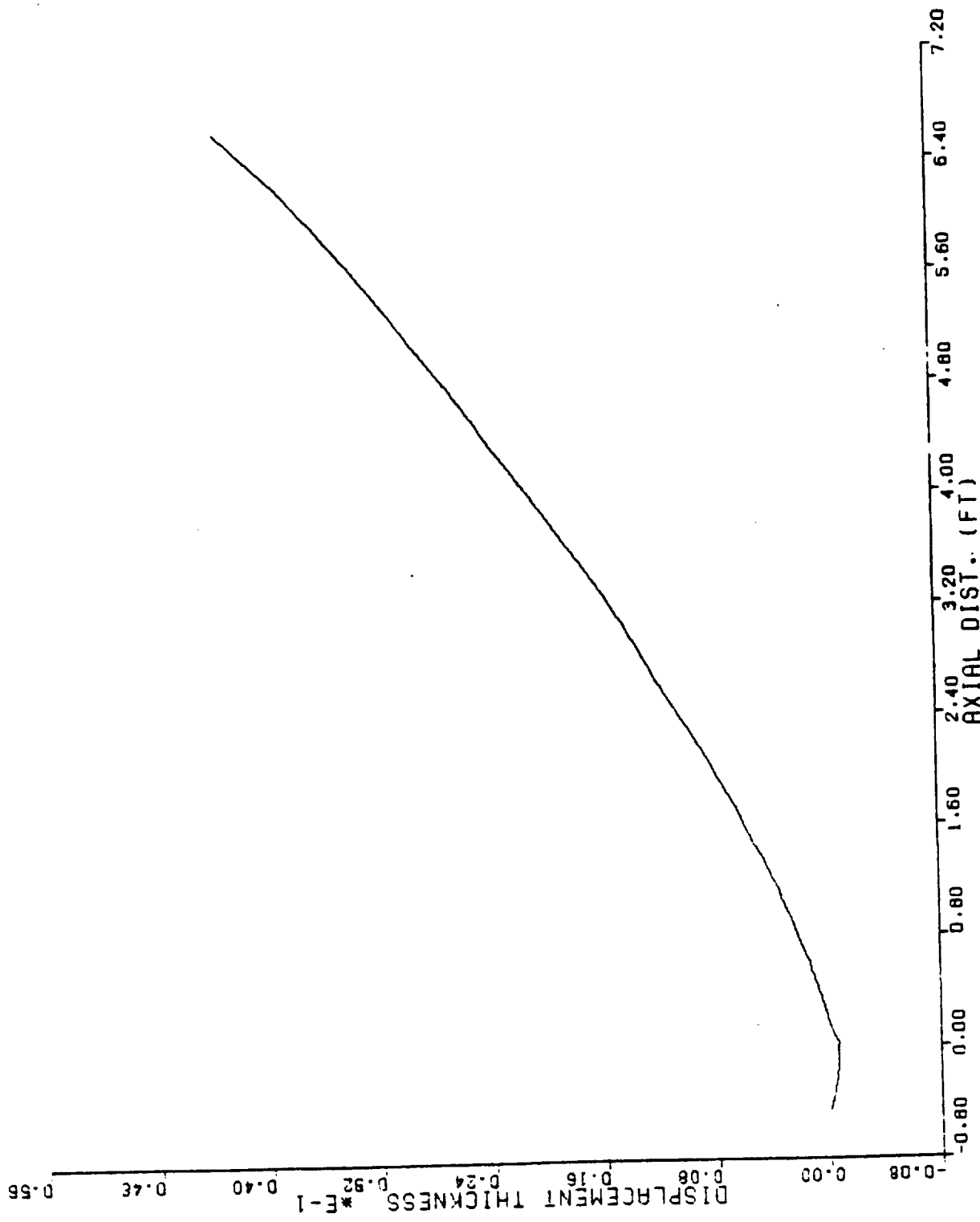


Figure 6-3: Boundary Layer Displacement Thickness vs Axial Position



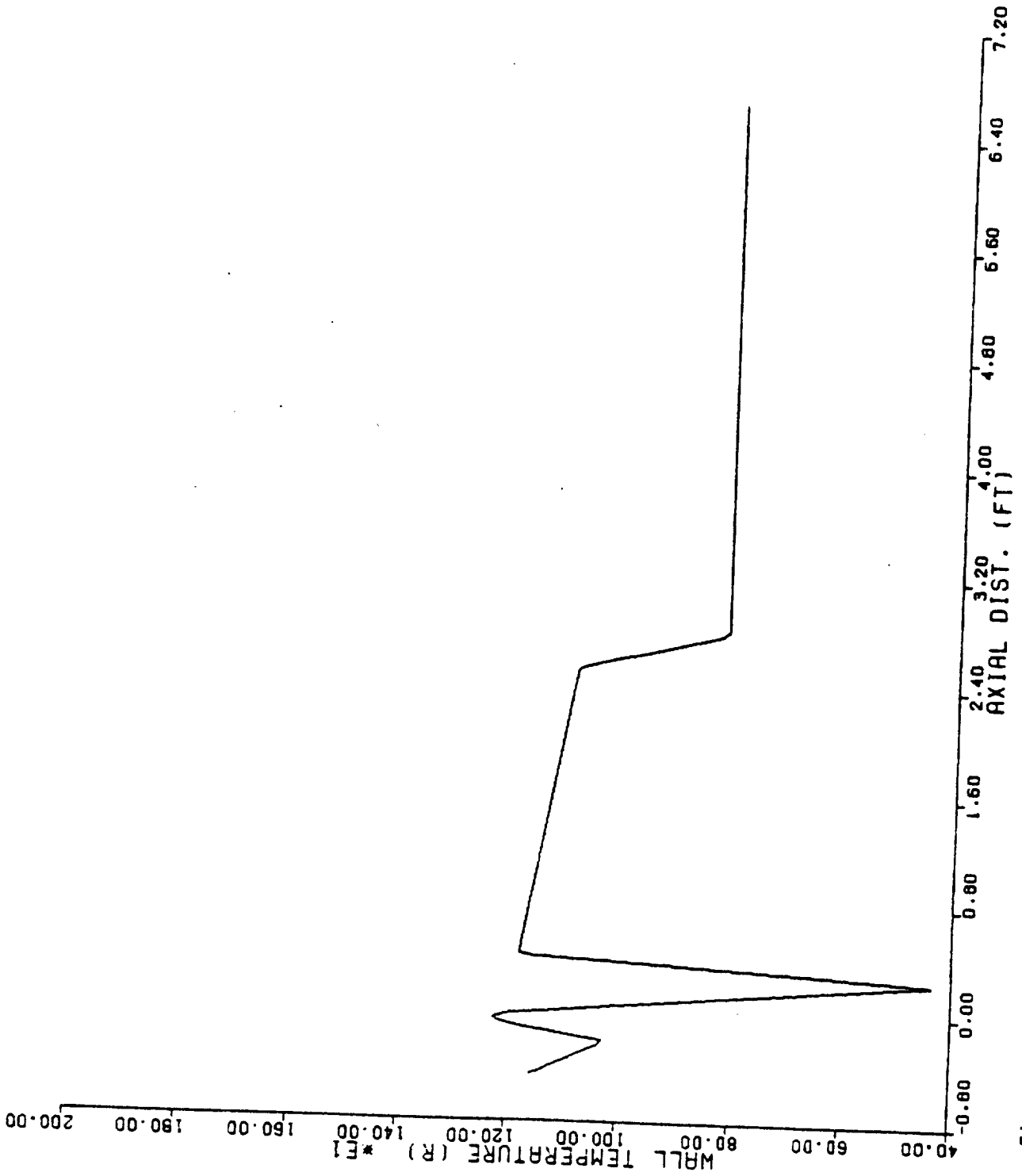


Figure 6-4: Wall Temperature (Input) vs Axial Position

TEMPERATURE PROFILE  
 EPS = 400.00  
 R = 2.090  
 Z = 6.626  
 TE = 1761.1  
 TH = 818.0  
 YE = 0.2689446

VELOCITY PROFILE  
 EPS = 400.00  
 R = 2.090  
 Z = 6.626  
 UE = 15079.1  
 YE = 0.2689446

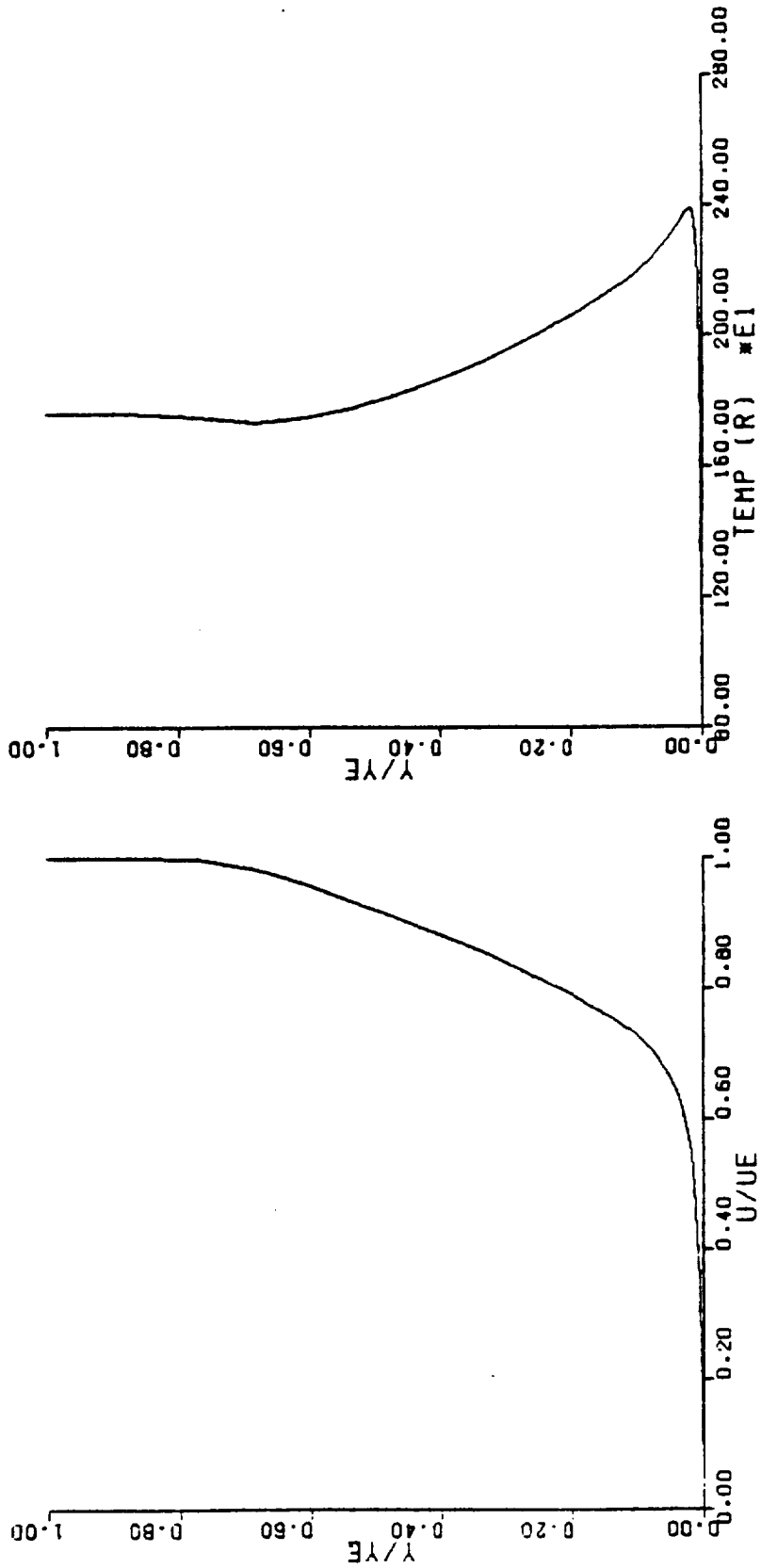


Figure 6-5: Velocity and Temperature Profiles at a Given Area Ratio

6.9 SPECIAL OPTIONS.

6.9.1 Constant Properties Gas Option.

The TDK program contains a useful option by which the real gas chemistry can be replaced by constant properties chemistry. Multiple zones can be calculated. The output includes the nozzle divergence efficiency,  $\eta_{DIV}$ , (see Section 5, subroutine PRINT).

The constant properties gas option is run by input of PFCOPT = 1 in \$DATA. Sample input data for the constant properties gas option is listed in Table 6-13.

Only the \$DATA, \$IRAN and \$MOC data sets are to be input. These data sets are input as described in Sections 6.3, 6.6 and 6.7, respectively, with the following required additions to the \$TRANS Namelist.

- G(1) = Value of specific heat ratio,  $\gamma$ , for each zone, inner to outer, the number of zones is specified in \$DATA.
- PSA = Chamber pressure in lbs/in<sup>2</sup>. (N/m<sup>2</sup> if SI units)
- XP(1) = (From Table 6-9) All assumed = 1, if not input.
- TC(1) = Chamber temperature,  $^{\circ}R$ , for each zone, inner to outer. ( $^{\circ}K$  if SI units)
- RGC(1) = Real gas constant, ft<sup>2</sup>/sec<sup>2</sup>  $^{\circ}R$ , (i.e.,  $49721/M_w = g \cdot J^* / 1.986/M_w$ ) for each zone, inner to outer. (m<sup>2</sup>/sec<sup>2</sup>  $^{\circ}K$  if SI units). Not needed if XMW is input
- XMW(1) = Gas Molecular Weight. If input then RGC(1) need not be input.

Table 6-13: Sample Case for the Constant Properties Gas Option.

TITLE SAMPLE CASE ONE

DATA

\$DATA

PFGOPT=1,

NZONES=1,

RSI=2,

RWTU=2, RNTD=.5,

THETA=35.6738,

IWALL=4,

NWS=11,

RS(2)= 1.16843, 1.26475, 1.47910, 1.73375, 2.04940, 2.45930,

3.68226, 4.84772, 5.79198, 6.32441,

ZS(2)= .39575, .53008, .82905, 1.19473, 1.66923, 2.32795,

4.68717, 7.68599, 10.9601, 13.3114.

THE=11.5813,

\$END

\$TRANS

G=1.23,

PSA=100,

TC=5500,

XMN=20,

XM=1,

ALI=0,

\$END

\$MOC

\$END

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6.10 INITIAL VALUES FOR THE \$ØDK, \$TRANS, AND \$STDK INPUTS

The following defines nominal values to which variables will be set if not input. If a variable is not listed, no nominal value is set. Variables are set in the subroutine containing the Namelist read..

\$ØDE, set in subroutine ØDES

DELH(I)	= 0.	, DELH1(I)	= 0
ECRAT	= 0.		
EQL	= .TRUE.		
EQTHST	= .FALSE.		
ERATIO	= .FALSE.		
FA	= .FALSE.		
FPCT	= .FALSE.		
FRØZ	= .TRUE.		
IØNS	= .FALSE.		
KASE	= 0		
LISTSP	= .FALSE.		
ØF	= .FALSE.		
ØFSKED(I)	= 0.		
P(I)	= 0.		
PCP(I)	= 0.		
PSIA	= .FALSE.		
RELERR	= .0005		
RKT	= .FALSE.		
SI	= .FALSE.		
SUBAR(I)	= 0.		
SUPAR(I)	= 0.		
WFLØW	= 0.		
XP(I)	= 1.		

**\$ØDK, set in subroutine ØDKINP**

CØNDEL = 1.0E-6  
DEL = .001  
EPS = 0.  
EPSEL = 1.0E-5  
HI = .01  
HMAX = .10001  
HMIN = .005  
IDYSCI = 0  
IWALL = 1  
JF = 0  
JPFLAG = 0  
JPRNT = -1  
  
TEXPLI = 0.  
XM (1) = 0.  
XMFTST = 1.0E-3

**\$TRANS, set in subroutine TRAN**

ALI = 0.  
IBUG = 0  
MP = 50  
PMCRIT = 1.  
PMDEG = 1.  
XM (1) = 0.

**\$TDK, set in subroutine CHAR**

DRPISP = 0.  
DS = .15  
DTWI = 2.  
DWWI = 3.  
EPW = .01  
ES = .0001

\$TDK (cont'd)

ETABAR	=	1.
ETHI	=	.25
IMAX	=	10
IMAXF	=	0
MASSFL	=	1
NC	=	0
NDS	=	1
N1	=	1000
N2	=	1000

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## 7. INPUT AND OUTPUT FOR SAMPLE CASES

In this section of the report input and output are presented for three engines, as follows:

- 1) the stratified flow engine.
- 2) the Pratt and Whitney RL-10 engine (prototype for OTV propulsion).
- 3) the Rocketdyne Advanced Space Engine, ASE, (prototype for OTV propulsion).

Complete input and output are given for the first case. For the next two cases only the program input and the summary output are given. All of the calculations were performed using a DEC PDP 11/750 VAX computer system.

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## 7.1 THE STRATIFIED FLOW ENGINE, CASE 1

This test case is the same one that has appeared in all earlier versions of the TDK program manual. It is similar to the Rocketdyne stratified flow engine that is presented in CPIA 246, Ref. 1.

On the following pages input and output for the problem are presented. The engine operates with liquid oxygen/gaseous hydrogen propellants. The injector is assumed to produce a stratified nozzle flow with a mixture ratio of 6.5 near the axis, 8.0 in the central zone, and 5.0 near the wall. Equal mass flow is assumed for each of these zones. Each zone is assumed to have a different stagnation pressure. The pressures are 300, 285, and 270 psia from axis to wall.

The modules used in performing the analysis are ODE, ODK, TDK, and BLM. A brief description of the computer output is presented below, followed by Table 7-1 which is a complete listing of the computer program print out.

The output sequence for case 1 is outlined below:

1. Program name.
2. All input data cards are listed.
3. ODE subprogram output.
  - a. Fuel/Oxidizer mixture description and list of species considered.
  - b. Equilibrium calculation output; Frozen calculation output.
  - c. Summary of Equilibrium Contraction Ratio conditions.
4. ODK subprogram output.
  - a. Listing of Reactions, etc., cards as they are read.
  - b. Species list from Reactions.
  - c. Reaction table.
  - d. Selected species list for kinetic expansion.

- e. Dissociation/Recombination reaction rate ratios.
  - f. Initial and Throat conditions for one dimensional ODK expansion.
5. 2 and 3 above are repeated for each zone with redundant print omitted.
  6. ODK  $I_{sp}$  summary.
  7. Inputs to the transonic calculations and the calculated results are printed. These include  $Y$ , mass flow for each zone and, the slipline locations,  $Y_n$ .
  8. Number of points on the initial line, characteristics mesh control parameters and table of  $x$  vs.  $r$  wall coordinates are printed. The wall table is used by TDK to define the nozzle wall downstream of the throat plane (see Subroutine WALL).
  9. A table of  $P$ ,  $\rho$ ,  $\theta$ ,  $V$ ,  $r$ ,  $x$ , and mass flow rate is printed corresponding to the initial data line for starting the method of characteristics calculations. The method used to calculate the mass flow rate,  $\dot{m}$ , and the characteristic velocity,  $C^*$ , (also printed) is described in Subroutine CHAR.
  10. Results of the method of characteristics calculations are then printed. The calculations begin at the initial data line (until the axis is reached) and follow each left running characteristic to the wall.
  11. TDK performance summary.
  12. BLM title page.  
BLM input geometry, and values of velocity, temperature, and pressure at the edge.
  13. Gas properties table supplied by the ODE module.
  14. BLM geometry and edge conditions that are equally spaced in  $X$ .
  15. BLM output data corresponding to 14, above.
  16. Nozzle wall geometry displaced inwards a distance  $\delta^*$  normal to the input wall contour.
  17. TDK performance summary, including the effects of the boundary layer.

TABLE 7-1. INPUT AND OUTPUT FOR THE STRATIFIED  
ENGINE TEST CASE (3 ZONES).

\$SET NOVERIFY

\*\*\*\*\*  
TWO DIMENSIONAL KINETIC PROGRAM (TDK), OCTOBER 1985 VERSION  
SOFTWARE AND ENGINEERING ASSOCIATES, INC.  
1050 E WILLIAM STREET, SUITE 402, CARSON CITY NEVADA 89701  
(702) 882 1966  
\*\*\*\*\*

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TITLE 3 ZONES TDK TEST CASE, LOX/GH2 - TDK MANUAL TEST CASE

DATA  
\$DATA  
NZONES=3, ODE=1, OOK=1, TDK=1, BLM=1,  
ECRAT=3, ASUB(1)=3, MASUB=1,  
ASUP(1)=2, 4, 10, 15, 20, 25, MASUP=1,  
RSI=2, RWID=1, RWID=1, THETA=30, RI=2.,  
IWALL=1, THETA=15.,  
EPS=2.,  
\$END  
REACTANTS  
H 2. 100. -2154.L 20.27F .0709  
O 2. 99.398 -3102.L 90.180 1.149  
N 2. .053 -2939.L 77.350 .808  
AR1. .549 -2607.L 90. 0

NAMLISTS  
\$CODE  
RKT=.TRUE.,  
P(1)=300., PSTIA=.TRUE.,  
XP(1)=1., .95, .9  
OFSKED(1)=6.5, 8., 5.,  
\$END  
REACTIONS  
H + H = H2 ,M1, A = 6.4E17, N = 1.0, B = 0.0, (AR) BAULCH 72 (A) 30U  
H + OH = H2O ,M2, A = 8.4E21, N = 2.0, B = 0.0, (AR) BAULCH 72 (A) 10U  
O + O = O2 ,M3, A = 1.9E13, N = 0.0, B = -1.79, (AR) BAULCH 76 (A) 10U  
O + H = OH ,M7, A = 3.62E18, N = 1.0, B = 0.0, (AR) JENSEN 78 (B) 30U  
END TBR REAX  
O2 + H = O + OH , A = 2.2E14, N = 0.0, B = 16.8, BAULCH 72 (A) 1.5U  
H2 + O = H + OH , A = 1.8E10, N = -1., B = 8.9, BAULCH 72 (A) 1.5U  
H2 + OH = H2O + H , A = 2.2E13, N = 0.0, B = 5.15, BAULCH 72 (A) 2U  
OH + OH = H2O + O , A = 6.3E12, N = 0.0, B = 1.09, BAULCH 72 (A) 3U  
LAST REAX

INERTS N2, AR, END  
THIRD BODY REAX RATE RATIOS  
M1 = 25\*H, 4\*H2, 10\*H2O, 25\*O, 25\*OH, 1.5\*O2,  
M2 = 12.5\*H, 5\*H2, 17\*H2O, 12.5\*O, 12.5\*OH, 6\*O2,  
M3 = 12.5\*H, 5\*H2, 5\*H2O, 12.5\*O, 12.5\*OH, 11\*O2,  
M7 = 12.5\*H, 5\*H2, 5\*H2O, 12.5\*O, 12.5\*OH, 5\*O2,  
LAST CARD  
\$BOOK  
JPRINT=-2,  
EP=2, XM=.3333, .3334, .3333, MAVISP=1,  
\$END  
\$TRANS  
MP=60,  
XM = .3333, .3333, .3334,  
\$END  
\$MOC  
NC=0,  
\$END,  
\$BLM  
I HFLAG=1,  
N SEGS=1  
\$END

TITLE 3 ZONES TDK TEST CASE, LOX/GH2 - TDK MANUAL TEST CASE

DATA

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\*\*\*\*\*  
CALCULATE ODE AREA RATIO AND PRESSURE SCHEDULES FOR ZONE 1  
\*\*\*\*\*

REACTANTS	0.0000	0.0000	0.0000	0.0000	0.0000	100.000000	-2154.00	L	20.270	F	0.07090
H	2.0000	0.0000	0.0000	0.0000	0.0000	99.398003	-3102.00	L	90.180	O	1.14900
O	2.0000	0.0000	0.0000	0.0000	0.0000	0.053000	-2939.00	L	77.350	O	0.80800
N	2.0000	0.0000	0.0000	0.0000	0.0000	0.549000	-2607.00	L	90.000	O	0.00000
AR	1.0000	0.0000	0.0000	0.0000	0.0000						
NAMELISTS											

SPECIES BEING CONSIDERED IN THIS SYSTEM  
 L 5/65 AR J 3/61 H2 J 3/61 N  
 J 6/63 NO J 6/74 H J 6/74 O J 9/65 O2  
 J 9/65 NH3 J 9/65 M2

OF = 6.500000

ENTHALPY (KG-MOL)(DEG K)/KG	EFFECTIVE FUEL HPP(2)	EFFECTIVE OXIDANT HPP(1)	MIXTURE HSUBO
-0.53769275E+03	-0.48698233E+02	-0.11389750E+03	
KG-ATOMS/KG	BOP(1,2)	BOP(1,1)	BOP(1)
H	0.99209303E+00	0.00000000E+00	0.13227907E+00
O	0.00000000E+00	0.62126074E-01	0.53842597E-01
N	0.00000000E+00	0.37839032E-04	0.32793829E-04
AR	0.00000000E+00	0.13742863E-03	0.11910484E-03

ENTHALPY IN BTU/LBM :  
 FROM REACTANTS : -407.3996  
 FROM DELH( ) : 0.0000  
 FROM DELH1( ) : 0.0000  
 TOTAL : -407.3996

C.S.

ZONE = 1  
THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC = 300.0 PSIA  
 CHEMICAL FORMULA  
 FUEL H 2.00000  
 OXIDANT O 2.00000  
 OXIDANT N 2.00000  
 OXIDANT AR 1.00000

O/F=0.6500E+01 PERCENT FUEL=0.0000E+00 EQUIVALENCE RATIO=0.1228E+01 STOIC MIXTURE RATIO=0.0000E+00 DENSITY=0.0000E+00

PC/P	CHAMBER	THROAT	EXIT	EXIT	WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
	1.0000	1.7268	1.0236	7.5244	1.00000	-2154.000	L	20.27	0.0709
P, PSIA	300.0	173.7	293.1	39.87	0.99398	-3102.000	L	90.18	1.1490
T, DEG R	6110	5821	6098	5093	0.00053	-2939.000	L	77.35	0.8080
H, BTU/LB	-407.4	-867.9	-427.6	-1976.5	0.00549	-2607.000	L	90.00	0.0000
S, BTU/(LB)(R)	4.2737	4.2737	4.2737	4.2737					
DEN (LBM/FT3)	0.639E-010	3.93E-010	6.25E-010	1.07E-01					
M, MOL WT	13.966	14.156	13.974	14.618					
(DLV/DLP)T	-1.04070	-1.03435	-1.04043	-1.01771					
(DLV/DLP)P	1.7427	1.6583	1.7393	1.3878					
CP, BTU/(LB)(R)	2.7889	2.6242	2.7827	1.9849					
CP GAS(SF)	0.8445	0.8383	0.8443	0.8194					
GAMMA GAS(SF)	1.2026	1.2011	1.2026	1.1989					
GAMMA (S)	1.1290	1.1271	1.1289	1.1289					
SOM VEL, FT/SEC	4955.8	4800.5	4948.9	4422.3					
MACH NUMBER	0.0000	1.0000	0.2034	2.0037					
AE/AT	1.0000	3.0001	2.0000						
CSTAR, FT/SEC	7355	7355	7355						
ICF VAC	1.232	3.068	1.471						
COI VAC, LBF-SEC/L	0.653	0.137	1.205						
I, LBF-SEC/LBM	281.59	701.30	336.17						
MOL WT(MIX)	149.20	31.28	275.41						
	13.966	14.156	13.974	14.618					

MOLE FRACTIONS

AR	0.001663	0.001686	0.001664	0.001741
H	0.046578	0.040226	0.046304	0.023887
H2	0.210243	0.204338	0.209987	0.190609
H2O	0.658171	0.685100	0.659338	0.750661
NO	0.000211	0.000176	0.000210	0.000082
N2	0.000123	0.000144	0.000124	0.000199
O	0.008472	0.006379	0.008377	0.002168
OH	0.063976	0.053383	0.063517	0.027171
O2	0.010562	0.008567	0.010478	0.003483
N	3.23E-07	1.96E-07	3.17E-07	3.70E-08
NH3	1.20E-07	7.84E-08	1.18E-07	2.50E-08

NOTE

WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS  
 (SF) STANDS FOR (SHIFTING FROZEN)



FROZEN TRANSPORT PROPERTIES CALCULATED FROM EQUILIBRIUM CONCENTRATIONS

STATION

CHAMBER	MU (LBF-SEC/FT**2)	K (LBF/SEC-DEG R)	PR
THROAT	0.19873776E-05	0.69233529E-01	0.60607994E+00
EXIT	0.19250290E-05	0.66055410E-01	0.61080652E+00
	0.17565214E-05	0.57863409E-01	0.62205720E+00

VISCOSITY EXPONENT (OMEGA) FOR THE FORM MU=MUREF\*(T/TREF)\*\*OMEGA IS 0.68215  
MUREF FOR INPUT TO BLM= 0.64018110E-04 LBM/(FT-SEC)

SPECIES CONSIDERED IN TRANSPORT PROPERTIES CALCULATIONS

AR			
H			
NO		H2	H2O
O2		N2	O
		NH3	

ZONE = 1  
THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN COMPOSITION DURING EXPANSION

PC = 300.0 PSIA  
 CHEMICAL FORMULA  
 FUEL H 2.00000  
 OXIDANT O 2.00000  
 OXIDANT N 2.00000  
 OXIDANT AR 1.00000  
 O/F=0.6500E+01 PERCENT FUEL=0.0000E+00 EQUIVALENCE RATIO=0.1228E+01 STOIC MIXTURE RATIO=0.0000E+00 DENSITY=0.0000E+00

CHAMBER	THROAT	EXIT	EXIT	WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
1.0000	1.7756	1.0248	8.4239	1.00000	-2154.000	L	20.27	0.0709
300.0	169.0	292.8	35.61	0.99398	-3102.000	L	90.18	1.1490
6110	5543	6085	4221	0.00053	-2939.000	L	77.35	0.8080
-407.4	-883.1	-428.6	-1959.2	0.00549	-2607.000	L	90.00	0.0000
4.2737	4.2737	4.2737	4.2737					
S, BTU/(LB)(R)	4.2737	4.2737	4.2737					
DEN (LBM/FT3)	0.639E-010	0.396E-010	0.626E-010					
M, MOL WT	13.966	13.966	13.966					
CP, BTU/(LB)(R)	0.8445	0.8440	0.7912					
GAMMA (S)	1.2026	1.2028	1.2193					
SON VEL, FT/SEC	5114.8	5104.6	4280.2					
MACH NUMBER	0.0000	0.2019	2.0588					
AE/AT	1.0000	2.9997	2.0000					
CSTAR, FT/SEC	7182	7182	7182					
CF VAC	1.243	3.071	1.464					
CF	0.679	0.143	1.227					
IVAC, LBF-SEC/L	277.36	685.46	326.89					
I, LBF-SEC/LBM	151.64	32.03	273.89					

MOLE FRACTIONS	H2	H2O	OH
AR	0.001663	0.210243	0.658171
NO	0.000211	0.008472	0.063976
O2	0.010562		
N			
NH3			

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .0000005 FOR ALL ASSIGNED CONDITIONS

NOTE WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

EQUILIBRIUM CONTRACTION CONDITIONS ZONE 1

TEMPERATURE (DEGR) 0.60978091E+04  
 PRESSURE (PSIA) 0.29308768E+03  
 VELOCITY (FT/S) 0.10067490E+04

SPECIES MOLE FRACTIONS

1 AR 0.16643750E-02  
 2 H 0.46303634E-01  
 3 H2 0.20998725E+00  
 4 H2O 0.65933824E+00  
 5 N 0.31651535E-06  
 6 NO 0.20977536E-03  
 7 N2 0.12402629E-03  
 8 O 0.83772782E-02  
 9 OH 0.63517161E-01  
 10 O2 0.10477899E-01  
 11 NH3 0.11762109E-06

ZONE = 1

REACTIONS

H + H = H2 ,M1, A = 6.4E17, N = 1.0, B = 0.0, (AR) BAULCH 72 (A) 30U  
 H + OH = H2O ,M2, A = 8.4E21, N = 2.0, B = 0.0, (AR) BAULCH 72 (A) 10U  
 O + O = O2 ,M3, A = 1.9E13, N = 0.0, B = -1.79, (AR) BAULCH 76 (A) 10U  
 O + H = OH ,M7, A = 3.62E18, N = 1.0, B = 0.0, (AR) JENSEN 78 (B) 30U  
 O2 + H = O + OH , A = 2.2E14, N = 0.0, B = 16.8, BAULCH 72 (A) 1.5U  
 H2 + O = H + OH , A = 1.8E10, N = -1, B = 8.9, BAULCH 72 (A) 1.5U  
 H2 + OH = H2O + H , A = 2.2E13, N = 0.0, B = 5.15, BAULCH 72 (A) 2U  
 OH + OH = H2O + O , A = 6.3E12, N = 0.0, B = 1.09, BAULCH 72 (A) 3U

THIRD BODY REAX RATE RATIOS

M1 = 25\*H, 4\*H2, 10\*H2O, 25\*O, 25\*OH, 1.5\*O2  
 M2 = 12.5\*H, 5\*H2, 17\*H2O, 12.5\*O, 12.5\*OH, 6\*O2  
 M3 = 12.5\*H, 5\*H2, 5\*H2O, 12.5\*O, 12.5\*OH, 11\*O2  
 M7 = 12.5\*H, 5\*H2, 5\*H2O, 12.5\*O, 12.5\*OH, 5\*O2,

INTERNAL SEQ NUM  
 \*\*REAX 1 \*\*\*  
 \*\*REAX 2 \*\*\*  
 \*\*REAX 3 \*\*\*  
 \*\*REAX 4 \*\*\*  
 \*\*REAX 5 \*\*\*  
 \*\*REAX 6 \*\*\*  
 \*\*REAX 7 \*\*\*  
 \*\*REAX 8 \*\*\*

ORIGINAL PAGE IS  
 OF POOR QUALITY

SELECTED SPECIES FOR KINETIC EXPANSION

ZONE = 1

	INERT SPECIES
1 AR	0.16643750E-02
2 H	0.46303634E-01
3 H2	0.20998725E+00
4 H2O	0.65933824E+00
7 M2	0.12402629E-03
8 O	0.83772782E-02
9 OH	0.63517161E-01
10 O2	0.10477899E-01

DISSOCIATION RECOMBINATION REACTION RATE RATIOS

ZONE = 1

1	0.10000E+01	0.25000E+02	0.40000E+01	0.10000E+02	0.10000E+01	0.25000E+02
	0.25000E+02	0.15000E+01				
2	0.10000E+01	0.12500E+02	0.50000E+01	0.17000E+02	0.10000E+01	0.12500E+02
	0.12500E+02	0.60000E+01				
3	0.10000E+01	0.12500E+02	0.50000E+01	0.50000E+01	0.10000E+01	0.12500E+02
	0.12500E+02	0.11000E+02				
4	0.10000E+01	0.12500E+02	0.50000E+01	0.50000E+01	0.10000E+01	0.12500E+02
	0.12500E+02	0.50000E+01				

ORIGINAL PAGE IS  
OF POOR QUALITY

INITIAL CONDITIONS KINETIC EXPANSION  
ZONE = 1 O/F = 6.5000

FLOW PROPERTIES

MACH NUMBER 0.19707128E+00  
VELOCITY (FT/SEC) 0.10067490E+04  
PRESSURE (PSIA) 0.29308768E+03  
DENSITY (LB/FT3) 0.62570341E-01  
TEMPERATURE (DEG-R) 0.60978091E+04  
ENTHALPY (BTU/LB) -0.42886520E+03  
GAS MOLECULAR WEIGHT 0.13979290E+02  
HEAT CAPACITY (BTU/LB-DEG-R) 0.84399462E+00  
GAMMA 0.12025388E+01

NOZZLE GEOMETRY

THROAT RADIUS (FT) 0.16666667E+00  
THROAT WALL RADIUS DNSTREAM 0.10000000E+01  
CONE ANGLE (DEG) 0.15000000E+02  
EXPANSION RATIO 0.20000000E+01  
CONTRACTION RATIO 0.30000982E+01  
INLET ANGLE (DEG) 0.30000000E+02  
INLET WALL RADIUS 0.20000000E+01  
THROAT WALL RADIUS UPSTREAM 0.10000000E+01

CHEMICAL COMPOSITION

NO.	SPECIES	MASS FRACTION	MOLE FRACTION	NO.	SPECIES	MASS FRACTION	MOLE FRACTION
1	AR	0.47601466E-02	0.16647248E-02	2	H	0.33414641E-02	0.46313372E-01
3	H2	0.30307118E-01	0.21003141E+00	4	H2O	0.85040307E+00	0.65947682E+00
5	N2	0.24874465E-03	0.12405239E-03	6	O	0.95957909E-02	0.83790403E-02
7	OH	0.77339672E-01	0.63530512E-01	8	O2	0.24003910E-01	0.10480101E-01

STEP SIZE SET TO HMIN AT THROAT, HMIN WAS TOO LARGE AND HAS BEEN RESET FROM 0.50000E-02 TO 0.25882E-03

THROAT CONDITIONS KINETIC EXPANSION  
ZONE = 1 O/F = 6.5000

FLOW PROPERTIES

MACH NUMBER 0.97005123E+00  
PRESSURE (PSIA) 0.17345639E+03  
VELOCITY (FT/SEC) 0.48069292E+04  
DENSITY (LB/FT3) 0.39317060E-01  
TEMPERATURE (DEG-R) 0.58181162E+04  
ENTHALPY (BTU/LB) -0.87000177E+03  
GAS MOLECULAR WEIGHT 0.14159413E+02  
HEAT CAPACITY (BTU/LB-DEG) 0.83800578E+00  
GAMMA 0.12011606E+01

PERFORMANCE PARAMETERS

VACUUM THRUST COEFFICIENT 0.12318200E+01  
VACUUM SPECIFIC IMPULSE (SEC) 0.28156735E+03  
CHARACTERISTIC VELOCITY (FT/SEC) 0.73542783E+04

INTEGRATION PARAMETERS

STEP SIZE 0.51763811E-03  
AXIAL POSITION 0.00000000E+00  
PERCENT ENTHALPY CHANGE 0.19432053E-01  
PERCENT MASS FRACTION CHANGE 0.29802322E-04

CHEMICAL COMPOSITION

NO.	SPECIES	MASS FRACTION	MOLE FRACTION	NO.	SPECIES	MASS FRACTION	MOLE FRACTION
1	AR	0.47601466E-02	0.16861745E-02	2	H	0.28714454E-02	0.40311620E-01
3	H2	0.29123077E-01	0.20442639E+00	4	H2O	0.87214732E+00	0.68505377E+00
5	N2	0.24874465E-03	0.12565080E-03	6	O	0.72312579E-02	0.63956906E-02
7	OH	0.64192802E-01	0.53410478E-01	8	O2	0.19424904E-01	0.85901842E-02

EXPANSION CONDITIONS KINETIC EXPANSION AREA RATIO 2.000  
 ZONE = 1 O/F = 6.5000

FLOW PROPERTIES

MACH NUMBER 0.19517127E+01  
 PRESSURE (PSIA) 0.39578793E+02  
 VELOCITY (FT/SEC) 0.86696348E+04  
 DENSITY (LB/FT3) 0.10652749E-01  
 TEMPERATURE (DEG-R) 0.50478320E+04  
 ENTHALPY (BTU/LB) -0.19796588E+04  
 GAS MOLECULAR WEIGHT 0.14589634E+02  
 HEAT CAPACITY(BTU/LB-DEG) 0.81788206E+00  
 GAMMA 0.1998068E+01  
 CURRENT RO\*V\*A 0.16490917E+02

PERFORMANCE PARAMETERS

VACUUM THRUST COEFFICIENT 0.14699095E+01  
 VACUUM SPECIFIC IMPULSE (SEC) 0.33598944E+03

INTEGRATION PARAMETERS

STEP SIZE 0.33128839E-01  
 AXIAL POSITION 0.16775185E+01  
 PERCENT ENTHALPY CHANGE 0.19197460E-01  
 PERCENT MASS FRACTION CHANGE 0.65565109E-04

CHEMICAL COMPOSITION

NO.	SPECIES	MASS FRACTION	MOLE FRACTION	NO. SPECIES	MASS FRACTION	MOLE FRACTION
1	AR	0.47601466E-02	0.17374079E-02	2	H	0.17749741E-02
3	H2	0.26431646E-01	0.19117150E+00	4	H2O	0.92249739E+00
5	N2	0.24874465E-03	0.12946859E-03	6	O	0.26705684E-02
7	OH	0.33039320E-01	0.28325036E-01	8	O2	0.85765254E-02

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CALCULATE ODE AREA RATIO AND PRESSURE SCHEDULES FOR ZONE 2

\*\*\*\*\*

SPECIES BEING CONSIDERED IN THIS SYSTEM

L 5/66 AR J 3/61 H2 J 3/61 N  
 J 6/63 NO J 6/74 O J 12/70 OH J 9/65 O2  
 J 9/65 NH3

OF = 8.000000

ENTHALPY (KG-MOL)(DEG K)/KG	EFFECTIVE FUEL HPP(2)	EFFECTIVE OXIDANT HPP(1)	MIXTURE HSUBO
-0.53769275E+03	-0.48698235E+02	-0.10303096E+03	
KG-ATOMS/KG	BOP(1,2)	BOP(1)	
H	0.99209303E+00	0.0000000E+00	0.11023256E+00
O	0.0000000E+00	0.62126074E-01	0.55223178E-01
N	0.0000000E+00	0.37839032E-04	0.33634697E-04
AR	0.0000000E+00	0.13742865E-03	0.12215880E-03

ENTHALPY IN BTU/LBM :

FROM REACTANTS : -368.5311  
 FROM DELH( ) : 0.0000  
 FROM DELH1( ) : 0.0000  
 TOTAL : -368.5311

OF POOR QUALITY

THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

ZONE = 2

PC = 285.0 PSIA

CHEMICAL FORMULA

FUEL H 2.00000  
 OXIDANT O 2.00000  
 OXIDANT N 2.00000  
 OXIDANT AR 1.00000

O/F=0.8000E+01 PERCENT FUEL=0.0000E+00

EQUIVALENCE RATIO=0.9981E+00 STOIC MIXTURE RATIO=0.0000E+00 DENSITY=0.0000E+00

PC/P	CHAMBER	THROAT	EXIT	EXIT	WT FRACTION	ENTHALPY	STATE	TEMP	DENSITY
P, PSIA	1.0000	1.7234	1.0235	7.4332	(SEE NOTE)	CAL/MOL		DEG K	G/CC
T, DEG R	285.0	165.4	278.5	38.34	1.00000	-2154.000	L	20.27	0.0709
H, BTU/LB	6164	5891	6152	5231	0.99398	-3102.000	L	90.18	1.1490
S, BTU/(LB)(R)	-368.5	-777.6	-386.5	-1764.9	0.00053	-2939.000	L	77.35	0.8080
DEN (LBM/FT3)	3.8898	3.8898	3.8898	3.8898	0.00549	-2607.000	L	90.00	0.0000
M, MOL WT	15.820	16.047	15.830	16.633					
(DLV/DLP)T	-1.05080	-1.04558	-1.05058	-1.03203					
(DLV/DLT)P	1.9200	1.8641	1.9178	1.6849					
CP, BTU/(LB)(R)	2.8639	2.7945	2.8614	2.4984					
CP GAS(SF)	0.7526	0.7476	0.7524	0.7332					
GAMMA GAS(SF)	1.2003	1.1985	1.2003	1.1947					
GAMMA (S)	1.1247	1.1216	1.1246	1.1157					
SON VEL, FT/SEC	4667.9	4524.4	4661.6	4176.8					
MACH NUMBER	0.0000	1.0000	0.2034	2.0013					
AE/AT	1.0000	3.0001	2.0000						
CSTAR, FT/SEC	6952	6952	6952						
CF VAC	1.231	3.068	1.471						
CF	0.651	0.136	1.202						
I VAC, LBF-SEC/L	266.00	662.83	317.95						
I I, LBF-SEC/LBM	140.62	29.47	259.81						
I MOL WT(MIX)	15.820	16.047	15.830	16.633					

MOLE FRACTIONS

AR	0.001933	0.001960	0.001934	0.002032
H	0.039486	0.034264	0.039258	0.021586
H2O	0.124454	0.115314	0.124069	0.089523
N2	0.679569	0.709230	0.680840	0.787126
N	0.000356	0.000329	0.000354	0.000243
O	0.000088	0.000105	0.000089	0.000158
OH	0.019219	0.015378	0.018092	0.008906
O2	0.023321	0.085588	0.095856	0.058605
NH3	3.26E-07	2.13E-07	0.039508	0.031821
NOTE	4.32E-08	2.65E-08	4.23E-08	0.00E+00

WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS  
 (SF) STANDS FOR (SHIFTING FROZEN)

FROZEN TRANSPORT PROPERTIES CALCULATED FROM EQUILIBRIUM CONCENTRATIONS

STATION MU (LBF-SEC/FT\*\*2) (LBF-SEC-DEG R) PR  
 CHAMBER 0.20423211E-05 0.60462840E-01 0.63557798E+00  
 THROAT 0.19826757E-05 0.5769757E-01 0.64230150E+00  
 EXIT 0.18295742E-05 0.50773460E-01 0.66048408E+00

VISCOSITY EXPONENT (OMEGA) FOR THE FORM MU=MUREF\*(T/TREF)\*\*OMEGA IS 0.67341  
 MUREF FOR INPUT TO BLM= 0.65770080E-04 LBM/(FT-SEC)

SPECIES CONSIDERED IN TRANSPORT PROPERTIES CALCULATIONS H2O  
 AR H H2  
 N NO N2  
 OH O2 OH3

THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN COMPOSITION DURING EXPANSION  
 ZONE = 2

PC = 285.0 PSIA  
 CHEMICAL FORMULA  
 FUEL H 2.00000  
 OXIDANT O 2.00000  
 OXIDANT N 2.00000  
 OXIDANT AR 1.00000

O/F=0.8000E+01 PERCENT FUEL=0.0000E+00 EQUIVALENCE RATIO=0.9981E+00 STOIC MIXTURE RATIO=0.0000E+00 DENSITY=0.0000E+00

CHAMBER	THROAT	EXIT	EXIT	WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
1.0000	1.7740	1.0247	8.3924	1.00000	-2154.000	L	20.27	0.0709
285.0	160.7	278.1	33.96	0.99398	-3102.000	L	90.18	1.1490
6164	5598	6139	4278	0.00053	-2939.000	L	77.35	0.8080
-368.5	-791.7	-387.4	-1750.9	0.00549	-2607.000	L	90.00	0.0000
3.8898	3.8898	3.8898	3.8898					
0.681E-010.423E-010.667E-010.117E-01								

M, MOL WT	15.820	15.820	15.820					
CP, BTU/(LB)(R)	0.7526	0.7423	0.7522					
GAMMA (S)	1.2003	1.2037	1.2005					
SON VEL, FT/SEC	4822.3	4601.9	4812.7					
MACH NUMBER	0.0000	1.0000	0.2019					
AE/AT	1.0000	3.0001	2.0000					
CSTAR, FT/SEC	6783	6783	6783					
CF VAC	1.242	3.071	1.464					
CF	0.678	0.143	1.226					
1VAC, LBF-SEC/L	261.86	647.40	308.75					
1, LBF-SEC/LBM	143.03	30.20	258.51					

MOLE FRACTIONS

AR	0.001933	H	0.039486	H2	0.124454	H2O	0.679569
NO	0.000356	N2	0.000088	O	0.018218	OH	0.096321
O2	0.039577						

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS  
 N NH3

NOTE WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS



EQUILIBRIUM CONTRACTION CONDITIONS ZONE 2

TEMPERATURE (DEGR) 0.61522261E+04  
 PRESSURE (PSIA) 0.27845251E+03  
 VELOCITY (FT/S) 0.94859015E+03

SPECIES MOLE FRACTIONS

1	AR	0.19337191E-02
2	H	0.39257679E-01
3	H2	0.12406919E+00
4	H2O	0.68083990E+00
5	N	0.31980758E-06
6	NO	0.35447202E-03
7	N2	0.88794040E-04
8	O	0.18091913E-01
9	OH	0.95856152E-01
10	O2	0.39507885E-01
11	NH3	0.42287063E-07

ZONE = 2

REACTIONS

H + H = H2  
 H + OH = H2O  
 O + O = O2  
 O + H = OH  
 O2 + H = O + OH  
 H2 + O = H + OH  
 H2 + OH = H2O + H  
 OH + OH = H2O + O

M1, A = 6.4E17, N = 1.0, B = 0.0, (AR) BAULCH 72 (A) 30U  
 M2, A = 8.4E21, N = 2.0, B = 0.0, (AR) BAULCH 72 (A) 10U  
 M3, A = 1.9E13, N = 0.0, B = -1.79, (AR) BAULCH 76 (A) 10U  
 M7, A = 3.62E18, N = 1.0, B = 0.0, (AR) JENSEN 78 (B) 30U  
 A = 2.2E14, N = 0.0, B = 16.8, BAULCH 72 (A) 1.5U  
 A = 1.8E10, N = -1., B = 8.9, BAULCH 72 (A) 1.5U  
 A = 2.2E13, N = 0.0, B = 5.15, BAULCH 72 (A) 2U  
 A = 6.3E12, N = 0.0, B = 1.09, BAULCH 72 (A) 3U

THIRD BODY REAX RATE RATIOS  
 M1 = 25\*H,4\*H2,10\*H2O,25\*O,25\*OH,1.5\*O2  
 M2 = 12.5\*H,5\*H2,17\*H2O,12.5\*O,12.5\*OH,6\*O2  
 M3 = 12.5\*H,5\*H2,5\*H2O,12.5\*O,12.5\*OH,11\*O2,  
 M7 = 12.5\*H,5\*H2,5\*H2O,12.5\*O,12.5\*OH,5\*O2,

INTERNAL SEQ NUM  
 \*\*REAX 1 \*\*  
 \*\*REAX 2 \*\*  
 \*\*REAX 3 \*\*  
 \*\*REAX 4 \*\*  
 \*\*REAX 5 \*\*  
 \*\*REAX 6 \*\*  
 \*\*REAX 7 \*\*  
 \*\*REAX 8 \*\*

SELECTED SPECIES FOR KINETIC EXPANSION

ZONE = 2

	INERT SPECIES
1 AR	0.19337191E-02
2 H	0.39257679E-01
3 H2	0.12406919E+00
4 H2O	0.68083990E+00
7 N2	0.88794040E-04
8 O	0.18091913E-01
9 OH	0.95856152E-01
10 O2	0.39507885E-01

DISSOCIATION RECOMBINATION REACTION RATE RATIOS

ZONE = 2

1	0.10000E+01	0.25000E+02	0.40000E+01	0.10000E+02	0.10000E+01	0.25000E+02
	0.25000E+02	0.15000E+01				
2	0.10000E+01	0.12500E+02	0.50000E+01	0.17000E+02	0.10000E+01	0.12500E+02
	0.12500E+02	0.60000E+01				
3	0.10000E+01	0.12500E+02	0.50000E+01	0.50000E+01	0.10000E+01	0.12500E+02
	0.12500E+02	0.11000E+02				
4	0.10000E+01	0.12500E+02	0.50000E+01	0.50000E+01	0.10000E+01	0.12500E+02
	0.12500E+02	0.50000E+01				

ORIGINAL PAGE IS  
OF POOR QUALITY

INITIAL CONDITIONS KINETIC EXPANSION  
ZONE = 2 O/F = 8.0000

FLOW PROPERTIES

MACH NUMBER 0.19693609E+00  
VELOCITY (FT/SEC) 0.94859015E+03  
PRESSURE (PSIA) 0.27845251E+03  
DENSITY (LB/FT3) 0.66738598E-01  
TEMPERATURE (DEG-R) 0.61522261E+04  
ENTHALPY (BTU/LB) -0.38846414E+03  
GAS MOLECULAR WEIGHT 0.15834289E+02  
HEAT CAPACITY (BTU/LB-DEG-R) 0.75226027E+00  
GAMMA 0.12002314E+01

NOZZLE GEOMETRY

THROAT RADIUS (FT) 0.16666667E+00  
THROAT WALL RADIUS DNSTREAM 0.10000000E+01  
COMB ANGLE (DEG) 0.15000000E+02  
EXPANSION RATIO 0.20000000E+01  
CONTRACTION RATIO 0.30000770E+01  
INLET ANGLE (DEG) 0.30000000E+02  
INLET WALL RADIUS 0.20000000E+01  
THROAT WALL RADIUS UPSTREAM 0.10000000E+01

CHEMICAL COMPOSITION

NO.	SPECIES	MASS FRACTION	MOLE FRACTION	NO.	SPECIES	MASS FRACTION	MOLE FRACTION
1	AR	0.48832833E-02	0.19344053E-02	2	H	0.25014721E-02	0.39271604E-01
3	H2	0.15811205E-01	0.12411321E+00	4	H2O	0.77537346E+00	0.68108147E+00
5	N2	0.15724363E-03	0.88825538E-04	6	O	0.18298339E-01	0.18098332E-01
7	OH	0.10305773E+00	0.95890157E-01	8	O2	0.79917319E-01	0.39521899E-01

STEP SIZE SET TO HMIN AT THROAT, HMIN WAS TOO LARGE AND HAS BEEN RESET FROM 0.50000E-02 TO 0.25882E-03

THROAT CONDITIONS KINETIC EXPANSION  
ZONE = 2 O/F = 8.0000

FLOW PROPERTIES

MACH NUMBER 0.96897125E+00  
PRESSURE (PSIA) 0.16504788E+03  
VELOCITY (FT/SEC) 0.45317544E+04  
DENSITY (LB/FT3) 0.41911609E-01  
TEMPERATURE (DEG-R) 0.58878354E+04  
ENTHALPY (BTU/LB) -0.78057233E+03  
GAS MOLECULAR WEIGHT 0.16050882E+02  
HEAT CAPACITY (BTU/LB-DEG) 0.74743026E+00  
GAMMA 0.11985229E+01

PERFORMANCE PARAMETERS

VACUUM THRUST COEFFICIENT 0.12309867E+01  
VACUUM SPECIFIC IMPULSE (SEC) 0.26598679E+03  
CHARACTERISTIC VELOCITY (FT/SEC) 0.69520313E+04

INTEGRATION PARAMETERS

STEP SIZE 0.10352762E-02  
AXIAL POSITION 0.00000000E+00  
PERCENT ENTHALPY CHANGE 0.15772091E-01  
PERCENT MASS FRACTION CHANGE 0.59604645E-05

CHEMICAL COMPOSITION

NO.	SPECIES	MASS FRACTION	MOLE FRACTION	NO.	SPECIES	MASS FRACTION	MOLE FRACTION
1	AR	0.48832833E-02	0.19608657E-02	2	H	0.21571529E-02	0.34329250E-01
3	H2	0.14505051E-01	0.11541778E+00	4	H2O	0.79663646E+00	0.70933062E+00
5	N2	0.15724363E-03	0.90040565E-04	6	O	0.15360956E-01	0.15400880E-01
7	OH	0.90759225E-01	0.85602134E-01	8	O2	0.75540572E-01	0.37868451E-01

EXPANSION CONDITIONS KINETIC EXPANSION AREA RATIO 2.000  
 ZONE = 2 O/F = 8.0000

FLOW PROPERTIES  
 MACH NUMBER 0.19404051E+01  
 PRESSURE (PSIA) 0.38096855E+02  
 VELOCITY (FT/SEC) 0.83668779E+04  
 DENSITY (LB/FT3) 0.11348549E-01  
 TEMPERATURE (DEG-R) 0.51903032E+04  
 ENTHALPY (BTU/LB) -0.17684902E+04  
 GAS MOLECULAR WEIGHT 0.16602911E+02  
 HEAT CAPACITY (BTU/LB-DEG) 0.73210776E+00  
 GAMMA 0.11954341E+01  
 CURRENT RO\*VFA 0.16572239E+02

PERFORMANCE PARAMETERS  
 VACUUM THRUST COEFFICIENT 0.14708618E+01  
 VACUUM SPECIFIC IMPULSE (SEC) 0.31781805E+03

INTEGRATION PARAMETERS  
 STEP SIZE 0.33128839E-01  
 AXIAL POSITION 0.16775185E+01  
 PERCENT ENTHALPY CHANGE 0.14661685E-01  
 PERCENT MASS FRACTION CHANGE 0.29802322E-04

CHEMICAL COMPOSITION

NO.	SPECIES	MASS FRACTION	MOLE FRACTION	NO.	SPECIES	MASS FRACTION	MOLE FRACTION
1	AR	0.48832833E-02	0.20283044E-02	2	H	0.13785680E-02	0.22693260E-01
3	H2	0.11080028E-01	0.91196798E-01	4	H2O	0.85020518E+00	0.78306454E+00
5	N2	0.15724363E-03	0.93137278E-04	6	O	0.89688255E-02	0.93013961E-02
7	OH	0.60542941E-01	0.59066691E-01	8	O2	0.62783629E-01	0.32555848E-01

\*\*\*\*\*  
 CALCULATE ODE AREA RATIO AND PRESSURE SCHEDULES FOR ZONE 3  
 \*\*\*\*\*

SPECIES BEING CONSIDERED IN THIS SYSTEM  
 L 5/65 AR J 6/74 H J 3/61 H2O J 3/61 N  
 J 6/63 NO J 9/65 N2 J 12/70 OH J 9/65 O2  
 J 9/65 NH3

OF =	5.000000	EFFECTIVE FUEL	EFFECTIVE OXIDANT	MIXTURE
ENTHALPY (KG-MOL)(DEG K)/KG	HPP(2)	-0.53769275E+03	HPP(1)	HSUBO
KG-ATOMS/KG	BOP(1,2)		BOP(1,1)	B0(1)
H	0.99209303E+00	0.0000000E+00	0.0000000E+00	0.16534894E+00
O	0.0000000E+00	0.62126074E-01	0.62126074E-01	0.51771730E-01
N	0.0000000E+00	0.37839032E-04	0.37839032E-04	0.31552527E-04
AR	0.0000000E+00	0.0000000E+00	0.13742865E-03	0.11452387E-03

ENTHALPY IN BTU/LBM :  
 FROM REACTANTS : -465.7024  
 FROM DELH( ) : 0.0000  
 FROM DELH1( ) : 0.0000  
 TOTAL : -465.7024

ZONE = 3  
THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC = 270.0 PSIA

CHEMICAL FORMULA

FUEL H 2.00000  
OXIDANT O 2.00000  
OXIDANT N 2.00000  
OXIDANT AR 1.00000

O/F=0.5000E+01 PERCENT FUEL=0.0000E+00 EQUIVALENCE RATIO=0.1597E+01 STOIC MIXTURE RATIO=0.0000E+00 DENSITY=0.0000E+00

PC/P	CHAMBER	THROAT	EXIT	EXIT	WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
P, PSIA	1.0000	1.7430	1.0239	7.9454	1.00000	-2154.000	L	20.27	0.0709
T, DEG R	270.0	154.9	263.7	33.98	0.99398	-3102.000	L	90.18	1.1490
H, BTU/LB	5728	5381	5714	4414	0.00053	-2939.000	L	77.35	0.8080
S, BTU/(LB)(R)	-4.8515	-987.9	-488.7	-2227.9	0.00549	-2607.000	L	90.00	0.0000
DEN (LBM/FT3)	0.513E-010	0.316E-010	0.502E-010	0.861E-02					
M, MOL WT	11.684	11.800	11.690	12.011					
(DLV/DLP)T	-1.01737	-1.01208	-1.01713	-1.00274					
(DLV/DLT)P	1.3315	1.2439	1.3277	1.0655					
CP, BTU/(LB)(R)	2.0622	1.8031	2.0513	1.1899					
CP GAS(SF)	0.9752	0.9648	0.9748	0.9279					
GAMMA GAS(SF)	1.2112	1.2115	1.2112	1.2170					
GAMMA (S)	1.1479	1.1526	1.1480	1.1836					
SOM VEL, FT/SEC	5289.6	5111.9	5281.9	4650.4					
MACH NUMBER	0.0000	1.0000	0.2031	2.0193					

AE/AT	CSTAR, FT/SEC	CF VAC	IVAC, LBF-SEC/L	I, LBF-SEC/LBM	MOL WT (MIX)
7730	1.0000	3.0001	2.0000	11.684	11.690
1.235	7730	7730	1.467	33.35	291.87
0.661	0.661	0.139	1.215	352.34	291.87
296.73	296.73	737.29	352.34	291.87	12.011
158.88	158.88	33.35	291.87	12.011	

MOLE FRACTIONS

AR	0.001338	0.001351	0.001339	0.001376
H	0.037138	0.028055	0.036744	0.008058
H2O	0.357397	0.360034	0.357496	0.368565
NO	0.578544	0.593816	0.579252	0.619108
N2	0.000057	0.000035	0.000056	0.000004
O	0.000155	0.000168	0.000156	0.000187
OH	0.001457	0.000744	0.001420	0.000039
O2	0.022967	0.015300	0.022613	0.002636
N	0.000946	0.000496	0.000924	0.000027
NH3	1.22E-07	5.16E-08	1.18E-07	0.00E+00
	3.02E-07	2.06E-07	2.97E-07	7.85E-08

NOTE

WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS  
(SF) STANDS FOR (SHIFTING FROZEN)

FROZEN TRANSPORT PROPERTIES CALCULATED FROM EQUILIBRIUM CONCENTRATIONS

STATION	MU (LBF-SEC/FT**2)	K (LBF/SEC-DEG R)	PR
CHAMBER	0.18288381E-05	0.77825621E-01	0.57290888E+00
THROAT	0.17521484E-05	0.73574215E-01	0.57443625E+00
EXIT	0.15203000E-05	0.61276197E-01	0.57555461E+00

VISCOSITY EXPONENT (OMEGA) FOR THE FORM MU=MUREF\*(T/TREF)\*\*OMEGA IS 0.71397  
MUREF FOR INPUT TO BLM= 0.58952501E-04 LBM/(FT-SEC)

SPECIES CONSIDERED IN TRANSPORT PROPERTIES CALCULATIONS

AR	H2O
N	O
OH	
	H2
	N2
	NH3
	O2

THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN COMPOSITION DURING EXPANSION

ZONE = 3

PC = 270.0 PSIA

CHEMICAL FORMULA

FUEL	H	2.00000	WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
OXIDANT O	2.00000	1.00000	-2154.000	L	20.27	0.0709	
OXIDANT N	2.00000	0.99398	-3102.000	L	90.18	1.1490	
OXIDANT AR	1.00000	0.00053	-2939.000	L	77.35	0.8080	
		0.00549	-2607.000	L	90.00	0.0000	

O/F=0.5000E+01 PERCENT FUEL=0.0000E+00 EQUIVALENCE RATIO=0.1597E+01 STOIC MIXTURE RATIO=0.0000E+00 DENSITY=0.0000E+00

PC/P	CHAMBER	THROAT	EXIT	EXIT
P, PSIA	1.0000	1.7814	1.0249	8.5450
T, DEG R	270.0	151.6	263.4	31.60
H, BTU/LB	5728	5175	5704	3888
S, BTU/(LB)(R)	-465.7	-1000.7	-489.6	-2202.6
DEN (LBM/FT3)	4.8515	4.8515	4.8515	4.8515
M, MOL WT	11.684	11.684	11.684	11.684
CP, BTU/(LB)(R)	0.9752	0.9588	0.9745	0.9043
GAMMA (S)	1.2112	1.2156	1.2114	1.2316
SON VEL, FT/SEC	5433.7	5174.0	5422.4	4514.0
MACH NUMBER	0.0000	1.0000	0.2017	2.0653
AE/AT	1.0000	3.0001	2.0000	
CSTAR, FT/SEC	7582	7582	7582	
CF VAC	1.244	3.072	1.464	
IVAC, LBF-SEC/L	0.682	0.144	1.230	
I, LBF-SEC/LBM	293.10	723.82	344.92	
	160.81	33.99	289.76	

AR	NO	O2	H2	OH
0.001338	0.037138	0.357397	0.578544	
0.000057	0.000155	0.001457	0.022967	
0.000946				

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .0000005 FOR ALL ASSIGNED CONDITIONS

NOTE WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

ORIGINAL PAGE IS OF POOR QUALITY

EQUILIBRIUM CONTRACTION CONDITIONS ZONE 3

TEMPERATURE (DEGR) 0.57135161E+04  
 PRESSURE (PSIA) 0.26368848E+03  
 VELOCITY (FT/S) 0.10733123E+04

SPECIES MOLE FRACTIONS

1 AR 0.13387334E-02  
 2 H 0.36743894E-01  
 3 H2 0.35749605E+00  
 4 H2O 0.57925242E+00  
 5 N 0.11801665E-06  
 6 NO 0.56386369E-04  
 7 N2 0.15590010E-03  
 8 O 0.14196864E-02  
 9 OH 0.22612970E-01  
 10 O2 0.92356431E-03  
 11 NH3 0.29670508E-06

ZONE = 3

REACTIONS  
 H + H = H2 ,M1, A = 6.4E17, N = 1.0, B = 0.0, (AR) BAULCH 72 (A) 30U  
 H + OH = H2O ,M2, A = 8.4E21, N = 2.0, B = 0.0, (AR) BAULCH 72 (A) 10U  
 O + O = O2 ,M3, A = 1.9E13, N = 0.0, B = -1.79, (AR) BAULCH 76 (A) 10U  
 O + H = OH ,M7, A = 3.62E18, N = 1.0, B = 0.0, (AR) JENSEN 78 (B) 30U  
 O2 + H = O + OH , A = 2.2E14, N = 0.0, B = 16.8, BAULCH 72 (A) 1.5U  
 H2 + O = H + OH , A = 1.8E10, N = -1., B = 8.9, BAULCH 72 (A) 1.5U  
 H2 + OH = H2O + H , A = 2.2E13, N = 0.0, B = 5.15, BAULCH 72 (A) 2U  
 OH + OH = H2O + O , A = 6.3E12, N = 0.0, B = 1.09, BAULCH 72 (A) 3U

THIRD BODY REAX RATE RATIOS

M1 = 25\*H,4\*H2,10\*H2O,25\*O,25\*OH,1.5\*O2,  
 M2 = 12.5\*H,5\*H2,17\*H2O,12.5\*O,12.5\*OH,6\*O2,  
 M3 = 12.5\*H,5\*H2,5\*H2O,12.5\*O,12.5\*OH,11\*O2,  
 M7 = 12.5\*H,5\*H2,5\*H2O,12.5\*O,12.5\*OH,5\*O2,

INTERNAL SEQ NUM  
 \*\*REAX 1 \*\*  
 \*\*REAX 2 \*\*  
 \*\*REAX 3 \*\*  
 \*\*REAX 4 \*\*  
 \*\*REAX 5 \*\*  
 \*\*REAX 6 \*\*  
 \*\*REAX 7 \*\*  
 \*\*REAX 8 \*\*



SELECTED SPECIES FOR KINETIC EXPANSION

ZONE = 3

		INERT SPECIES	INERT SPECIES
1	AR	0.13387334E-02	
2	H	0.36743894E-01	
3	H2	0.35749605E+00	
4	H2O	0.57925242E+00	
7	N2	0.15590010E-03	INERT SPECIES
8	O	0.14196864E-02	
9	OH	0.22612970E-01	
10	O2	0.92356431E-03	

DISSOCIATION RECOMBINATION REACTION RATE RATIOS

ZONE = 3

1	0.10000E+01	0.25000E+02	0.40000E+01	0.10000E+02	0.10000E+01	0.25000E+02
	0.25000E+02	0.15000E+01				
2	0.10000E+01	0.12500E+02	0.50000E+01	0.17000E+02	0.10000E+01	0.12500E+02
	0.12500E+02	0.60000E+01				
3	0.10000E+01	0.12500E+02	0.50000E+01	0.50000E+01	0.10000E+01	0.12500E+02
	0.12500E+02	0.11000E+02				
4	0.10000E+01	0.12500E+02	0.50000E+01	0.50000E+01	0.10000E+01	0.12500E+02
	0.12500E+02	0.50000E+01				

INITIAL CONDITIONS KINETIC EXPANSION

ZONE = 3 O/F = 5.0000

FLOW PROPERTIES

MACH NUMBER 0.19782001E+00  
 VELOCITY (FT/SEC) 0.10735123E+04  
 PRESSURE (PSIA) 0.26348848E+03  
 DENSITY (LB/FT3) 0.50266068E-01  
 TEMPERATURE (DEG-R) 0.57135161E+04  
 ENTHALPY (BTU/LB) -0.48887775E+03  
 GAS MOLECULAR WEIGHT 0.11695736E+02  
 HEAT CAPACITY (BTU/LB-DEG-R) 0.97425121E+00  
 GAMMA 0.12112339E+01

NOZZLE GEOMETRY

THROAT RADIUS (FT) 0.16666667E+00  
 THROAT WALL RADIUS DNSTREAM 0.10000000E+01  
 COME ANGLE (DEG) 0.15000000E+02  
 EXPANSION RATIO 0.20000000E+01  
 CONTRACTION RATIO 0.30000784E+01  
 INLET ANGLE (DEG) 0.30000000E+02  
 INLET WALL RADIUS 0.20000000E+01  
 THROAT WALL RADIUS UPSTREAM 0.10000000E+01

CHEMICAL COMPOSITION

NO.	SPECIES	MASS FRACTION	MOLE FRACTION	NO.	SPECIES	MASS FRACTION	MOLE FRACTION
1	AR	0.45756646E-02	0.13388094E-02	2	H	0.31688218E-02	0.36745980E-01
3	H2	0.61661471E-01	0.35751635E+00	4	H2O	0.89284354E+00	0.57928526E+00
5	N2	0.37366056E-03	0.15590896E-03	6	O	0.19433954E-02	0.14197669E-02
7	OH	0.32904841E-01	0.22614254E-01	8	O2	0.25285168E-02	0.92361670E-03

STEP SIZE SET TO HMIN AT THROAT, HMIN WAS TOO LARGE AND HAS BEEN RESET FROM 0.50000E-02 TO 0.25882E-03

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THROAT CONDITIONS KINETIC EXPANSION

ZONE = 3 O/F = 5.0000

FLOW PROPERTIES

MACH NUMBER 0.97714138E+00  
 PRESSURE (PSIA) 0.15462626E+03  
 VELOCITY (FT/SEC) 0.51191938E+04  
 DENSITY (LB/FT3) 0.31627599E-01  
 TEMPERATURE (DEG-R) 0.53742822E+04  
 ENTHALPY (BTU/LB) -0.98919781E+03  
 GAS MOLECULAR WEIGHT 0.11802890E+02  
 HEAT CAPACITY(BTU/LB-DEG) 0.96414113E+00  
 GAMMA 0.12115697E+01

PERFORMANCE PARAMETERS

VACUUM THRUST COEFFICIENT 0.12352805E+01  
 VACUUM SPECIFIC IMPULSE (SEC) 0.29863614E+03  
 CHARACTERISTIC VELOCITY (FT/SEC) 0.77261567E+04

INTEGRATION PARAMETERS

STEP SIZE 0.10352762E-02  
 AXIAL POSITION 0.00000000E+00  
 PERCENT ENTHALPY CHANGE 0.68588299E-02  
 PERCENT MASS FRACTION CHANGE 0.00000000E+00

CHEMICAL COMPOSITION

NO.	SPECIES	MASS FRACTION	MOLE FRACTION	NO.	SPECIES	MASS FRACTION	MOLE FRACTION
1	AR	0.45756646E-02	0.13510754E-02	2	H	0.24232785E-02	0.28358039E-01
3	H2	0.61514165E-01	0.35992998E+00	4	H2O	0.90647423E+00	0.59351736E+00
5	N2	0.37366056E-03	0.15733739E-03	6	O	0.10286119E-02	0.75834757E-03
7	OH	0.22233596E-01	0.15420306E-01	8	O2	0.13767871E-02	0.50752045E-03

EXPANSION CONDITIONS KINETIC EXPANSION AREA RATIO 2.000  
 ZONE = 3 O/F = 5.0000

FLOW PROPERTIES

MACH NUMBER 0.2004303E+01  
 PRESSURE (PSIA) 0.33545719E+02  
 VELOCITY (FT/SEC) 0.94009004E+04  
 DENSITY (LB/FT<sup>3</sup>) 0.86109657E-02  
 TEMPERATURE (DEG-R) 0.43445571E+04  
 ENTHALPY (BTU/LB) -0.22308054E+04  
 GAS MOLECULAR WEIGHT 0.11975692E+02  
 HEAT CAPACITY(BTU/LB-DEG) 0.92458695E+00  
 GAMMA 0.12187207E+01  
 CURRENT RO\*V\*A 0.14128585E+02

PERFORMANCE PARAMETERS

VACUUM THRUST COEFFICIENT 0.14652495E+01  
 VACUUM SPECIFIC IMPULSE (SEC) 0.35186014E+03  
 INTEGRATION PARAMETERS  
 STEP SIZE 0.33128839E-01  
 AXIAL POSITION 0.16775185E+01  
 PERCENT ENTHALPY CHANGE 0.56242407E-02  
 PERCENT MASS FRACTION CHANGE -0.83446503E-04

CHEMICAL COMPOSITION

NO.	SPECIES	MASS FRACTION	MOLE FRACTION	NO.	SPECIES	MASS FRACTION	MOLE FRACTION
1	AR	0.45756646E-02	0.13708560E-02	2	H	0.11136207E-02	0.13222769E-01
3	H2	0.61593093E-01	0.36566815E+00	4	H2O	0.92614126E+00	0.61527246E+00
5	N2	0.37366056E-03	0.15964088E-03	6	O	0.13606373E-03	0.10178208E-03
7	OH	0.58691776E-02	0.41302163E-02	8	O2	0.19835548E-03	0.74189629E-04

ODK ISP SUMMARY

ZONE	ODK ISP	ZONE MASS FLOW
1	335.989	0.33330
2	317.818	0.33340
3	351.860	0.33330

MASS AVERAGED ISP = 335.221

MASS AVERAGED O/F = 6.29744

DATA FOR ODE/ODK SAVED ON UNIT 15

TRANSONIC ANALYSIS SUBPROGRAM

3 ZONE(S) SPECIFIED

THROAT UPSTREAM RADIUS OF CURVATURE = 1.00000  
THROAT DOWNSTREAM RADIUS OF CURVATURE = 1.00000  
NUMBER OF POINTS ON INITIAL LINE (MP) = 60

SINUSOIDAL DISTRIBUTION FOR INITIAL LINE

ZONE	GAMMA	MASS FLOW THRU ZONE
1	1.12875	0.33330
2	1.12153	0.33330
3	1.16325	0.33340

\*\*\*\*\* CD = 0.99559

TWO DIMENSIONAL KINETIC ANALYSIS SUBPROGRAM

NUMBER OF POINTS ON INITIAL LINE = 59

CHARACTERISTICS MESH CONTROL PARAMETERS  
(SEE SECTION 5.9.3 TDK MANUAL)

INSERTION CONTROL, STREAMLINE POINT SEPARATION (DS) = 0.150  
INSERTION CONTROL, NOZZLE END POINT TOLERANCE (EPW) = 0.010  
INSERTION CONTROL, FLOW ANGLE CHANGE (DTWI) = 2.000  
INSERTION CONTROL, WALL ANGLE CHANGE (DWMI) = 3.000  
EDIT CONTROL, CHARACTERISTICS POINT SEPARATION (ES) = 0.000  
EDIT CONTROL, CHARACTERISTICS POINT ANGLE CHANGE (ETHI) = 0.250  
  
IWALL = 1 OPTION SPECIFIED

ORIGINAL PAGE IS  
OF POOR QUALITY

WALL COORDINATES

1 R/R*	1.00000	1.00000	1.00005	1.00009	1.00012	1.00017	1.00022	1.00028	1.00034
1 X/R*	0.00524	0.00785	0.01047	0.01309	0.01571	0.01832	0.02094	0.02356	0.02618
SLOPE(DEG)	0.07566	0.37569	0.52440	0.67573	0.82445	0.97579	1.12453	1.27588	1.42463
12 R/R*	1.00058	1.00067	1.00077	1.00088	1.00099	1.00111	1.00124	1.00137	1.00151
12 X/R*	0.03403	0.03664	0.03926	0.04188	0.04449	0.04711	0.04972	0.05234	0.05495
SLOPE(DEG)	1.87356	2.02496	2.17638	2.32260	2.47666	2.62551	2.77439	2.92589	3.07481
23 R/R*	1.00181	1.00214	1.00232	1.00250	1.00269	1.00288	1.00308	1.00329	1.00351
23 X/R*	0.06018	0.06560	0.06802	0.07063	0.07324	0.07585	0.07846	0.08107	0.08368
SLOPE(DEG)	3.37531	3.67590	3.82494	3.97401	4.12569	4.27481	4.42654	4.57313	4.72493
34 R/R*	1.00396	1.00444	1.00469	1.00494	1.00521	1.00548	1.00576	1.00604	1.00633
34 X/R*	0.08889	0.09150	0.09671	0.09932	0.10192	0.10453	0.10713	0.10973	0.11234
SLOPE(DEG)	4.87677	5.02345	5.17534	5.32469	5.47666	5.62348	5.77554	5.92502	6.07455
45 R/R*	1.00693	1.00724	1.00789	1.00822	1.00856	1.00890	1.00925	1.00961	1.00998
45 X/R*	0.11754	0.12014	0.12533	0.12793	0.13053	0.13312	0.13572	0.13831	0.14090
SLOPE(DEG)	6.67571	6.82546	6.97527	7.12510	7.27496	7.42491	7.57495	7.72494	7.87506
56 R/R*	1.01035	1.01111	1.01191	1.01231	1.01272	1.01314	1.01357	1.01400	1.01444
56 X/R*	0.14349	0.14867	0.15126	0.15643	0.15902	0.16160	0.16419	0.16677	0.16935
SLOPE(DEG)	8.17539	8.32307	8.47600	8.62636	8.77418	8.92468	9.07528	9.22583	9.37597
67 R/R*	1.01489	1.01534	1.01627	1.01723	1.01771	1.01821	1.01871	1.01921	1.01973
67 X/R*	0.17193	0.17451	0.17708	0.18224	0.18481	0.18738	0.18995	0.19252	0.19509
SLOPE(DEG)	9.82379	9.97471	10.12569	10.27673	10.42281	10.57652	10.72523	10.87400	11.02545
78 R/R*	1.02025	1.02078	1.02131	1.02185	1.02240	1.02295	1.02352	1.02408	1.02466
78 X/R*	0.20022	0.20279	0.20535	0.20791	0.21047	0.21303	0.21559	0.21814	0.22070
SLOPE(DEG)	11.47501	11.62416	11.77592	11.92521	12.07469	12.22411	12.37621	12.52329	12.67560
89 R/R*	1.02642	1.02702	1.02763	1.02824	1.02887	1.02949	1.03013	1.03077	1.03142
89 X/R*	0.22835	0.23090	0.23345	0.23599	0.23853	0.24108	0.24362	0.24615	0.24869
SLOPE(DEG)	13.12519	13.27533	13.42546	13.57313	13.72603	13.87386	14.02699	14.17498	14.32320
100 R/R*	1.03340	1.03407	1.03472	1.03537	1.03602	1.03667	1.03732	1.03797	1.03862
100 X/R*	0.25629	0.25882	1.67752	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
SLOPE(DEG)	14.77328	14.92570	15.00000						

P (PSIA)	RHO (LB/FT <sup>3</sup> )	THETA (DEG)	VEL (FT/SEC)	R	X	MASS FLOW RATE
0.13069E+03	0.27351E-01	0.00000E+00	0.58091E+04	0.10000E+01	0.00000E+00	0.00000E+00
0.13132E+03	0.27465E-01	0.88066E-01	0.57906E+04	0.98981E+00	0.55602E-02	0.28126E+00
0.13160E+03	0.27515E-01	0.12655E+00	0.57825E+04	0.98535E+00	0.79807E-02	0.40387E+00
0.13192E+03	0.27573E-01	0.17181E+00	0.57731E+04	0.98008E+00	0.10821E-01	0.54785E+00
0.13229E+03	0.27639E-01	0.28224E+00	0.57624E+04	0.97402E+00	0.14071E-01	0.71277E+00
0.13270E+03	0.27714E-01	0.41832E+00	0.57504E+04	0.96717E+00	0.17719E-01	0.89809E+00
0.13316E+03	0.27796E-01	0.57879E+00	0.57372E+04	0.95953E+00	0.21753E-01	0.11032E+01
0.13365E+03	0.27981E-01	0.86190E+00	0.57228E+04	0.95113E+00	0.26158E-01	0.13275E+01
0.13419E+03	0.28083E-01	0.95559E+00	0.57073E+04	0.94196E+00	0.30920E-01	0.15703E+01
0.13476E+03	0.28191E-01	0.66770E+00	0.56908E+04	0.93204E+00	0.36020E-01	0.18307E+01
0.13536E+03	0.28305E-01	0.76215E+00	0.56733E+04	0.92138E+00	0.41441E-01	0.21079E+01
0.13599E+03	0.28423E-01	0.86190E+00	0.56550E+04	0.90999E+00	0.47165E-01	0.24011E+01
0.13655E+03	0.28546E-01	0.96674E+00	0.56360E+04	0.89788E+00	0.53172E-01	0.27091E+01
0.13733E+03	0.28672E-01	0.10764E+01	0.56162E+04	0.88504E+00	0.59440E-01	0.30311E+01
0.13804E+03	0.28801E-01	0.11908E+01	0.55958E+04	0.87156E+00	0.65949E-01	0.33660E+01
0.13876E+03	0.28933E-01	0.13095E+01	0.55750E+04	0.85739E+00	0.72674E-01	0.37125E+01
0.13950E+03	0.29067E-01	0.14323E+01	0.55538E+04	0.84254E+00	0.79595E-01	0.40696E+01
0.14024E+03	0.29201E-01	0.15590E+01	0.55322E+04	0.82706E+00	0.86686E-01	0.44361E+01
0.14100E+03	0.29337E-01	0.16894E+01	0.55105E+04	0.81095E+00	0.93924E-01	0.48107E+01
0.14175E+03	0.30593E-01	0.18951E+01	0.54887E+04	0.79423E+00	0.10128E+00	0.51921E+01
0.14248E+03	0.32666E-01	0.19285E+01	0.54643E+04	0.77747E+00	0.10851E+00	0.56268E+01
0.14327E+03	0.34788E-01	0.19595E+01	0.54404E+04	0.76018E+00	0.11581E+00	0.60661E+01
0.14405E+03	0.36940E-01	0.17403E+01	0.54174E+04	0.74237E+00	0.12315E+00	0.65086E+01
0.14483E+03	0.37653E-01	0.18594E+01	0.54009E+04	0.72407E+00	0.13051E+00	0.69529E+01
0.14561E+03	0.37826E-01	0.18951E+01	0.53899E+04	0.70529E+00	0.13788E+00	0.73977E+01
0.14638E+03	0.37996E-01	0.18951E+01	0.53792E+04	0.68605E+00	0.14522E+00	0.78415E+01
0.14713E+03	0.38161E-01	0.18951E+01	0.53701E+04	0.66638E+00	0.15252E+00	0.82829E+01
0.14787E+03	0.38321E-01	0.19285E+01	0.53633E+04	0.64630E+00	0.15975E+00	0.87207E+01
0.14859E+03	0.38476E-01	0.19881E+01	0.53582E+04	0.62582E+00	0.16689E+00	0.91534E+01
0.14930E+03	0.38624E-01	0.20376E+01	0.53535E+04	0.60498E+00	0.17393E+00	0.95797E+01
0.15062E+03	0.34692E-01	0.20141E+01	0.53528E+04	0.58380E+00	0.18084E+00	0.99984E+01
0.15140E+03	0.34999E-01	0.18723E+01	0.53520E+04	0.56230E+00	0.18760E+00	0.10408E+02
0.15213E+03	0.35144E-01	0.18176E+01	0.53508E+04	0.54305E+00	0.18760E+00	0.10408E+02
0.15284E+03	0.35416E-01	0.17582E+01	0.53492E+04	0.53287E+00	0.19455E+00	0.10825E+02
0.15418E+03	0.35543E-01	0.16941E+01	0.53484E+04	0.52249E+00	0.20130E+00	0.11229E+02
0.15480E+03	0.35663E-01	0.15529E+01	0.53477E+04	0.51597E+00	0.20783E+00	0.11620E+02
0.15539E+03	0.35777E-01	0.14763E+01	0.53471E+04	0.49240E+00	0.21410E+00	0.11995E+02
0.15595E+03	0.35883E-01	0.13959E+01	0.53465E+04	0.46859E+00	0.22012E+00	0.12356E+02
0.15648E+03	0.35982E-01	0.13122E+01	0.53459E+04	0.44459E+00	0.22585E+00	0.12699E+02
0.15742E+03	0.36159E-01	0.12254E+01	0.53453E+04	0.42042E+00	0.22887E+00	0.13025E+02
0.15783E+03	0.36236E-01	0.11361E+01	0.53447E+04	0.39613E+00	0.23129E+00	0.13333E+02
0.15855E+03	0.36305E-01	0.10446E+01	0.53441E+04	0.37175E+00	0.24125E+00	0.13622E+02
0.15886E+03	0.36366E-01	0.95132E+00	0.53435E+04	0.34731E+00	0.24574E+00	0.13891E+02
0.15913E+03	0.36421E-01	0.85682E+00	0.53429E+04	0.32287E+00	0.24990E+00	0.14140E+02
0.15936E+03	0.36467E-01	0.76160E+00	0.53423E+04	0.29846E+00	0.25373E+00	0.14369E+02
0.15955E+03	0.36507E-01	0.66621E+00	0.53417E+04	0.27413E+00	0.25721E+00	0.14577E+02
0.15971E+03	0.36540E-01	0.57123E+00	0.53411E+04	0.24992E+00	0.26034E+00	0.14765E+02
0.15984E+03	0.36566E-01	0.47733E+00	0.53405E+04	0.22588E+00	0.26314E+00	0.14932E+02
0.15994E+03	0.36585E-01	0.38522E+00	0.53400E+04	0.20208E+00	0.26559E+00	0.15079E+02
0.16001E+03	0.36599E-01	0.29573E+00	0.53394E+04	0.17540E+00	0.26772E+00	0.15206E+02
0.16005E+03	0.36608E-01	0.20992E+00	0.53388E+04	0.15540E+00	0.26951E+00	0.15314E+02
0.16007E+03	0.36612E-01	0.12926E+00	0.53382E+04	0.13268E+00	0.27099E+00	0.15402E+02
0.16008E+03	0.36615E-01	0.56314E-01	0.53376E+04	0.11048E+00	0.27217E+00	0.15473E+02
		0.00000E+00	0.51361E+04	0.88907E-01	0.27307E+00	0.15564E+02
				0.68109E-01	0.27370E+00	0.15688E+02
				0.51378E+04	0.27410E+00	0.15800E+02
				0.29697E-01	0.27430E+00	0.15860E+02
				0.12926E+00	0.27430E+00	0.15860E+02
				0.51362E+04	0.27434E+00	0.15860E+02
				0.12932E-01		
				0.00000E+00		

MASS FLOW RATE (LB/SEC) = 15.6027      CSTAR (FT/SEC) = 6996.46      INITIAL THRUST (LBF) = 4395.54

LRC ID    R    X    MACH    THETA T (DEG.R)    P (PSI)    DENSITY    VELOCITY    CF    ISP    IT    ZONE

0 15    1.00000    0.00000    1.122    0.000    5264.60    130.69    0.27351E-01    5809.73    1.2955    281.716    0

ORIGINAL DATA  
OF ROOF

LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
1	1	0.98981	1.118	0.088	5267.78	131.32	0.27465E-01	5791.21	0.0000	0.000	0	3
1	5	1.00001	1.130	0.309	5256.82	129.31	0.27105E-01	5850.36	1.2955	281.719	2	3
1	5	1.00006	1.139	0.620	5249.17	127.94	0.26860E-01	5890.66	1.2956	281.728	4	3
MASS FLOW POINT 1 = 2.812945E-01 DELTA FLOWRATE = 1.532142E+01 PERCENT DELTA = 9.819714E+01 AREA RATIO = 1.000117E+00												
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
2	1	0.98535	1.116	0.127	5269.16	131.60	0.27515E-01	5783.18	0.0000	0.000	0	3
2	5	1.00012	1.147	0.895	5242.62	126.76	0.26648E-01	5925.42	1.2956	281.741	4	3
MASS FLOW POINT 2 = 4.039025E-01 DELTA FLOWRATE = 1.519881E+01 PERCENT DELTA = 9.741134E+01 AREA RATIO = 1.000244E+00												
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
3	1	0.98008	1.114	0.172	5270.77	131.92	0.27573E-01	5773.77	0.0000	0.000	0	3
3	5	1.00023	1.155	1.220	5234.96	125.38	0.26400E-01	5966.18	1.2957	281.763	4	3
MASS FLOW POINT 3 = 5.478930E-01 DELTA FLOWRATE = 1.505482E+01 PERCENT DELTA = 9.648848E+01 AREA RATIO = 1.000454E+00												
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
4	1	0.97402	1.112	0.224	5272.61	132.29	0.27639E-01	5763.04	0.0000	0.000	0	3
4	5	1.00039	1.165	1.596	5226.27	123.80	0.26115E-01	6012.51	1.2959	281.795	4	3
MASS FLOW POINT 4 = 7.127798E-01 DELTA FLOWRATE = 1.488993E+01 PERCENT DELTA = 9.543169E+01 AREA RATIO = 1.000776E+00												
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
5	1	0.96717	1.109	0.282	5274.65	132.70	0.27714E-01	5751.02	0.0000	0.000	0	3
5	5	1.00062	1.177	2.023	5216.42	122.04	0.25796E-01	6064.76	1.2961	281.842	4	3
MASS FLOW POINT 5 = 8.981084E-01 DELTA FLOWRATE = 1.470460E+01 PERCENT DELTA = 9.424390E+01 AREA RATIO = 1.001247E+00												
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
6	1	0.95953	1.106	0.347	5276.90	133.16	0.27796E-01	5737.79	0.0000	0.000	0	3
6	5	1.00095	1.189	2.501	5205.45	120.10	0.25444E-01	6122.64	1.2964	281.906	4	3
MASS FLOW POINT 6 = 1.103257E+00 DELTA FLOWRATE = 1.469945E+01 PERCENT DELTA = 9.292907E+01 AREA RATIO = 1.001906E+00												
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
7	1	0.95113	1.103	0.418	5279.34	133.65	0.27885E-01	5723.40	0.0000	0.000	0	3
7	5	1.00116	1.196	2.764	5199.45	119.04	0.25251E-01	6154.12	1.2966	281.947	2	3
7	5	1.00140	1.203	3.029	5193.40	117.98	0.25059E-01	6185.64	1.2968	281.991	3	3
MASS FLOW POINT 7 = 1.327569E+00 DELTA FLOWRATE = 1.427314E+01 PERCENT DELTA = 9.149142E+01 AREA RATIO = 1.002796E+00												
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
8	1	0.94196	1.100	0.496	5281.95	134.19	0.27981E-01	5707.92	0.0000	0.000	0	3
8	5	1.00168	1.210	3.317	5186.79	116.83	0.24850E-01	6219.89	1.2970	282.044	2	3
8	5	1.00198	1.218	3.607	5180.13	115.69	0.24641E-01	6254.17	1.2973	282.101	3	3
MASS FLOW POINT 8 = 1.570325E+00 DELTA FLOWRATE = 1.403239E+01 PERCENT DELTA = 8.993556E+01 AREA RATIO = 1.003965E+00												
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
9	1	0.93204	1.097	0.579	5284.72	134.76	0.28083E-01	5691.42	0.0000	0.000	0	3
9	5	1.00234	1.226	3.919	5172.92	114.46	0.24417E-01	6291.04	1.2976	282.168	2	3
9	5	1.00273	1.234	4.234	5165.64	113.24	0.24193E-01	6327.97	1.2979	282.239	3	3
MASS FLOW POINT 9 = 1.830737E+00 DELTA FLOWRATE = 1.377197E+01 PERCENT DELTA = 8.826655E+01 AREA RATIO = 1.005465E+00												
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
10	1	0.92138	1.093	0.668	5287.64	135.36	0.28191E-01	5673.98	0.0000	0.000	0	3
10	5	1.00318	1.243	4.570	5157.79	111.94	0.23954E-01	6367.43	1.2983	282.321	2	3
10	5	1.00367	1.252	4.909	5149.86	110.63	0.23715E-01	6406.98	1.2987	282.409	3	3
MASS FLOW POINT 10 = 2.107963E+00 DELTA FLOWRATE = 1.349475E+01 PERCENT DELTA = 8.648976E+01 AREA RATIO = 1.007350E+00												
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
11	1	0.90999	1.089	0.762	5290.69	135.99	0.28305E-01	5655.68	0.0000	0.000	0	3
11	5	1.00423	1.261	5.269	5141.36	109.26	0.23463E-01	6448.96	1.2991	282.508	2	3
11	5	1.00483	1.270	5.632	5132.74	107.88	0.23209E-01	6491.11	1.2996	282.614	3	3
MASS FLOW POINT 11 = 2.401087E+00 DELTA FLOWRATE = 1.320162E+01 PERCENT DELTA = 8.461109E+01 AREA RATIO = 1.009677E+00												
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
12	1	0.89788	1.088	0.862	5293.85	136.65	0.28423E-01	5636.60	0.0000	0.000	0	3





MASS FLOW POINT 22 = 6.068181E+00 DELTA FLOWRATE = 9.534531E+00 PERCENT DELTA = 6.110817E+01 AREA RATIO = 1.074506E+00

Table with columns: LRC ID, R, X, MACH, THETA, T (DEG.R), P (PSI), DENSITY, VELOCITY, CF, ISP, IT, ZONE. Includes data for points 22, 23, and 24.

MASS FLOW POINT 23 = 6.509702E+00 DELTA FLOWRATE = 9.093010E+00 PERCENT DELTA = 5.827840E+01 AREA RATIO = 1.086609E+00

Table with columns: LRC ID, R, X, MACH, THETA, T (DEG.R), P (PSI), DENSITY, VELOCITY, CF, ISP, IT, ZONE. Includes data for points 23, 24, and 25.

MASS FLOW POINT 24 = 6.953610E+00 DELTA FLOWRATE = 8.649102E+00 PERCENT DELTA = 5.543333E+01 AREA RATIO = 1.098859E+00

Table with columns: LRC ID, R, X, MACH, THETA, T (DEG.R), P (PSI), DENSITY, VELOCITY, CF, ISP, IT, ZONE. Includes data for points 24, 25, and 26.

MASS FLOW POINT 25 = 7.398190E+00 DELTA FLOWRATE = 8.204522E+00 PERCENT DELTA = 5.258395E+01 AREA RATIO = 1.111247E+00

Table with columns: LRC ID, R, X, MACH, THETA, T (DEG.R), P (PSI), DENSITY, VELOCITY, CF, ISP, IT, ZONE. Includes data for points 25, 26, and 27.

MASS FLOW POINT 26 = 7.841299E+00 DELTA FLOWRATE = 7.761413E+00 PERCENT DELTA = 4.974400E+01 AREA RATIO = 1.123764E+00

Table with columns: LRC ID, R, X, MACH, THETA, T (DEG.R), P (PSI), DENSITY, VELOCITY, CF, ISP, IT, ZONE. Includes data for points 26, 27, and 28.

MASS FLOW POINT 27 = 8.282604E+00 DELTA FLOWRATE = 7.320107E+00 PERCENT DELTA = 4.691561E+01 AREA RATIO = 1.136406E+00

Table with columns: LRC ID, R, X, MACH, THETA, T (DEG.R), P (PSI), DENSITY, VELOCITY, CF, ISP, IT, ZONE. Includes data for points 27, 28, and 29.

MASS FLOW POINT 28 = 8.720003E+00 DELTA FLOWRATE = 6.882709E+00 PERCENT DELTA = 4.411226E+01 AREA RATIO = 1.149176E+00

Table with columns: LRC ID, R, X, MACH, THETA, T (DEG.R), P (PSI), DENSITY, VELOCITY, CF, ISP, IT, ZONE. Includes data for points 28, 29, and 30.

MASS FLOW POINT 29 = 9.152867E+00 DELTA FLOWRATE = 6.449844E+00 PERCENT DELTA = 4.133797E+01 AREA RATIO = 1.162081E+00

Table with columns: LRC ID, R, X, MACH, THETA, T (DEG.R), P (PSI), DENSITY, VELOCITY, CF, ISP, IT, ZONE. Includes data for points 29, 30, and 31.

MASS FLOW POINT 31 = 9.998495E+00 DELTA FLOWRATE = 5.604217E+00 PERCENT DELTA = 3.591822E+01 AREA RATIO = 1.188193E+00

LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
31 1	0.56230	0.18760	1.052	2.038	5842.33	150.62	0.38624E-01	4895.31	0.0000	0.000	0	2
31 4	0.81229	0.30646	1.307	8.273	5681.18	108.36	0.28805E-01	5969.21	0.0000	0.000	2	2
31 4	0.81229	0.30646	1.267	8.273	5140.56	108.36	0.23282E-01	6479.37	0.0000	0.000	2	3
31 5	1.09610	0.49031	1.539	15.000	4890.06	72.424	0.16442E-01	7657.27	1.3555	294.757	3	3

MASS FLOW POINT 32 = 1.040845E+01 DELTA FLOWRATE = 5.194263E+00 PERCENT DELTA = 3.329077E+01 AREA RATIO = 1.201439E+00

LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
32 1	0.56230	0.18760	1.094	2.038	5743.63	150.62	0.34692E-01	5375.42	0.0000	0.000	0	1
32 1	0.53929	0.19455	1.089	1.922	5746.33	151.40	0.34850E-01	5356.17	0.0000	0.000	0	1
32 4	0.56294	0.20427	1.108	2.341	5734.58	147.87	0.34125E-01	5442.46	0.0000	0.000	8	1
32 4	0.56294	0.20427	1.068	2.341	5833.54	147.87	0.37992E-01	4962.36	0.0000	0.000	8	2
32 4	0.81604	0.33110	1.332	9.007	5663.65	104.57	0.27906E-01	6072.42	0.0000	0.000	2	2
32 4	0.81604	0.33110	1.294	9.007	5116.39	104.57	0.22583E-01	6597.66	0.0000	0.000	2	3
32 5	1.10004	0.50501	1.542	15.000	4887.29	72.070	0.16372E-01	7670.23	1.3578	295.260	3	3
32 5	1.10398	0.51971	1.545	15.000	4884.45	71.717	0.16303E-01	7683.21	1.3601	295.763	3	3

MASS FLOW POINT 34 = 1.082411E+01 DELTA FLOWRATE = 4.778598E+00 PERCENT DELTA = 3.062671E+01 AREA RATIO = 1.218770E+00

LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
33 1	0.51597	0.20130	1.085	1.872	5748.88	152.13	0.34999E-01	5337.96	0.0000	0.000	0	1
33 4	0.56368	0.22127	1.122	2.671	5726.01	145.33	0.33605E-01	5504.94	0.0000	0.000	2	1
33 4	0.56368	0.22127	1.082	2.671	5825.40	145.33	0.37410E-01	5024.06	0.0000	0.000	2	2
33 4	0.82002	0.35526	1.357	9.720	5646.16	100.92	0.27040E-01	6173.53	0.0000	0.000	2	2
33 4	0.82002	0.35526	1.320	9.720	5092.18	100.92	0.21908E-01	6713.05	0.0000	0.000	2	3
33 5	1.10779	0.53392	1.548	15.000	4881.59	71.375	0.16236E-01	7695.99	1.3623	296.248	3	3
33 5	1.11159	0.54812	1.551	15.000	4878.68	71.028	0.16167E-01	7708.82	1.3646	296.733	3	3

MASS FLOW POINT 35 = 1.122801E+01 DELTA FLOWRATE = 4.374704E+00 PERCENT DELTA = 2.803810E+01 AREA RATIO = 1.235640E+00

LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
34 1	0.49240	0.20783	1.082	1.818	5751.33	152.84	0.35144E-01	5320.37	0.0000	0.000	0	1
34 4	0.56454	0.23858	1.137	3.005	5716.49	142.71	0.33068E-01	5571.03	0.0000	0.000	4	1
34 4	0.56454	0.23858	1.097	3.005	5816.47	142.71	0.36809E-01	5088.93	0.0000	0.000	4	2
34 4	0.82433	0.37952	1.382	10.432	5628.39	97.346	0.26186E-01	6273.91	0.0000	0.000	2	2
34 4	0.82433	0.37952	1.346	10.432	5067.48	97.346	0.21243E-01	6827.76	0.0000	0.000	2	3
34 5	1.11537	0.56222	1.554	15.000	4875.64	70.682	0.16099E-01	7721.90	1.3668	297.213	3	3
34 5	1.11915	0.57631	1.557	15.000	4872.55	70.329	0.16030E-01	7735.03	1.3690	297.692	3	3

MASS FLOW POINT 36 = 1.161917E+01 DELTA FLOWRATE = 3.983541E+00 PERCENT DELTA = 2.553108E+01 AREA RATIO = 1.252490E+00

LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
35 1	0.46859	0.21410	1.078	1.758	5753.67	153.52	0.35283E-01	5303.46	0.0000	0.000	0	1
35 4	0.56552	0.25616	1.152	3.335	5706.92	140.10	0.32530E-01	5636.74	0.0000	0.000	2	1
35 4	0.56552	0.25616	1.112	3.335	5807.54	140.10	0.36206E-01	5153.07	0.0000	0.000	2	2
35 4	0.82898	0.40393	1.407	11.141	5610.20	93.817	0.25340E-01	6374.65	0.0000	0.000	2	2
35 4	0.82898	0.40393	1.377	11.141	5042.15	93.817	0.20584E-01	6942.50	0.0000	0.000	2	3
35 5	1.12291	0.59035	1.561	15.000	4869.29	69.968	0.15960E-01	7748.60	1.3712	298.168	3	3
35 5	1.12667	0.60438	1.564	15.000	4865.99	69.604	0.15888E-01	7762.20	1.3733	298.644	3	3

MASS FLOW POINT 37 = 1.199530E+01 DELTA FLOWRATE = 3.607415E+00 PERCENT DELTA = 2.312044E+01 AREA RATIO = 1.269381E+00

LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
36 1	0.44459	0.22012	1.074	1.694	5755.91	154.18	0.35416E-01	5287.27	0.0000	0.000	0	1
36 4	0.56660	0.27397	1.167	3.660	5696.86	137.45	0.31986E-01	5704.46	0.0000	0.000	3	1
36 4	0.56660	0.27397	1.128	3.660	5798.00	137.45	0.35599E-01	5220.25	0.0000	0.000	3	2
36 4	0.83398	0.42853	1.432	11.849	5591.54	90.337	0.24502E-01	6475.66	0.0000	0.000	2	2
36 4	0.83398	0.42853	1.398	11.849	5016.12	90.337	0.19931E-01	7056.88	0.0000	0.000	2	3
36 5	1.13447	0.61839	1.567	15.000	4862.53	69.232	0.15816E-01	7776.21	1.3755	299.118	3	3
36 5	1.13417	0.63240	1.571	15.000	4859.04	68.859	0.15743E-01	7790.27	1.3777	299.590	3	3

MASS FLOW POINT 38 = 1.235581E+01 DELTA FLOWRATE = 3.246900E+00 PERCENT DELTA = 2.080984E+01 AREA RATIO = 1.286353E+00

LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
37 1	0.42042	0.22585	1.071	1.626	5758.04	154.80	0.35543E-01	5271.84	0.0000	0.000	0	1
37 4	0.56781	0.29201	1.182	3.982	5686.85	134.82	0.31442E-01	5771.31	0.0000	0.000	2	1

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LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
37 4	0.56781	0.29201	1.143	3.982	5788.68	134.82	0.34990E-01	5285.63	0.0000	0.000	0.000	2
37 4	0.83934	0.45331	1.458	12.551	5572.36	86.905	0.23673E-01	6577.17	0.0000	0.000	0.000	2
37 4	0.83934	0.45331	1.425	12.551	4989.35	86.905	0.19284E-01	7171.58	0.0000	0.000	0.000	2
37 5	1.13793	0.64640	1.574	15.000	4855.34	68.472	0.15667E-01	7804.90	1.3799	300.062	3	3
37 5	1.14168	0.66040	1.578	15.000	4851.61	68.085	0.15591E-01	7819.56	1.3820	300.532	3	3
MASS FLOW POINT 39 = 1.269941E+01 DELTA FLOWRATE = 2.903298E+00 PERCENT DELTA = 1.860765E+01 AREA RATIO = 1.303427E+00												
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
38 1	0.39613	0.23129	1.068	1.553	5760.05	155.39	0.35663E-01	5257.21	0.0000	0.000	0.000	1
38 4	0.56913	0.31023	1.197	4.302	5676.53	132.18	0.30896E-01	5838.91	0.0000	0.000	0.000	1
38 4	0.56913	0.31023	1.159	4.302	5779.06	132.18	0.34378E-01	5351.74	0.0000	0.000	0.000	2
38 4	0.84505	0.47825	1.483	13.240	5552.99	83.565	0.22863E-01	6677.77	0.0000	0.000	0.000	2
38 4	0.84505	0.47825	1.452	13.240	4962.18	83.565	0.18652E-01	7285.07	0.0000	0.000	0.000	2
38 5	1.14542	0.67438	1.582	15.000	4847.73	67.688	0.15514E-01	7834.62	1.3842	301.000	3	3
38 5	1.14917	0.68835	1.585	15.000	4843.83	67.293	0.15436E-01	7849.71	1.3863	301.467	3	3
MASS FLOW POINT 40 = 1.302545E+01 DELTA FLOWRATE = 2.577257E+00 PERCENT DELTA = 1.651801E+01 AREA RATIO = 1.320586E+00												
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
39 1	0.37175	0.23643	1.065	1.476	5761.94	155.95	0.35777E-01	5243.40	0.0000	0.000	0.000	1
39 4	0.57056	0.32859	1.212	4.617	5665.94	129.53	0.30347E-01	5907.26	0.0000	0.000	0.000	1
39 4	0.57056	0.32859	1.174	4.617	5769.21	129.53	0.33763E-01	5418.34	0.0000	0.000	0.000	2
39 4	0.85110	0.50334	1.508	13.892	5534.16	80.388	0.22088E-01	6774.70	0.0000	0.000	0.000	2
39 4	0.85110	0.50334	1.478	13.892	4935.40	80.388	0.18047E-01	7394.75	0.0000	0.000	0.000	2
39 5	1.15291	0.70232	1.589	15.000	4839.76	66.886	0.15357E-01	7865.26	1.3885	301.933	3	3
39 5	1.15665	0.71629	1.593	15.000	4835.66	66.480	0.15277E-01	7880.85	1.3906	302.397	3	3
MASS FLOW POINT 41 = 1.333325E+01 DELTA FLOWRATE = 2.269464E+00 PERCENT DELTA = 1.454531E+01 AREA RATIO = 1.337849E+00												
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
40 1	0.34731	0.24125	1.062	1.396	5763.71	156.48	0.35883E-01	5230.46	0.0000	0.000	0.000	1
40 4	0.57210	0.34710	1.228	4.930	5655.14	126.88	0.29798E-01	5975.99	0.0000	0.000	0.000	1
40 4	0.57210	0.34710	1.190	4.930	5759.15	126.88	0.33148E-01	5485.37	0.0000	0.000	0.000	2
40 4	0.85747	0.52854	1.531	14.474	5516.82	77.482	0.21374E-01	6864.44	0.0000	0.000	0.000	2
40 4	0.85747	0.52854	1.502	14.474	4910.21	77.482	0.17490E-01	7496.65	0.0000	0.000	0.000	2
40 5	1.16413	0.74421	1.601	15.000	4827.12	65.648	0.15115E-01	7912.96	1.3949	303.321	3	3
MASS FLOW POINT 42 = 1.362206E+01 DELTA FLOWRATE = 1.980650E+00 PERCENT DELTA = 1.269427E+01 AREA RATIO = 1.355209E+00												
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
41 1	0.32287	0.24574	1.059	1.312	5765.35	156.97	0.35982E-01	5218.39	0.0000	0.000	0.000	1
41 4	0.57376	0.36569	1.244	5.239	5644.13	124.24	0.29248E-01	6045.06	0.0000	0.000	0.000	1
41 4	0.57376	0.36569	1.202	5.239	5748.89	124.24	0.32533E-01	5552.83	0.0000	0.000	0.000	2
41 4	0.86411	0.55383	1.552	14.952	5501.83	74.933	0.20743E-01	6943.87	0.0000	0.000	0.000	2
41 4	0.86411	0.55383	1.524	14.952	4887.77	74.933	0.16997E-01	7587.35	0.0000	0.000	0.000	2
41 5	1.17161	0.77212	1.609	15.000	4818.15	64.793	0.14947E-01	7946.17	1.3991	304.238	3	3
MASS FLOW POINT 43 = 1.389131E+01 DELTA FLOWRATE = 1.711402E+00 PERCENT DELTA = 1.096862E+01 AREA RATIO = 1.372676E+00												
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
42 1	0.29846	0.24990	1.057	1.225	5766.87	157.42	0.36074E-01	5207.22	0.0000	0.000	0.000	1
42 4	0.57552	0.38435	1.259	5.545	5632.96	121.62	0.28701E-01	6114.16	0.0000	0.000	0.000	1
42 4	0.57552	0.38435	1.222	5.545	5738.51	121.62	0.31920E-01	5620.20	0.0000	0.000	0.000	2
42 4	0.87095	0.57913	1.569	15.308	5489.58	72.779	0.20206E-01	7011.51	0.0000	0.000	0.000	2
42 4	0.87095	0.57913	1.543	15.308	4868.76	72.779	0.16578E-01	7664.98	0.0000	0.000	0.000	2
42 5	1.17908	0.79999	1.618	15.000	4808.84	63.921	0.14776E-01	7980.28	1.4033	305.148	3	3
MASS FLOW POINT 44 = 1.414055E+01 DELTA FLOWRATE = 1.462163E+00 PERCENT DELTA = 9.371210E+00 AREA RATIO = 1.390229E+00												
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
43 1	0.27413	0.25373	1.055	1.136	5768.26	157.83	0.36159E-01	5196.97	0.0000	0.000	0.000	1
43 4	0.57738	0.40305	1.275	5.847	5621.63	119.02	0.28157E-01	6183.26	0.0000	0.000	0.000	1
43 4	0.57738	0.40305	1.238	5.847	5727.98	119.02	0.31311E-01	5687.61	0.0000	0.000	0.000	2
43 4	0.87792	0.60438	1.584	15.543	5479.99	71.003	0.19760E-01	7067.58	0.0000	0.000	0.000	2
43 4	0.87792	0.60438	1.558	15.543	4853.26	71.003	0.16230E-01	7729.66	0.0000	0.000	0.000	2
43 5	1.18653	0.82778	1.627	15.000	4799.19	63.035	0.14602E-01	8015.20	1.4074	306.049	3	3
MASS FLOW POINT 45 = 1.436951E+01 DELTA FLOWRATE = 1.233202E+00 PERCENT DELTA = 7.903767E+00 AREA RATIO = 1.407849E+00												
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE

44	1	0.24992	0.25721	1.052	1.045	5769.52	158.21	0.36236E-01	5187.63	0.0000	0.000	0
44	4	0.57935	0.42176	1.291	6.144	5610.17	116.44	0.27616E-01	6252.18	0.0000	0.000	2
44	4	0.57935	0.42176	1.255	6.144	5717.32	116.44	0.30706E-01	5754.91	0.0000	0.000	2
44	4	0.88495	0.62954	1.596	15.670	5472.52	69.550	0.19393E-01	7113.79	0.0000	0.000	3
44	4	0.88495	0.62954	1.571	15.670	4840.83	69.550	0.15943E-01	7783.09	0.0000	0.000	3
44	5	1.19396	0.85551	1.636	15.000	4789.25	62.138	0.14426E-01	8050.82	1.4115	306.941	3

MASS FLOW POINT 46 = 1.457803E+01  
 DELTA FLOWRATE = 1.024679E+00  
 PERCENT DELTA = 6.567315E+00  
 AREA RATIO = 1.425536E+00

LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
45	1	0.22588	0.26034	0.951	5770.66	158.55	0.36305E-01	5179.22	0.0000	0.000	0	1
45	4	0.58140	0.44043	1.307	6.436	5598.58	113.89	0.27082E-01	6320.84	0.0000	0.000	2
45	4	0.58140	0.44043	1.271	6.436	5706.55	113.89	0.30108E-01	5821.99	0.0000	0.000	2
45	4	0.89197	0.65454	1.606	15.710	5466.43	68.350	0.19088E-01	7152.81	0.0000	0.000	2
45	4	0.89197	0.65454	1.582	15.710	4830.82	68.350	0.15704E-01	7827.55	0.0000	0.000	2
45	5	1.20135	0.88311	1.645	15.000	4779.05	61.233	0.14248E-01	8087.02	1.4155	307.820	3

MASS FLOW POINT 47 = 1.476592E+01  
 DELTA FLOWRATE = 8.367891E-01  
 PERCENT DELTA = 5.363101E+00  
 AREA RATIO = 1.443248E+00

LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
46	1	0.20208	0.26314	0.857	5771.67	158.86	0.36366E-01	5171.74	0.0000	0.000	0	1
46	4	0.58355	0.45903	1.323	6.724	5586.93	111.39	0.26555E-01	6388.91	0.0000	0.000	2
46	4	0.58355	0.45903	1.287	6.724	5695.76	111.39	0.29518E-01	5888.34	0.0000	0.000	2
46	4	0.89894	0.67932	1.614	15.687	5461.39	67.339	0.18831E-01	7185.94	0.0000	0.000	2
46	4	0.89894	0.67932	1.591	15.687	4822.58	67.339	0.15502E-01	7865.26	0.0000	0.000	2
46	5	1.20870	0.91052	1.654	15.000	4768.73	60.332	0.14070E-01	8123.35	1.4195	308.687	3

MASS FLOW POINT 48 = 1.493324E+01  
 DELTA FLOWRATE = 6.694727E-01  
 PERCENT DELTA = 4.290746E+00  
 AREA RATIO = 1.460949E+00

LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
47	1	0.17856	0.26559	0.762	5772.55	159.13	0.36421E-01	5165.16	0.0000	0.000	0	1
47	4	0.58577	0.47751	1.338	7.005	5575.22	108.94	0.26037E-01	6456.38	0.0000	0.000	2
47	4	0.58577	0.47751	1.303	7.005	5684.93	108.94	0.28938E-01	5954.06	0.0000	0.000	2
47	4	0.90580	0.70382	1.622	15.621	5456.90	66.459	0.18607E-01	7215.08	0.0000	0.000	2
47	4	0.90580	0.70382	1.599	15.621	4815.47	66.459	0.15325E-01	7898.31	0.0000	0.000	2
47	5	1.21598	0.93770	1.663	15.000	4758.31	59.436	0.13893E-01	8159.74	1.4234	309.539	3

MASS FLOW POINT 49 = 1.508026E+01  
 DELTA FLOWRATE = 5.224562E-01  
 PERCENT DELTA = 3.348496E+00  
 AREA RATIO = 1.478606E+00

LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
48	1	0.15540	0.26772	0.666	5773.32	159.36	0.36467E-01	5159.47	0.0000	0.000	0	1
48	4	0.58806	0.49580	1.354	7.281	5563.55	106.54	0.25530E-01	6522.76	0.0000	0.000	2
48	4	0.58806	0.49580	1.319	7.281	5674.12	106.54	0.28371E-01	6018.79	0.0000	0.000	2
48	4	0.91252	0.72793	1.629	15.529	5452.64	65.668	0.18407E-01	7241.61	0.0000	0.000	2
48	4	0.91252	0.72793	1.606	15.529	4809.05	65.668	0.15166E-01	7928.20	0.0000	0.000	2
48	5	1.22316	0.96450	1.672	15.000	4747.89	58.555	0.13719E-01	8195.82	1.4273	310.371	3

MASS FLOW POINT 50 = 1.520722E+01  
 DELTA FLOWRATE = 3.954868E-01  
 PERCENT DELTA = 2.534731E+00  
 AREA RATIO = 1.496123E+00

LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
49	1	0.13268	0.26951	1.045	5773.96	159.55	0.36507E-01	5154.66	0.0000	0.000	0	1
49	4	0.59041	0.51384	1.369	7.550	5551.92	104.21	0.25035E-01	6587.99	0.0000	0.000	2
49	4	0.59041	0.51384	1.334	7.550	5663.36	104.21	0.27817E-01	6082.39	0.0000	0.000	2
49	4	0.91908	0.75161	1.635	15.422	5448.40	64.934	0.18220E-01	7266.55	0.0000	0.000	2
49	4	0.91908	0.75161	1.613	15.422	4802.94	64.934	0.15018E-01	7956.16	0.0000	0.000	2
49	5	1.23024	0.99090	1.682	15.000	4737.50	57.689	0.13547E-01	8231.55	1.4310	311.183	3

MASS FLOW POINT 51 = 1.531470E+01  
 DELTA FLOWRATE = 2.880116E-01  
 PERCENT DELTA = 1.845907E+00  
 AREA RATIO = 1.513478E+00

LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
50	1	0.11048	0.27099	1.044	5774.49	159.71	0.36540E-01	5150.69	0.0000	0.000	0	1
50	4	0.59281	0.53159	1.384	7.811	5540.39	101.95	0.24555E-01	6651.80	0.0000	0.000	2
50	4	0.59281	0.53159	1.350	7.811	5652.70	101.95	0.27280E-01	6144.61	0.0000	0.000	2
50	4	0.92545	0.77478	1.641	15.310	5444.10	64.239	0.18045E-01	7290.45	0.0000	0.000	2
50	4	0.92545	0.77478	1.620	15.310	4796.99	64.239	0.14878E-01	7982.82	0.0000	0.000	2
50	5	1.23717	1.01680	1.691	15.000	4727.22	56.845	0.13379E-01	8266.66	1.4346	311.973	3

MASS FLOW POINT 52 = 1.540332E+01  
 DELTA FLOWRATE = 1.993933E-01  
 PERCENT DELTA = 1.277940E+00  
 AREA RATIO = 1.530602E+00

LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE
49	1	0.13268	0.26951	1.045	5773.96	159.55	0.36507E-01	5154.66	0.0000	0.000	0	1
49	4	0.59041	0.51384	1.369	7.550	5551.92	104.21	0.25035E-01	6587.99	0.0000	0.000	2
49	4	0.59041	0.51384	1.334	7.550	5663.36	104.21	0.27817E-01	6082.39	0.0000	0.000	2
49	4	0.91908	0.75161	1.635	15.422	5448.40	64.934	0.18220E-01	7266.55	0.0000	0.000	2
49	4	0.91908	0.75161	1.613	15.422	4802.94	64.934	0.15018E-01	7956.16	0.0000	0.000	2
49	5	1.23024	0.99090	1.682	15.000	4737.50	57.689	0.13547E-01	8231.55	1.4310	311.183	3

51	1	0.08891	0.27217	1.044	0.385	5774.92	159.84	0.36566E-01	5147.53	0.0000	0.000	0	1	1.547407E+00
51	4	0.59522	0.54894	1.399	8.063	5528.99	99.772	0.24090E-01	6713.98	0.0000	0.000	2	1	
51	4	0.59522	0.54894	1.365	8.063	5642.19	99.772	0.26759E-01	6205.15	0.0000	0.000	2	1	
51	4	0.93160	0.79734	1.648	15.197	5439.73	63.573	0.17876E-01	7313.65	0.0000	0.000	2	2	
51	5	1.24395	1.04208	1.699	15.000	4717.09	56.026	0.14744E-01	8008.56	0.0000	0.000	2	2	
MASS FLOW POINT 53 = 1.547390E+01 DELTA FLOWRATE = 1.288071E-01 PERCENT DELTA = 8.255428E-01 AREA RATIO = 1.4382 312.757 3														
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE		
52	1	0.06811	0.27307	1.043	0.296	5775.24	159.94	0.36585E-01	5145.13	0.0000	0.000	0	3	1.563700E+00
52	4	0.59764	0.56573	1.413	8.305	5517.93	97.698	0.23647E-01	6773.64	0.0000	0.000	2	1	
52	4	0.59764	0.56573	1.379	8.305	5632.00	97.698	0.26264E-01	6263.26	0.0000	0.000	2	1	
52	4	0.93747	0.81905	1.653	15.089	5435.36	62.936	0.17716E-01	7336.01	0.0000	0.000	2	2	
52	5	1.25048	1.06646	1.632	15.089	4785.23	62.936	0.14616E-01	8033.34	0.0000	0.000	2	2	
MASS FLOW POINT 54 = 1.552747E+01 DELTA FLOWRATE = 7.523823E-02 PERCENT DELTA = 4.822125E-01 AREA RATIO = 1.563700E+00														
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE		
53	1	0.04827	0.27370	1.043	0.210	5775.46	160.01	0.36599E-01	5143.44	0.0000	0.000	0	3	1.579443E+00
53	4	0.60003	0.58189	1.427	8.536	5507.18	95.728	0.23225E-01	6830.86	0.0000	0.000	2	1	
53	4	0.60003	0.58189	1.393	8.536	5622.09	95.728	0.25792E-01	6319.02	0.0000	0.000	2	1	
53	4	0.94307	0.83988	1.659	14.985	5431.02	62.325	0.17562E-01	7357.61	0.0000	0.000	2	2	
53	5	1.25676	1.08989	1.638	14.985	4779.44	62.325	0.14493E-01	8057.24	0.0000	0.000	2	2	
MASS FLOW POINT 55 = 1.556536E+01 DELTA FLOWRATE = 5.4.498 DELTA = 2.393612E-01 AREA RATIO = 1.579443E+00														
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE		
54	1	0.02970	0.27410	1.042	0.129	5775.61	160.05	0.36608E-01	5142.37	0.0000	0.000	0	3	1.594303E+00
54	4	0.60234	0.59709	1.440	8.750	5497.01	93.902	0.22833E-01	6884.39	0.0000	0.000	2	1	
54	4	0.60234	0.59709	1.406	8.750	5612.73	93.902	0.25353E-01	6371.13	0.0000	0.000	2	1	
54	4	0.94828	0.85941	1.665	14.890	5426.82	61.752	0.17417E-01	7378.05	0.0000	0.000	2	2	
54	5	1.26266	1.11190	1.644	14.890	4773.86	61.752	0.14378E-01	8079.83	0.0000	0.000	2	2	
MASS FLOW POINT 56 = 1.558911E+01 DELTA FLOWRATE = 1.360416E-02 PERCENT DELTA = 8.719102E-02 AREA RATIO = 1.594303E+00														
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE		
55	1	0.01293	0.27430	1.042	0.056	5775.68	160.07	0.36612E-01	5141.85	0.0000	0.000	0	3	1.607861E+00
55	4	0.60449	0.61093	1.451	8.944	5487.71	92.264	0.22481E-01	6932.80	0.0000	0.000	2	1	
55	4	0.60449	0.61093	1.418	8.944	5604.18	92.264	0.24959E-01	6418.26	0.0000	0.000	2	1	
55	4	0.95297	0.87712	1.670	14.806	5422.92	61.231	0.17286E-01	7396.72	0.0000	0.000	2	2	
55	5	1.26801	1.13190	1.649	14.806	4768.67	61.231	0.14274E-01	8100.44	0.0000	0.000	2	2	
MASS FLOW POINT 57 = 1.560079E+01 DELTA FLOWRATE = 1.916885E-03 PERCENT DELTA = 1.4504 315.595 3														
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE		
56	13	0.00000	0.27434	1.042	0.000	5775.69	160.08	0.36613E-01	5141.72	0.0000	0.000	0	3	1.618425E+00
56	4	0.60620	0.62169	1.460	9.093	5480.46	91.006	0.22210E-01	6970.25	0.0000	0.000	2	1	
56	4	0.60620	0.62169	1.427	9.093	5597.52	91.006	0.24656E-01	6454.71	0.0000	0.000	2	1	
56	4	0.95659	0.89085	1.673	14.742	5419.85	60.826	0.17184E-01	7411.29	0.0000	0.000	2	2	
56	5	1.27217	1.14742	1.653	14.742	4764.56	60.826	0.14193E-01	8116.53	0.0000	0.000	2	2	
MASS FLOW POINT 58 = 1.560344E+01 DELTA FLOWRATE = 7.247925E-04 PERCENT DELTA = 4.645298E-03 AREA RATIO = 1.618425E+00														
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE		
57	3	0.00000	0.28236	1.051	0.000	5770.20	158.44	0.36283E-01	5181.81	0.0000	0.000	2	3	1.640140E+00
57	4	0.60979	0.64373	1.479	9.392	5465.47	88.475	0.21663E-01	7046.66	0.0000	0.000	2	1	
57	4	0.60979	0.64373	1.445	9.392	5583.79	88.475	0.24045E-01	6529.02	0.0000	0.000	2	1	
57	4	0.96393	0.91886	1.681	14.612	5413.49	60.004	0.16977E-01	7441.18	0.0000	0.000	2	2	
57	5	1.28068	1.17916	1.661	14.612	4755.99	60.004	0.14028E-01	8149.47	0.0000	0.000	2	2	
MASS FLOW POINT 58 = 1.560351E+01 DELTA FLOWRATE = 7.991791E-04 PERCENT DELTA = 5.122053E-03 AREA RATIO = 1.640140E+00														
LRC ID	R	X	MACH	THETA	T (DEG.R)	P (PSI)	DENSITY	VELOCITY	CF	ISP	IT	ZONE		
58	1	0.00000	0.28236	1.051	0.000	5770.20	158.44	0.36283E-01	5181.81	0.0000	0.000	2	3	1.640140E+00
58	4	0.60979	0.64373	1.479	9.392	5465.47	88.475	0.21663E-01	7046.66	0.0000	0.000	2	1	
58	4	0.60979	0.64373	1.445	9.392	5583.79	88.475	0.24045E-01	6529.02	0.0000	0.000	2	1	
58	4	0.96393	0.91886	1.681	14.612	5413.49	60.004	0.16977E-01	7441.18	0.0000	0.000	2	2	
58	5	1.28068	1.17916	1.661	14.612	4755.99	60.004	0.14028E-01	8149.47	0.0000	0.000	2	2	
MASS FLOW POINT 58 = 1.560351E+01 DELTA FLOWRATE = 7.991791E-04 PERCENT DELTA = 5.122053E-03 AREA RATIO = 1.640140E+00														

58 3 0.00000 0.29116 1.061 0.000 5764.36 156.69 0.35926E-01 5224.80 0.000 0.000 2  
 58 4 0.61369 0.66694 1.498 9.701 5449.70 85.883 0.21102E-01 7125.99 0.000 0.000 2  
 58 4 0.61369 0.66694 1.465 9.701 5569.37 85.883 0.23417E-01 6606.07 0.000 0.000 2  
 58 4 0.97154 0.94820 1.690 14.482 5406.70 59.144 0.16760E-01 7472.76 0.000 0.000 2  
 58 4 0.97154 0.94820 1.670 14.482 4746.75 59.144 0.13856E-01 8184.28 0.000 0.000 2  
 58 5 1.28961 1.21249 1.760 15.000 4647.47 50.715 0.12150E-01 8530.86 1.4610 317.705 3  
 MASS FLOW POINT 58 = 1.560348E+01 DELTA FLOWRATE = -7.696152E-04 PERCENT DELTA = -4.932573E-03 AREA RATIO = 1.663090E+00

LRC ID R X MACH THETA T (DEG.R) P (PSI) DENSITY VELOCITY CF ISP IT ZONE  
 59 3 0.00000 0.30071 1.071 0.000 5758.17 154.83 0.35548E-01 5270.32 0.000 0.000 2  
 59 4 0.61792 0.69127 1.518 10.017 5433.16 83.248 0.20530E-01 7207.80 0.000 0.000 3  
 59 4 0.61792 0.69127 1.485 10.017 5554.28 83.248 0.22776E-01 6685.48 0.000 0.000 2  
 59 4 0.97940 0.97879 1.699 14.351 5399.48 58.248 0.16534E-01 7505.98 0.000 0.000 2  
 59 4 0.97940 0.97879 1.679 14.351 4736.84 58.248 0.13677E-01 8220.86 0.000 0.000 2  
 59 5 1.29427 1.22990 1.766 15.000 4640.31 50.199 0.12046E-01 8553.92 1.4633 318.195 3  
 59 5 1.29894 1.24731 1.772 15.000 4633.07 49.684 0.11942E-01 8577.11 1.4655 318.681 3  
 MASS FLOW POINT 58 = 1.560343E+01 DELTA FLOWRATE = -7.190704E-04 PERCENT DELTA = -4.608625E-03 AREA RATIO = 1.687242E+00

LRC ID R X MACH THETA T (DEG.R) P (PSI) DENSITY VELOCITY CF ISP IT ZONE  
 60 3 0.00000 0.31100 1.081 0.000 5751.83 152.92 0.35158E-01 5317.06 0.000 0.000 2  
 60 4 0.62247 0.71662 1.539 10.336 5415.93 80.591 0.19950E-01 7291.64 0.000 0.000 3  
 60 4 0.62247 0.71662 1.506 10.336 5538.57 80.591 0.22128E-01 6766.82 0.000 0.000 2  
 60 4 0.98748 1.01052 1.708 14.222 5391.85 57.320 0.16299E-01 7540.77 0.000 0.000 2  
 60 4 0.98748 1.01052 1.689 14.222 4726.27 57.320 0.13491E-01 8259.16 0.000 0.000 2  
 60 5 1.30379 1.26541 1.778 15.000 4625.62 49.157 0.11835E-01 8600.92 1.4678 319.184 3  
 60 5 1.30864 1.28351 1.785 15.000 4618.07 48.632 0.11729E-01 8624.87 1.4701 319.683 3  
 MASS FLOW POINT 58 = 1.560341E+01 DELTA FLOWRATE = -6.942749E-04 PERCENT DELTA = -4.449707E-03 AREA RATIO = 1.712536E+00

LRC ID R X MACH THETA T (DEG.R) P (PSI) DENSITY VELOCITY CF ISP IT ZONE  
 61 3 0.00000 0.32202 1.092 0.000 5745.18 150.95 0.34756E-01 5365.57 0.000 0.000 2  
 61 4 0.62737 0.74306 1.560 10.656 5398.05 77.926 0.19367E-01 7377.20 0.000 0.000 3  
 61 4 0.62737 0.74306 1.527 10.656 5522.31 77.926 0.21475E-01 6849.81 0.000 0.000 2  
 61 4 0.99578 1.04343 1.718 14.095 5383.77 56.358 0.16055E-01 7577.19 0.000 0.000 2  
 61 4 0.99578 1.04343 1.699 14.095 4715.03 56.358 0.13298E-01 8299.21 0.000 0.000 2  
 61 5 1.31368 1.30233 1.791 15.000 4610.30 48.096 0.11619E-01 8649.43 1.4725 320.198 3  
 61 5 1.31872 1.32115 1.798 15.000 4602.43 47.561 0.11511E-01 8674.15 1.4748 320.709 3  
 MASS FLOW POINT 58 = 1.560340E+01 DELTA FLOWRATE = -6.904602E-04 PERCENT DELTA = -4.425258E-03 AREA RATIO = 1.739035E+00

LRC ID R X MACH THETA T (DEG.R) P (PSI) DENSITY VELOCITY CF ISP IT ZONE  
 62 3 0.00000 0.33374 1.103 0.000 5738.23 148.92 0.34340E-01 5415.72 0.000 0.000 2  
 62 4 0.63261 0.77051 1.581 10.973 5379.67 75.277 0.18785E-01 7463.75 0.000 0.000 3  
 62 4 0.63261 0.77051 1.549 10.973 5505.62 75.277 0.20824E-01 6933.73 0.000 0.000 2  
 62 4 1.00428 1.07742 1.728 13.971 5375.31 55.369 0.15804E-01 7615.07 0.000 0.000 2  
 62 4 1.00428 1.07742 1.710 13.971 4703.15 55.369 0.13100E-01 8340.86 0.000 0.000 2  
 62 5 1.32394 1.34062 1.805 15.000 4594.40 47.019 0.11400E-01 8699.30 1.4772 321.234 3  
 62 5 1.32916 1.36010 1.812 15.000 4586.26 46.478 0.11290E-01 8724.62 1.4796 321.756 3  
 MASS FLOW POINT 58 = 1.560336E+01 DELTA FLOWRATE = -6.475449E-04 PERCENT DELTA = -4.150207E-03 AREA RATIO = 1.766670E+00

LRC ID R X MACH THETA T (DEG.R) P (PSI) DENSITY VELOCITY CF ISP IT ZONE  
 63 3 0.00000 0.34618 1.114 0.000 5731.04 146.84 0.33916E-01 5467.15 0.000 0.000 2  
 63 4 0.63823 0.79906 1.603 11.282 5360.84 72.654 0.18205E-01 7551.08 0.000 0.000 3  
 63 4 0.63823 0.79906 1.571 11.282 5488.56 72.654 0.20177E-01 7018.35 0.000 0.000 2  
 63 4 1.01299 1.11259 1.739 13.851 5366.40 54.349 0.15545E-01 7654.57 0.000 0.000 2  
 63 4 1.01299 1.11259 1.721 13.851 4690.57 54.349 0.12895E-01 8384.26 0.000 0.000 2  
 63 5 1.33457 1.38029 1.819 15.000 4577.93 45.929 0.11177E-01 8750.43 1.4821 322.292 3  
 63 5 1.33998 1.40049 1.826 15.000 4569.48 45.382 0.11065E-01 8776.43 1.4845 322.824 3  
 MASS FLOW POINT 58 = 1.560334E+01 DELTA FLOWRATE = -6.237030E-04 PERCENT DELTA = -3.997401E-03 AREA RATIO = 1.795558E+00

LRC ID R X MACH THETA T (DEG.R) P (PSI) DENSITY VELOCITY CF ISP IT ZONE  
 64 3 0.00000 0.35932 1.126 0.000 5723.53 144.72 0.33479E-01 5520.18 0.000 0.000 2  
 64 4 0.64422 0.82872 1.625 11.578 5341.70 70.076 0.17635E-01 7638.55 0.000 0.000 3  
 64 4 0.64422 0.82872 1.593 11.578 5471.27 70.076 0.19538E-01 7103.02 0.000 0.000 2

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64 4 1.02191 1.14893 1.750 13.736 5357.05 53.300 0.15278E-01 7695.65 0.0000 0.000 2  
 64 4 1.02191 1.14893 1.733 13.736 4677.31 53.300 0.12684E-01 8429.38 0.0000 0.000 2  
 64 5 1.34559 1.42141 1.833 15.000 4560.87 44.829 0.10952E-01 8802.84 1.4871 323.371 3  
 MASS FLOW POINT 58 = 1.560333E+01 DELTA FLOWRATE = -6.170273E-04 PERCENT DELTA = -3.954616E-03 AREA RATIO = 1.825723E+00  
 LRC ID R X MACH THETA T (DEG.R) P (PSI) DENSITY VELOCITY CF ISP IT ZONE  
 65 3 0.00000 0.37316 1.138 0.000 5715.77 142.54 0.33033E-01 5574.41 0.0000 0.000 2  
 65 4 0.65061 0.85950 1.647 11.856 5322.41 67.561 0.17076E-01 7725.55 0.0000 0.000 3  
 65 4 0.65061 0.85950 1.615 11.856 5453.86 67.561 0.18912E-01 7187.24 0.0000 0.000 3  
 65 4 1.03104 1.18647 1.762 13.626 5347.25 52.224 0.15003E-01 7738.31 0.0000 0.000 2  
 65 5 1.35699 1.18647 1.745 13.626 4663.33 52.224 0.12467E-01 8476.22 0.0000 0.000 2  
 65 5 1.36279 1.48561 1.848 15.000 4543.24 43.720 0.10724E-01 8856.44 1.4921 324.470 3  
 MASS FLOW POINT 58 = 1.560330E+01 DELTA FLOWRATE = -5.865097E-04 PERCENT DELTA = -3.759024E-03 AREA RATIO = 1.857199E+00

LRC ID R X MACH THETA T (DEG.R) P (PSI) DENSITY VELOCITY CF ISP IT ZONE  
 66 3 0.00000 0.38771 1.150 0.000 5707.66 140.32 0.32576E-01 5630.32 0.0000 0.000 2  
 66 4 0.65738 0.89141 1.669 12.110 5303.06 65.126 0.16532E-01 7811.65 0.0000 0.000 2  
 66 4 0.65738 0.89141 1.637 12.110 5436.41 65.126 0.18304E-01 7270.71 0.0000 0.000 2  
 66 4 1.04040 1.2521 1.774 13.522 5336.99 51.123 0.14722E-01 7782.53 0.0000 0.000 2  
 66 5 1.36879 1.2521 1.758 13.522 4648.65 51.123 0.12244E-01 8524.75 0.0000 0.000 2  
 66 5 1.37479 1.50799 1.863 15.000 4525.03 42.604 0.10494E-01 8911.17 1.4972 325.587 3  
 MASS FLOW POINT 58 = 1.560329E+01 DELTA FLOWRATE = -5.798340E-04 PERCENT DELTA = -3.716239E-03 AREA RATIO = 1.890036E+00

LRC ID R X MACH THETA T (DEG.R) P (PSI) DENSITY VELOCITY CF ISP IT ZONE  
 67 3 0.00000 0.40295 1.163 0.000 5699.31 138.06 0.32110E-01 5687.29 0.0000 0.000 2  
 67 4 0.66455 0.92451 1.691 12.334 5283.89 62.784 0.16006E-01 7896.11 0.0000 0.000 2  
 67 4 0.66455 0.92451 1.659 12.334 5419.18 62.784 0.17716E-01 7352.51 0.0000 0.000 2  
 67 4 1.04998 1.26521 1.787 13.424 5326.29 50.000 0.14434E-01 7828.28 0.0000 0.000 2  
 67 5 1.38099 1.26521 1.771 13.424 4633.28 50.000 0.12017E-01 8574.91 0.0000 0.000 2  
 67 5 1.38719 1.57667 1.886 15.000 4496.66 40.925 0.10262E-01 8966.99 1.5025 326.723 3  
 MASS FLOW POINT 58 = 1.560325E+01 DELTA FLOWRATE = -5.369186E-04 PERCENT DELTA = -3.441188E-03 AREA RATIO = 1.924302E+00

LRC ID R X MACH THETA T (DEG.R) P (PSI) DENSITY VELOCITY CF ISP IT ZONE  
 68 3 0.00000 0.41889 1.176 0.000 5690.68 135.76 0.31636E-01 5745.47 0.0000 0.000 2  
 68 4 0.67210 0.95879 1.712 12.523 5265.07 60.552 0.15503E-01 7978.28 0.0000 0.000 2  
 68 4 0.67210 0.95879 1.680 12.523 5402.31 60.552 0.17153E-01 7432.05 0.0000 0.000 2  
 68 4 1.05979 1.30647 1.800 13.331 5315.14 48.857 0.14140E-01 7875.48 0.0000 0.000 2  
 68 5 1.05979 1.30647 1.785 13.331 4617.22 48.857 0.11785E-01 8626.60 0.0000 0.000 2  
 68 5 1.39360 1.60059 1.894 15.000 4486.94 40.363 0.10029E-01 9023.82 1.5078 327.877 3  
 MASS FLOW POINT 58 = 1.560325E+01 DELTA FLOWRATE = -5.359650E-04 PERCENT DELTA = -3.435076E-03 AREA RATIO = 1.960033E+00

LRC ID R X MACH THETA T (DEG.R) P (PSI) DENSITY VELOCITY CF ISP IT ZONE  
 69 3 0.00000 0.43534 1.189 0.000 5681.78 133.44 0.31154E-01 5804.77 0.0000 0.000 2  
 69 4 0.68004 0.99429 1.733 12.671 5246.74 58.436 0.15023E-01 8057.76 0.0000 0.000 2  
 69 4 0.68004 0.99429 1.701 12.671 5385.94 58.436 0.16617E-01 7508.96 0.0000 0.000 2  
 69 4 1.06985 1.34906 1.814 13.243 5303.55 47.698 0.13842E-01 7924.09 0.0000 0.000 2  
 69 5 1.06985 1.34906 1.799 13.243 4600.48 47.698 0.11549E-01 8679.79 0.0000 0.000 2  
 69 5 1.40664 1.64925 1.911 15.000 4467.04 39.240 0.97945E-02 9081.68 1.5132 329.047 3  
 MASS FLOW POINT 58 = 1.560325E+01 DELTA FLOWRATE = -5.359650E-04 PERCENT DELTA = -3.435076E-03 AREA RATIO = 1.960033E+00

TDK PERFORMANCE SUMMARY : 3 ZONES TDK TEST CASE, LOX/GH2 - TDK MANUAL TEST CASE

I SP (SEC)	329.633
F (LBF)	5143.17
MASS FLOW (LB/SEC)	15.6027
CD	0.995554
C* (FT/SEC)	6996.46
CF	1.51585



TDK PERFORMANCE SUMMARY : 3 ZONES TDK TEST CASE, LOX/GH2 - TDK MANUAL TEST CASE  
 REAL WALL CONTOUR 3 ZONES

	FIRST TDK SOLUTION
CHAMBER PRESS [PSIA]	300.0000
CHAMBER TEMP [R]	6001.056
MIXTURE RATIO [-]	6.297435
EP (NOZZLE) [-]	2.000000
H (OXID) [CAL/MOLE]	-3099.196
H (FUEL) [CAL/MOLE]	-2154.000
HCHAM (ODE) [BTU/LB]	-413.8725
DELH (AVERAGE) [BTU/LB]	0.000000E+00
DELH1 (AV) [BTU/LB]	0.000000E+00
ECRAT [-]	3.000000
RSTAR	2.000000
RWTD [-]	1.000000
RWTU [-]	1.000000
THE	0.000000E+00
THETA [DEGREES]	15.00000
THETA1 [DEGREES]	30.00000
RI [-]	2.000000
MIT [-]	59.00000
ISP (ODE) [SECONDS]	335.4859
ISP (ODF) [SECONDS]	326.8484
ISP (OOK) [SECONDS]	335.2208
ISP (TDK) [SECONDS]	329.6333
THRUST (TDK) [POUNDS]	5143.173
WDOT (TDK) [LB/SEC]	15.60271
CSTAR (TDK) [FT/SEC]	6996.465
CF (TDK) [-]	1.515854
CD [-]	0.9955939
P (AXIS,EXIT) [PSIA]	0.000000E+00
P (WALL,EXIT) [PSIA]	38.67983
T (WALL,EXIT) [R]	4456.856
V (WALL,EXIT) [FT/SEC]	9110.994
MA (WALL,EXIT) [-]	1.918942
SHOCK STRENGTH [-]	0.000000E+00
SHOCK (X/R*) [-]	0.000000E+00
SHOCK (R/R*) [-]	0.000000E+00
XA (X/R*) [-]	0.000000E+00
XB (X/R*) [-]	0.000000E+00

\*\*\*\*\*  
 BOUNDARY LAYER MODULE ( BLM )  
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3 ZONES TDK TEST CASE, LOX/GH2 - TDK MANUAL TEST CASE

ORIGINAL PAGE IS  
 OF POOR QUALITY

INPUT GEOMETRY

I	X(FT)	R(FT)	S(FT)	UE(FT/SEC)	TE(DEG. R)	PE(LB.-F/FT2)	HSE(FT2/SEC2)
1	-3.45300E-01	2.88675E-01	0.00000E+00	1.07331E+03	5.71352E+03	3.79711E+04	
2	-3.25315E-01	2.88075E-01	1.99940E-02	1.07911E+03	5.71346E+03	3.79617E+04	
3	-2.42048E-01	2.72280E-01	1.04746E-01	1.21460E+03	5.70943E+03	3.77194E+04	
4	-1.67107E-01	2.37362E-01	1.87423E-01	1.63275E+03	5.69394E+03	3.68027E+04	
5	-1.13816E-01	2.06595E-01	2.48958E-01	2.25131E+03	5.66253E+03	3.50142E+04	
6	-6.71857E-02	1.80808E-01	3.02243E-01	3.24766E+03	5.58988E+03	3.12172E+04	
7	-7.23290E-03	1.66823E-01	3.63805E-01	4.90616E+03	5.40456E+03	2.33375E+04	
8	0.00000E+00	1.66667E-01	3.71040E-01	5.89066E+03	5.26460E+03	1.88189E+04	
9	1.80460E-03	1.66677E-01	3.74589E-01	5.96618E+03	5.24917E+03	1.84234E+04	
10	3.54942E-03	1.66705E-01	3.75683E-01	6.01251E+03	5.23496E+03	1.80546E+04	
11	4.64293E-03	1.66732E-01	3.76831E-01	6.06476E+03	5.22627E+03	1.78278E+04	
12	5.88402E-03	1.66770E-01	3.76925E-01	6.12264E+03	5.21642E+03	1.75739E+04	
13	7.27195E-03	1.66825E-01	3.78314E-01	6.18564E+03	5.20545E+03	1.72938E+04	
14	8.80657E-03	1.66900E-01	3.79850E-01	6.25417E+03	5.19340E+03	1.69890E+04	
15	1.04842E-02	1.66997E-01	3.81531E-01	6.32797E+03	5.18013E+03	1.66592E+04	
16	1.23036E-02	1.67122E-01	3.83354E-01	6.40698E+03	5.16564E+03	1.63064E+04	
17	1.42620E-02	1.67278E-01	3.85319E-01	6.49111E+03	5.14986E+03	1.59313E+04	
18	1.63560E-02	1.67472E-01	3.87422E-01	6.58020E+03	5.13274E+03	1.55353E+04	
19	1.85813E-02	1.67705E-01	3.89660E-01	6.67416E+03	5.11424E+03	1.51196E+04	
20	2.09335E-02	1.67987E-01	3.92028E-01	6.77286E+03	5.09429E+03	1.46857E+04	
21	2.34073E-02	1.68318E-01	3.94524E-01	6.87286E+03	5.07283E+03	1.42351E+04	
22	2.59977E-02	1.68707E-01	3.97144E-01	6.98409E+03	5.04979E+03	1.37691E+04	
23	2.86995E-02	1.69157E-01	3.99883E-01	7.10881E+03	5.02513E+03	1.32897E+04	
24	3.15083E-02	1.69672E-01	4.02738E-01	7.24327E+03	4.99871E+03	1.27979E+04	
25	3.44188E-02	1.70260E-01	4.05708E-01	7.33429E+03	4.97049E+03	1.22956E+04	
26	3.74235E-02	1.70923E-01	4.08785E-01	7.49141E+03	4.94039E+03	1.17850E+04	
27	4.1057E-02	1.71815E-01	4.12573E-01	7.60108E+03	4.90808E+03	1.11373E+04	
28	4.46977E-02	1.72763E-01	4.16288E-01	7.75272E+03	4.88445E+03	1.04944E+04	
29	4.8243E-02	1.73667E-01	4.20185E-01	7.86088E+03	4.85999E+03	1.00230E+04	
30	5.17949E-02	1.7463E-01	4.2413E-01	7.94088E+03	4.83566E+03	9.80424E+03	
31	5.5352E-02	1.75667E-01	4.2813E-01	8.0085E+03	4.81161E+03	9.69018E+03	
32	5.89180E-02	1.76778E-01	4.3228E-01	8.0685E+03	4.78925E+03	9.57313E+03	
33	6.25031E-01	1.77978E-01	4.3659E-01	8.1202E+03	4.76873E+03	9.45325E+03	
34	6.61106E-01	1.79280E-01	4.4106E-01	8.1729E+03	4.74991E+03	9.33019E+03	
35	6.97426E-01	1.80687E-01	4.4575E-01	8.2240E+03	4.73255E+03	9.20465E+03	
36	7.34073E-01	1.8226E-01	4.5068E-01	8.2772E+03	4.7172E+03	9.07710E+03	
37	7.71067E-01	1.8392E-01	4.5584E-01	8.3321E+03	4.7030E+03	8.94790E+03	
38	8.08425E-01	1.8568E-01	4.6125E-01	8.3882E+03	4.6899E+03	8.81757E+03	
39	8.46287E-01	1.8755E-01	4.6694E-01	8.4455E+03	4.6779E+03	8.68775E+03	
40	8.8464E-01	1.8953E-01	4.7298E-01	8.5040E+03	4.6673E+03	8.55877E+03	
41	9.2351E-01	1.9168E-01	4.7932E-01	8.5640E+03	4.6581E+03	8.43185E+03	
42	9.6294E-01	1.9399E-01	4.8608E-01	8.6255E+03	4.6499E+03	8.30720E+03	
43	1.00400E-01	1.9642E-01	4.9333E-01	8.6885E+03	4.6428E+03	8.18564E+03	
44	1.04400E-01	1.9899E-01	5.0084E-01	8.7535E+03	4.6366E+03	8.06773E+03	
45	1.08942E-01	2.01718E-01	5.0860E-01	8.8202E+03	4.6315E+03	7.95506E+03	
46	1.14000E-01	2.0463E-01	5.1650E-01	8.8885E+03	4.6274E+03	7.84771E+03	
47	1.19500E-01	2.0763E-01	5.2459E-01	8.9582E+03	4.6242E+03		
48	1.25500E-01	2.1075E-01	5.3275E-01	9.0292E+03	4.6220E+03		
49	1.32000E-01	2.1400E-01	5.4106E-01	9.1018E+03	4.6208E+03		
50	1.39000E-01	2.1743E-01	5.4959E-01	9.1755E+03	4.6200E+03		
51	1.46600E-01	2.2103E-01	5.5830E-01	9.2503E+03	4.6192E+03		

ORIGINAL PAGE IS  
OF POOR QUALITY

3 ZONES TDK TEST CASE, LOX/GH2 - TDK MANUAL TEST CASE

INPUT GEOMETRY

I	X(FT)	R(FT)	S(FT)	UE(FT/SEC)	TE(DEG. R)	PE(LB-F/FT2)	HSE(FT2/SEC2)
1	3.45300E-01	2.88675E-01	0.00000E+00	1.07331E+03	5.71352E+03	3.79711E+04	
2	3.25315E-01	2.88075E-01	1.99940E-02	1.07911E+03	5.71346E+03	3.79617E+04	
3	2.42048E-01	2.72800E-01	1.04746E-01	1.21460E+03	5.70943E+03	3.77194E+04	
4	1.67107E-01	2.37362E-01	1.87423E-01	1.63275E+03	5.69394E+03	3.68027E+04	
5	1.13816E-01	2.06595E-01	2.48958E-01	2.25131E+03	5.66253E+03	3.50142E+04	
6	6.71857E-02	1.80808E-01	3.02243E-01	3.24766E+03	5.58988E+03	3.12172E+04	
7	7.23290E-03	1.66823E-01	3.63805E-01	4.90616E+03	5.40456E+03	2.33375E+04	
8	0.00000E+00	1.66667E-01	3.71040E-01	5.80973E+03	5.26460E+03	1.88189E+04	
9	1.80460E-03	1.66677E-01	3.72844E-01	5.89066E+03	5.24917E+03	1.84234E+04	
10	3.54942E-03	1.66705E-01	3.74589E-01	5.96618E+03	5.23496E+03	1.80546E+04	
11	4.64293E-03	1.66732E-01	3.75683E-01	6.01251E+03	5.22627E+03	1.78278E+04	
12	5.88402E-03	1.66770E-01	3.76925E-01	6.06476E+03	5.21642E+03	1.75739E+04	
13	7.27195E-03	1.66823E-01	3.78314E-01	6.12264E+03	5.20545E+03	1.72938E+04	
14	8.80657E-03	1.66900E-01	3.79850E-01	6.18564E+03	5.19340E+03	1.69890E+04	
15	1.04842E-02	1.66997E-01	3.81531E-01	6.25417E+03	5.18013E+03	1.66592E+04	
16	1.23036E-02	1.67122E-01	3.83354E-01	6.32797E+03	5.16564E+03	1.63064E+04	
17	1.42620E-02	1.67278E-01	3.85319E-01	6.40698E+03	5.14986E+03	1.59313E+04	
18	1.63560E-02	1.67472E-01	3.87422E-01	6.49111E+03	5.13274E+03	1.55353E+04	
19	1.85813E-02	1.67705E-01	3.89660E-01	6.58020E+03	5.11424E+03	1.51196E+04	
20	2.09335E-02	1.67987E-01	3.92028E-01	6.67416E+03	5.09429E+03	1.46857E+04	
21	2.34073E-02	1.68318E-01	3.94524E-01	6.77286E+03	5.07283E+03	1.42351E+04	
22	2.59977E-02	1.68707E-01	3.97144E-01	6.87624E+03	5.04979E+03	1.37691E+04	
23	2.86995E-02	1.69157E-01	4.02738E-01	6.98409E+03	5.02513E+03	1.32897E+04	
24	3.15083E-02	1.69672E-01	4.05708E-01	7.10232E+03	4.97049E+03	1.22956E+04	
25	3.44188E-02	1.70260E-01	4.08785E-01	7.2327E+03	4.9039E+03	1.17850E+04	
26	3.74235E-02	1.70923E-01	4.12573E-01	7.33429E+03	4.84088E+03	1.11373E+04	
27	4.1057E-02	1.71815E-01	4.17573E-01	7.49141E+03	4.8084E+03	1.08016E+04	
28	4.46977E-02	1.72763E-01	4.2388E-01	7.7272E+03	4.8599E+03	1.04944E+04	
29	6.67243E-02	1.78667E-01	4.3092E-01	7.60108E+03	4.89808E+03	1.06544E+04	
30	7.79495E-02	1.81673E-01	4.3907E-01	7.68321E+03	4.89311E+03	1.03273E+04	
31	8.66180E-02	1.83997E-01	4.59688E-01	7.75503E+03	4.87255E+03	1.00230E+04	
32	9.60525E-02	1.86525E-01	4.69455E-01	7.79027E+03	4.85904E+03	9.91570E+03	
33	1.00731E-01	1.87778E-01	4.74298E-01	7.81956E+03	4.85161E+03	9.80424E+03	
34	1.05400E-01	1.89028E-01	4.79132E-01	7.84971E+03	4.84383E+03	9.69018E+03	
35	1.10067E-01	1.90280E-01	4.83964E-01	7.84971E+03	4.83566E+03	9.57313E+03	
36	1.14726E-01	1.91528E-01	4.88787E-01	7.84971E+03	4.82712E+03	9.45325E+03	
37	1.19382E-01	1.92775E-01	4.93608E-01	7.91296E+03	4.81815E+03	9.33019E+03	
38	1.24035E-01	1.94022E-01	4.98425E-01	7.94617E+03	4.80884E+03	9.20465E+03	
39	1.28687E-01	1.95268E-01	5.03240E-01	7.98028E+03	4.79919E+03	9.07710E+03	
40	1.33331E-01	1.96513E-01	5.08049E-01	8.01520E+03	4.78925E+03	8.94790E+03	
41	1.37964E-01	1.97755E-01	5.12845E-01	8.05082E+03	4.77905E+03	8.81757E+03	
42	1.42586E-01	1.98993E-01	5.17630E-01	8.08702E+03	4.76873E+03	8.68775E+03	
43	1.47185E-01	2.00225E-01	5.22391E-01	8.12335E+03	4.75831E+03	8.55877E+03	
44	1.51754E-01	2.01450E-01	5.27121E-01	8.15974E+03	4.74789E+03	8.43185E+03	
45	1.56283E-01	2.02663E-01	5.31810E-01	8.19582E+03	4.73750E+03	8.30720E+03	
46	1.60750E-01	2.03860E-01	5.36435E-01	8.23155E+03	4.72722E+03	8.18564E+03	
47	1.65150E-01	2.05040E-01	5.40990E-01	8.26666E+03	4.71709E+03	8.06773E+03	
48	1.69467E-01	2.06195E-01	5.45459E-01	8.30099E+03	4.70727E+03	7.95506E+03	
49	1.73680E-01	2.07325E-01	5.49821E-01	8.33405E+03	4.69779E+03	7.84771E+03	
50	1.77743E-01	2.08413E-01	5.54028E-01	8.36579E+03			
51	1.81648E-01	2.09460E-01	5.58070E-01				

INPUT GEOMETRY

I	X(FT)	R(FT)	S(FT)	UE(FT/SEC)	TE(DEG. R)	PE(LB-F/FT2)	HSE(FT2/SEC2)
52	1.85317E-01	2.10443E-01	5.61868E-01	8.39559E+03	4.68883E+03	7.74763E+03	
53	1.88650E-01	2.11335E-01	5.65319E-01	8.42252E+03	4.68069E+03	7.65778E+03	
54	1.96527E-01	2.13447E-01	5.73474E-01	8.48626E+03	4.66123E+03	7.44772E+03	
55	2.02082E-01	2.14955E-01	5.79224E-01	8.53086E+03	4.64747E+03	7.30300E+03	
56	2.07885E-01	2.16490E-01	5.85232E-01	8.57711E+03	4.63307E+03	7.15454E+03	
57	2.13918E-01	2.18107E-01	5.91479E-01	8.62487E+03	4.61807E+03	7.00308E+03	
58	2.20192E-01	2.19787E-01	5.97973E-01	8.67415E+03	4.60243E+03	6.84881E+03	
59	2.26683E-01	2.21527E-01	6.04694E-01	8.72462E+03	4.58626E+03	6.69289E+03	
60	2.33415E-01	2.23303E-01	6.11663E-01	8.77643E+03	4.56948E+03	6.53507E+03	
61	2.40387E-01	2.25198E-01	6.18881E-01	8.82944E+03	4.55213E+03	6.37589E+03	
62	2.47602E-01	2.27132E-01	6.26350E-01	8.88363E+03	4.53421E+03	6.21562E+03	
63	2.55062E-01	2.29132E-01	6.34074E-01	8.93893E+03	4.51572E+03	6.05460E+03	
64	2.62778E-01	2.31198E-01	6.42062E-01	8.99527E+03	4.49666E+03	5.89316E+03	
65	2.70753E-01	2.33335E-01	6.50318E-01	9.05262E+03	4.47705E+03	5.73157E+03	
66	2.78998E-01	2.35545E-01	6.58855E-01	9.11099E+03	4.45686E+03	5.56989E+03	

GAS PROPERTIES TABLES

I	T DEG R	HS FT2/SEC2	MU LBM/FT-SEC	K LBM-FT/S3-DEGR	CP FT2/SEC2-DEGR	GAMMA	RGAS LBF-FT/LBM-DEGR
1	1.0000E+02	-1.4180E+08	3.2758E-06	9.0999E-02	1.5915E+04	1.3501E+00	1.2803E+02
2	6.0000E+02	-1.3385E+08	1.1773E-05	3.2705E-01	1.5915E+04	1.3501E+00	1.2803E+02
3	8.0000E+02	-1.3064E+08	1.4458E-05	4.0778E-01	1.6159E+04	1.3422E+00	1.2804E+02
4	1.0000E+03	-1.2738E+08	1.6953E-05	4.8903E-01	1.6525E+04	1.3321E+00	1.2804E+02
5	1.2000E+03	-1.2403E+08	1.9312E-05	5.7095E-01	1.6938E+04	1.3214E+00	1.2804E+02
6	1.4000E+03	-1.2060E+08	2.1559E-05	6.5441E-01	1.7391E+04	1.3104E+00	1.2804E+02
7	1.6000E+03	-1.1707E+08	2.3713E-05	7.3981E-01	1.7872E+04	1.2996E+00	1.2804E+02
8	1.8000E+03	-1.1345E+08	2.5796E-05	8.2715E-01	1.8371E+04	1.2891E+00	1.2804E+02
9	2.0000E+03	-1.0972E+08	2.7811E-05	9.1795E-01	1.8910E+04	1.2786E+00	1.2804E+02
10	2.2000E+03	-1.0589E+08	2.9769E-05	1.0090E+00	1.9417E+04	1.2693E+00	1.2804E+02
11	2.4000E+03	-1.0196E+08	3.1677E-05	1.1001E+00	1.9897E+04	1.2611E+00	1.2804E+02
12	2.6000E+03	-9.7930E+07	3.3540E-05	1.1918E+00	2.0358E+04	1.2633E+00	1.2804E+02
13	2.8000E+03	-9.3814E+07	3.5363E-05	1.2849E+00	2.0816E+04	1.2538E+00	1.2804E+02
14	3.0000E+03	-8.9606E+07	3.7148E-05	1.3810E+00	2.1298E+04	1.2470E+00	1.2805E+02
15	3.2000E+03	-8.5301E+07	3.8900E-05	1.4831E+00	2.1843E+04	1.2405E+00	1.2805E+02
16	3.4000E+03	-8.0886E+07	4.0621E-05	1.5954E+00	2.2501E+04	1.2339E+00	1.2807E+02
17	3.6000E+03	-7.6341E+07	4.2313E-05	1.7233E+00	2.3333E+04	1.2193E+00	1.2807E+02
18	3.8000E+03	-7.1635E+07	4.3978E-05	1.8733E+00	2.4404E+04	1.2111E+00	1.2813E+02
19	4.0000E+03	-6.6732E+07	4.5619E-05	2.0526E+00	2.5778E+04	1.2023E+00	1.2832E+02
20	4.2000E+03	-6.1593E+07	4.7236E-05	2.2678E+00	2.7506E+04	1.1932E+00	1.2849E+02
21	4.4000E+03	-5.6175E+07	4.8831E-05	2.5250E+00	2.9623E+04	1.1842E+00	1.2872E+02
22	4.6000E+03	-5.0443E+07	5.0406E-05	2.8284E+00	3.2148E+04	1.1758E+00	1.2903E+02
23	4.8000E+03	-4.4369E+07	5.1961E-05	3.1796E+00	3.5058E+04	1.1682E+00	1.2942E+02
24	5.0000E+03	-3.7937E+07	5.3497E-05	3.5773E+00	3.8310E+04	1.1617E+00	1.2990E+02
25	5.2000E+03	-3.1150E+07	5.5017E-05	4.0169E+00	4.1829E+04	1.1564E+00	1.3047E+02
26	5.4000E+03	-2.4020E+07	5.6519E-05	4.4905E+00	4.5518E+04	1.1523E+00	1.3112E+02
27	5.6000E+03	-1.6576E+07	5.8006E-05	4.9882E+00	4.9267E+04	1.1493E+00	1.3184E+02
28	5.8000E+03	-8.8673E+06	5.9478E-05	5.4959E+00	5.2939E+04	1.1473E+00	1.3263E+02
29	6.0000E+03	-7.1460E+06	6.0935E-05	6.0066E+00	5.6474E+04	1.1461E+00	1.3348E+02
30	6.2000E+03	-5.3004E+06	6.2378E-05	6.5082E+00	5.9774E+04	1.1457E+00	1.3437E+02
31	6.4000E+03	-3.4335E+06	6.3808E-05	6.9923E+00	6.2781E+04	1.1458E+00	1.3529E+02
32	6.6000E+03	-1.5526E+06	6.5226E-05	7.4524E+00	6.5458E+04	1.1465E+00	1.3624E+02
33	6.8000E+03	3.2423E+07	6.6631E-05	7.8844E+00	6.7792E+04	1.1475E+00	1.3721E+02
34	7.0000E+03	4.0960E+07	6.8024E-05	8.2859E+00	6.9781E+04	1.1488E+00	1.3818E+02

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BOUNDARY CONDITIONS (INFLAG = 1)

CON(LBM/FTZ/SEC)

QW(BTU/IN2/S)

HSE(FTZ/SEC2)

PE(LB-F/FTZ)

TE(DEG. R)

UE(FT/SEC)

S(FT)

R(FT)

X(FT)

I	X(FT)	R(FT)	S(FT)	UE(FT/SEC)	TE(DEG. R)	PE(LB-F/FTZ)	HSE(FTZ/SEC2)	QW(BTU/IN2/S)	CON(LBM/FTZ/SEC)
1	-0.34530	0.28868	0.00000E+00	1.07331E+03	5.71352E+03	3.79711E+04	-1.22003E+07	0.00000E+00	0.00000E+00
2	-0.33886	0.28848	6.44534E-03	1.07518E+03	5.71350E+03	3.79681E+04	-1.22011E+07	0.00000E+00	0.00000E+00
3	-0.33757	0.28844	1.07555E+03	1.07550E+03	5.71350E+03	3.79674E+04	-1.22012E+07	0.00000E+00	0.00000E+00
4	-0.33435	0.28835	1.09571E-02	1.07649E+03	5.71349E+03	3.79659E+04	-1.22016E+07	0.00000E+00	0.00000E+00
5	-0.32791	0.28815	1.74024E-02	1.07836E+03	5.71347E+03	3.79629E+04	-1.22024E+07	0.00000E+00	0.00000E+00
6	-0.31259	0.28566	3.29427E-02	1.09981E+03	5.71284E+03	3.79247E+04	-1.22264E+07	0.00000E+00	0.00000E+00
7	-0.30612	0.28463	3.95313E-02	1.11034E+03	5.71253E+03	3.79058E+04	-1.22385E+07	0.00000E+00	0.00000E+00
8	-0.29965	0.28321	4.61198E-02	1.12088E+03	5.71222E+03	3.78870E+04	-1.22505E+07	0.00000E+00	0.00000E+00
9	-0.29317	0.28198	5.27084E-02	1.13141E+03	5.71190E+03	3.78682E+04	-1.22626E+07	0.00000E+00	0.00000E+00
10	-0.28670	0.28075	5.92969E-02	1.14194E+03	5.71159E+03	3.78493E+04	-1.22747E+07	0.00000E+00	0.00000E+00
11	-0.28023	0.27952	6.58855E-02	1.15248E+03	5.71128E+03	3.78305E+04	-1.22868E+07	0.00000E+00	0.00000E+00
12	-0.27375	0.27829	7.24740E-02	1.16301E+03	5.71096E+03	3.78116E+04	-1.22988E+07	0.00000E+00	0.00000E+00
13	-0.26728	0.27707	7.90626E-02	1.17354E+03	5.71065E+03	3.77928E+04	-1.23109E+07	0.00000E+00	0.00000E+00
14	-0.26081	0.27584	8.56511E-02	1.18407E+03	5.71034E+03	3.77740E+04	-1.23230E+07	0.00000E+00	0.00000E+00
15	-0.25434	0.27461	9.22396E-02	1.19461E+03	5.71002E+03	3.77551E+04	-1.23351E+07	0.00000E+00	0.00000E+00
16	-0.24786	0.27338	9.88282E-02	1.20514E+03	5.70971E+03	3.77363E+04	-1.23471E+07	0.00000E+00	0.00000E+00
17	-0.24144	0.27210	1.05417E-01	1.21567E+03	5.70940E+03	3.77175E+04	-1.23592E+07	0.00000E+00	0.00000E+00
18	-0.23547	0.26921	1.12005E-01	1.22620E+03	5.70909E+03	3.76987E+04	-1.23713E+07	0.00000E+00	0.00000E+00
19	-0.22950	0.26643	1.18594E-01	1.23673E+03	5.70878E+03	3.76800E+04	-1.23834E+07	0.00000E+00	0.00000E+00
20	-0.22352	0.26365	1.25182E-01	1.24726E+03	5.70847E+03	3.76613E+04	-1.23955E+07	0.00000E+00	0.00000E+00
21	-0.21755	0.26087	1.31771E-01	1.25779E+03	5.70816E+03	3.76426E+04	-1.24076E+07	0.00000E+00	0.00000E+00
22	-0.21158	0.25808	1.38359E-01	1.26832E+03	5.70785E+03	3.76239E+04	-1.24197E+07	0.00000E+00	0.00000E+00
23	-0.20561	0.25530	1.44948E-01	1.27885E+03	5.70754E+03	3.76052E+04	-1.24318E+07	0.00000E+00	0.00000E+00
24	-0.19964	0.25252	1.51537E-01	1.28938E+03	5.70723E+03	3.75865E+04	-1.24439E+07	0.00000E+00	0.00000E+00
25	-0.19366	0.24974	1.58125E-01	1.29991E+03	5.70692E+03	3.75678E+04	-1.24560E+07	0.00000E+00	0.00000E+00
26	-0.18769	0.24695	1.64714E-01	1.31044E+03	5.70661E+03	3.75491E+04	-1.24681E+07	0.00000E+00	0.00000E+00
27	-0.18172	0.24417	1.71302E-01	1.32097E+03	5.70630E+03	3.75304E+04	-1.24802E+07	0.00000E+00	0.00000E+00
28	-0.17575	0.24139	1.77891E-01	1.33150E+03	5.70599E+03	3.75117E+04	-1.24923E+07	0.00000E+00	0.00000E+00
29	-0.16977	0.23860	1.84479E-01	1.34203E+03	5.70568E+03	3.74930E+04	-1.25044E+07	0.00000E+00	0.00000E+00
30	-0.16395	0.23584	1.91068E-01	1.35256E+03	5.70537E+03	3.74743E+04	-1.25165E+07	0.00000E+00	0.00000E+00
31	-0.15824	0.23325	1.97656E-01	1.36309E+03	5.70506E+03	3.74556E+04	-1.25286E+07	0.00000E+00	0.00000E+00
32	-0.15254	0.22895	2.04245E-01	1.37362E+03	5.70475E+03	3.74369E+04	-1.25407E+07	0.00000E+00	0.00000E+00
33	-0.14683	0.22566	2.10833E-01	1.38415E+03	5.70444E+03	3.74182E+04	-1.25528E+07	0.00000E+00	0.00000E+00
34	-0.14113	0.22236	2.17422E-01	1.39468E+03	5.70413E+03	3.73995E+04	-1.25649E+07	0.00000E+00	0.00000E+00
35	-0.13542	0.21907	2.24011E-01	1.40521E+03	5.70382E+03	3.73808E+04	-1.25770E+07	0.00000E+00	0.00000E+00
36	-0.12971	0.21577	2.30599E-01	1.41574E+03	5.70351E+03	3.73621E+04	-1.25891E+07	0.00000E+00	0.00000E+00
37	-0.12401	0.21248	2.37188E-01	1.42627E+03	5.70320E+03	3.73434E+04	-1.26012E+07	0.00000E+00	0.00000E+00
38	-0.11830	0.20919	2.43776E-01	1.43680E+03	5.70289E+03	3.73247E+04	-1.26133E+07	0.00000E+00	0.00000E+00
39	-0.11258	0.20591	2.50365E-01	1.44733E+03	5.70258E+03	3.73060E+04	-1.26254E+07	0.00000E+00	0.00000E+00
40	-0.10682	0.20273	2.56953E-01	1.45786E+03	5.70227E+03	3.72873E+04	-1.26375E+07	0.00000E+00	0.00000E+00
41	-0.10105	0.19954	2.63542E-01	1.46839E+03	5.70196E+03	3.72686E+04	-1.26496E+07	0.00000E+00	0.00000E+00
42	-0.09529	0.19635	2.70130E-01	1.47892E+03	5.70165E+03	3.72499E+04	-1.26617E+07	0.00000E+00	0.00000E+00
43	-0.08952	0.19316	2.76719E-01	1.48945E+03	5.70134E+03	3.72312E+04	-1.26738E+07	0.00000E+00	0.00000E+00
44	-0.08375	0.18997	2.83307E-01	1.49998E+03	5.70103E+03	3.72125E+04	-1.26859E+07	0.00000E+00	0.00000E+00
45	-0.07799	0.18678	2.89896E-01	1.51051E+03	5.70072E+03	3.71938E+04	-1.26980E+07	0.00000E+00	0.00000E+00
46	-0.07222	0.18359	2.96485E-01	1.52104E+03	5.70041E+03	3.71751E+04	-1.27101E+07	0.00000E+00	0.00000E+00
47	-0.06638	0.18062	3.03073E-01	1.53157E+03	5.70010E+03	3.71564E+04	-1.27222E+07	0.00000E+00	0.00000E+00
48	-0.05996	0.17912	3.09662E-01	1.54210E+03	5.70000E+03	3.71377E+04	-1.27343E+07	0.00000E+00	0.00000E+00
49	-0.05354	0.17763	3.16250E-01	1.55263E+03	5.70000E+03	3.71190E+04	-1.27464E+07	0.00000E+00	0.00000E+00
50	-0.04713	0.17613	3.22839E-01	1.56316E+03	5.70000E+03	3.71003E+04	-1.27585E+07	0.00000E+00	0.00000E+00
51	-0.04071	0.17463	3.29427E-01	1.57369E+03	5.70000E+03	3.70816E+04	-1.27706E+07	0.00000E+00	0.00000E+00

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BOUNDARY CONDITIONS (IHFLAG = 1)  
I X(FT) R(FT) S(FT) UE(FT/SEC) TE(DEG. R) PE(LB-F/FT2) HSE(FT2/SEC2) QW(BTU/IN2/S) CQM(LBM/FT2/SEC)

52	-0.03430	0.17314	3.36016E-01	4.15751E+03	5.48821E+03	2.68944E+04	-2.07366E+07	0.00000E+00	0.00000E+00
53	-0.02788	0.17164	3.42604E-01	4.33501E+03	5.46838E+03	2.60511E+04	-2.14748E+07	0.00000E+00	0.00000E+00
54	-0.02146	0.17014	3.49193E-01	4.51251E+03	5.44855E+03	2.52078E+04	-2.22131E+07	0.00000E+00	0.00000E+00
55	-0.01505	0.16865	3.55781E-01	4.69000E+03	5.42871E+03	2.43645E+04	-2.29513E+07	0.00000E+00	0.00000E+00
56	-0.00863	0.16715	3.62370E-01	4.86750E+03	5.40888E+03	2.35212E+04	-2.36896E+07	0.00000E+00	0.00000E+00
57	-0.00208	0.16671	3.68959E-01	5.04598E+03	5.38986E+03	2.26818E+04	-2.44281E+07	0.00000E+00	0.00000E+00
58	0.00451	0.16673	3.75547E-01	5.22355E+03	5.37146E+03	2.18360E+04	-2.51766E+07	0.00000E+00	0.00000E+00
59	0.01109	0.16704	3.82136E-01	5.40219E+03	5.35426E+03	2.10742E+04	-2.59351E+07	0.00000E+00	0.00000E+00
60	0.02419	0.16761	3.88724E-01	5.58084E+03	5.33712E+03	2.03118E+04	-2.67036E+07	0.00000E+00	0.00000E+00
61	0.03068	0.16844	3.95313E-01	5.75969E+03	5.32000E+03	1.95494E+04	-2.74821E+07	0.00000E+00	0.00000E+00
62	0.03714	0.16952	4.01901E-01	5.93854E+03	5.30288E+03	1.87868E+04	-2.82706E+07	0.00000E+00	0.00000E+00
63	0.04353	0.17086	4.08490E-01	6.11739E+03	5.28576E+03	1.80242E+04	-2.90591E+07	0.00000E+00	0.00000E+00
64	0.04989	0.17245	4.15078E-01	6.29624E+03	5.26864E+03	1.72616E+04	-2.98476E+07	0.00000E+00	0.00000E+00
65	0.05626	0.17416	4.21667E-01	6.47510E+03	5.25152E+03	1.64990E+04	-3.06361E+07	0.00000E+00	0.00000E+00
66	0.06262	0.17586	4.28255E-01	6.65396E+03	5.23440E+03	1.57364E+04	-3.14246E+07	0.00000E+00	0.00000E+00
67	0.06898	0.17757	4.34844E-01	6.83282E+03	5.21728E+03	1.49738E+04	-3.22131E+07	0.00000E+00	0.00000E+00
68	0.07535	0.17927	4.41433E-01	7.01168E+03	5.20016E+03	1.42112E+04	-3.30016E+07	0.00000E+00	0.00000E+00
69	0.08171	0.18098	4.48021E-01	7.18604E+03	5.18304E+03	1.34486E+04	-3.37901E+07	0.00000E+00	0.00000E+00
70	0.08808	0.18268	4.54610E-01	7.36040E+03	5.16592E+03	1.26860E+04	-3.45786E+07	0.00000E+00	0.00000E+00
71	0.09444	0.18439	4.61198E-01	7.53476E+03	5.14880E+03	1.19234E+04	-3.53671E+07	0.00000E+00	0.00000E+00
72	0.10080	0.18609	4.67787E-01	7.70912E+03	5.13168E+03	1.11608E+04	-3.61556E+07	0.00000E+00	0.00000E+00
73	0.10717	0.18780	4.74375E-01	7.88348E+03	5.11456E+03	1.03982E+04	-3.69441E+07	0.00000E+00	0.00000E+00
74	0.11353	0.18950	4.80964E-01	8.05784E+03	5.09744E+03	9.6356E+03	-3.77326E+07	0.00000E+00	0.00000E+00
75	0.11990	0.19121	4.87552E-01	8.23220E+03	5.08032E+03	8.8718E+03	-3.85211E+07	0.00000E+00	0.00000E+00
76	0.12626	0.19291	4.94141E-01	8.40656E+03	5.06320E+03	8.1080E+03	-3.93096E+07	0.00000E+00	0.00000E+00
77	0.13263	0.19462	5.00729E-01	8.58092E+03	5.04608E+03	7.3442E+03	-4.00981E+07	0.00000E+00	0.00000E+00
78	0.13899	0.19632	5.07318E-01	8.75528E+03	5.02896E+03	6.5794E+03	-4.08866E+07	0.00000E+00	0.00000E+00
79	0.14535	0.19803	5.13907E-01	8.92964E+03	5.01184E+03	5.8146E+03	-4.16751E+07	0.00000E+00	0.00000E+00
80	0.15172	0.19973	5.20495E-01	9.10400E+03	5.00000E+03	5.0498E+03	-4.24636E+07	0.00000E+00	0.00000E+00
81	0.15808	0.20144	5.27084E-01	9.27836E+03	4.98816E+03	4.2850E+03	-4.32521E+07	0.00000E+00	0.00000E+00
82	0.16445	0.20315	5.33672E-01	9.45272E+03	4.97632E+03	3.5192E+03	-4.40406E+07	0.00000E+00	0.00000E+00
83	0.17081	0.20485	5.40261E-01	9.62708E+03	4.96448E+03	2.7534E+03	-4.48291E+07	0.00000E+00	0.00000E+00
84	0.17717	0.20656	5.46849E-01	9.80144E+03	4.95264E+03	1.9876E+03	-4.56176E+07	0.00000E+00	0.00000E+00
85	0.18354	0.20826	5.53438E-01	9.97580E+03	4.94080E+03	1.2218E+03	-4.64061E+07	0.00000E+00	0.00000E+00
86	0.18990	0.20997	5.60026E-01	10.15016E+03	4.92896E+03	4.4601E+02	-4.71946E+07	0.00000E+00	0.00000E+00
87	0.19627	0.21167	5.66615E-01	10.32452E+03	4.91712E+03	3.6943E+02	-4.79831E+07	0.00000E+00	0.00000E+00
88	0.20263	0.21338	5.73203E-01	10.49888E+03	4.90528E+03	2.9285E+02	-4.87716E+07	0.00000E+00	0.00000E+00
89	0.20899	0.21508	5.79792E-01	10.67324E+03	4.89344E+03	2.1627E+02	-4.95601E+07	0.00000E+00	0.00000E+00
90	0.21536	0.21679	5.86381E-01	10.84760E+03	4.88160E+03	1.3969E+02	-5.03486E+07	0.00000E+00	0.00000E+00
91	0.22172	0.21849	5.92969E-01	11.02196E+03	4.86976E+03	6.4144E+01	-5.11371E+07	0.00000E+00	0.00000E+00
92	0.22809	0.22020	5.99558E-01	11.19632E+03	4.85792E+03	3.6444E+01	-5.19256E+07	0.00000E+00	0.00000E+00
93	0.23445	0.22190	6.06146E-01	11.37068E+03	4.84608E+03	2.8786E+01	-5.27141E+07	0.00000E+00	0.00000E+00
94	0.24081	0.22361	6.12735E-01	11.54504E+03	4.83424E+03	2.1128E+01	-5.35026E+07	0.00000E+00	0.00000E+00
95	0.24718	0.22531	6.19323E-01	11.71940E+03	4.82240E+03	1.3470E+01	-5.42911E+07	0.00000E+00	0.00000E+00
96	0.25354	0.22702	6.25912E-01	11.89376E+03	4.81056E+03	5.9100E+00	-5.50796E+07	0.00000E+00	0.00000E+00
97	0.25991	0.22872	6.32500E-01	12.06812E+03	4.79872E+03	3.1440E+00	-5.58681E+07	0.00000E+00	0.00000E+00
98	0.26627	0.23043	6.39089E-01	12.24248E+03	4.78688E+03	1.3780E+00	-5.66566E+07	0.00000E+00	0.00000E+00
99	0.27263	0.23213	6.45677E-01	12.41684E+03	4.77504E+03	5.9200E-01	-5.74451E+07	0.00000E+00	0.00000E+00
100	0.27900	0.23384	6.52266E-01	12.59120E+03	4.76320E+03	3.1540E-01	-5.82336E+07	0.00000E+00	0.00000E+00
101	0.28536	0.23555	6.58855E-01	12.76556E+03	4.75136E+03	1.3880E-01	-5.90221E+07	0.00000E+00	0.00000E+00

OUTPUT DATA ( SEGMENT 1 )

NX	X FT	X/R*	DELTA* FT	THETA FT	H	CF	R DELT*	REX	TW DEG R	DF LBF	SQM BTU/SEC
1	-0.34530	-2.07180	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	5.7276E+03	0.0000E+00	0.0000E+00
2	-0.33886	-2.03315	1.4563E-04	5.6108E-05	2.5955E+00	8.6546E-03	1.3368E+02	5.9167E+03	5.7253E+03	-9.8341E+00	0.0000E+00
3	-0.33757	-2.02541	1.5925E-04	6.1444E-05	2.5918E+00	7.9279E-03	1.4624E+02	7.1024E+03	5.7251E+03	-1.0752E+01	0.0000E+00
4	-0.33435	-2.00609	1.8549E-04	7.3380E-05	2.5278E+00	7.0346E-03	1.7047E+02	1.0070E+04	5.7249E+03	-1.2512E+01	0.0000E+00
5	-0.32791	-1.96743	2.1621E-04	9.5636E-05	2.2608E+00	7.2411E-03	1.9904E+02	1.6020E+04	5.7249E+03	-1.6512E+01	0.0000E+00
6	-0.31259	-1.87556	2.7954E-04	1.4393E-04	1.9422E+00	7.5660E-03	2.6225E+02	3.0905E+04	5.7252E+03	-1.8242E+01	0.0000E+00
7	-0.30612	-1.83672	3.0732E-04	1.6294E-04	1.8861E+00	7.3029E-03	2.9096E+02	3.7426E+04	5.7253E+03	-1.9905E+01	0.0000E+00
8	-0.29965	-1.79788	3.3353E-04	1.8077E-04	1.8451E+00	7.0424E-03	3.1864E+02	4.4061E+04	5.7253E+03	-2.1473E+01	0.0000E+00
9	-0.29317	-1.75904	3.5821E-04	1.9765E-04	1.8124E+00	6.8481E-03	3.4530E+02	5.0809E+04	5.7253E+03	-2.2926E+01	0.0000E+00
10	-0.28670	-1.72020	3.8189E-04	2.1368E-04	1.7872E+00	6.6458E-03	3.7140E+02	5.7669E+04	5.7253E+03	-2.4298E+01	0.0000E+00
11	-0.28023	-1.68137	4.0411E-04	2.2893E-04	1.7652E+00	6.4888E-03	3.9648E+02	6.4642E+04	5.7252E+03	-2.5563E+01	0.0000E+00
12	-0.27375	-1.64253	4.2527E-04	2.4358E-04	1.7459E+00	6.3415E-03	4.2089E+02	7.1728E+04	5.7252E+03	-2.6744E+01	0.0000E+00
13	-0.26728	-1.60369	4.4536E-04	2.5768E-04	1.7284E+00	6.2211E-03	4.4459E+02	7.8926E+04	5.7252E+03	-2.7844E+01	0.0000E+00
14	-0.26081	-1.56485	4.6475E-04	2.7130E-04	1.7130E+00	6.1059E-03	4.6971E+02	8.6237E+04	5.7252E+03	-2.8886E+01	0.0000E+00
15	-0.25434	-1.52601	4.8327E-04	2.8448E-04	1.6988E+00	6.0037E-03	4.9071E+02	9.3660E+04	5.7251E+03	-2.9862E+01	0.0000E+00
16	-0.24786	-1.48717	5.0008E-04	2.9682E-04	1.6848E+00	5.9447E-03	5.1205E+02	1.0119E+05	5.7251E+03	-3.0641E+01	0.0000E+00
17	-0.24144	-1.44864	5.1620E-04	3.0259E-04	1.6610E+00	6.2237E-03	5.1986E+02	1.0904E+05	5.7251E+03	-2.9510E+01	0.0000E+00
18	-0.23547	-1.41281	4.7931E-04	2.9929E-04	1.6349E+00	6.5208E-03	5.1915E+02	1.1884E+05	5.7249E+03	-2.7125E+01	0.0000E+00
19	-0.22950	-1.37697	4.6729E-04	2.9136E-04	1.6038E+00	6.6433E-03	5.2056E+02	1.2946E+05	5.7245E+03	-2.5134E+01	0.0000E+00
20	-0.22352	-1.34114	4.6205E-04	2.8969E-04	1.5881E+00	6.6211E-03	5.2692E+02	1.5027E+05	5.7241E+03	-2.4476E+01	0.0000E+00
21	-0.21755	-1.30531	4.5924E-04	2.8917E-04	1.5824E+00	6.5092E-03	5.4671E+02	1.6145E+05	5.7240E+03	-2.3956E+01	0.0000E+00
22	-0.21158	-1.26948	4.5829E-04	2.8961E-04	1.5824E+00	6.4368E-03	5.5937E+02	1.8473E+05	5.7238E+03	-2.3537E+01	0.0000E+00
23	-0.20561	-1.19781	4.5885E-04	2.9089E-04	1.5729E+00	6.3588E-03	5.7362E+02	1.9689E+05	5.7237E+03	-2.2922E+01	0.0000E+00
24	-0.19964	-1.16198	4.6364E-04	2.9558E-04	1.5687E+00	6.2753E-03	5.8933E+02	2.2218E+05	5.7235E+03	-2.2699E+01	0.0000E+00
25	-0.19366	-1.12615	4.6753E-04	2.9880E-04	1.5647E+00	6.1901E-03	6.0639E+02	2.532E+05	5.7232E+03	-2.2518E+01	0.0000E+00
26	-0.18769	-1.09031	4.7228E-04	3.0258E-04	1.5608E+00	6.1041E-03	6.2473E+02	2.8507E+05	5.7230E+03	-2.1661E+01	0.0000E+00
27	-0.18172	-1.05448	4.7672E-04	3.0328E-04	1.5519E+00	6.2027E-03	6.3472E+02	3.0328E+05	5.7226E+03	-1.9961E+01	0.0000E+00
28	-0.17575	-1.01865	4.7067E-04	2.9537E-04	1.5364E+00	6.4997E-03	6.1965E+02	3.2830E+05	5.7221E+03	-1.8276E+01	0.0000E+00
29	-0.16977	-0.98370	4.5381E-04	2.8323E-04	1.5232E+00	6.6942E-03	6.1965E+02	3.5390E+05	5.7216E+03	-1.7039E+01	0.0000E+00
30	-0.16395	-0.94946	4.3142E-04	2.7247E-04	1.5166E+00	6.7280E-03	6.1360E+02	3.7321E+05	5.7211E+03	-1.6090E+01	0.0000E+00
31	-0.15824	-0.91523	4.1323E-04	2.6475E-04	1.5146E+00	6.6846E-03	6.1473E+02	3.8618E+05	5.7207E+03	-1.5334E+01	0.0000E+00
32	-0.15254	-0.88099	3.9290E-04	2.5941E-04	1.5146E+00	6.6096E-03	6.2105E+02	3.9368E+05	5.7207E+03	-1.4721E+01	0.0000E+00
33	-0.14683	-0.84676	3.9290E-04	2.5603E-04	1.5155E+00	6.5134E-03	6.4589E+02	4.0821E+05	5.7198E+03	-1.4217E+01	0.0000E+00
34	-0.14113	-0.81252	3.8802E-04	2.5426E-04	1.5168E+00	6.4053E-03	6.4589E+02	4.2674E+05	5.7194E+03	-1.3796E+01	0.0000E+00
35	-0.13542	-0.77829	3.8543E-04	2.5385E-04	1.5183E+00	6.2797E-03	6.5400E+02	4.4757E+05	5.7189E+03	-1.3362E+01	0.0000E+00
36	-0.12971	-0.74405	3.8433E-04	2.5339E-04	1.5168E+00	6.2510E-03	6.7909E+02	4.7090E+05	5.7189E+03	-1.2491E+01	0.0000E+00
37	-0.12401	-0.70982	3.8433E-04	2.5339E-04	1.5168E+00	6.2510E-03	6.7909E+02	4.9557E+05	5.7181E+03	-1.199E+01	0.0000E+00
38	-0.11830	-0.67551	3.7026E-04	2.4565E-04	1.4983E+00	6.5400E-03	6.7373E+02	5.2002E+05	5.7169E+03	-1.1199E+01	0.0000E+00
39	-0.11258	-0.64091	3.4733E-04	2.3182E-04	1.4983E+00	6.7784E-03	6.5905E+02	5.4914E+05	5.7145E+03	-9.2293E+00	0.0000E+00
40	-0.10682	-0.60632	3.2849E-04	2.1944E-04	1.4969E+00	6.8107E-03	6.4880E+02	5.8618E+05	5.7133E+03	-8.5652E+00	0.0000E+00
41	-0.10105	-0.57172	3.1679E-04	2.110E-04	1.5079E+00	6.7300E-03	6.5719E+02	6.1978E+05	5.7121E+03	-8.0305E+00	0.0000E+00
42	-0.09529	-0.53713	3.1024E-04	2.0268E-04	1.5216E+00	6.4723E-03	6.7220E+02	6.5368E+05	5.7110E+03	-7.5671E+00	0.0000E+00
43	-0.08952	-0.50254	3.0727E-04	2.0150E-04	1.5218E+00	6.3424E-03	6.9144E+02	6.8782E+05	5.7098E+03	-7.2195E+00	0.0000E+00
44	-0.08376	-0.46794	3.0664E-04	2.0150E-04	1.5272E+00	6.2242E-03	7.1383E+02	7.285E+05	5.7082E+03	-7.0457E+00	0.0000E+00
45	-0.07799	-0.43335	3.0770E-04	2.0147E-04	1.5272E+00	6.3390E-03	7.2151E+02	7.7059E+05	5.7078E+03	-6.6668E+00	0.0000E+00
46	-0.07222	-0.39826	3.0251E-04	1.9809E-04	1.5290E+00	6.4750E-03	7.1542E+02	8.0058E+05	5.7035E+03	-5.7272E+00	0.0000E+00
47	-0.06638	-0.35926	2.9068E-04	1.9011E-04	1.5290E+00	6.4679E-03	7.1542E+02	8.3801E+05	5.7011E+03	-5.1400E+00	0.0000E+00
48	-0.05996	-0.32127	2.8159E-04	1.8334E-04	1.5359E+00	6.4679E-03	7.2836E+02	8.7428E+05	5.6987E+03	-4.6153E+00	0.0000E+00
49	-0.05354	-0.28277	2.754E-04	1.7917E-04	1.5490E+00	6.3810E-03	7.2042E+02	9.1961E+05	5.6987E+03	-4.1400E+00	0.0000E+00
50	-0.04713	-0.24427	2.7597E-04	1.7698E-04	1.5593E+00	6.2972E-03	7.3241E+02	9.7428E+05	5.6987E+03	-3.6153E+00	0.0000E+00
51	-0.04071	-0.20427	2.7597E-04	1.7698E-04	1.5593E+00	6.2972E-03	7.3241E+02	10.2972E+05	5.6987E+03	-3.1400E+00	0.0000E+00



OUTPUT DATA ( SEGMENT 1 )

MX	X FT	X/R*	DELTA* FT	THETA FT	H	CF	R DELT*	REX	TW DEG R	DF LBF	SON BTU/SEC
52	-0.03430	-0.20577	2.7699E-04	1.7638E-04	1.5705E+00	6.2070E-03	7.4954E+02	9.0925E+05	5.6964E+03	-4.1507E+00	0.0000E+00
53	-0.02788	-0.16728	2.8013E-04	1.7705E-04	1.5822E+00	6.0991E-03	7.7083E+02	9.4275E+05	5.6940E+03	-3.7269E+00	0.0000E+00
54	-0.02146	-0.12878	2.8492E-04	1.7877E-04	1.5939E+00	5.9960E-03	7.9523E+02	9.7462E+05	5.6915E+03	-3.3278E+00	0.0000E+00
55	-0.01503	-0.09028	2.9120E-04	1.8139E-04	1.6054E+00	5.8906E-03	8.2231E+02	1.0047E+06	5.6890E+03	-2.9457E+00	0.0000E+00
56	-0.00863	-0.05178	2.7368E-04	1.7135E-04	1.5972E+00	6.6066E-03	7.7998E+02	1.0328E+06	5.6835E+03	-2.3409E+00	0.0000E+00
57	-0.00208	-0.01248	2.4965E-04	1.5264E-04	1.6355E+00	7.1628E-03	7.1867E+02	1.0621E+06	5.6684E+03	-8.2395E-01	0.0000E+00
58	0.00451	0.02704	2.4946E-04	1.4786E-04	1.6871E+00	6.8687E-03	7.0842E+02	1.0665E+06	5.6564E+03	1.2292E-01	0.0000E+00
59	0.01109	0.06653	2.6486E-04	1.5270E-04	1.7345E+00	6.4401E-03	7.4131E+02	1.0695E+06	5.6520E+03	2.1265E-01	0.0000E+00
60	0.01765	0.10591	2.8305E-04	1.5927E-04	1.8142E+00	6.1135E-03	7.7736E+02	1.0608E+06	5.6472E+03	5.5208E-01	0.0000E+00
61	0.02419	0.14512	3.0100E-04	1.6591E-04	1.8378E+00	6.0690E-03	8.2908E+02	1.0492E+06	5.6355E+03	9.0102E-01	0.0000E+00
62	0.03068	0.18411	3.1757E-04	1.7279E-04	1.8886E+00	5.9478E-03	8.6270E+02	1.0332E+06	5.6293E+03	1.2751E+00	0.0000E+00
63	0.04333	0.26217	3.4108E-04	1.8060E-04	1.9328E+00	5.6172E-03	9.1232E+02	1.0175E+06	5.6253E+03	1.5827E+00	0.0000E+00
64	0.04989	0.29936	4.0494E-04	1.9255E-04	1.9328E+00	5.6172E-03	9.1232E+02	1.0175E+06	5.6253E+03	1.8930E+00	0.0000E+00
65	0.05626	0.33754	4.3707E-04	2.0722E-04	1.9541E+00	5.1586E-03	9.8554E+02	1.0263E+06	5.6279E+03	2.0370E+00	0.0000E+00
66	0.06898	0.37572	4.6577E-04	2.195E-04	1.9692E+00	4.8647E-03	1.0600E+03	1.0386E+06	5.6324E+03	2.1643E+00	0.0000E+00
67	0.08171	0.41391	4.9172E-04	2.3550E-04	1.9778E+00	4.6884E-03	1.1255E+03	1.0508E+06	5.6349E+03	2.2953E+00	0.0000E+00
68	0.09228	0.45209	5.0970E-04	2.5966E-04	1.9825E+00	4.5788E-03	1.1837E+03	1.0627E+06	5.6366E+03	2.4386E+00	0.0000E+00
69	0.10871	0.49028	5.2866E-04	2.803E-04	1.9825E+00	4.5788E-03	1.2219E+03	1.0740E+06	5.6376E+03	2.6704E+00	0.0000E+00
70	0.12626	0.52846	5.6060E-04	2.8111E-04	1.9929E+00	4.3936E-03	1.2713E+03	1.0846E+06	5.6382E+03	2.8360E+00	0.0000E+00
71	0.14444	0.56665	5.7610E-04	2.8111E-04	1.9942E+00	4.3691E-03	1.3304E+03	1.0945E+06	5.6383E+03	2.9478E+00	0.0000E+00
72	0.16333	0.60483	5.9638E-04	2.9105E-04	1.9942E+00	4.3691E-03	1.3595E+03	1.1039E+06	5.6381E+03	3.1957E+00	0.0000E+00
73	0.18266	0.64302	6.1651E-04	3.002E-04	1.9886E+00	4.3477E-03	1.3990E+03	1.128E+06	5.6379E+03	3.3864E+00	0.0000E+00
74	0.20263	0.68120	6.3613E-04	3.1002E-04	1.9886E+00	4.3477E-03	1.4371E+03	1.128E+06	5.6379E+03	3.5811E+00	0.0000E+00
75	0.22263	0.71938	6.553E-04	3.1909E-04	1.9936E+00	4.3114E-03	1.4729E+03	1.128E+06	5.6379E+03	3.7814E+00	0.0000E+00
76	0.24263	0.75757	6.7424E-04	3.2790E-04	1.9986E+00	4.2876E-03	1.5065E+03	1.128E+06	5.6379E+03	3.9871E+00	0.0000E+00
77	0.26263	0.79575	6.9289E-04	3.3649E-04	2.0038E+00	4.2512E-03	1.5383E+03	1.128E+06	5.6379E+03	4.1981E+00	0.0000E+00
78	0.28263	0.83394	7.1133E-04	3.4508E-04	2.0092E+00	4.2349E-03	1.5682E+03	1.128E+06	5.6379E+03	4.4136E+00	0.0000E+00
79	0.30263	0.87212	7.2978E-04	3.5308E-04	2.0166E+00	4.2291E-03	1.5965E+03	1.128E+06	5.6379E+03	4.6346E+00	0.0000E+00
80	0.32263	0.91030	7.4856E-04	3.6119E-04	2.0205E+00	4.2188E-03	1.6234E+03	1.128E+06	5.6379E+03	4.8589E+00	0.0000E+00
81	0.34263	0.94849	7.673E-04	3.7118E-04	2.0275E+00	4.2131E-03	1.6500E+03	1.128E+06	5.6379E+03	5.0822E+00	0.0000E+00
82	0.36263	0.98667	7.8679E-04	3.8512E-04	2.0352E+00	4.2034E-03	1.6761E+03	1.128E+06	5.6379E+03	5.3069E+00	0.0000E+00
83	0.38263	1.02486	8.0611E-04	3.9303E-04	2.0430E+00	4.1955E-03	1.7013E+03	1.128E+06	5.6379E+03	5.5333E+00	0.0000E+00
84	0.40263	1.06304	8.2559E-04	4.0097E-04	2.0509E+00	4.1860E-03	1.7259E+03	1.128E+06	5.6379E+03	5.7616E+00	0.0000E+00
85	0.42263	1.10123	8.4531E-04	4.0890E-04	2.0590E+00	4.1792E-03	1.7498E+03	1.128E+06	5.6379E+03	5.9907E+00	0.0000E+00
86	0.44263	1.13941	8.6522E-04	4.1683E-04	2.0673E+00	4.1693E-03	1.7732E+03	1.128E+06	5.6379E+03	6.2212E+00	0.0000E+00
87	0.46263	1.17759	8.8537E-04	4.2477E-04	2.0757E+00	4.1629E-03	1.7961E+03	1.128E+06	5.6379E+03	6.4520E+00	0.0000E+00
88	0.48263	1.21578	9.0573E-04	4.3273E-04	2.0844E+00	4.1542E-03	1.8184E+03	1.128E+06	5.6379E+03	6.6829E+00	0.0000E+00
89	0.50263	1.25396	9.2635E-04	4.4072E-04	2.0931E+00	4.1466E-03	1.8404E+03	1.128E+06	5.6379E+03	6.9150E+00	0.0000E+00
90	0.52263	1.29215	9.4718E-04	4.4873E-04	2.1019E+00	4.1367E-03	1.8621E+03	1.128E+06	5.6379E+03	7.1467E+00	0.0000E+00
91	0.54263	1.33033	9.6823E-04	4.5676E-04	2.1108E+00	4.1281E-03	1.8834E+03	1.128E+06	5.6379E+03	7.3785E+00	0.0000E+00
92	0.56263	1.36852	9.8948E-04	4.6481E-04	2.1198E+00	4.1189E-03	1.9042E+03	1.128E+06	5.6379E+03	7.6101E+00	0.0000E+00
93	0.58263	1.40670	1.0110E-03	4.7288E-04	2.1288E+00	4.109E-03	1.9246E+03	1.128E+06	5.6379E+03	7.8413E+00	0.0000E+00
94	0.60263	1.44489	1.0331E-03	4.8096E-04	2.1379E+00	4.0938E-03	1.9446E+03	1.128E+06	5.6379E+03	8.0719E+00	0.0000E+00
95	0.62263	1.48307	1.0602E-03	4.8920E-04	2.1479E+00	4.0789E-03	1.9651E+03	1.128E+06	5.6379E+03	8.2978E+00	0.0000E+00
96	0.64263	1.52125	1.0788E-03	4.9744E-04	2.1579E+00	4.0629E-03	1.9846E+03	1.128E+06	5.6379E+03	8.5285E+00	0.0000E+00
97	0.66263	1.55944	1.1020E-03	5.0572E-04	2.1687E+00	4.0479E-03	2.0071E+03	1.128E+06	5.6379E+03	8.7583E+00	0.0000E+00
98	0.68263	1.59762	1.1256E-03	5.1404E-04	2.1792E+00	4.0692E-03	2.0277E+03	1.128E+06	5.6379E+03	8.9730E+00	0.0000E+00
99	0.70263	1.63581	1.1494E-03	5.2239E-04	2.1897E+00	4.0600E-03	2.0480E+03	1.128E+06	5.6379E+03	9.1959E+00	0.0000E+00
100	0.72263	1.67399	1.1734E-03	5.3076E-04	2.2003E+00	4.0520E-03	2.0680E+03	1.128E+06	5.6379E+03	9.4178E+00	0.0000E+00
101	0.74263	1.71217	1.1971E-03	5.3913E-04	2.2108E+00	4.0424E-03	2.0875E+03	1.128E+06	5.6379E+03	9.6385E+00	0.0000E+00

MEAN FREE PATH (FT) = 0.1493001E-05  
 REFINARIZATION PARAMETER (KE AND KW) = 0.4218829E-06  
 MASS FLOW (LBM/SEC) = 15.40270  
 DELTA ISP (SEC) = 0.6177459

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NEW VALUES OF NOZZLE GEOMETRY PARAMETERS  
(NEGATIVE DISPLACEMENT)

RST = 1.9970 INCH RTU = 1.0030 RMTD = 1.0030 EPS = 1.9841 THE = 14.800 DEG

N	R/R*	X/R*	SLOPE(DEG)
1	1.034176	0.2595955	15.000
2	1.054212	0.3387269	14.208
3	1.074391	0.4152935	14.765
4	1.094643	0.4918421	14.819
5	1.114889	0.5683912	14.814
6	1.135145	0.6449372	14.822
7	1.155410	0.7214797	14.829
8	1.175689	0.7980213	14.839
9	1.195971	0.8745610	14.842
10	1.216242	0.9511083	14.832
11	1.236510	1.027650	14.831
12	1.256779	1.104194	14.832
13	1.277043	1.180739	14.828
14	1.297296	1.257285	14.820
15	1.317544	1.333833	14.816
16	1.337786	1.410382	14.812
17	1.357997	1.486941	14.788
18	1.378251	1.563488	14.820
19	1.398467	1.640051	14.791
20	1.408579	1.678324	14.800

TDK PERFORMANCE SUMMARY : 3 ZONES TDK TEST CASE, LOX/GH2 - TDK MANUAL TEST CASE

TDK	TDK / BLM
ISP (SEC)	DISP(BLM) 0.617748
F (LBF)	DF OPT(BLM) 18.9816
MASS FLOW (LB/SEC)	*DF(BLM) 9.63854
CD	ISP(TDK-BLM) 329.016
C* (FT/SEC)	F (TDK-BLM) 5133.53
CF	CF (TDK-BLM) 1.5130
	329.633
	5143.17
	15.6027
	0.995594
	6996.46
	1.51585

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TDK PERFORMANCE SUMMARY : 3 ZONES TDK TEST CASE, LOX/GH2 - TDK MANUAL TEST CASE  
REAL WALL CONTOUR 3 ZONES ADIABATIC

FIRST  
TDK/BLM SOLUTION

CHAMBER PRESS [PSIA]	300.0000
CHAMBER TEMP [R]	6001.056
MIXTURE RATIO [-]	6.297435
EP (NOZZLE) [-]	2.000000
H (OXID) [CAL/MOLE]	-3099.196
H (FUEL) [CAL/MOLE]	-2154.000
HCHAM (ODE) [BTU/LB]	-413.8725
DELH (AVERAGE) [BTU/LB]	0.000000E+00
DELH1 (AV) [BTU/LB]	0.000000E+00
ECRAT [-]	3.000000
RSTAR	2.000000
RWTD [-]	1.000000
RWTD [-]	1.000000
THE [DEGREES]	1.000000
THETA [DEGREES]	0.000000E+00
THETA1 [DEGREES]	15.00000
RI [-]	30.00000
NIT [-]	2.000000
ISP (ODE) [SECONDS]	59.00000
ISP (ODF) [SECONDS]	335.4859
ISP (ODK) [SECONDS]	326.8484
ISP (TDK) [SECONDS]	335.2208
THRUST (TDK) [POUNDS]	329.6333
WDOT (TDK) [LB/SEC]	5143.173
CSTAR (TDK) [FT/SEC]	15.60271
CF (TDK) [-]	6996.465
P (AXIS,EXIT) [PSIA]	1.515854
P (WALL,EXIT) [PSIA]	0.9955939
T (WALL,EXIT) [R]	0.000000E+00
V (WALL,EXIT) [FT/SEC]	38.67983
MA (WALL,EXIT) [-]	4456.856
SHOCK STRENGTH [-]	9110.994
SHOCK (X/R*) [-]	1.918942
SHOCK (R/R*) [-]	0.000000E+00
XA (X/R*) [-]	0.000000E+00
XB (X/R*) [-]	0.000000E+00
DFORT (BLME) [POUNDS]	0.000000E+00
DF (BLME) [POUNDS]	18.98157
DISP (BLME) [SECONDS]	9.638544
THET (EXIT) [FEET]	0.6177480
DEL* (EXIT) [-]	0.5307631E-03
EP (REGEN) [-]	0.1173430E-02
SODOT (REGEN) [BTU/SEC]	0.000000E+00
SODOT (ODS) [BTU/SEC]	0.000000E+00
FWDOT (IC) [POUNDS]	0.000000E+00
ISF (IC) [SECONDS]	5133.535
CF (IC) [-]	329.0155
	1.513014

FORTRAN STOP  
LANH

job terminated at 26-OCT-1985 04:11:30.46

Accounting information:

Buffered I/O count: 120

Direct I/O count: 1087

Page faults: 3758

Elapsed CPU time: 0 00:11:03.34

Peak working set size: 500

Peak page file size: 2331

Mounted volumes: 0

Elapsed time: 0 00:11:30.37

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## 7.2 PRATT AND WHITNEY TEST ENGINE FOR RL-10 OTV PROPULSION

This engine uses a hydrogen expander cycle with oxygen preheating and a nozzle that is regeneratively cooled with hydrogen. A flow schematic for the engine which was taken from Reference 25 is shown in Figure 7-1. The engine is sized to produce a nominal vacuum thrust of 15,500 pounds when operated at a chamber pressure of 394 psia and an expansion ratio of 205:1. Complete input for the case is presented in Table 7-2. This input has been prepared by SEA, Inc. from data provided by NASA MSFC. The complete output for the case is rather lengthy and is not given here. It is available from SEA, Inc. However, the output summary table is given in Table 7-3.

The calculations were carried out using the TDK shock option (SHOCK=1). An induced shock wave was found that originated from the wall inflection point just downstream of the throat. The shock was found to be weak,  $(P_2 - P_1)/P_1 = .03$ , within the domain of influence for the nozzle wall.

The sequence of calculations is as follows:

- 1) ODE calculation with the system enthalpy set at the propellant tank values, i.e., liquid oxygen and liquid hydrogen at their normal boiling points.
- 2) ODK calculation starting from the above ODE results at a chamber contraction ratio of 3.98, corresponding to the chamber diameter.
- 3) TDK calculation using the above ODE and ODK results.
- 4) BLM calculation using the above ODE, ODK, and TDK results. A new wall geometry is calculated by displacing the wall inward a distance of  $\delta^*$  normal to the real wall. This new wall defines the boundary of the inviscid core flow. BLM calculated that 5288 BTU/LBM were picked up through the wall by the regen cooling circuit. Since the nozzle mass flow was found by TDK to be 33.82 lb/sec, the propellant enthalpy was increased by 156.3 BTU/LB.
- 5) ODE calculation with the increased propellant enthalpy. The expansion ratio of the inviscid core flow is automatically placed in the ODE output schedule.

- 6) ODK calculation using the above ODE results, including the new expansion ratio.
- 7) TDK calculation using the above ODE and ODK results, including the new wall contour.
- 8) Output summary table.

The total number of flow field points computed by the MOC was more than 65,000 for each pass. Computer execution time for the case was 2 hours and 50 minutes using a DEC PDP 11/750 VAX computer system.

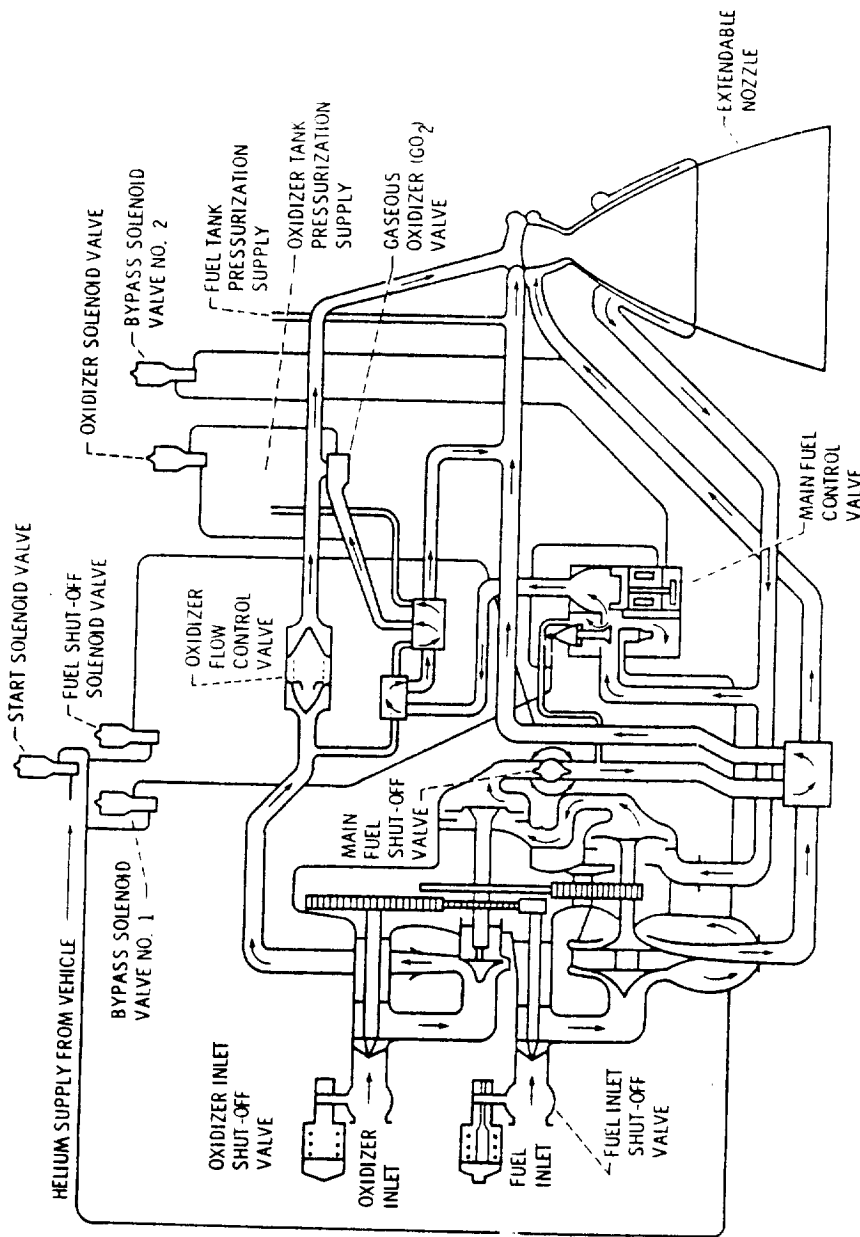


Figure 7-1. Flow schematic, Pratt & Whitney advanced OTV propulsion concept.

Table 7-2. TDK Input for the RL-10 OTV Test Engine.

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TITLE 1 ZONE RL-10 (WITH SHOCK SIMULATION)
DATA
$DATA
ODE=1, ODK=1, NZONES=1, TDK=1, BLM=1, IRPEAT=1,
SHOCK=1,
PFGOPT=0,
ECRAT=3.98, ASUB=10.089, 5.845, 4.538, 3.234, 3.982, MASUB=5,
ASUP = 40, 56.9, 100., 197.8, 205.03, MASUP=5,
ASUB = 4, 3.982, 2, 1.5, 1.25, MASUB = 5
RS1=2.57, RWTD=2.0623, RWTD=.190, THETA=26.25, RI=1.7899,
IMALL=4, THE=11.56, THETA=30,
NWS=29,
RS = .0, 1.0967, 1.3149, 1.6292, 2.2540, 3.2560, 4.1825, 4.8385,
5.5335, 6.3720, 7.0654, 7.2630, 7.8181, 8.0758, 9.6218,
9.8795, 10.3681, 10.6064, 11.7979, 12.0362,
12.1807, 12.1990, 12.2166, 12.2337, 12.2501,
12.4710, 12.6755,
14.1073, 14.3190,
14.1073, 14.3190, .5787, 1.0747, 2.1000, 3.9424, 5.9743, 7.6537,
ZS = .0, 9.7136, 12.6486, 15.5584, 16.4883, 19.0000, 20.0000, 26.0000,
27.0000, 29.0000, 30.0000, 35.0000, 36.0000,
36.6064, 36.6846, 36.7629, 36.8413, 36.9199,
38.0000, 39.0000,
46.0000, 47.0350,
EPS=205.05376,
IOFF=3,
$END
REACTANTS
H 2.
O 2.
NAMELISTS
1 $CODE
1 RKT=.TRUE.,
P(1)=394.3, PSIA=.TRUE., XP=1.,
OFKED(1)=5.035244,
$END
REACTIONS
M1, A = 6.4E17, N = 1.0, B = 0.0, (AR) BAULCH 72 (A) 30U
M2, A = 8.4E21, N = 2.0, B = 0.0, (AR) BAULCH 72 (A) 10U
M3, A = 1.9E13, N = 0.0, B = -1.79, (AR) BAULCH 76 (A) 10U
M7, A = 3.62E18, N = 1.0, B = 0.0, (AR) JENSEN 78 (B) 30U
END TBR REAX
O2 + H = O + OH, A = 2.2E14, N = 0.0, B = 16.8, BAULCH 72 (A) 1.5U
H2 + O = H + OH, A = 1.8E10, N = -1., B = 8.9, BAULCH 72 (A) 1.5U
H2 + OH = H2O + H, A = 2.2E13, N = 0.0, B = 5.15, BAULCH 72 (A) 2U
OH + OH = H2O + O, A = 6.3E12, N = 0.0, B = 1.09, BAULCH 72 (A) 3U
THIRD BODY REAX RATE RATIOS
M1 = 25*H, 4*H2, 10*H2O, 25*O, 25*OH, 1.5*O2,
M2 = 12.5*H, 5*H2, 17*H2O, 12.5*O, 12.5*OH, 6*O2,
M3 = 12.5*H, 5*H2, 5*H2O, 12.5*O, 12.5*OH, 11*O2,
M7 = 12.5*H, 5*H2, 5*H2O, 12.5*O, 12.5*OH, 5*O2,
LAST END
$END
MP=200, XM=1,
$MOC
NC=0, ISHCK=2,

```

100. -2154.L 20.56F .0709  
100. -3102.L 90.110 1.149



Table 7-2. (Continued).

```

$END
$BLM
IPRNT=0,
XINO = -4.28, -3.89, -3.50,
RINO = 3*1.995,
UEO = 190, 380, 570,
TEO = 5917, 5915, 5913,
PEO = 393, 392, 391,
OFC = 2, DISTRB = 0,
XCO = -4.28,
XCE = 18.1,
INFLAG = 0,
NTQW = 14,
XTQW = -3, -1, 0, 1, 2, 4, 6, 8, 10, 12, 14, 18, 19, 47,
TQW = 1800, 2000, 2200, 1500, 1300, 1200, 1050, 800, 650, 500,
425, 350, 750, 800,
NSEGS=10,
APROF=75, 150, 200, NPROF=0,
KDTPLT=0, KMTPLT=0, KTMPLT=0,
$END

```

Table 7-3. TDK Performance Summary: RL10 Engine.

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TDK PERFORMANCE SUMMARY : 1 ZONE RL-10 (WITH SHOCK SIMULATION)  
REAL WALL CONTOUR 1 ZONES WALL TEMP  
INDUCED SHOCK AFTER XA

	FIRST TDK/BLM SOLUTION	SECOND TDK/BLM SOLUTION
CHAMBER PRESS [PSIA]	394.3000	394.3000
CHAMBER TEMP [R]	5815.918	5892.477
MIXTURE RATIO [-]	5.035244	5.035244
EP (NOZZLE) [-]	205.0338	194.0614
H (OXID) [CAL/MOLE]	-3102.000	-3102.000
H (FUEL) [CAL/MOLE]	-2154.000	-2154.000
HCHAM (ODE) [BTU/LB]	-464.2563	-307.9082
DELH (AVERAGE) [BTU/LB]	0.000000E+00	0.000000E+00
DELH1 (AV) [BTU/LB]	0.000000E+00	156.3460
ECRAT [-]	3.980000	3.969802
RSTAR [INCHES]	2.570000	2.573304
RWTD [-]	0.1900000	0.1884720
RWTU [-]	2.062300	2.058368
THE [DEGREES]	11.56000	10.6555
THETA [DEGREES]	30.00000	30.00000
THETA1 [DEGREES]	26.25000	26.25000
RI [-]	1.789900	1.789900
NIT [-]	196.0000	196.0000
ISP (ODE) [SECONDS]	477.5184	483.3437
ISP (ODF) [SECONDS]	456.1371	459.4965
ISP (ODK) [SECONDS]	474.4465	479.8922
ISP (TDK) [SECONDS]	469.6459	475.5385
THRUST (TDK) [POUNDS]	15885.27	15972.03
WDOT (TDK) [LB/SEC]	33.82393	33.58724
CSTAR (TDK) [FT/SEC]	7782.584	7857.594
CF (TDK) [-]	1.941564	1.952167
CD [-]	0.9963781	0.9989328
P (AXIS,EXIT) [PSIA]	0.000000E+00	0.000000E+00
P (WALL,EXIT) [PSIA]	0.7859458E-01	0.8903214E-01
T (WALL,EXIT) [R]	1177.088	1257.314
V (WALL,EXIT) [FT/SEC]	14947.51	15101.62
MA (WALL,EXIT) [-]	5.909647	5.784453
SHOCK STRENGTH [-]	0.3437161E-01	0.9015918E-02
SHOCK (X/R*) [-]	8.749036	1.162930
SHOCK (R/R*) [-]	1.110723	9.098541
XA (X/R*) [-]	0.9500000E-01	0.9500000E-01
XB (X/R*) [-]	0.0000000E+00	0.0000000E+00
DFOPT (BLME) [POUNDS]	412.6425	436.4781
DF (BLME) [POUNDS]	395.3395	417.3250
OTSP (BLME) [SECONDS]	11.68816	12.42511
THET (EXIT) [FEET]	0.4160833E-01	0.4160833E-01
THETA (EXIT) [FEET]	0.8098879E-01	0.8098879E-01
EC (REGENT) [BTU/SEC]	57.88868	57.88868
SODOT (REGENT) [BTU/SEC]	5288.230	5288.230
SODOT (LOSS) [BTU/SEC]	1214.000	1214.000
THRUST (TC) [POUNDS]	15489.93	15554.70
ISP (TC) [SECONDS]	457.9577	463.1133
CF (TC) [-]	1.893244	1.901160

### 7.3 ROCKETDYNE PROTOTYPE ADVANCED SPACE ENGINE FOR OTV PROPULSION

This engine uses a hydrogen expander cycle with oxygen preheating and a nozzle that is regeneratively cooled with hydrogen. A flow schematic for the engine which was taken from Reference 25 is shown in Figure 7-2. The engine is sized to produce a nominal vacuum thrust of 22,500 pounds when operated at a chamber pressure of 2300 psia and an expansion ratio of 400:1.

Complete input for the case is given in Table 7-4. This input has been prepared by SEA, Inc., from data provided by NASA MSFC. The complete output for the case is lengthy and is not given here. It is available from SEA, Inc.. However, the output summary table is given in Table 7-5.

As with the RL-10 engine discussed in the previous subsection, 7.2, the calculations were carried out using the TDK shock option (SHOCK=1). The sequence of calculations is the same as given in subsection 7.1. An induced shock wave was found that originated from the wall inflection point just downstream of the throat. The shock strength at the last left running characteristic surface inside the nozzle (i.e., on the boundary of the domain of influence for the nozzle wall) was found to be  $(P_2 - P_1) / P_1 = .12$ .

The total number of flow field points computed by the MOC was more than 95,000 for each pass. Computer execution time for the case was 3 hours and 38 minutes using a DEC PDP 11/750 VAX computer system.

The ASE engine was also run using the TDE option (no shocks allowed); i.e., the two-dimensional expansion was assumed to be

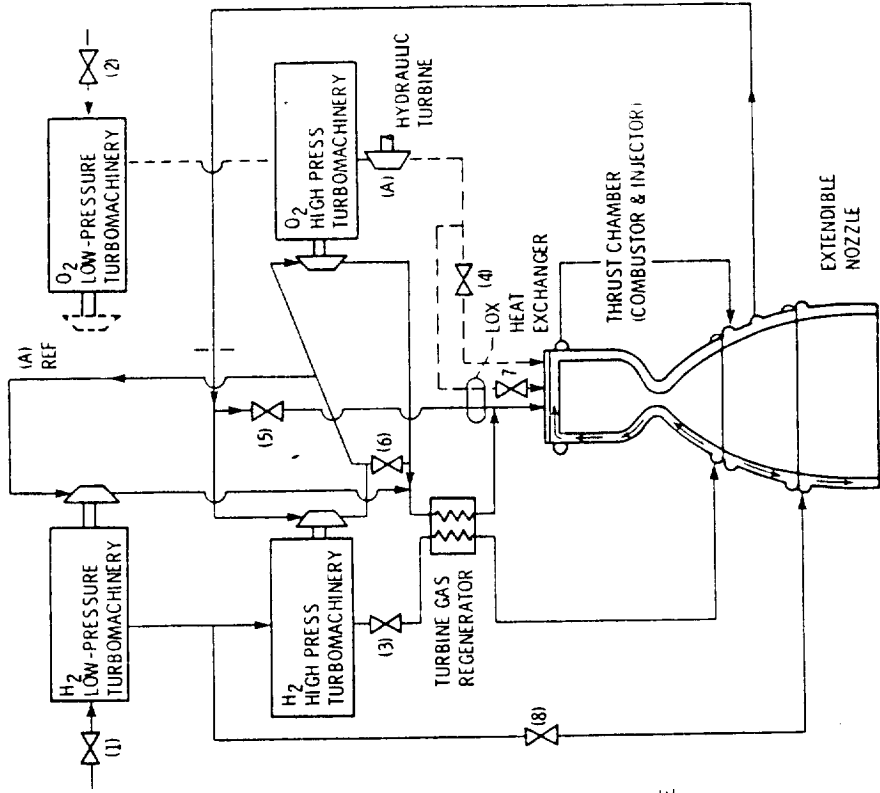
in a state of chemical equilibrium. A complete input data listing for the case is presented in Table 7-6. The boundary layer plots given in Section 6.8.5 were obtained for this case by input of APROF = 400, NPROF = 1, KDTPLT = 1, KMTPLT = 1, and KTWPLT = 1 in \$BLM. The sequence of calculations for TDE is as follows:

- 1) ODE calculation with the system enthalpy set at the propellant tank values, i.e., liquid oxygen and liquid hydrogen at their normal boiling points.
- 2) ODE calculation to generate the TDE gas tables (see Table 7-7 for this output), and the BLM gas tables.
- 3) TDE calculation using the TDE gas tables.
- 4) BLM calculations using the above ODE, TDE results. A new wall geometry is calculated by displacing the wall inwards a distance of  $\delta^*$  normal to the real wall. This new wall defines the boundary of the inviscid core flow. BLM calculated that a total of 10592.2 BTU/sec. were conducted through the nozzle wall. Of this amount a total of 8333.8 BTU/sec. were picked up by the two regen cooling circuits, the remainder being lost from the system. Since the nozzle mass flow was found by TDE to be 47.75 lbm/sec, the propellant enthalpy was increased by 174.5 BTU/lbm.
- 5) ODE calculation with the increased propellant enthalpy. The expansion ratio of the inviscid core flow is automatically placed in the ODE output schedule.
- 6) ODE calculation to generate the TDE gas tables.
- 7) TDE calculation using the above ODE results, including the new wall contour.
- 8) Output summary table, see Table 7-8.

With the TDE option the flow field is constructed using a left running characteristics procedure, and shock waves from the wall are suppressed. Results obtained from the calculations are given in the output summary table, Table 7-8. These results can be compared with those given in Table 7-5 for the same engine but with full kinetics and shock tracing. The difference in predicted specific impulse is

$$I_{sp_{TDE}} - I_{sp_{TRK}} = 475.6 - 474.1 = 1.5 \text{ sec.}$$

Computer execution time for this case was 39 minutes using a DEC PDP 11/750 VAX computer system.



ENGINE CONTROLS

- (1) IFV - INLET FUEL VALVE
- (2) IOV - INLET OXIDIZER VALVE
- (3) MFV - MAIN FUEL VALVE
- (4) MOV - MAIN OXIDIZER VALVE
- (5) TBV - TURBINE BYPASS VALVE
- (6) OTBV - OXIDIZER TURBINE BYPASS VALVE
- (7) GOV - GASEOUS OXIDIZER VALVE
- (8) DFV - DUMP FUEL VALVE
- (A) FULL FLOW HYDRAULIC TURBINE FOR LOW PRESSURE LOX PUMP

Figure 7-2. Flow schematic; Rocketdyne advanced OTV propulsion concept.

Table 7-4. TDK Input for the ASE OTV Test Engine.

```

TITLE 1 ZONE ASE (WITH SHOCK SIMULATION)
DATA
$DATA
OOE=1, OOK=1, NZONES=1, TDK=1, BUM=1, IRPEAT=1, IRSTR=0,
SHOCK = 1,
ECRAT=3.6629,
ASUB=10,5,4,3.6629,3,2,1.5,
NASUB=7,
ASUP = 2,4,6,8,10,15,20,25,30,40,50,75,100,125,150,175,200,
225,250,275,300,325,350,375,400,400.7148,
NASUP=26,
RS1=1.254, RVTU=1, RMTD=.3429, THETA1=17, RI=8.3732,
IWall=4, THE=6.5036, THETA=41,
NUS=14,
RS = 0, 2.1934, 3.3462, 5.0972, 6.7240, 8.4642, 9.7250, 11.0935,
12.5699, 14.1654, 15.8849, 18.6739, 21.6611, 25.1027,
ZS = 0, 1.2654, 2.6315, 4.9818, 7.5269, 10.6702, 13.2392, 16.3252,
20.0311, 24.5243, 30.0103, 40.6593, 55.3049, 79.7103,
RZNORM=1.254,
EPS=400.7248,
IOFF=4,
$END
REACTANTS
H 2.
O 2.
NAMELISTS
$CODE
RKT=.TRUE.
P(1)=2287, PSIA=.TRUE., XP=1.,
OFSKED(1)=6.3780,
$END
REACTIONS
H + H = H2 ,M1, A = 6.4E17, N = 1.0, B = 0.0, (AR) BAULCH 72 (A) 30U
H + OH = H2O ,M2, A = 8.4E21, N = 2.0, B = 0.0, (AR) BAULCH 72 (A) 10U
O + O = O2 ,M3, A = 1.9E13, N = 0.0, B = -1.79, (AR) BAULCH 76 (A) 10U
O + H = OH ,M7, A = 3.62E18, N = 1.0, B = 0.0, (AR) JENSEN 78 (B) 30U
END TBR REAX
O2 + H = O + OH , A = 2.2E14, N = 0.0, B = 16.8, BAULCH 72 (A) 1.5U
H2 + O = H + OH , A = 1.8E10, N = -1., B = 8.9, BAULCH 72 (A) 1.5U
H2 + OH = H2O + H , A = 2.2E13, N = 0.0, B = 5.15, BAULCH 72 (A) 2U
OH + OH = H2O + O , A = 6.3E12, N = 0.0, B = 1.09, BAULCH 72 (A) 3U
LAST REAX
THIRD BODY REAX RATE RATIOS
M1 = 25*H,4*H2,10*H2O,25*O,25*OH,1.5*O2,
M2 = 12.5*H,5*H2,17*H2O,12.5*O,12.5*OH,6*O2,
M3 = 12.5*H,5*H2,5*H2O,12.5*O,12.5*OH,11*O2,
M7 = 12.5*H,5*H2,5*H2O,12.5*O,12.5*OH,5*O2,
LAST CARO
$BOOK
JPRNT =,EP=400.7148,
$END
$TRANS
M=200,
XM(1)=1.,
$END
$SHOC
NC=0,
I$HCK=2,
$END
$BLM
I$PRNT=0,
XINO = -5.778, -5.582, -5.183, -4.749,

```

Table 7-4. (Continued).

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RINO = 4\*1.9138,  
UEO = 309, 533, 689, 856  
PEO = 2282, 2273, 2264, 2251,  
TEO = 6661, 6658, 6655, 6651,  
OFC = 2.2,  
DISTRB=0,  
XCO = -6.7780, 3.1901,  
XCE = 3.1901, 25.9644,  
IHFLAG = 0,  
NTQW = 11,  
XTQW = -6.7780, -5.1834, -1.9936, -.7974, -.4785, -.3987, -.1595,  
2.3928, 3.9872, 25.3589, 25.9968, 63.5649,  
TQW = 910, 1200, 1020, 1210, 1210, 1230, 1210, 430, 1180, 1080,  
818, 657,  
NSEGS=7,  
APROF=2, 10, 50, 100, 200, 300, 390, 400, NPROF=0,  
KDTPLT=0, KMTPLT=0, KTWPLT=0,  
\$END

Table 7-5. TDK Performance Summary: ASE Engine.

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TDK PERFORMANCE SUMMARY : 1 ZONE ASE (WITH SHOCK SIMULATION)  
REAL WALL CONTOUR 1 ZONES WALL TEMP  
INDUCED SHOCK AFTER XA

	FIRST TDK/BLM SOLUTION	SECOND TDK/BLM SOLUTION
CHAMBER PRESS [PSIA]	2287.000	2287.000
CHAMBER TEMP [R]	6556.935	6642.703
MIXTURE RATIO [-]	6.378000	6.378000
EP (NOZZLE) [-]	400.7248	384.4752
H (OXID) [CAL/MOLE]	-3102.000	-3102.000
H (FUEL) [CAL/MOLE]	-2154.000	-2154.000
HCHAM (ODE) [BTU/LB]	-411.5210	-236.9780
DELH (AVERAGE) [BTU/LB]	0.000000E+00	0.000000E+00
DELH1 (AV) [BTU/LB]	0.000000E+00	174.5418
ECRAT [-]	3.662900	3.646226
RSTAR [INCHES]	1.254000	1.256817
RWTD [-]	0.3429000	0.3398899
RWTU [-]	1.000000	0.995171
THE [DEGREES]	6.503600	6.029917
THETA [DEGREES]	41.00000	41.00000
THTAI [DEGREES]	17.00000	17.00000
RI [-]	8.373200	8.373200
NIT [-]	196.0000	196.0000
ISP (ODE) [SECONDS]	485.5364	491.9677
ISP (ODF) [SECONDS]	457.5597	461.1883
ISP (ODK) [SECONDS]	484.1301	490.3438
ISP (TDK) [SECONDS]	481.4474	487.9469
THRUST (TDK) [POUNDS]	22981.83	23173.47
WDOT (TDK) [LB/SEC]	47.73488	47.49179
CSTAR (TDK) [FT/SEC]	7615.182	7688.589
CF (TDK) [-]	2.034106	2.051068
CD [-]	0.9896481	0.9940407
P (AXIS,EXIT) [PSIA]	0.1151442E-01	0.1154842E-01
P (WALL,EXIT) [PSIA]	0.4545023	0.4803083
T (WALL,EXIT) [R]	1690.341	1780.143
V (WALL,EXIT) [FT/SEC]	15046.61	15231.09
MA (WALL,EXIT) [-]	5.594438	5.527072
SHOCK STRENGTH [-]	0.1198294	0.4595399E-02
SHOCK (X/R*) [-]	17.87842	18.09883
SHOCK (R/R*) [-]	4.474361	4.548824
XA (X/R*) [-]	0.2249627	0.2249627
XB (X/R*) [-]	0.000000E+00	0.000000E+00
DFOPT (BLME) [POUNDS]	683.8337	691.0768
DF (BLME) [POUNDS]	650.9324	656.9037
DISP (BLME) [SECONDS]	13.63641	13.83194
THET (EXIT) [FEET]	0.1998608E-01	0.1998608E-01
DELTA (EXIT) [FEET]	0.3850399E-01	0.3850399E-01
DELTA (WALL) [FEET]	175.4796	175.4796
SURF (BLME) [BTU/SEC]	8331.736	8331.736
SURF1 (BLME) [BTU/SEC]	2289.264	2289.264
THRUST (TC) [POUNDS]	22330.90	22516.57
ISP (TC) [SECONDS]	467.8110	474.1150
CF (TC) [-]	1.976493	1.992926



Table 7-6. TDK Input for the ASE OTV Test Engine.

```

TITLE 1 ZONE ASE - TDE OPTION
DATA
$DATA
ODE=1, ODK=0, NZONES=1, TDE=1, BLM=1, IRPEAT=1,
ECRAT=3.6629,
ASUB=10, 5.4, 3.6629, 3, 2, 1.5,
NASUB=7
ASUP = 2, 6, 8, 10, 15, 20, 25, 30, 40, 50, 75, 100, 125, 150, 175, 200,
225, 250, 275, 300, 325, 350, 375, 400, 400.7148,
MASUP=26
RSI=1.254, RWTD=1, RWTD=.3429, THETA=17, RI=8.3732,
IWALL=4, THE=6.5036, THETA=41,
NWS=14,
RS = .0, 2.1934, 3.3462, 5.0972, 6.7240, 8.4642, 9.7250, 11.0935,
12.5699, 14.1654, 15.8849, 18.6739, 21.6611, 25.1027,
ZS = .0, 1.2654, 2.6375, 4.9818, 7.5269, 10.6702, 13.2392, 16.3252,
20.0311, 24.5243, 30.0103, 40.6593, 55.3049, 79.7103,
RZNMORF=1.254,
EPS=400.7248,
IOFF=4,
$END
REACTANTS
H 2.
O 2.
NAMELISTS
$CODE
RKT=.TRUE.
P(1)=2287, PSIA=.TRUE., XP=1.,
OFSKED(1)=6.3780,
$END
$TRANS
MP=200,
I XM(1)=1.,
$END
$SMOC
NC=0,
ISHCK=2,
$END
$BLM
IPRNT=0,
XTMO = -5.778, -5.582, -5.183, -4.749,
RINO = 4*1.9138,
UEO = 309, 533, 689, 856,
PEO = 2282, 2273, 2264, 2251,
TEO = 6661, 6658, 6655, 6651,
OFC = 2, 2,
DISTRB=0,
XCO = -6.7780, 3.1901,
XCE = 3.1901, 25.9644,
IHFLAG = 0,
NTOW = 11,
XTOW = 5.778, 5.1934, 1.9936, -.7974, -.4785, -.3987, -.1595,
2.5229, 3.9872, 25.3589, 25.9968, 63.5649,
TOW = 910, 1200, 1020, 1210, 1210, 1230, 1210, 430, 1180, 1080,
818, 657,
NSEGS=7,
APROF=2, 10, 50, 100, 200, 300, 390, 400, NPROF=0,
KDTPLT=0, KMTPLT=0, KTHPLT=0,
$END

```

Table 7-7. Gas Properties Table Prepared for TDE.

TDE GAS TABLES FOR ZONE 1

I	PRESSURE (PSI)	MOL WT	GAMMA	TEMPERATURE (DEG R)	ENTHALPY (FT2/SEC2)	MACH NO
1	2287.000	14.14817	1.141751	6556.935	-0.1030305E+08	0.0000000E+00
1	1317.704	14.30514	1.141197	6192.129	-0.2259110E+08	1.000000
2	1142.505	14.34392	1.141336	6100.000	-0.2564447E+08	1.127213
3	976.4395	14.38510	1.141634	6000.000	-0.2892166E+08	1.253724
4	833.8527	14.42552	1.142116	5900.000	-0.3216584E+08	1.371666
5	711.2675	14.46485	1.142796	5800.000	-0.3536805E+08	1.482871
6	606.2949	14.50296	1.143696	5700.000	-0.3852501E+08	1.588694
7	516.4310	14.53959	1.144831	5600.000	-0.4163028E+08	1.689988
8	374.2011	14.60774	1.147869	5400.000	-0.4766850E+08	1.881458
9	271.4484	14.66821	1.152025	5200.000	-0.5345665E+08	2.060988
10	197.2862	14.71997	1.157297	5000.000	-0.5897009E+08	2.230871
11	143.8113	14.76264	1.163571	4800.000	-0.6420190E+08	2.393127
12	56.45561	14.84074	1.185546	4200.000	-0.7834301E+08	2.855202
13	21.80071	14.87303	1.205911	3600.000	-0.9075598E+08	3.328062
14	7.756236	14.87359	1.223118	3000.000	-0.1021462E+09	3.868471
15	2.376307	14.87360	1.242535	2400.000	-0.1127972E+09	4.533237
16	0.5785754	14.87360	1.270487	1800.000	-0.1226660E+09	5.420125
17	0.9463301E-01	14.87360	1.305148	1200.000	-0.1316647E+09	6.806742
18	0.5593139E-02	14.87360	1.339089	600.0000	-0.1398936E+09	9.820318
19	0.5423629E-05	14.87360	1.349951	100.0000	-0.1463893E+09	24.55089

Table 7-8. TDK Performance Summary: ASE Engine (TDE).

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TDK PERFORMANCE SUMMARY : 1 ZONE ASE - TDE OPTION  
REAL WALL CONTOUR 1 ZONES WALL TEMP

	FIRST TDK/BLM SOLUTION	SECOND TDK/BLM SOLUTION
CHAMBER PRESS [PSIA]	2287.000	2287.000
CHAMBER TEMP [R]	6556.935	6642.690
MIXTURE RATIO [-]	6.378000	6.378000
EP (NOZZLE) [-]	400.7248	384.2064
H (OXID) [CAL/MOLE]	-3102.000	-3102.000
H (FUEL) [CAL/MOLE]	-2154.000	-2154.000
HCHAM (ODE) [BTU/LB]	-411.5210	-237.0014
DELH (AVERAGE) [BTU/LB]	0.0000000E+00	0.0000000E+00
DELH1 (AV) [BTU/LB]	0.0000000E+00	174.5199
ECRAT [-]	3.662900	3.646455
RSTAR [INCHES]	1.254000	1.256778
RJWD [-]	0.3429000	0.3399320
RWTU [-]	1.000000	0.9955798
THE [DEGREES]	6.503600	5.728948
THETA [DEGREES]	41.00000	41.00000
THETA1 [DEGREES]	17.00000	17.00000
RI [-]	8.373200	8.373200
MIT [-]	192.0000	192.0000
ISP (ODE) [SECONDS]	485.5364	491.9593
ISP (OOF) [SECONDS]	457.5597	461.1822
ISP (OOK) [SECONDS]	0.0000000E+00	0.0000000E+00
ISP (TDE) [SECONDS]	482.9971	489.6729
THRUST (TDE) [POUNDS]	23064.45	23248.76
WDOT (TDE) [LB/SEC]	47.75277	47.47814
CSTAR (TDE) [FT/SEC]	7612.330	7690.318
CF (TDE) [-]	2.041418	2.057731
CD [-]	0.9894340	0.9937611
P (AXIS,EXIT) [PSIA]	0.0000000E+00	0.0000000E+00
P (WALL,EXIT) [PSIA]	0.4573059	0.5004708
T (WALL,EXIT) [R]	1711.442	1820.351
V (WALL,EXIT) [FT/SEC]	15082.84	15258.59
MA (WALL,EXIT) [-]	5.582643	5.488873
SHOCK STRENGTH [-]	0.0000000E+00	0.0000000E+00
SHOCK (X/R*) [-]	0.0000000E+00	0.0000000E+00
SHOCK (R/R*) [-]	0.0000000E+00	0.0000000E+00
XA (X/R*) [-]	0.0000000E+00	0.0000000E+00
XB (X/R*) [-]	0.0000000E+00	0.0000000E+00
DFOPT (BLME) [POUNDS]	681.5857	705.2800
DF (BLME) [POUNDS]	647.8039	668.9509
DISP (BLME) [SECONDS]	13.56579	14.08966
THET (EXIT) [DEG]	0.1994434E-01	0.1994434E-01
ET (EXIT) [FEET]	0.3928238E-01	0.3928238E-01
ET (REGEN) [FEET]	175.4854	175.4854
SODOT (REGEN) [BTU/SEC]	8333.813	8333.813
SODOT (LOSS) [BTU/SEC]	2258.387	2258.387
THRUST (TC) [POUNDS]	22416.64	22579.80
ISP (TC) [SECONDS]	469.4313	475.5832
CF (TC) [-]	1.984082	1.998522

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#### 7.4 DISCUSSION OF SUMMARY OUTPUT

At the end of each computer run, the TDK program prints a table of summary output. Examples of this output are given in Table 7-1, and Tables 7-3, 7-5, and 7-8. As can be seen from Table 7-8, the first item printed is the title

TDK PERFORMANCE SUMMARY: (title)

where the title is taken from the input data last title card (see Table 7-2, first card image).

Next, performance parameters summarizing the results of the calculations are printed in three columns. The left hand column identifies each item to be printed and its units. The first column of results is for the first MOC/BLM solution, and second column of results is for the second MOC/BLM solution.

The items labeled ISP(TDK), THRUST(TDK), WDOT(TDK), CD, CSTAR(TDK), and CF(TDK) are defined as:

<u>Name</u>	<u>Units</u>	<u>Definition</u>
ISP(TDK)	sec	Specific Impulse, $I_{sp,2D}$
THRUST(TDK)	lbf	Thrust, $F_{2D}$
WDOT(TDK)	lbm/sec	Mass Flow, $\dot{m}_{2D}$
CD	-	Flow coefficient, $C_{D,2D}$
CSTAR(TDK)	ft/sec	Characteristic Velocity, $C^*_{2D}$
CF(TDK)	-	Thrust coefficient, $C_{F,2D}$

If a TDF or TDE calculation was made rather than TDK, then these items will be relabeled.

The values given for  $I_{sp,2D}$  and  $\dot{m}_{2D}$  are obtained by evaluating the integrals discussed in the documentation for MOC module subroutine CHAR. The mass flow integral is evaluated across the MOC initial data line. The  $I_{sp}$  integral is evaluated across the initial data line, plus the integral of the axial component of wall pressure from the initial data line to the nozzle end point. The thrust is

$$F_{2D} = I_{sp,2D} \dot{m}_{2D}$$

The nozzle flow coefficient is calculated as

$$C_{D,2D} = \dot{m}_{2D} / \dot{m}_{1D}$$

where

$$\dot{m}_{1D} = \rho_{1D}^* V_{1D}^* A^*$$

is obtained from ODE.  $A^*$  is the geometric throat area.

The characteristic velocity,  $C^*$ , is calculated as

$$C_{2D}^* = I_{sp,2D} g / C_{F,2D}$$

where the thrust coefficient,  $C_F$ , is defined by

$$C_{F,2D} = F_{2D} / P_c A^*$$

Again,  $A^*$ , is the geometric throat area.

The items labeled DISP(BLME), DFOPT(BLME), DF(BLME), ISP(TC), THRUST(TC), and CF(TC) are defined as follows:

<u>Name</u>	<u>Units</u>	<u>Definition</u>
DISP(BLME)	sec	$\Delta I_{sp, BLM}$
DFOPT(BLME)	lbf	$\Delta F_{BLM}$ for $P_e = P_{amb}$
DF(BLME)	lbf	$\Delta F_{BLM}$

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<u>Name</u>	<u>Units</u>	<u>Definition</u>
ISP(TC)	sec	$I_{sp,2D,BLM}$
THRUST(TC)	lbf	$F_{2D,BLM}$
CF(TC)	-	$C_{F,2D,BLM}$

In the above, the thrust loss calculated by the BLM is given by the following relation:

$$\Delta F_{BLM} = 2\pi r_e \cos \alpha_e * \rho_e U_e^2 \theta_{BLM} - 2\pi r_e \cos \alpha_e * (P_e - P_{amb}) \delta_{BLM}^*$$

The additional items, printed are

$$\begin{aligned} \Delta I_{sp,BLM} &= \Delta F_{BLM} / \dot{m}_{2D} \\ I_{sp,2D,BLM} &= (F_{2D} - \Delta F_{BLM}) / \dot{m}_{2D} \\ F_{2D,BLM} &= F_{2D} - \Delta F_{BLM} \\ C_{F,2D,BLM} &= F_{2D,BLM} / P_c A^* \end{aligned}$$

Performance parameters summarizing the results of the second MOC/BLM calculation differ from the first set printed as follows:

- 1) The TDK and ODE results are for the second (inviscid core) run have a modified wall contour, throat area, and expansion ratio. Note that the system enthalpy is different than used in the first run if the BLM wall calculation is not adiabatic.
- 2) The BLM results are re-calculated using edge conditions from the second TDK run. BLM itself is not re-run, and the values of  $\delta^*$  and  $\theta$  are not changed.

The equations used are the same as given above.

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## 8. ERROR DIAGNOSTICS

### 8.1 DISCUSSION OF PROGRAM USAGE

Error diagnostics\* are printed by the program when it has either found an input card error or is unable to continue with its computations because it has obtained an impossible result. The analysis performed by the computer program is limited by the physical assumptions used in its development and by the numerical methods used. Consequently, an understanding of these assumptions and of the numerical methods that have been applied is necessary in order to correctly run cases using the computer program. Although the computer program contains many error diagnostics, it is not possible to diagnose all errors.

Input values given for the sample cases (see Section 7) can be used as a guide in preparing data for similar calculations. Special care must be taken, however, to avoid errors of the type given below:

8.1.1 The computer program will not give valid results if the input kinetic reaction rate parameters are unrealistic. A common mistake is to input an implied third body reaction rate backwards; which gives a very large error. Tables 6-10 and 6-11 can be used as guides in preparing reaction rate data. It should be remembered that the computer program automatically calculates equilibrium constants from the input JANAF thermochemical data.

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\* Error diagnostics can also be given by the computer system subroutines. These vary with the operating system and are not discussed here.

8.1.2 Although the ØDK and TDK calculations allow condensed phases to be present in the flow, no mass transfer between phases is allowed.

8.1.3 A common mistake in using the computer program is to input inlet and throat geometry parameters that are physically impossible when compared with Figure 6-1.

8.1.4 A value  $RWTU > .5$  should be used because of inaccuracies which can occur as a result of the transonic method of solution<sup>9</sup>.

8.1.5 For some chemical systems (e.g., H-F) it is possible that the two-dimensional throat Mach number will be subsonic as a result of the kinetic process. In this case the initial data line can be displaced downstream, increasing the Mach number, by use of the input parameter ALI (see Section 6.6). If ALI is input greater than zero, a symmetric throat is required and it is necessary that RWTU be set to the same value as RWTU.

8.1.6 An important consideration in preparing data for all but ØDE calculations concerns input of the nozzle wall. The derivative of the wall contour has an important effect on the nozzle flow field and it is required that wall derivatives vary slowly with respect to the local characteristic mesh spacing. In this respect the TDK program is no different than any other method of characteristics calculation. Usually the most satisfactory method of specifying a nozzle wall contour is through the use of the spline fit contour option (IWALL=4). Too many points should not be input when using this option since a bad derivative could result. Never place points close together. Although the initial section of the contour is assumed to be a circular arc, a small value of THETA can be used if necessary.

In case of difficulty with the method of characteristics calculations, a useful procedure is to plot the (r,x) coordinates of mesh points in the region of difficulty. A plot of this type will frequently locate the cause of the problem. For this purpose it is necessary to print each calculated mesh point (i.e., N1=1 and N2=1).

## 8.2 LISTING OF ERROR DIAGNOSTICS

Errors printed by the program are listed in Table 8-1 in alphabetical order. The subroutine printing the error message is listed in Table 8-1 in parenthesis at the right of each message. Table 8-2 and the write-up for the subroutine printing the error message should be referred to when the message is encountered.

Suggested corrective action for some of the errors listed in Table 8-1 is given in Table 8-2.

Error diagnostics consist of two types: fatal errors and nonfatal errors. A fatal error will terminate the case being executed and the program will proceed to the next case. The case may not be immediately terminated. For example, in processing input data cards the program will attempt to find as many input card errors as possible before terminating the case. A nonfatal error serves only as a warning and the program will continue the case. If the error diagnostic is of the nonfatal type the symbol (NF) appears in the explanation.

TABLE 8-1: LIST OF ERROR DIAGNOSTICS

ORIGINAL PAGE IS  
OF POOR QUALITY

3 PHASES OF A CONDENSED SPECIES ARE OUT OF ORDER (EQLBRM)  
 35 ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREMENTS FOR THE POINT (EQLBRM)  
 ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .0000005 FOR ALL ASSIGNED CONDITIONS (OUT1)  
 ALL REACTION RATE RATIOS INPUT AS 1.0 (PACK)  
 BLM MODULE COULD NOT FIND DATA FROM ODE MODULE -- WILL ASSUME DATA TO BE READ IN \$BLM (READAT)  
 CALCULATIONS WERE STOPPED BECAUSE NEXT POINT IS MORE THAN 50 DEG BELOW TEMP RANGE OF A CONDENSED SPECIES (ROCKET)  
 CANNOT FIND POINT 4 FOR 2ND RRS CALCULATION (SHCKA)  
 CANNOT FIND POINT 4 FOR LRS CALCULATION (CNTR13)  
 CANNOT FIND POINT 4 FOR RRS CALCULATION (CNTR12)  
 CANNOT FIND POINT 4 FOR RRS CALCULATION (CNTR14)  
 CANNOT FIND POINT 4 FOR RRS CALCULATION (CNTR22)  
 CANNOT FIND POINT 4 FOR RRS CALCULATION (CNTR24)  
 CANNOT FIND POINT 5 FOR 2ND RRS (CNTR22)  
 CANNOT FIND POINT 5 FOR 2ND RRS (SHCKA)  
 CANNOT FIND THETA FOR WALL OPTION 5 - RUN ABORTED IN OOKINP (OOKINP)  
 CANT FIND MATCHING PHASE FOR TMELT= 0.0000000E+00 CURRENT TEMP= 0.0000000E+00 (MAIN1D)  
 COMPUTED HS = 0.000000E+00 AT J = 0 IS OUT OF GIVEN RANGE. (COEF1)  
 CONDENSED REACTANTS NOT PERMITTED IN DETN OR SHOCK PROBLEMS (ODES)  
 CONSERVATION EQNS WERE NOT SATISFIED IN 8 ITERATIONS (DETOM)  
 COULD NOT LOCATE PRES 0.000000E+00 FOR ZONE 0 AND POINT 0 IN OOK GENERATED TRANSONIC TABLES (GETIL)  
 DATA FROM MODULE OUT OF ORDER IN MODULE BLM. CARD 0 HAS SEQ. NO. 0 (READAT)  
 DERIVATIVE MATRIX SINGULAR (EQLBRM)  
 DID NOT CONVERGE FOR AREA RATIO = 0.00000 (ROCKET)  
 DID NOT CONVERGE FOR U1= 0.00 ANSWERS PROBABLY NOT RELIABLE SOLUTION MAY NOT EXIST (SHCK)  
 DID NOT CONVERGE ON ELECTRON BALANCE (EQLBRM)  
 DIMENSIONS IN/SPECIES/TOO SMALL TO CONSIDER (SEARCH)  
 END OF FILE ENCOUNTERED WHILE READING PROFILE PLOT FILE IN BLPLTS - RUN CONTINUES (BLPLTS)  
 END OF LRC CONSTRUCTION FROM CNTR41 (CNTR41)  
 END OF NOZZLE DETECTED (CNTR91)  
 END OF RRC CONSTRUCTION FROM CNTR21 (CNTR31)  
 ENTIRE TRANSONIC TABLE FILE HAS BEEN READ (GETIL)  
 EP NOT REACHED (MAIN1D)  
 ERROR - THE WALL TEMPERATURE/HEAT FLUX TABLE MUST CONTAIN AT LEAST 4 POINTS WHEN CUBIC INTERPOLATION IS USED (INPUTB)  
 ERROR DETECTED DURING INPUT PROCESSING (REAXIN)  
 ERROR DETECTED DURING TRANSONIC CALC (TRAN)  
 ERROR DURING LOW T THERMO EVAL, T= 0.0000000 E+00 (SKPB1)  
 ERROR DURING LOW T THERMO EVAL, T= 0.0000000 E+00 (THERM)  
 ERROR DURING LOW T THERMO EVAL, T= 0.00000000E+00 (CPHS)  
 ERROR FOR SKEWED PARABOLA OPTION - STOP (SKPB1)  
 ERROR FROM BANDI- (BANDI)  
 ERROR IN ABOVE CARD. CONTENTS IGNORED. (ODES)  
 ERROR IN ATSHCK (ATSHCK)  
 ERROR IN BLW WHILE READING LINKAGE DATA (BLTK)  
 ERROR IN BLW WHILE READING LINKAGE DATA (BLW)  
 ERROR IN BLW, NWS EXCEEDS 50 (BLW)  
 ERROR IN CNTR21, CROSSING OF RRC SHOULD HAVE BEEN TERMINATED IN CNTRL1 (CNTR21)  
 ERROR IN CNTR21, CROSSING OF RRC SHOULD HAVE BEEN TERMINATED IN CNTRL1 (CNTR31)  
 ERROR IN CNTR91- END OF RRC AND NO SHOCK OR END OF NOZZLE DETECTED (NTR91)  
 ERROR IN CNTRL1, INSERTION TABLE EXCEEDS MAXIMUM (CNTRL1)  
 ERROR IN CNTRL1, INSERTION TABLE EXCEEDS MAXIMUM (CNTRL2)  
 ERROR IN CNTRL1, IP= 0 EXCEEDS MAXIMUM= 0 (CNTR21)  
 ERROR IN CNTRL1, IP= 0 EXCEEDS MAXIMUM= 0 (CNTR31)  
 ERROR IN CNTRL1, IP= 0 EXCEEDS MAXIMUM= 0 (CNTRL1)  
 ERROR IN CNTRL1, IP= 0 EXCEEDS MAXIMUM= 0 (CNTRL2)  
 ERROR IN FINDT (FINDT)  
 ERROR IN GAUELM. UNABLE TO FIND PIVOT FOR LINE 0 EPSILON=0.00E+00 (GAUELM)  
 ERROR IN GETPT, ID= 0 (GETPT)  
 ERROR IN GETPT- POINT NOT PREVIOUSLY WRITTEN (GETPT)  
 ERROR IN IVPL, NP EXCEEDS NPT (IVPL)  
 ERROR IN ODWALL, IWALL= 0 RUN ABORTED (ODWALL)  
 ERROR IN ORDER OF CARDS FOR (TTAPE)  
 ERROR IN RBL WHILE READING FILE 0 (RBL)  
 ERROR IN REACTANT CARDS (ODES)

ORIGINAL PAGE IS  
OF POOR QUALITY

ERROR IN SAVPT, ID= 0 (SAVPT)  
 ERROR IN SHCKA, ITERATION FOR REFLECTED SHOCK ANGLE FAILED, DLT3A= 0.0000 DLT3B= 0.0000 DEG (SHCKA)  
 ERROR IN SHCKW, ITERATION FOR REFLECTED SHOCK ANGLE FAILED, DLT3A= 0.0000 DLT3B= 0.0000 DEG (SHCKW)  
 ERROR IN THE CALCULATION OF 2ND SHOCK, X3 = 0.00000E+00 X4 = 0.00000E+00 (CNTR16)  
 ERROR MESSAGE FROM BLTABL - THE REQUESTED TABLE SIZE OF 0 EXCEEDED THE INTERNAL DIMENSIONS OF 0 (BLTABL)  
 ERROR OCCURS WHILE POSITIONING BLM TAPE FOR RESTART (READAT)  
 ERROR TYPE= 0 IN CNTR12 (CNTR12)  
 ERROR TYPE= 0 IN CNTR13 (CNTR13)  
 ERROR( ) .... (ERRORZ)  
 ERROR( 2) OR ( 4) THE PROGRAM IS ATTEMPTING TO INSERT AN EXCESSIVE NUMBER OF FLOWFIELD POINTS. (ERRORZ)  
 ERROR( 6) THE LRC INSERTION TABLE HAS OVERFLOWED. (ERRORZ)  
 ERROR( 7) THE MAXIMUM NO. OF POINTS FOR A LRC HAS BEEN EXCEEDED. (ERRORZ)  
 ERROR( 8) THE PROGRAM IS ATTEMPTING TO LOCATE A WALL POINT UPSTREAM  
 OF THE 1ST POINT IN THE WALL TABLE. (ERRORZ)  
 ERROR( 9) OR (10) THE PROGRAM IS UNABLE TO LOCATE POINT 1 IN SUBROUTINE INPT (ERRORZ)  
 ERROR(11) OR (12) THE PROGRAM IS UNABLE TO LOCATE POINT 1 IN SUBROUTINE DSPT (ERRORZ)  
 ERROR(50) AN IMPROPER INITIAL LINE POINT IS SOUGHT. (ERRORZ)  
 ERROR(13) THE CALCULATION FOR THE LAST POINT EXCEEDED MAXIMUM ITERATIONS (ERRORZ)  
 ERROR(14) NO MORE THAN 275 POINTS MAY BE INPUT ON INITIAL LINE (ERRORZ)  
 ERROR(15) SUM OF INPUT SPECIES CONCENTRATIONS FOR ABOVE POINTS NOT ONE. (ERRORZ)  
 ERROR(16) WALL TABLE VIOLATES INSERTION ANGLE CRITERION (ERRORZ)  
 ERROR(17) INCOMPLETE TDK INITIAL LINE HAS BEEN GENERATED (ERRORZ)  
 EXIT PLANE OPTION REQUIRES GREATER WALL EXTENSION (CNTRL)  
 EXIT PLANE OPTION REQUIRES LARGER NCHMXE,NPTMXE (CNTRL)  
 FAILED TO CONVERGE IN IVPL (IVPL)  
 FATAL ERROR ENCOUNTERED DURING REACTION PROCESSING DUE TO ABOVE CARD (REAXIN)  
 FATAL ERROR ENCOUNTERED WHILE PROCESSING THIRD BODY REACTION RATE RATIOS - ERROR ON ABOVE CARD (REAXIN)  
 FIND\* VAR OUTSIDE TABLE (FIND)  
 FROZEN DID NOT CONVERGE IN 8 ITERATIONS (FROZEN)  
 ILL-CONDITIONED MATRIX IN ROUTINE SKPB ERROR = 0.00000E+00 -STOP- (SKPB1)  
 INERT NOT IN MASTER SPECIES TABLE (SEARCH)  
 INERT SPECIES (SEARCH)  
 INERTS FOUND IN TDK PROBLM, INERTS NOT SPECIFIED, CANNOT USE RELATIVE  
 SELECTION CRITERION FOR TDK CASE (SELECT)  
 INFINITELY WEAK SHOCK BT1 M1 M1\*ABS(SIN(BT1))= 0.000000E+00 0.000000E+00 0.000000E+00 (SHOCK)  
 INLET GEOMETRY INCOMPATIBLE WITH INITIAL CONDITIONS (PRES)  
 INTERNAL SEQ NUM (REAXIN)  
 ITERATIONS EXCEEDED ITMAX (BLSEGE)  
 KIN EXPN CODE DIMENSIONED FOR MAX. OF 40 SPECIES, CURRENT CASE USES (SELECT)  
 LOW T THERMO EXTENSION AT T= DEG-K (THERM)  
 LOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE BEEN INCLUDED ON AN INSERT CARD, RESTART (EQLBRM)  
 LRS PT IS OUTSIDE THE NOZZLE (CNTR13)  
 MACH NUMBER CONVERGENCE FAILED, ZONE= 0 CONV CRIT = 0.00E+00 CONV OBTAINED = 0.00E+00 (PRINT)  
 MACH NUMBER CONVERGENCE FAILED, ZONE= 0 CONV CRIT = 0.00E+00 CONV OBTAINED = 0.00E+00 (PRINTS)  
 MASS FRACTION SUM NOT 1. (OUT1)  
 MASS OF MOLE FRACTIONS NOT SPECIFIED MASS FRACTIONS ASSUMED (REAXIN)  
 MAXIMUM ITERATION REACHED- RUN IS TERMINATED (PRINTS)  
 MORE THAN 12 CHARACTERS SPECIFIED FOR AN INERT SPECIES NAME (REAXIN)  
 NE DID NOT CONVERGE (PRES)  
 NO \$ODE VALUE GIVEN FOR OF,ECRAT,FA,OR FPCT (ODES)  
 NO ECRAT SPECIFIED FOR OOK START-RUN ABORTED (ODES)  
 NO LINKAGE DATA FOUND, EXPECT MANUAL INPUT (READAT)  
 NO MATCH FOR SPECIES NAME (REAXIN)  
 NO MATCH FOUND FOR SPECIES NAME (STORNU)  
 NON-NUMERIC ENCOUNTERED IN ECVN WHILE DECODING... (ECVN)  
 NONCONVERGENCE IN ENCALC, T1 T11= 0.0000000E+00 0.0000000E+00 (ENCALC)  
 NONCONVERGENCE IN TSCALC, T P S S0= 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 (TSCALC)  
 NOT ENOUGH POINTS FOR SECOND SPLINE (WALL)  
 NOZZLE PWZS COORDINATES NOT MONOTONIC INCREASING AT PT 0 (PACK)  
 NP EXCEEDED NPT -- PROGRAM TERMINATED (BLMAIN)  
 NUMBER OF SHOCK REFLECTIONS EXCEEDS MAXIMUM= 0 (CNTR91)  
 NUMBER OF SPECIES TOO LARGE FOR TABLES, MUST REDIMENSION (REAXIN)  
 NUMBER OF TEMP VALUES OUTSIDE RANGE (LTCPHS)

## TABLE 8-1: CONTINUED

POOR CONVERGENCE - STOP - (SKPB1)  
 PRESSURE = 0.000000E+00 IS OUT OF RANGE FOR STREAMLINE = 0 (FINDT)  
 PROG NOT DIMENSIONED FOR 0 POINTS AND 0 ZONES (XPIL)  
 PTB(0) = 0.000000E+00, DID NOT CONVERGE (PRES)  
 REACTANT 0 IS NOT IN THERMO DATA (HCALC)  
 REACTANT TEMPERATURE OUT OF RANGE OF THERMO DATA (HCALC)  
 REACTION 0 HAS MASS IMBALANCE OF 0.000000E+00 (PACK)  
 REACTION CARDS (REAXIN)  
 REACTION EXTENDS BEYOND CARD COL 80 (REAXIN)  
 REGULAR REFLECTION IS NOT POSSIBLE (CNTR12)  
 REGULAR REFLECTION IS NOT POSSIBLE (CNTR14)  
 REGULAR REFLECTION IS NOT POSSIBLE (CNTR22)  
 REGULAR REFLECTION IS NOT POSSIBLE (CNTR24)  
 REGULAR REFLECTION NOT POSSIBLE (CNTR12)  
 REGULAR REFLECTION NOT POSSIBLE (CNTR22)  
 REGULAR REFLECTION NOT POSSIBLE (SHCKA)  
 REQ AREA RATIO 0 0.000000E+00 DELETED (OOKINP)  
 RESTART (EQLBRM)  
 RIGHT RUNNING SHOCK DETECTED (CNTR31)  
 RIGHT RUNNING SHOCK DETECTED (CNTR41)  
 RRS PT IS OUTSIDE THE NOZZLE (CNTR12)  
 RRS PT IS OUTSIDE THE NOZZLE (CNTR14)  
 RRS PT IS OUTSIDE THE NOZZLE (CNTR22)  
 RRS PT IS OUTSIDE THE NOZZLE (CNTR24)  
 SHOCK DETECTED ON RRC FROM INITIAL LINE (CNTR11)  
 SHOCK DETECTED ON RRC FROM INITIAL LINE (CNTR21)  
 SHOCK DETECTED ON RRC FROM INITIAL LINE (CNTR31)  
 SHOCK-SHOCK INTERSECTION DETECTED- RUN ABORTED (CNTR22)  
 SHOCK-SHOCK INTERSECTION DETECTED- RUN ABORTED (SHCKA)  
 SHOCKED GAS (2)--INCIDENT--EQUILIBRIUM (SHCK)  
 SHOCKED GAS (2)--INCIDENT--FROZEN (SHCK)  
 SHOCKED GAS (5)--REFLECTED--EQUILIBRIUM (SHCK)  
 SHOCKED GAS (5)--REFLECTED--FROZEN (SHCK)  
 SINGULAR MATRIX (EQLBRM)  
 SINGULARITY, K,A(K,K) 0 0.000000E+00 (LESK)  
 SINGULARITY, N,A(N,N) 0 0.000000E+00 (LESK)  
 SPECIES REQUIRES ELEMENT THIS ELEMENT IS NOT IN ELEMENT TABLE (PACK)  
 SPECIES NO. 0 NOT CONTAINED IN MASTER EQUILIBRIUM SPECIES TABLE (SEARCH)  
 SPECIES NOT ON THERMO TAPE (PACK)  
 SUM OF INPUT MOLE OR MASS FRACTIONS NOT ONE. THE SUM IS = 0.000000E+00 NO. SPECIES = 0 (OOKINP)  
 TEMPERATURE IS OUT OF RANGE OF THE THERMO DATA (SHCK)  
 THE FOLLOWING CARD WAS IGNORED (REAXIN)  
 THE REPEAT OPTION SHOULD NOT BE USED WITH A POTENTIAL WALL (PROBLM)  
 THE SUM OF THE STOICHIOMETRIC COEFFICIENTS FOR THE REACTANTS OR/AND PRODUCTS EXCEEDS 10 (PREAX)  
 THE TEMPERATURE= IS OUT OF RANGE FOR POINT (EQLBRM)  
 THIRD BODY REAX RATE RATIOS ENCOUNTERED BEFORE LAST REAX CARD (REAXIN)  
 TRY REMOVING CONDENSED SPECIES (EQLBRM)  
 UNEXPECTED END DURING INERTS PROCESSING LAST CARD ENCOUNTERED BEFORE END SPECIFICATION (REAXIN)  
 WALL TABLE ERROR ON 2ND SPLINE ... (R,X)= 0.0000E+00 0.0000E+00 (WALL)  
 WALL TABLE ERROR... (R,X)= 0.0000E+00 0.0000E+00 (WALL)  
 WALL TABLE REQUIRES TOO MANY PTS ON 2ND SPLINE (WALL)  
 WALL TABLE REQUIRES TOO MANY PTS. (WALL)  
 WARNING CARD SEQUENCE ERRORS (LTCPHS)  
 WARNING IN INTEXT, Z1 ZEXIT Z2= 0.000000E+00 0.000000E+00 0.000000E+00 (INTEXT)  
 WARNING IN RBL, XFIRST = 0.000000E+00 XI = 0.000000E+00 (RBL)  
 WARNING IN RBL, XLAST = 0.000000E+00 XI = 0.000000E+00 (RBL)  
 WARNING, TBL TABLES EXCEED THEIR DIMENSIONS IN OUT1 (OUT1)  
 WARNING, UNABLE TO POSITION BLM TAPE FOR RESTART (READAT)  
 WEIGHT FLOW DID NOT CONVERGE (CHAR)  
 XTEST=0.000000E+00 ERROR IN TCALC, RUN ABORTED (TCALC)  
 Z OUTSIDE NOZZLE WALL TABLE, Z AND JNOZ ARE 0.000000E+00 0 (FLU)  
 Z OUTSIDE PRESSURE TABLE (FLU)

TABLE 8-2: ERROR MESSAGES, POSSIBLE CORRECTIVE ACTION

DIAGNOSTIC	EXPLANATION OR POSSIBLE CORRECTIVE ACTION	SUBROUTINE
ALL REACTION RATE RATIOS INPUT AS 1.0	(NF) Informative, no action necessary.	PACK
AN IMPROPER INITIAL LINE POINT IS SOUGHT CALCULATIONS WERE STOPPED BECAUSE NEXT POINT IS MORE THAN 50 DEG. BELOW TEMP. RANGE OF A CONDENSED SPECIES	Check input of nozzle throat geometry. (NF)ØDE frozen calculation can not be con- tinued. No action required.	ERRORZ RØCKET
CONDENSED REACTANTS NOT PERMITTED IN DETN OR SHOCK PROBLEMS	Only gaseous reactants are permitted (see Ref. 3 , pg. 70).	ØDES
CONSERVATION EQNS WERE NOT SATISFIED IN 8 ITERATIONS	On detonation option convergence is usually obtained in 3 or 4 iterations (see Ref. 3 , pg 70).	DETNØN
COULD NOT LOCATE PRES _____ FOR ZONE AND POINT _____ IN ØDK GENERATED TRANSONIC TABLES	Check nozzle throat geometry and the initial line flow MACH number.	GETIL
DID NOT CONVERGE FOR AREA RATIO= _____	(NF) The area ratio is probably too close to 1.0 the usual number of iterations is less than 6. Here it exceeded 10. (see Ref. 3 , pg. 71).	RØCKET
DID NOT CONVERGE FOR U1= _____ ANSWERS PROBABLY NOT RELIABLE SOLUTION MAY NOT EXIST	U1 was probably less than the minimum value re- quired for shock to occur (see Ref. 3 , pg. 71).	SHCK
DID NOT CONVERGE ON ELECTRON BALANCE	Check input charge balance.	EQLBRM

TABLE 8-2: CONTINUED

DIAGNOSTIC	EXPLANATION OR POSSIBLE CORRECTIVE ACTION	SUBROUTINE
DIMENSIONS IN/SPECIES/TOO SMALL TO CONSIDER	Too many species are possible for the system being input. Use OMIT cards or recompile program dimensions.	SEARCH
ENTIRE TRANSONIC TABLE FILE HAS BEEN READ	Occurs while constructing initial line for the method of characteristics. Check throat geometry.	GETIL
EP NOT REACHED	Refer to section 6.5.3.1 and discussion of EP	MAIN1D
ERRØR DETECTED DURING INPUT PROCESSING	Check input for bad reaction card.	REAXIN
ERRØR DURING LOW T THERMO EVAL, T=_____	Low temperature out of range. Check LØW T CPHS input if used (see section 6.1.1.1).	THERM
ERRØR IN ABOVE CARD. CONTENTS IGNORED	A card is missing, extraneous, or in error (see Ref. 3, pg. 71).	ØDES
ERRØR IN ORDER OF CARDS FOR _____	THERMØ data cards for this species are out of order (see Ref. 3, pg. 71).	TTAPE
ERRØR IN REACTANT CARDS	Chemical symbol not left-justified, or not included in BLØCK DATA program (see Ref. 3, pg. 71).	ØDES
EXIT PLANE OPTION REQUIRES GREATER WALL EXTENSION	Check nozzle wall input, section 6.3.1.	CNTRL



TABLE 8-2: CONTINUED

DIAGNOSTIC	EXPLANATION OR POSSIBLE CORRECTIVE ACTION	SUBROUTINE
FATAL ERROR ENCOUNTERED WHILE PROCESSING PROBLEM CARD-PROCESSED TO NEXT CASE	Correct bad problem card.	DRIVER
*FIND* VAR OUTSIDE TABLE	Interpolation was requested outside of the range of the input tables. Check input tables for range of independent variable.	FIND
FRØZEN DID NOT CONVERGE IN 8 ITERATIONS	ØDE could not converge in frozen calculations. If desired add more area and/or pressure ratios (see Ref. 3, pg. 71).	FRØZEN
INCOMPLETE TDK INITIAL LINE HAS BEEN GENERATED	Check STRANS input, section 6.6.	ERRØRZ
INERT _____ NOT IN MASTER SPECIES TABLE	Species not in thermo file, check species name and correct.	SELECT
INERTS FOUND IN TDK PROBLEM, INERTS NOT SPECIFIED, CAN NOT USE RELATIVE SELECTION CRITERION FOR TDK CASE	See section 6.5.3.4 for explanation of species selection.	SELECT
INLET GEOMETRY INCOMPATIBLE WITH INITIAL CONDITIONS	$\sqrt{EC} < 1 + (R_u + R_i) (1 - \cos\theta_i)$ see 5.3.25.	PRES
35 ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREMENTS FOR THE POINT _____	Check output for cause of non-convergence. If not obvious, re-run with intermediate output (see Ref. 3, pg. 73).	EQLBRM
KIN EXPN CODE DIMENSIONED FOR MAX. OF 40 SPECIES, CURRENT CASE USES _____	More than 40 species found. Check input	SELECT
LOW T THERMO EXTENSION AT T= _____ DEG-K	(NF) LØW T CPHS input is being used, section 6.1.1.	THERM
LOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE BEEN INCLUDED ON AN INSERT CARD, RESTART	An important condensed species has been omitted causing unrealistically low combustion temperature (see Ref. 3, pg. 72).	EQLBRM
MASS FRACTION SUM NOT 1	$ 1 - \sum c_i  < .01$ the ØDK output subroutine has detected an error in mass conservation.	ØUTPUT

DIAGNOSTIC	EXPLANATION OR POSSIBLE CORRECTIVE ACTION	SUBROUTINE
MASS OR MOLE FRACTIONS NOT SPECIFIED, MASS FRACTIONS ASSUMED	(NF) Informative - mass or mole fractions not specified on species card.	REAXIN
MORE THAN 12 CHARACTERS SPECIFIED FOR AN INERT SPECIES NAME	Check inert species names (see section 6.5.2.2).	REAXIN
NE DID NOT CONVERGE	Unable to find an expansion coefficient, $N_e'$ when PRES generating ØDK pressure table (see section 5.3.2.5)	
NØ ECRAT SPECIFIED FOR ØDK START-RUN ABORTED	Initial contraction ratio must be input (see section 5.3.2.5).	ØDES
NØ MORE THAN 275 POINTS MAY BE INPUT ON INITIAL LINE	Check input initial line and modify for 275 or less points.	ERRØRZ
NØ \$ØDE VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT	Input the desired value as true in \$ØDE.	ØDES
NON-NUMERIC ENCOUNTERED IN ECVN WHILE DECODING. . . _____	Fatal error, correct bad number in data field.	ECNV
NOZZLE PWZS COORDINATES NOT MONOTONIC INCREASING AT PT _____	Check input of nozzle wall and correct error (see section 6.3.3.1).	PACK
NUMBER OF SPECIES TOO LARGE FOR TABLES, MUST REDIMENSION	The ØDK program allows only 40 species per re-action. If possible omit unimportant species. Check input. If program is to be modified to allow more species various arrays must be redimensioned.	REAXIN
NUMBER OF TEMP VALUES OUTSIDE RANGE	Temperature below range specified in LØW T CPHS input, section 6.1.1.	LTCPHS
PRØG NOT DIMENSIONED FOR _____ POINTS AND _____ ZONES	The maximum number of initial line points (275) and/or mixture ratio zones (50) has been exceeded.	XPIL
PTB (____) = _____ DID NOT CONVERGE	Unable to calculate $P/P_e$ vs. area table entry in ØDK. See 5.3.3.5.	PRES

## DIAGNOSTIC

EXPLANATION OR POSSIBLE  
CORRECTIVE ACTION

## SUBROUTINE

REACTANT \_\_\_\_\_ IS NOT IN THERMØDATA

Enthalpy can be computed only for those reactants included as reaction species in thermodynamic data (see Ref. 3, pg. 72). HCALC

REACTANT TEMPERATURE OUT OF RANGE OF THERMØ DATA

Assigned temperature is more than 20% beyond temperature range over which thermodynamic data have been fitted (see Ref. 3, pg. 72). HCALC

REACTION \_\_\_\_\_ HAS MASS IMBALANCE OF \_\_\_\_\_

Fatal error: either stoichiometric coefficients do not match or a reaction or molecular weight input incorrectly in thermo data. PACK

REACTION EXTENDS BEYOND CARD COL. 80

SINGULARITY \_\_\_\_\_

Ending comma left out of a reaction card. REAXIN

SINGULAR MATRIX

(NF) Numerical singularity in matrix solution of  $Ax=b$ . Solution may be in error. LESK, NESK

SPECIES NO. \_\_\_\_\_ NOT CONTAINED IN MASTER EQUILIBRIUM SPECIES TABLE

Assign a slightly modified equivalence ratio or O/F ratio (see Ref. 3 pg. 73). EQLBRM

\_\_\_\_\_ SPECIES NOT ON THERMØ TAPE

Check reaction species names against thermodynamic data species names. SELECT

SPECIES \_\_\_\_\_ REQUIRES ELEMENT

Check reaction species names against thermodynamic data species names. PACK

THIS ELEMENT IS NOT IN ELEMENT TABLE

Check input for misspelled species or element name. PACK

SUM OF INPUT SPECIES CONCENTRATIONS FOR ABOVE POINTS NOT ONE

If INLINF option was input in #TRK, check input data for MAX initial data line points. ERRØRZ

SUM OF MOLE FRACTIONS OF SELECTED SPECIES NOT ONE, THEIR SUM IS= \_\_\_\_\_

See detailed discussion in section 6.5.3.4. SELECT

TEMPERATURE IS OUT OF RANGE OF THE THERMØ DATA

Converged temperature for a shock problem is beyond  $TLØW/1.5 > T > 1.25 * THIGH$ . Results may be inaccurate (see Ref. pg. 73). SHCK

EXPLANATION OR POSSIBLE  
CORRECTIVE ACTION

## DIAGNOSTICS

ERRØRZ

THE CALCULATION FOR THE LAST POINT EX-  
CEEDED MAXIMUM ITERATIONS

Check MOC output to see if run is in error. If no input errors are found and run is to be continued either increase IMAX and/or set IMAXF=0 (see 6.7.1).

REAXIN

THE FOLLOWING CARD WAS IGNORED \_\_\_\_\_

(NF) Check this card for error.

ERRØRZ

THE LRC INSERTION TABLE HAS OVERFLOWED

The calculation has inserted more than 20 left running characteristics. Try more points on the initial line (see section 6.6).

ERRØRZ

THE MAXIMUM NO. OF POINTS FOR A LRC HAS  
BEEN EXCEEDED

More than 275 points are on the initial data line. Reduce by modifying \$TRANS input (see section 6.6).

ERRØRZ

THE PROGRAM IS ATTEMPTING TO INSERT AN  
EXCESSIVE NUMBER OF FLOWFIELD POINTS

Probable cause is too few points on the initial line upstream of the region being computed. Try more points or a redistribution of points on the initial line (see section 6.6).

ERRØRZ

THE PROGRAM IS ATTEMPTING TO LOCATE A  
WALL POINT UPSTREAM OF THE 1ST POINT IN  
THE WALL TABLE

Check input of initial line (see section 6.6) and nozzle wall (see section 6.3.3.1).

ERRØRZ

THE PROGRAM IS UNABLE TO LOCATE POINT 1  
IN SUBROUTINE DSPT

Check input to be sure a value given in XM is not too small. If XM value is  $< .05$ , eliminate this zone and adjust mixture ratios.

ERRØRZ

THE PROGRAM IS UNABLE TO LOCATE POINT 1  
IN SUBROUTINE INPT

Error in MOC. All \$TRANS and \$MOC input should be checked.

EQLBRM

THE TEMPERATURE=\_\_\_\_\_ IS OUT OF RANGE FOR  
POINT\_\_\_\_\_

Converged temperature input on card following THERMØ card is beyond the allowed range:  $TLØW/1.5 > T > 1.25 * THIGH$  (see Ref. 3, pg. 73).

REAXIN

THIRD BODY REAX RATE RATIOS BEFORE END OF  
REAX

LAST REAX card was left out. Check for a mistake in reaction order.

EQLBRM

THREE PHASES OF A CONDENSED SPECIES ARE  
OUT OF ORDER

THERMØ data for condensed species must be in either increasing or decreasing order depending on their temperature intervals (see Table 6-2).

EQLBRM

TRY REMOVING CONDENSED SPECIES

Use ØN.IT cards on trace condensed species.

TABLE 8-2: CONTINUED

DIAGNOSTIC	EXPLANATION OR POSSIBLE OR CORRECTIVE	SUBROUTINE
UNEXPECTED END DURING INERTS PROCESSING LAST CARD ENCOUNTERED BEFORE END SPECIFICATION	Self explanatory, check reaction input.	REAXIN
WALL TABLE VIOLATES INSERTION ANGLE CRITERION	The program calculates wall angles from point to point and prints them and the wall table points. (e.g. see pg 7-29). If the difference of any adjacent slopes exceed DWWI this error is printed. Modify the wall input .	ERRØRZ
WARNING CARD SEQUENCE ERRORS	(NF) Check input LØW T CPHS cards for proper order (see section 6.1.1).	LTCPHS
WEIGHT FLOW DID NOT CONVERGE	Specified weight flow option. Input value estimated by the program for chamber pressure, PEST, into P(1) of \$ØDE and rerun (unless run is obviously in error).	CHAR
XMØØT= _____ PEST= _____ WFLØW= _____ ERRØR OF _____ PERCENT		

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## REFERENCES

ORIGINAL PAGE 13  
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APPENDIX A

REACTION RATE DATA

NOVEMBER 1984

PREPARED BY:

GARY R. NICKERSON  
THUAN K. NGUYEN

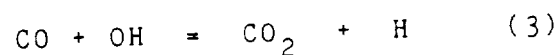
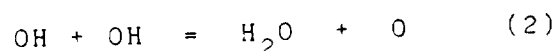
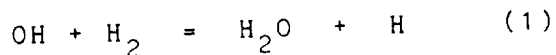
## REACTION RATE DATA

Reactions and reaction rates for determining loss in performance due to chemical kinetics are presented in Reference 1, which is CPIA 246, the JANNAF Rocket Engine Performance and Evaluation Manual (see Section 6.2, titled Reaction Rate Data.) The reactions and reaction rates presented in CPI 246 were revised by Kushida in Reference 2 in 1976. Until the present time, no further revisions have been made.

A literature review through June 1984 has now been carried out by SEA, Inc. The review includes the systems discussed by Kushida, i.e. those containing the elements CHNO and FHN. The result of this study shows almost no change in the CHNO system and minor changes in the FHN system. A revised uncertainty factor, U, is given for each rate coefficient such that  $k \times U$  and  $k/U$  provide probable approximate upper and lower bounds respectively to  $k$  for temperatures within the range 250 to 3000 °K.

Tables 1 and 2 give reactions and rates for the CHNO system, and correspond to Tables I and II of Reference 2 except that the species  $\text{HO}_2$  and  $\text{N}_2\text{O}$  have been deleted. These species are not considered important for engine performance prediction. Although there are no changes in the rate data, new information regarding some of the reactions have been obtained that suggest a change in the form of the rate expression.

For certain reactions involving the OH radical, in particular the reactions,



The rate data do not conform to an Arrhenius plot<sup>3</sup>. For reaction (3), the experimental results are now numerous and precise enough to confirm the deviation from the Arrhenius form at low and high temperature. The form that fits the data adequately over the temperature range 250-2500 °K is,

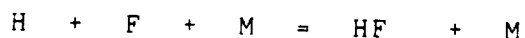
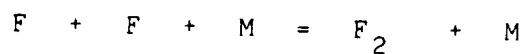
$$\log_{10} k = 10.83 + 3.94 \times 10^{-4} T.$$

The present form of the rate data,  
 $k = 1.5 \times 10^7 T^{1.3} \exp(765./RT).$

is in close agreement with the above expression up to 2000 °k. In addition, it is necessary for use in the existing computer programs.

Tables 3 and 4 give reactions and rates for the FHN system, and correspond to Tables III and IV of Reference 2.

For the two reactions,



the rate coefficient expressions are completely different than those listed in Table III of Reference 2. These new expressions give a much higher rate at low temperature, but about the same value in the high temperature range.

As in Reference 2, the tables given here define the rates in the form accepted by the TDK computer program, i.e., the constants A, N, and B are given for the expression

$$k = AT^{-N} e^{-(1000B/RT)}; \text{in units of cc, } ^\circ\text{K, mole, sec.}$$

The reference for each reaction is listed in the tables, e.g. BAULCH 72 is Reference 7. The uncertainty estimate is also given; e.g. 30 U is an uncertainty factor of 30.

TABLE 1. Reaction Rate Data for the CHON System:

For Chemical Reactions between species, CO, CO<sub>2</sub>, H, H<sub>2</sub>, H<sub>2</sub>O, N, NO, N<sub>2</sub>, O, OH, and O<sub>2</sub> in initial equilibrium expanding through an adiabatic nozzle.

$$k = A T^{-N} \exp(-1000B/RT); \text{in units of cc, } ^\circ\text{K, mole, sec.}$$

REACTIONS

H + H = H <sub>2</sub>	, A = 6.4E17, N = 1.0, B = 0.0	, M = AR, BAULCH 72 (A) 30U
H + OH = H <sub>2</sub> O	, A = 8.4E21, N = 2.0, B = 0.0	, M = AR, BAULCH 72 (A) 10U
O + O = O <sub>2</sub>	, A = 1.9E13, N = 0.0, B = -1.79	, M = AR, BAULCH 76 (A) 10U
N + O = NO	, A = 6.4E16, N = 0.5, B = 0.0	, M = N2, BAULCH 73 (C) 10U
N + N = N <sub>2</sub>	, A = 3.0E14, N = 0.0, B = -0.99	, M = N2, BAULCH 73 (C) 10U
CO + O = CO <sub>2</sub>	, A = 1.0E14, N = 0.0, B = 0.0	, M = AR, BAULCH 76 (B) 30U
O + H = OH	, A = 3.62E18, N = 1.0, B = 0.0	, M = AR, JENSEN 78 (B) 30U

END TBR REAX

O <sub>2</sub> + H = O + OH	, A = 2.2E14, N = 0.0, B = 16.8	, BAULCH 72 (A) 1.5U
H <sub>2</sub> + O = H + OH	, A = 1.8E10, N = -1.0, B = 8.9	, BAULCH 72 (A) 1.5U
H <sub>2</sub> + OH = H <sub>2</sub> O + H	, A = 2.2E13, N = 0.0, B = 5.15	, BAULCH 72 (A) 2 U
OH + OH = H <sub>2</sub> O + O	, A = 6.3E12, N = 0.0, B = 1.0	, BAULCH 72 (A) 3 U
CO + OH = CO <sub>2</sub> + H	, A = 1.5E7, N = -1.3, B = -0.765	, BAULCH 74 (A) 3 U
N <sub>2</sub> + O = NO + N	, A = 7.6E13, N = 0.0, B = 75.5	, BAULCH 73 (C) 3 U
O <sub>2</sub> + N = NO + O	, A = 6.4E9, N = -1.0, B = 6.25	, BAULCH 73 (C) 2 U
CO + O = CO <sub>2</sub>	, A = 2.5E6, N = 0.0, B = 3.18	, BAULCH 76 (B) 2 U
CO <sub>2</sub> + O = CO + O <sub>2</sub>	, A = 1.7E13, N = 0.0, B = 52.7	, BAULCH 76 (B) 3 U

LAST REAX

TABLE 2. Third Body Recombination Efficiency Ratio for CHON System:  
 (as recommended by Kushida, Reference 2)

Species	H + H	H + OH	O + O	N + O	N + N	CO + O	O + H
AR	1.	1.	1.	.8	1.	1.	1.
CO	1.5	3.	4.	1.	1.	1.	4.
CO <sub>2</sub>	6.4	4.	8.	3.	2.	5.	5.
H	25.	12.5	12.5	10.	10.	1.	12.5
H <sub>2</sub>	4.	5.	5.	2.	2.	1.	5.
H <sub>2</sub> O	10.	17.	5.	7.	3.	1.	5.
N	1.	1.	10.	10.	10.	1.	1.
NO	1.5	3.	4.	1.	1.	1.	4.
N <sub>2</sub>	1.5	3.	4.	1.	1.	2.	4.
O	25.	12.5	12.5	10.	10.	1.	12.5
OH	25.	12.5	12.5	10.	10.	1.	12.5
O <sub>2</sub>	1.5	6.	11.	1.	1.	25.	5.

TABLE 3. Recommended Reaction Data (HFN System): For chemical reactions between species F, F<sub>2</sub>, H, HF, H<sub>2</sub>, N, and N<sub>2</sub> in initial equilibrium expand through an adiabatic nozzle.

$$k = AT^{-N} e^{(-1000B/RT)}; \text{ in units of cc, } ^\circ\text{K, mole, sec.}$$

REACTIONS:

H + H = H<sub>2</sub> , A = 6.4E17, N = 1.0, B = 0. , BAULCH 72, M = AR (A) 30 U

F + F = F<sub>2</sub> , A = 3.25E8, N = -1.0, B = -6.38, BAULCH 81, M = AR (A) 10 U

H + F = HF , A = 7.5E12, N = 0.0, B = -35.13, BAULCH 81, M = AR (A) 30 U

N + N = N<sub>2</sub> , A = 3.0E14, N = 0.0, B = -0.99, BAULCH 73, M = N<sub>2</sub> (A) 10 U

END TBR REAX

F + H<sub>2</sub> = HF + H , A = 9.2E13, N = 0.0 B = 1.08, FOON 75 , (A) 30 U

H + F<sub>2</sub> = HF + F , A = 8.8E13, N = 0.0, B = 2.40, BAULCH 81, (A) 10 U

LAST REAX

TABLE 4. Third Body Reaction Rate Ratios (H F N System)  
(as recommended by Kushida, Reference 2)

REACTION		H + H	F + F	H + F	N + N
SPECIES	H <sub>2</sub> ,	4.	1.	8.	2.
SPECIES	F <sub>2</sub> ,	1.	2.4	1.	1.
SPECIES	HF,	2.	1.	2.	1.
SPECIES	N <sub>2</sub> ,	1.5	1.	2.8	1.
SPECIES	N ,	1.	1.	1.	10.
SPECIES	F ,	4.	2.4	4.	1.
SPECIES	H ,	25.	1.	20.	10.

## Other Elemental Systems

Consideration was given to expanding the reaction set of Reference 2 to other elemental systems. Tables 5 and 6 have been prepared to indicate liquid propellant rocket engine systems of possible interest. This approach leads to 11 combinations of the elements C, Cl, F, H, N, and O, which are listed alphabetically in Table 6. Sets 3, 4, 7, 8, 10, and 11 are covered by the reactions presented in Tables 1 through 4. There is presently a lack of interest in the oxidizer/fuel combinations that require sets 1, 2, 5, 6, and 9. However, screening studies, such as References 4, 5, and 6, have indicated the species and reactions that control these systems. The additional species required are: Cl, Cl<sub>2</sub>, ClF, HCl. The additional reactions required are presented in Table 7.

Many of the rates given in Table 7 are estimates rather than measured values. The reaction set given in Table 7 must be considered preliminary.

The reaction numbers used in Reference 1 are indicated in Table 7. For example, the first three reactions in Table 7 are the reactions numbered 13, 12, and 11 in Reference 1.

Good measured data are now available for the Cl + Cl recombination reaction. The reaction rate for the reaction H + Cl + M = HCl + M is obtained from the data for the reverse reaction and the equilibrium constant. The third body efficiencies for the reactions listed in Table 7 are given in Table 8. For the reaction Cl + Cl + M = Cl<sub>2</sub> + M with M = Cl<sub>2</sub> an efficiency ratio of about 5 is reported from 4 sets of experiments. A value of unity is used for the other third body efficiencies because of a lack of data.

Measured data was found for reactions 29 and 31 of Reference 1. Reaction 30 of Reference 1, i.e.

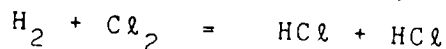


Table 5. Oxidizers and Fuels for Liquid Rocket Propellants  
Containing Elements C, Cl, F, H, N, O

Oxidizers Containing Elements Cl, F, H, N, O Formula, Name	Fuels Containing Elements C, H, N Formula, Name
<p><math>\text{ClF}_3</math> , Chlorine Trifluoride</p> <p><math>\text{ClO}_3\text{F}</math> , Perchloryl Flouride</p> <p><math>\text{F}_2</math> , Flourine</p> <p><math>\text{HNO}_3</math> , Nitric Acid</p> <p><math>\text{N}_2\text{O}_4</math> , Nitrogen Tetroxide</p> <p><math>\text{O}_2</math> , Oxygen</p> <p><math>\text{OF}_2</math> , Oxygen Difluoride</p>	<p><math>\text{CH}_4</math> , Methane</p> <p><math>\text{C}_2\text{H}_2</math> , Acetylene</p> <p><math>\text{C}_2\text{H}_4</math> , Ethylene</p> <p><math>\text{C}_2\text{H}_6</math> , Ethane</p> <p><math>\text{C}_3\text{H}_8</math> , Propane</p> <p><math>\text{C}_7\text{H}_{16}</math> , Heptane</p> <p><math>(\text{CH}_2)_n</math> , RP-1 or JP-4</p> <p><math>\text{CH}_6\text{N}_2</math> , Monomethyl - Hydrazine</p> <p><math>\text{C}_2\text{H}_8\text{N}_2</math> , Unsymmetrical Dimethyl - Hydrazine (UDMH)</p> <p><math>\text{H}_2</math> , Hydrogen</p> <p><math>\text{NH}_3</math> , Ammonia</p> <p><math>\text{N}_2\text{H}_4</math> , Hydrazine</p>



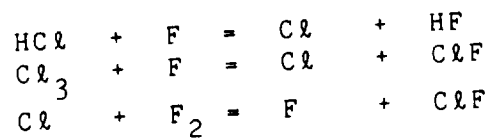
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Table 6. Elemental Compositions for Oxidizer/Fuel Combinations used in Liquid Rocket Engines

Elemental Composition	Example Propellants
1. C, F, H, N	$F_2/CH_4N_2$ , $F_2/C_2H_8N_2$
2. C, F, H, N, O	$OF_2/N_2H_4-C_2H_8N_2$
3. C, H, O	$O_2/RP-1$ , $O_2/CH_4$ , $O_2/C_3H_8$
4. C, H, N, O	$N_2O_4/CH_6N_2$ , $N_2O_4/C_2H_8N_2$
5. Cl, F, H, N	$ClF_3/N_2H_4$
6. Cl, F, H, N, O	$ClO_3F/N_2H_4$
7. F, H	$F_2/H_2$
8. F, H, N	$F_2/N_2H_4$
9. F, H, N, O	$OF_2/N_2H_4$
10. H, N, O	$N_2O_4/N_2H_4$
11. H, O	$O_2/H_2$

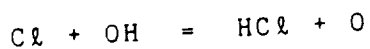
was deleted as unimportant. Reactions 11, 32, 33, 34, 35, 36, 37, 38, 39, 40, 52, and 53 with their estimated rates, were taken from Reference 1.

There are some scattered data reported for the reactions 32, 33, and 34, i.e.



These data are within a factor of 10 of the estimated values. No other data was found for these reactions.

Two reactions were added to the system that did not appear in Reference 1, but are believed to be important (for example see References 4, 5, and 6). Measured data is available for these reactions, which are:



and

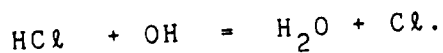
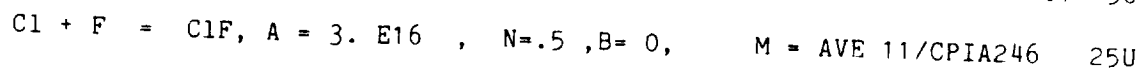
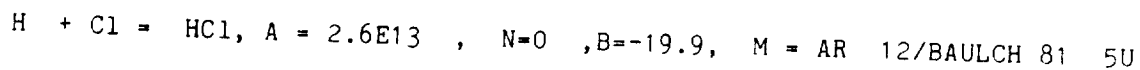
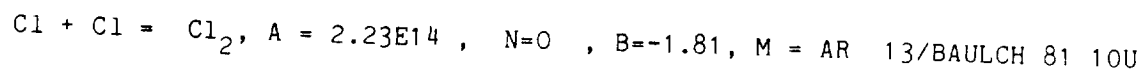


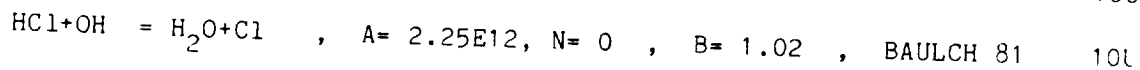
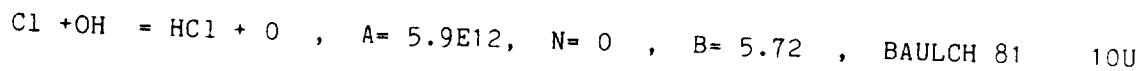
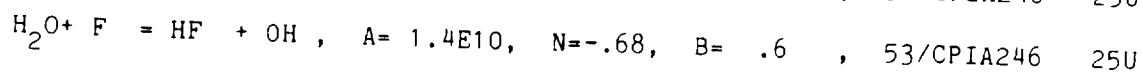
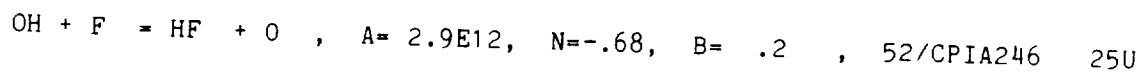
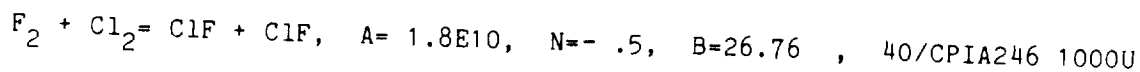
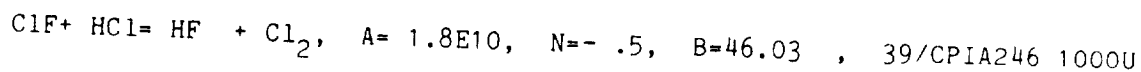
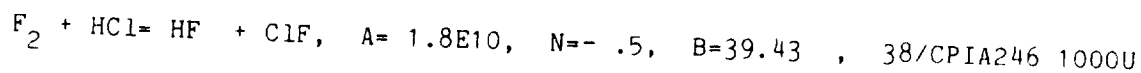
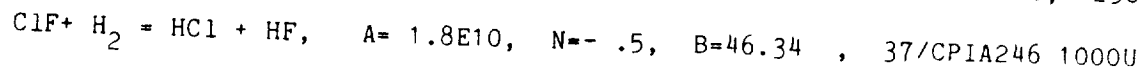
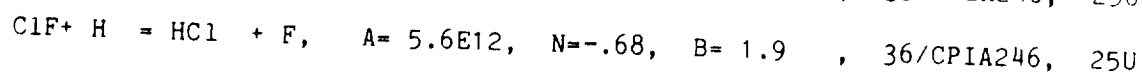
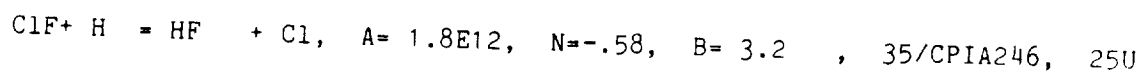
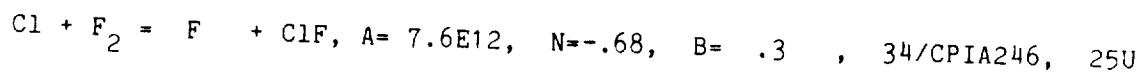
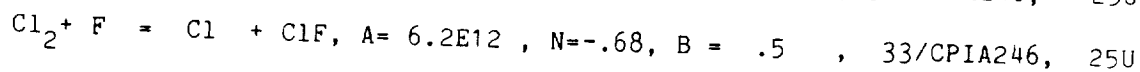
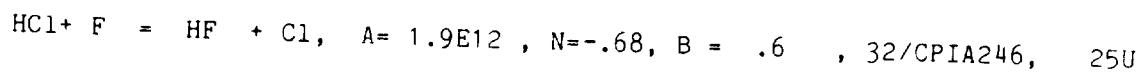
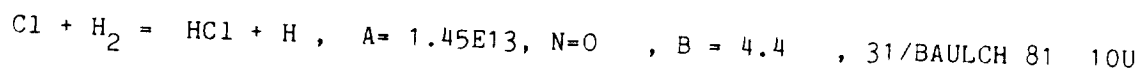
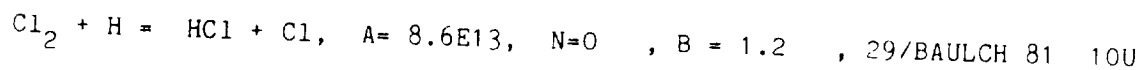
TABLE 7. Additional Chemical Reactions of Importance in C, Cl, F, H, N, O Systems

$$k = AT^{-N}e^{(-1000B/RT)}; \text{ in units of cc, }^\circ\text{K, mole, sec.}$$

REACTIONS



END TBR REAX



LAST REAX

TABLE 8. Third Body Reaction Rate Ratio

REACTION		H + Cl	Cl + Cl
SPECIES Ar		1	1
SPECIES HCl		1	1
SPECIES Cl <sub>2</sub>		1	5
SPECIES Cl		1	1

APPENDIX A -- REFERENCES

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- Ref.12. Foon, R., Kaufman, M., "Kinetics of Gaseous Fluorine Reactions," Prog. in Reaction Kinetics 8:2, 81-160, (1975).

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