SN-55

# FINAL REPORT

# A SHOCK WAVE CAPABILITY

# FOR THE IMPROVED

# TWO-DIMENSIONAL KINETICS (TDK)

# Computer Program

Contract Number NAS8-34974

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Prepared For

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## FORWARD

This report describes work performed by Software and Engineering Associates, Inc. (SEA) under NASA contract NAS8-34974 "A Shock Wave Capability for the Improved Two-Dimensional Kinetics (TDK) Computer Program". The TDK computer program is a primary tool in applying the JANNAF liquid rocket engine performance prediction procedures. The purpose of this contract has been to improve the TDK computer program so that it can be applied to rocket engine designs of advanced type. In particular, future orbit transfer vehicles (OTV) will require rocket engines that operate at high expansion ratio, i.e. in excess of 200:1. Because only a limited length is available in the space shuttle bay, it is possible that OTV nozzles will be designed with both relatively short length and high expansion ratio. In this case, a shock wave may be present in the flow. An objective of the present study has been to modify the TDK computer program to include the simulation of shock waves in the supersonic nozzle flow field. The shocks induced by the wall contour can produce strong perturbations of the flow, affecting downstream conditions which need to be considered for thrust chamber performance calculations. Project manager for this project has been Mr. Gary R. Nickerson. Dr. Lanh Dang has performed the computer programming and has provided engineering support. The project was very much aided by the helpful support of the contract monitor, Mr. Klaus W. Gross, and by Mr. A. Kresbach.

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## ABBREVIATIONS

| | |
|---|---|
| BLM | Boundary Layer Module, computer program |
| JANNAF | Joint Army-Navy-NASA-Air Force |
| MØC | Method of Characteristics, module of TDK |
| ØDE | One-Dimensional Equilibrium, module of TDK |
| ODK | One-Dimensional Kinetics, module of TDK |
| OTV | Orbit Transfer Vehicle(s) |
| PSS | Performance Standardizatin Subcommittee of JANNAF |
| SEA | Software and Engineering Associates, Inc. |
| TDE | Two-Dimensional Equilibrium, module of TDK |
| TDK | Two-Dimensional Kinetics, JANNAF computer program |

## 1. INTRODUCTION

The Two-Dimensional Kinetics (TDK)[1] computer program is a primary tool in applying the JANNAF liquid rocket thrust chamber performance prediction methodology.[2] 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 OTV design, has required an extension of the analytical methods used by the TDK computer program. The primary objective of the study reported here has been to equip the TDK computer program with the capability of simulating a shock wave induced by curvature of the nozzle wall contour. This capability includes the effects of chemical reaction kinetics. For example when Hydrogen and Oxygen are used as propellants, the dissociation of water behind an oblique shock front is simulated.

In order to accomodate variation in mixture ratio from streamline to streamline within the flow, it has been necessary to revise the transonic analysis method used by TDK. No attempt has been made to treat mixture ratio variation along streamline, i.e. mass addition or diffusion effects. No attempt has been

Ref. 1. Nickerson, G. R., Coats, D. E., and Bartz, J. L. "The Two-Dimensional Kinetic (TDK) Reference Computer Program," Engineering and Programming Manual, Ultrasytems, Inc., December 1973, prepared for Contract No. NAS9-12652, NASA JSC.

Ref. 2. "JANNAF Rocket Engine Performance Prediction and Calculation Manual", CPIA 246, April 1975.

made to treat the interaction of shockwaves with slip discontinuities. Instead, the approach has been to allow a continuous variation in mixture ratio to be specified transverse to the flow, and to trace by construction methods the shock path and flow interaction.

The work carried out in the study is summarized below:

a) In the TDK program, the existing slip line method has been converted to a streamline method to avoid unrealistic shock interaction with the slip line. Each streamline is assigned a specific mixture ratio. Completely coupled two-dimensional flow with finite rate chemical kinetics is computed.

b) The existing TDK transonic model[1] has been modified to analyze flow with variable mixture ratio.

c) The method of characteristic (MOC) concept has been modified to utilize the varying properties of the streamlines.

d) Various techniques for constructing the supersonic flow field with the MOC concept have been investigated, and several shock construction methods have been examined. The most efficient ones were selected for incorporation into the TDK program.

e) A set of supersonic flow control subroutines were written to construct the supersonic flow field with shock waves included.

f) The TDK program with shocks was checked out 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.

g) The TDK program, coupled with a boundary layer module, was adjusted such that the effect of a shock wave undergoing regular reflection at the nozzle wall was accounted for.

h) Techniques were introduced for reducing computer time.

## 2. METHOD OF APPROACH

The TDK computer program described in Reference 1 is the JANNAF approved computer program used for the purpose of calculating two-dimensional rocket nozzle flows. The program is highly accurate and contains many useful features. However, no provisions have been made for including the effects on nozzle performance caused by the occurrance of strong shock waves. Previously, it had been assumed that a nozzle wall which induces a strong shock in the flow should be considered a poor design and, thus, not a design of interest. More recently, nozzles containing shock waves have become important. There are several reasons for this. The foremost reason is that the engines required for Orbit Transfer Vehicle (OTV) propulsion feature unusually high expansion ratios ($A/A^* > 200$). In an effort to shorten the length of these nozzles, designs are being proposed that induce shocks in the flow. If the shock strength is everywhere small, then the flow streamlines remains isentropic and the TDK program will accurately compute the nozzle performance. The basic reason for this is that the shock strength, $\beta$, defined as:

$$\beta \equiv (P_2 - P_1)/P_1$$

effects a change in entropy in accordance with the following well-known expression:

$$\Delta S/R = \frac{\gamma + 1}{12\,\gamma^2}\,\beta^3 + \text{higher order terms.}$$

Thus, weak shocks are essentially isentropic.

According to Hoffman (Reference 3, Volume II, page 140), the method used by TDK will yield "reasonable" results even for relatively strong shocks, i.e. shocks such that $\beta < 4$.

Ref.3 Zucrow, M.J., and Hoffman, J.D., Gas Dynamics, Volume I and II, John Wiley & Sons, Inc., New York, 1976.

Nevertheless, since OTV Mission requirements are highly sensitive to the engines delivered specific impulse, it is crucial that TDK be able to accurately compute the effects of shock waves on performance. Nozzle shock waves are inherently two-dimensional in their character; so that it is necessary that a two-dimensional analysis be used to compute their effects. Since TDK is the approved JANNAF program for calculating the effects of two-dimensional phenomenon on nozzle performance (see Reference 4), it is appropriate that it be extended to include shock waves. The method of approach used for achieving this objective is presented below.

It is required that TDK be able to accurately assess the effects on performance of shock waves that are induced by a nozzle wall. This accuracy requirement was an overriding consideration when selecting the approach to be used. Thus, the numerical solution selected is based on the Method of Characteristics (MOC), since it represents the most accurate method available. Shock tracing (as opposed to shock capturing) was also selected for reasons of accuracy.

Although accurate, the MOC with shock tracing is not suitable for flows that feature many shocks, since the logic to treat the reflection, intersection, and coalescence of many shocks is intractable. It was assumed, however, that only a few strong shocks are present, and that these originate from the wall. Multiple regular reflections from the flow axis and the nozzle wall (see Figure 1a) were treated. Mach reflections from the flow axis or the nozzle wall (see Figure 1b) were not treated. It was assumed that Mach shocks, which include a

Ref.4 "JANNAF" Rocket Engine Performance Prediction and Evaluation Manual," CPIA Publication 246, April, 197 .

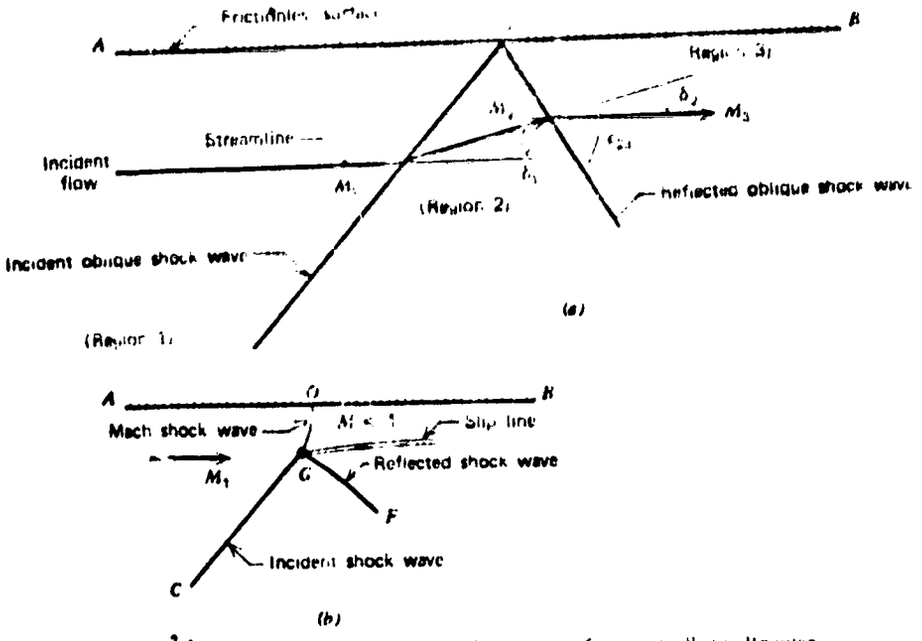



Figure 1: Reflection of an oblique shock wave from a wall. (a) Regular reflection (b) Mach reflection

region of subsonic flow, will not effect nozzle performance. That is, if a Mach shock occurs, it is assumed that its' domain of dependance does not include the nozzle wall.

In the present study, it is also assumed that a shock originates by the coelescence of Right Running Characteristics (RRCs) due to flow angle gradient change, or turning, at the nozzle wall. The case where the shock starts attached to the wall, due to an abrupt discontinuity in wall slope, is not treated at this time. Only the more difficult induced shock case is treated.

Since the shock wave is very thin, it is assumed that the chemical composition across the shock will be frozen. On the downstream side of the shock, the reacting flow will relax towards a new equilibrium state at increased pressure. If the flow is near equilibrium, this process can occur extremely fast, causing numerical difficulties that can be severe. This problem has been solved by utilizing a fully implicit numerical integration method.

The version of TDK that is described in Reference 5 was taken as the starting point for the present program. All of the capabilities described in Reference 5 have been included in the newer program.

Ref.5 Nickerson, G.R. and Dang, L.D., "Improved Two-Dimensional Kinetics (TDK) Computer Program", SEA Inc., Final Report, SN58, NAS8-35406, October 1983.

## 3. TECHNICAL DISCUSSION

The technical effort is discussed under the four topics given below:

Transonic Model with Mixture Ratio Variation,
Selections of Shock Methods,
Shock Construction Methods, and
Techniques for Reducing Computer Time

### 3.1 Transonic Model with Mixture Ratio Variation

The transonic model used by TDK is described in References 1 and 6. It is a first-order perturbation analysis that is based on the method of Sauer[7]. The method 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 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 sing 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 ) as a function of pressure. These tables span the nozzle throat region. An average expansion coefficient is computed using these tables as

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

---


Ref.6 Nickerson, G. R., "Striated Flow in a Converging-Diverging Nozzle", Dynamic Science Report CS-2/71-1, prepared for NASA JSC, February 1971.

Ref.7 Sauer, R. "General Characteristics of the Flow Through Nozzles at Near Critical Speeds", NACA Tech. Note No. 1147 (1947).

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

$$\Upsilon_n = (\bar{\Upsilon}_n + \bar{\Upsilon}_{n-1})/2 \qquad n = 1,2,\ldots N$$

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

$$Y_0 = 0,\ Y_1,\ Y_2,\ \ldots Y_N = Y_{wall}.$$

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

$$r_0,\ r_1,\ r_2,\ldots . r_N$$

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 ($B_{0_n}$, $B_{1_n}$, $C_{1_n}$, $C_{2_n}$). These are used to compute P(X,Y) and $\theta$ (X,Y) in the transonic region (see Reference 1, pp.2-20) at points n=0,1...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:

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

where

r is the mixture ratio at position Y, and

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

## 3.2 Selection of Shock Methods

Several techniques were investigated for constructing the supersonic flow field using the Method of Characteristics (MOC) concept. The MOC construction methods considered were:

1) Combinations of RRC, LRC, and Streamline tracing,
2) Streamline Normal method,
3) Hartree scheme[8].

It was determined that streamline tracing must be used because of the numerically stiff behavior of the finite rate chemistry. Streamlines must be traced and a fully-implicit integration method must be used in order to accurately compute the reacting flow chemistry while maintaining a reasonable integration step size.

Since the shock waves to be analyzed come from the nozzle wall, it is necessary to trace Right Running Characteristics (RRC's). A shock wave is inititiated when adjacent RRC's cross-over. Since computing the effect of these shock waves on nozzle performance is a primary objective of the study, a RRC construction method was considered to be necessary. Since the Streamline Normal Method and the Hartree scheme use interpolation formulas to locate characteristic lines, those methods were considered to be less accurate than RRC tracing.

It was concluded that Method 1, (combinations of RRC, LRC, and Streamline tracing), must be used if the effect of an oblique shock on engine performance is to be accurately estimated.

Two shock construction methods were investigated:

a) Shock capturing, and
b) Shock tracing.

It was concluded that Method a, above, must be used, again for reasons of numerical accuracy.

Ref.8 Fox, L., Numerical Solution of Ordinary and Partial Differential Equations, Pergamon Press, 1962.

## 3.3 Shock Construction Methods

In order to construct supersonic nozzle flow fields containing shock waves, a set of logic control subroutines and a set of point calculation procedure subroutines were developed. The flow field point calculation subroutines are:

| | |
|---|---|
| SHØCK | Basic running interior point |
| INPTR | Right running interior point |
| SHCKR | Right running shock point |
| SHCKA | Axis shock reflection point |
| SHCKA1 | Off-axis shock reflection point |
| SHCKL | Left running shock point |
| SHCKW | Wall shock reflection point |
| SHCKW1 | Off-wall shock reflection point |

The flow field construction procedure is outlined below.

The mesh construction begins at the intersection of the initial data line and the nozzle wall and RRC's are constructed. After the nozzle wall is reached, succesive 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 first 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.

An example calculation is shown in Figure 2, which presents the mesh construction for a source flow with 1 1/4 degree cone half angle that enters a right regular cylinder. A Right Running Shock (RRS) wave occurs at the intersection of the cone and cylinder. In Figure 2 the shock is attached to the wall. If the induced shock option is used (rather than the attached shock option) a shock will be detected when the first RRC from the cylinder crosses the RRC that is immediately upstream. The control subroutine detects this crossing and inserts a RRS point. The RRS is traced to the axis, reflected, and then traced as a Left Running Shock (LRS) to the wall, reflected, etc. Four axis reflections and three wall reflections are shown in Figure 2.

Strictly speaking, regular reflection from the axis cannot occur in axisymmetric flow. This is because the term $(\sin \theta)/r$ in the MOC relations becomes infinite behind the first shock front; i.e., r is zero, but $\theta$ is not zero. Thus a Mach shock will occur. However, as a practical matter, unless the shock is strong, the Mach disk is very small and can be ignored. In the computer program the Mach disk is ignored by reflecting the shock based on assuming that the incident shock angle at the axis is the same as at the previously calculated off axis shock point.

The flow axis can be thought of as being a right cylinder with zero radius. If the radius of this cylinder were non-zero, regular reflection would be possible only if the radius exceeded some minimum value. At each RRS point this condition is checked, i.e. the Mach number is calculated behind a reflected shock resulting in zero flow angle. The value must be greater than one for the calculations to continue.

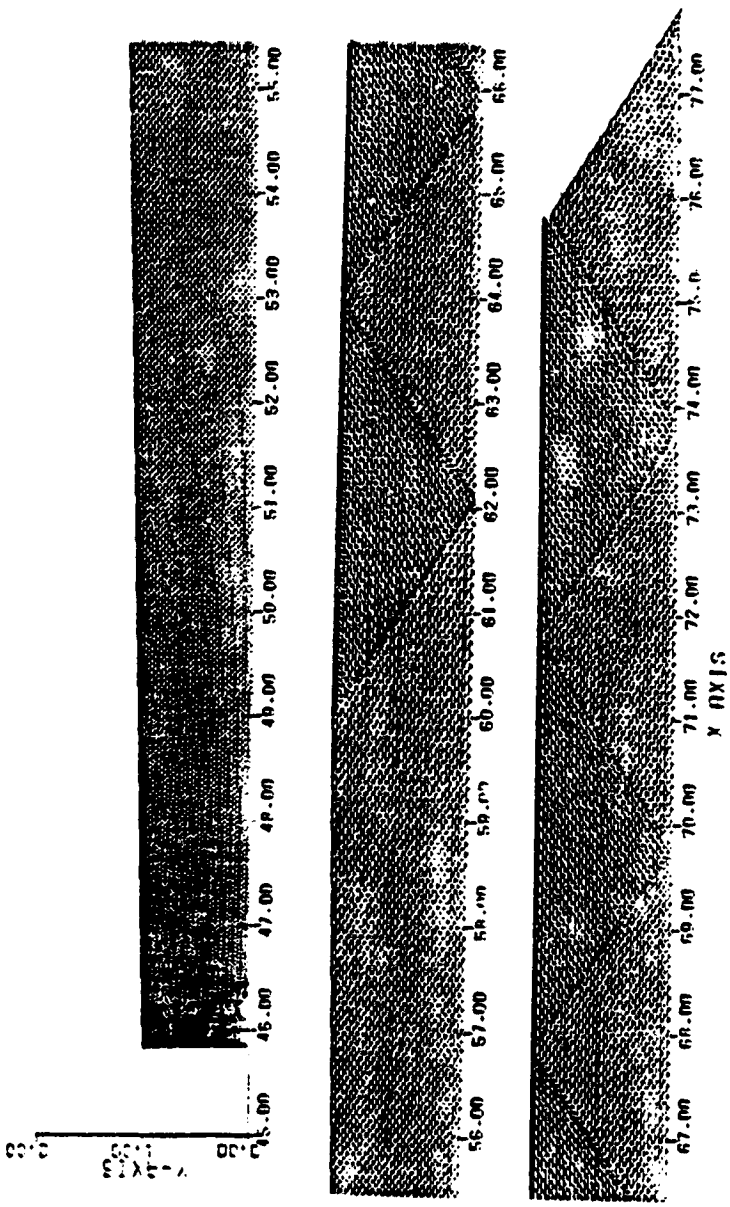



Figure: 2

Figure 3 shows Mach number vs distance for three streamlines: the wall streamline, the median streamline, and the axis. It can be seen that the shock is much stronger at axis than at the wall. The strongest shock occurs at the first axis reflection. The Mach number behind the reflection is 1.58. A very rapid steepening of the shock occurs near the axis, such that in actuality, there is a Mach disk at the axis with subsonic flow downstream. This small region is ignored by the computer program.

Figure 4 shows pressure versus distance for the same streamlines as shown in Figure 3. It can be seen from these two figures that there is a weakening of the shock front as the flow progresses down the cylinder. Eventually, the flow in the duct will be at constant pressure.

The shock wave is constructed using the point calculations listed at the beginning of this section. Details of two of the subroutines are presented below. The basic shock wave calculation, subroutine SHØCK, is used to compute properties across an oblique shock front that is inclined at an angle, $\beta$, with respect to the approach streamline. Subroutine SHØCK is described in Section 3.3.1. The Right Running shock point calculation, subroutine SHCKR, is described Section 3.3.2. It is used for shock initiation, as well as for RRS point calculation.

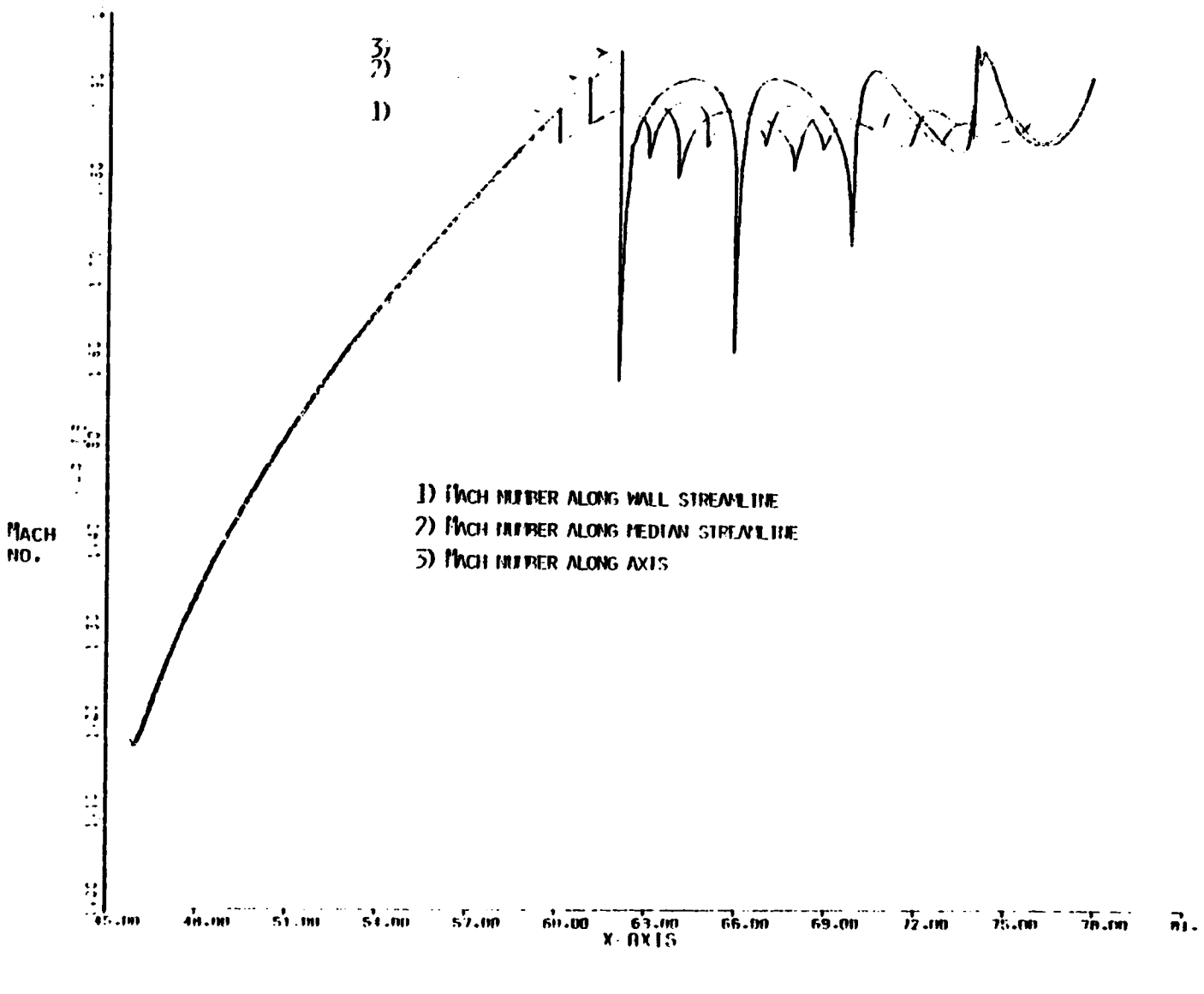



Figure 3: Mach Number versus Distance for 3 Streamlines

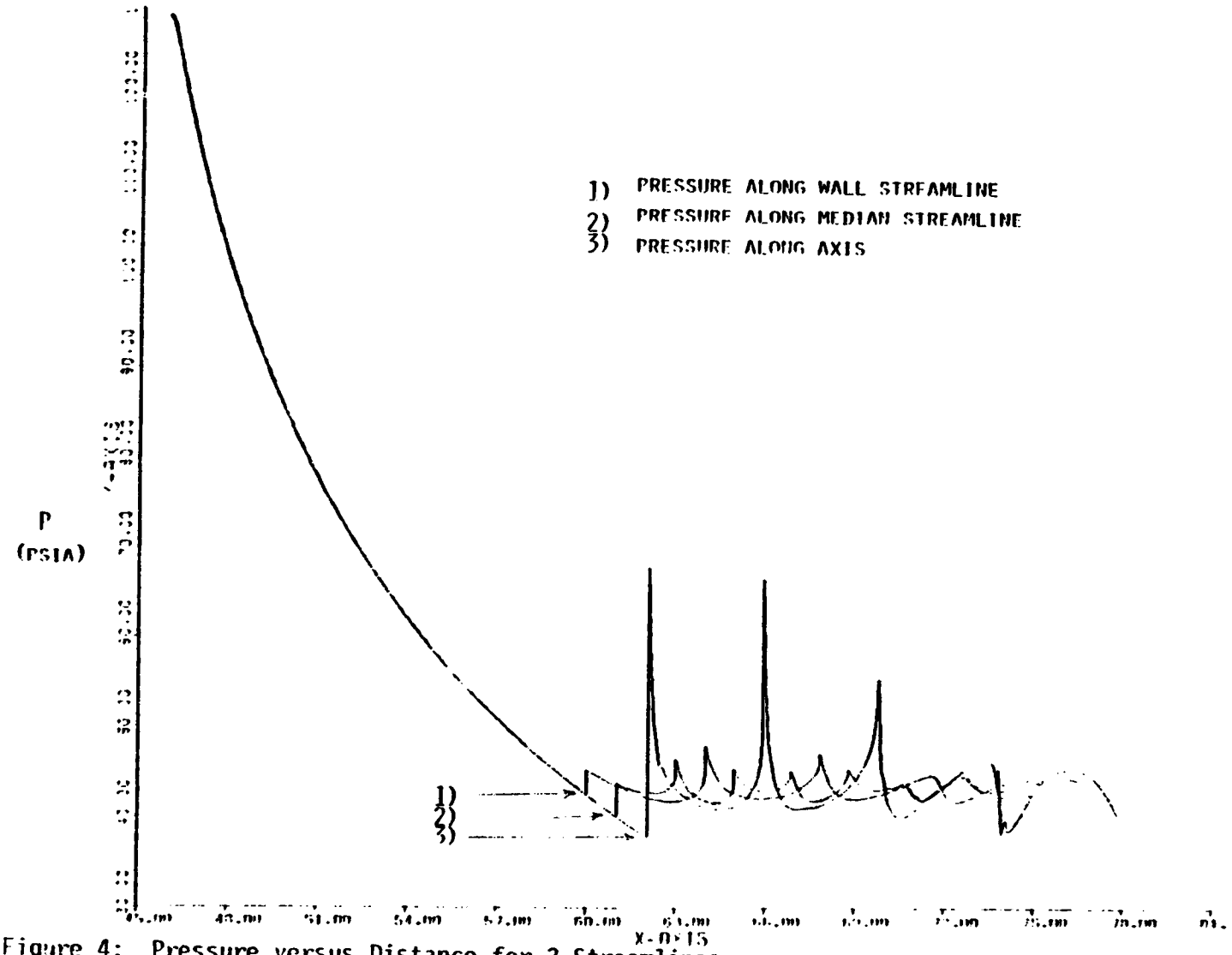



Figure 4: Pressure versus Distance for 3 Streamlines

### 3.3.1 Subroutine SHOCK

Given the shock angle, $\beta$, and the properties at point 1, this subroutine finds all values at point 2 behind the oblique shock front, see figures 5a and 5b, below.

(Step 1)
The quantities $\tilde{u}$, $\tilde{v}$, and M, are calculated as

$$\tilde{u}_1 = V_1 \sin\beta$$

$$\tilde{v}_1 = V_1 \cos\beta$$

$$M_1 = V_1 / (\gamma_1 R T_1)^{1/2} .$$

The Mach number, $M_1$, is used to obtain a first estimate for $P_2^{(i)}$ as follows (equation 128 of NACA 1135):

$$P_2^{(1)} = P_1 \left\{ 2\gamma_1 M_1^2 \sin^2\beta - (\gamma_1 - 1) \right\} / (\gamma_1 + 1).$$

(Step 2)
Using the relations,

$\rho_1\tilde{u}_1 = \rho_2\tilde{u}_2$ Mass Conservation (1)

$P_1 + \rho_1\tilde{u}_1^2 = P_2 + \rho_2\tilde{u}_2^2$ Normal Momentum (2)

$\rho_1\tilde{u}_1\tilde{v}_1 = \rho_2\tilde{u}_2\tilde{v}_2$ Tangential Momentum

$\frac{1}{2}\tilde{u}_1^2 + h_1 = \frac{1}{2}\tilde{u}_2^2 + h_2$ Energy Conservation (3)

$P/\rho = RT$ , $R = \mathcal{R}/M_w$ Gas law (4)

and

$h = h(T)$ Gas Properties (5)

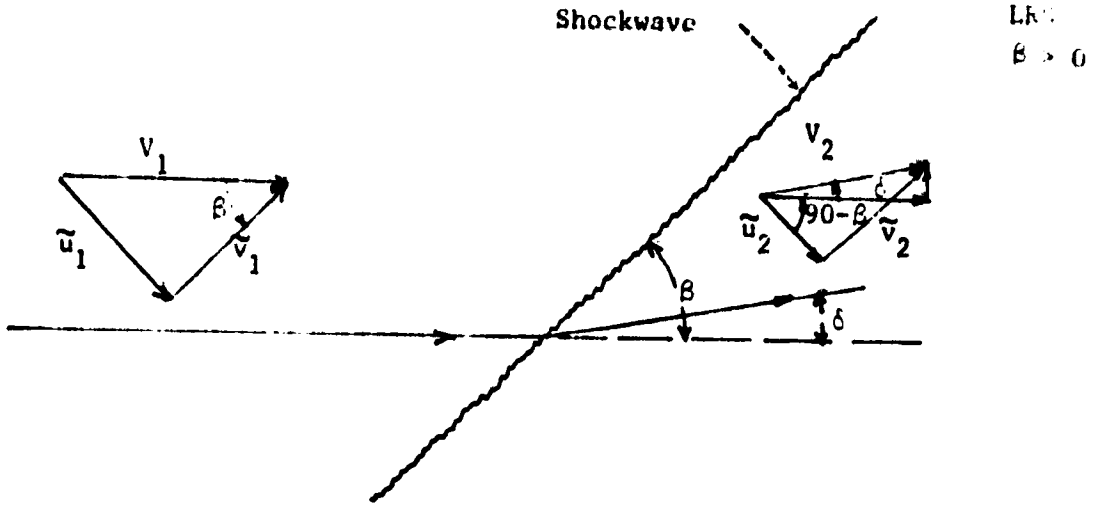



FIGURE 5a Notation for Oblique Shock Wave, Left Running.

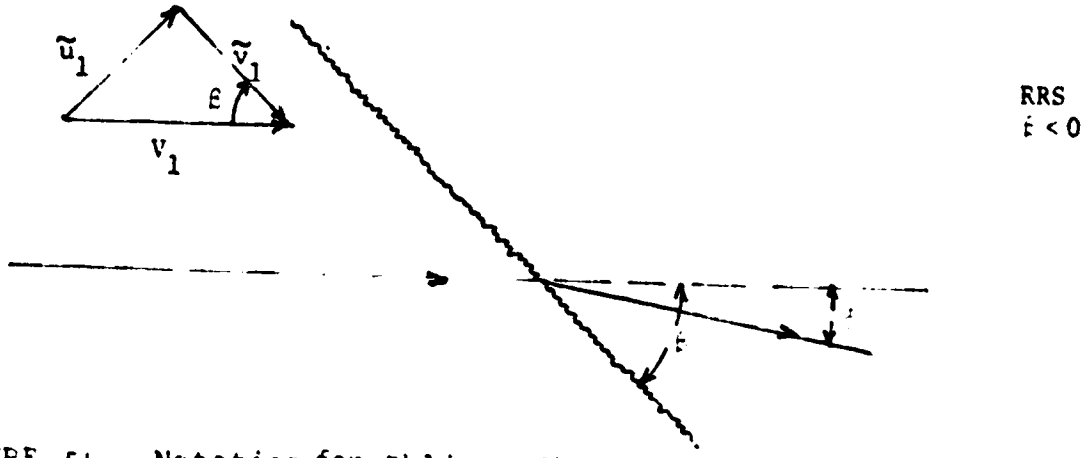



FIGURE 5b Notation for Oblique Shock Wave, Right Running.

The following are calculated:

from (1) and (2)

$$\tilde{u}_2 = (P_1 - P_2 + \rho_1 \tilde{u}_1^2)/\rho_1 \tilde{u}_1$$

from (3)

$$h_2 = \tfrac{1}{2}\,\tilde{u}_1^2 + h_1 - \tfrac{1}{2}\,\tilde{u}_2^2$$

from (5) using subroutine TCALC

$$T_2 = T_2\,(h_2)$$

from (1)

$$\rho_2 = \rho_1\,\tilde{u}_1/\tilde{u}_2$$

from (4)

$$P_2^{(i+1)} = \rho_2\,R\,T_2$$

Iterate on $P_2$ until

$$\left| P_2^{(i+1)} - P_2^{(i)} \right| / P_2^{(i)} < \epsilon .$$

(Step 3)

Values at point 2 are calculated as follows:

$$\delta = \arctan(\tilde{v}_2/\tilde{u}_2) - \arctan(\tilde{v}_1/\tilde{u}_1)$$

$$\theta_2 = \theta_1 + \delta$$

$$V_2 = (\tilde{u}_2^2 + \tilde{v}_2^2)^{1/2}$$

All other properties are obtained from Subroutine GPF.

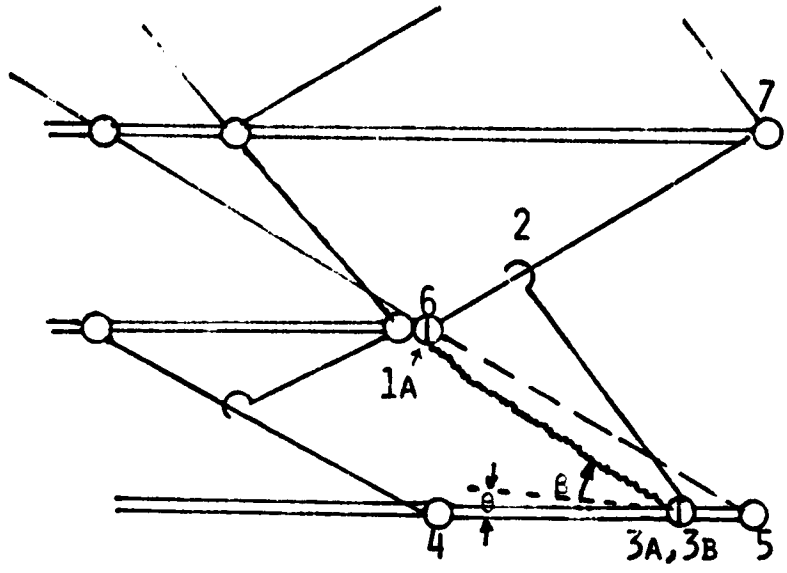
If $M_2$ is returned from GPF such that

$M_2 < 1 + \epsilon_m$ , nominally $\epsilon_m = .2$,

an error message is printed and the run terminated.

### 3.3.2 Subroutine SHCKR

This subroutine calculates a pair of right-running shock points, 3a and 3b, using the known points 1a, 1b, 4, 5, 6, and 7 shown in the figure below.




The procedure used consists of 8 steps, as follows:

1) Use point 5 if available, otherwise calculate from 1a and 4, using INPTRS.

2) Using 4 and 1a, including $\beta_1$, locate point 3 on line 4-5*.

3) Interpolate along 4-5 for all properties at 3a.

4) Use shock subroutine to calculate properties at 3b from 3a.

---

* For the first shock point that is computed, set $\beta = -\alpha$ where $\alpha$ = arc sin 1/M evaluated at the average of the folded back point and point 1a.

5) Interpolate for point 2 between points 6 and 7. Set point 6 as 1b for first estimate.

6) Relocate point 3 by intersection of RRC line 2-3b and streamline 4-3a.

7) Calculate $\beta$ from slope of line 1-3.

8) Return to step 3 and iterate until convergence.

Details of this procedure are given below.

Step 1)
Point 5 is calculated (unless available) from points 1a and 4 using subroutine INPTR just before entering this subroutine.

Points 1a, 1b, 4, 5, 6 and 7 are known points and points 3a and 3b are the unknown points to be computed. Initial values (i=0) at point 3a for A, B, $\alpha$, $\gamma$, and $\theta$ are taken as the values at point 4.

Double subscripts imply averaged values, e.g.

$$\theta_{45} = \frac{1}{2} (\theta_4 + \theta_5) ,$$

$$\left(\frac{A}{\cos\theta}\right)_{43a} = \frac{1}{2}\left(\frac{A_4}{\cos\theta_4} + \frac{A_{3a}}{\cos\theta_{3a}}\right), \text{ etc.}$$

Step 2)
Using points 4 and 1a, point 3 is located on the line 4-5.

$$x_3^{(i)} = \frac{r_1 - x_1 \tan(\beta_1 + \theta_{1a}) - r_4 + x_4 \tan \theta_{45}}{\tan \theta_{45} - \tan(\beta_1 + \theta_{1a})}$$

$$r_3^{(i)} = r_4 + (x_3^{(i)} - x_4) \tan \theta_{45}$$

Step 3)
Properties at point 3a are determined by interpolation and integration along the line 4-5, as follows:

$$C = (x_3 - x_4) / (x_5 - x_4)$$

$$\theta_{3a}^{(i+1)} = \theta_4 + C(\theta_5 - \theta_4)$$

$$P_{3a}^{(i+1)} = P_4 + C(P_5 - P_4)$$

$$\rho_{3a}^{(i+1)} = \rho_4 \left[\frac{P_{3a}^{(i+1)}}{P_4}\right]^{\left[\frac{1}{\gamma}\right]_{43a}^{(i)}} \exp\left\{ - \left(\frac{A}{\cos\theta}\right)_{43a}^{(i)} \left(x_{3a}^{(i+1)} - x_4\right)\right\}$$

$$T_{3a}^{(i+1)} = T_4 \left[\frac{P_{3a}^{(i+1)}}{P_4}\right]^{\left[\frac{\gamma-1}{\gamma}\right]_{43a}^{(i)}} \exp\left\{ - \left(\frac{B}{\cos\theta}\right)_{43a}^{(i)} \left(x_{3a}^{(i+1)} - x_4\right)\right\}$$

Next the gas velocity is calculated as

$$N^{(i+1)} = \frac{\ln\left(P_{3a}^{(i+1)}/P_4\right)}{\ln\left(\rho_{3a}^{(i+1)}/\rho_4\right)}$$

$$V_{3a}^{(i+1)} = \left( V_4^2 + \frac{2N^{(i+1)}}{N^{(i+1)} - 1} \frac{P_4}{\rho_4} \left\{ 1 - \left[\frac{P_{3a}^{(i+1)}}{P_4}\right]^{\frac{N^{(i+1)}-1}{N^{(i+1)}}} \right\} \right)^{1/2}$$

The species concentrations at point 3a, $c_{i_{3a}}^{(i+1)}$, are calculated using the Species Integration Subroutine, SINT, and the gas properties at point 3a, $A_{3a}^{(i+1)}$, $B_{3a}^{(i+1)}$, $F_{3a}^{(i+1)}$, $G_{3a}^{(i+1)}$, $H_{3a}^{(i+1)}$, $\alpha_{3a}^{(i+1)}$, $\gamma_{3a}^{(i+1)}$, are calculated using the GPF subroutine.

Step 4)

Calculate all properties at point 3b from 3a using the shock wave subroutine, SHOCK.

Step 5)

Values at point 2 are determined by interpolation between points 6 and 7. Points 6 is initially assumed to be point 1b and point 7 is the next point on the back LRC data line.

The radial location of point 2 is calculated from

$$r_2^{(i+1)} = \frac{r_3^{(i+1)} - \left[\frac{x_7 - x_6}{r_7 - r_6} r_6 + x_3^{(i+1)} - x_6\right] \tan\frac{1}{2}\left[\theta_2^{(i)} + \theta_{3b}^{(i)} - \alpha_2^{(i)} - \alpha_{3b}^{(i)}\right]}{1 - \frac{x_7 - x_6}{r_7 - r_6} \tan\frac{1}{2}\left[\theta_2^{(i)} + \theta_{3b}^{(i)} - \alpha_2^{(i)} - \alpha_{3b}^{(i)}\right]}$$

If $r_2^{(i)} > r_7$, point 7 becomes point 6 and the next point on the back data line is point 7. The above calculation is repeated until $r_6 < r_2^{(i+1)} < r_7$.

The axial location, flow angles, and Mach angle of point 2 are calculated from

$$C_2 = \frac{r_2^{(i+1)} - r_6}{r_7 - r_6}$$

$$x_2^{(i+1)} = x_6 + C_2 (x_7 - x_6)$$

$$\theta_2^{(i+1)} = \theta_6 + C_2\,(\theta_7 - \theta_6)$$

$$\alpha_2^{(i+1)} = \alpha_6 + C_2\,(\alpha_7 - \alpha_6)$$

Step 6)
Relocate point 3 by the intersection of RRC line 2-3b and streamline 4-5

$$x_3^{(i+1)} = \frac{-r_2 + x_2 \tan \frac{1}{2}(\theta_2 - \alpha_2 + \theta_{3b} - \alpha_{3b}) + r_4 - x_4 \tan \theta_{45}}{\tan \frac{1}{2}(\theta_2 - \alpha_2 + \theta_{3b} - \alpha_{3b}) - \tan \theta_{45}}$$

$$r_3^{(i+1)} = r_4 + (x_3^{(i+1)} - x_4) \tan \theta_{45}$$

Step 7)
The revised shock angle is calculated from

$$\beta_{13}^{(i+1)} = -\theta_{13a} + \arctan \left| (r_1 - r_3^{(i+1)})/(x_1 - x_3^{(i+1)}) \right|$$

$$\beta_3 = 2\beta_{13} - \beta_1$$

where $|\beta_3| \geq \alpha_3$

Step 8)
Return to Step 3.

The above integration equations are iterated (i=1,...) until $r_3$, $x_3$, $\theta_3$, $P_3$, $\rho_3$, $T_3$, and $V_3$ converge to the required accuracy.

## 3.4 Techniques for Reducing Computer Time

Work was carried out on the ODK and TDK modules for the purpose of reducing computer run time. Three separate tasks were carried out 1) single precision in ODK versus double precision, 2) modification of the matrix inversion method, and 3) modifications to the chemical reaction decoding subroutine STØICC. Each task is discussed below.

### 3.4.1 ODK Precision

It was found that double precision is not needed in the linear equation solver, LESK, when using DEC 32 bit word computers. The program was run with and without double precision for a test case with high expansion ratio. The results showed no appreciable differences. The change from double precision to single precision in ODK saved about 30% of execution time.

### 3.4.2 TDK Matrix Inversion Procedure

The linear equation solver used by TDK is subroutine NESK. It is used to solve the linear equation $\bar{\bar{A}}\bar{X}=\bar{b}$ where the vector, $\bar{X}$, is the chemical species mass fractions. In an attempt to reduce computer time the procedure was changed so that $\bar{\bar{A}}^{-1}$ was found and saved for use on sucessive iterations. Two methods were investigated.

In the first method $\bar{\bar{A}}^{-1}$ is computed by Gaussian elimination and saved for successive iteration. This method has

the advantage of being conceptually clear. However, it pays off only if there are at least some minimum number of iterations, depending on the size of the linear system. The approximate number of operations for the $\bar{\bar{A}}\bar{X}=\bar{b}$ method and for the $\bar{\bar{A}}^{-1}$ method are, respectively, $\frac{kn^3}{3}$ and $\frac{5n^3}{6} + (k-1)n^2$, where n is the size linear system (i.e., the number of species) and k is the number of iterations. Thus, for a system of 10 species, at least 4 iterations must be made before execution time is reduced.

A second method was investigated in which the sequence of row exchanges and row operations in the Gaussian eliminations were saved the first time, and the same sequence of operation were applied to $\bar{b}$ on successive iterations. This method is slightly more complex than the previous one, but has the advantage that execution time is always equal to or less than that of the straight Gaussian elimination at every iteration. Morever, additional savings in execution time can be achieved by using scaled Gaussian elimination instead of unscaled Gaussian elimination.

The following table shows the timing of the different methods for our test case.

| METHOD | TIMING (sec.) | % SAVING |
|---|---|---|
| Present Method | 164 | |
| Method 1 | 162 | 1.2% |
| Method 2 (unscaled Gaussian) | 158 | 3.7% |
| Method 2 (scaled Gaussian) | 152 | 7.3% |

The drawback of the new methods is that they have not yet taken into account the slight dependence of A on the step size, which is variable. Although this adjustment can be done, the added complexity and risk involved outweighs the small saving in execution time. Thus, it was decided to leave the linear equation solver in TDK the way it is.

### 3.4.3 Modifications to Subroutine STØICC

In order to reduce the number of calls to subroutine STØICC, the stoichiometric coefficients are obtained at the beginning of the run and then stored in various arrays. With this change, the subroutines DERIV, SDERIV, EF and EF2D do not need to call STØICC repeatedly and, therefore, the execution time is reduced. In our test cases the saving was about 5%.

## 4. Conclusions

The TDK computer program that is described in Reference 5 has been modified to incorporate the work items a) through h) listed in Section 1. All of the capabilities described in Reference 5 have been retained.

The TDK program has been given the capability to detect an oblique shock wave induced by curvature of the nozzle wall. The shock is detected by a crossing of right running chracteristics. The shock is traced through the flow field, including multiple regular reflections from the nozzle axis and wall. Only one such shock wave is allowed. Mach shocks are not allowed.

The chemistry of the flow with a shock can be either a) constant properties, or b) frozen chemical composition or c) finite rate kinetics. Equilibrium chemistry with a shock wave is not allowed. TDK has not been provided with a exit plane option for flows with shock waves.

Straited flow (i.e. dividing the flow into regions of constant mixture ratio separated by sliplines) is not allowed with a shock wave. This is because shock-slipline interaction is not provided in the program. The program can, however, be run with a continuous variation in mixture ratio from streamline to streamline. The transonic analysis has been modified to provide this capability.

Modifications were made to the computer program to reduce computer run time and also to improve accuracy. Only a modest (on the order of 5%) improvement in run time was achieved. Program accuracy was increased by several means. Complete energy conservation was achieved along streamlines in the MOC module by computing the gas velocity directly from the energy equation. The Bernoulli equation was used for a first estimate. Conservation of mass flow was forced by adjusting the flow pressure across each complete characteristic surface. The gas density was then adjusted using the gas law. These measures

served to conserve energy flux and momentum flux across the flow. Accuracy was also improved by distributing points along the MOC initial data line using a sinusoidal distribution function. This method provided an improved MOC grid spacing.

A revised User's Manual for TDK (i.e. Section 6 of Reference 1) has been prepared. This document has been attached as Appendix A. The revised computer program and manual render obsolete the earlier versions presented in Reference 5.

## REFERENCES


1) 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.

2) "JANNAF Rocket Engine Performance Prediction and Calculation Manual", CPIA 246, April 1975.

3) Zucrow, M.J., and Hoffman, J.D., Gas Dynamics, Volume I and II, John Wiley & Sons, Inc., New York, 1976.

4) "JANNAF" Rocket Engine Performance Prediction and Evaluation Manual," CPIA Publications 246, April 1975.

5) Nickerson, G.R. and Dang, L.D., "Improved Two-Dimensional Kinetics (TDK) Computer Program", SEA Inc., Final Report, SN58, NAS8-35406, October 1983.

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7) Sauer, R. "General Characteristics of the Flow Through Nozzles at Near Critical Speeds", NACA Tech. Note No. 1147 (1947).

8) Fox, L., Numerical Solution of Ordinary and Partial Differential Equations, Pergamon Press, 1962.

APPENDIX A - Revised TDK User's Manual

# Section 6
# Engineering and Programming Manual
( Revised 3/84 )

# TDK

## Two-Dimensional Kinetic Reference Computer Program

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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

| Card Input | Section No., | Description |
|---|---|---|
| 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 namelist for module selection, 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) |
| . | | |
| . | | |

| Card Input | Section No., | Description |
|---|---|---|
| THIRD BODY | 6.5.2.7, | reaction rate ratios for third bodies |
| . | | |
| . | | |
| LAST CARD | | |
| $ODK | 6.5.3 | ØDK module namelist |
| $END | | |
| $TRANS | 6.6 | TRANS module namelist |
| $END | | |
| $MOC | 6.7 | MØC module namelist |
| $END | | |
| $BLM | 6.8 | BLM module namelist |
| $END | | |

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 logicial 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 9).

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 22).

The thermodynamic data (i.e. $C^o_{p_T}$, 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:

$$\frac{C^o_{p_T}}{R} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$\frac{H^o}{R} = a_1 + \frac{a_2T}{2} + \frac{a_3T^2}{3} + \frac{a_4T^3}{4} + \frac{a_5T^4}{5} + \frac{a_6}{T}$$

$$\frac{S^o_T}{R} = a_1 \ln T + a_2T + \frac{a_3T^2}{2} + \frac{a_4T^3}{3} + \frac{a_5T^4}{4} + a_7$$

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 9 the lower temperature interval is 300° to 1000°K and the upper temperature interval is 1000°K to 5000°K.

---

Ref. 22. 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, $H_2$, $H_2O$, $N_2$, O, OH, and $O_2$ 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.

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 |
| | Integer 1 | I15 | 80 |
| 4 | Coefficients $a_i'$ (i = 1 to 5) in equations (6-1) to (6-3) (for upper temperature interval) | 5(E15.8) | 1 to 75 |
| | Integer 2 | I5 | 80 |
| 5 | 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(E15.8) | 1 to 75 |
| | Integer 3 | I5 | 80 |
| 6 | 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 |
| | 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 |

[a]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 $O_2/H_2$ PROPELLANT

(Species AR, H, $H_2$, $H_2O$, $N_2$, O, OH, and $O_2$)

```
THERMO
   300.000  1000.000  5000.000
AR                  L 5/66AR  100  000  000  0G   300.000  5000.000
 0.25000000E 01 0.                    0.                   0.                   0.
-0.74537502E 03 0.43660006E 01 0.25000000E 01 0.                   0.
 0.                0.                   -0.74537498E 03 0.43660006E 01
H                   J 9/65H   100  000  000  0G   300.000  5000.000
 0.25000000E 01 0.                    0.                   0.                   0.
 0.25471627E 05-0.46011763E 00 0.25000000E 01 0.                   0.
 0.                0.                   0.25471627E 05-0.46011762E 00
H2                  J 3/61H   20   00   00   0G   300.000  5000.000
 0.31001901E 01 0.51119464E-03 0.52644210E-07-0.34909973E-10 0.36945345E-14
-0.87738042E 03-0.19629421E 01 0.30574451E 01 0.26765200E-02-0.58099162E-05
 0.55210391E-08-0.18122739E-11-0.98890474E 03-0.22997056E 01
H2O                 J 3/61H   20   100  000  0G   300.000  5000.000
 0.27167633E 01 0.29451374E-02-0.80224374E-06 0.10226682E-09-0.48472145E-14
-0.29905826E 05 0.66305671E 01 0.40701275E 01-0.11084499E-02 0.41521180E-05
-0.29637404E-08 0.80702103E-12-0.30279722E 05-0.32270046E 00
N2                  J 9/65N   20   00   00   0G   300.000  5000.000
 0.28963194E 01 0.15154866E-02-0.57235277E-06 0.99807393E-10-0.65223555E-14
-0.90586184E 03 0.61615148E 01 0.36748261E 01-0.12081500E-02 0.23240102E-05
-0.63217559E-09-0.22577253E-12-0.10611588E 04 0.23580424E 01
O                   J 6/620   100  000  000  0G   300.000  5000.000
 0.25420596E 01-0.27550619E-04-0.31028033E-08 0.45510674E-11-0.43680515E-15
 0.29230803E 05 0.49203080E 01 0.29464287E 01-0.16381665E-02 0.24210316E-05
-0.16028432E-08 0.38906964E-12 0.29147644E 05 0.29639949E 01
OH                  J 3/660   1H   100  000  0G   300.000  5000.000
 0.29106427E 01 0.95931650E-03-0.19441702E-06 0.13756646E-10 0.14224542E-15
 0.39353815E 04 0.54423445E 01 0.38375943E 01-0.10778858E-02 0.96830378E-06
 0.18713972E-09-0.22571094E-12 0.36412823E 04 0.49370009E 00
O2                  J 9/650   20   00   00   0G   300.000  5000.000
 0.36219535E 01 0.73618264E-03-0.19652228E-06 0.36201558E-10-0.28945627E-14
-0.12019825E 04 0.36150960E 01 0.36255985E 01-0.18782184E-02 0.70554544E-05
-0.67635137E-08 0.21555993E-11-0.10475226E 04 0.43052778E 01
END
```

Table 6-4. SPECIES WITH THERMODYNAMIC DATA PROVIDED

| | | | | | |
|---|---|---|---|---|---|
| AL(S) | BCL | BEO(S) | C2H | FECL2(S) | KOH |
| AL(L) | BCL+ | BEO(L) | C2HF | FECL2(L) | KOH(S) |
| AL | BCLF | BEO | C2H2 | FECL2 | KOH(L) |
| AL+ | BCL2 | BEOH | C2H4 | FECL3(S) | K2 |
| ALBO2 | BCL2+ | BEOH+ | C2N | FECL3(L) | K2O(S) |
| ALCL | BCL2- | BEO2H2 | C2N2 | FECL3 | LI(S) |
| ALCL+ | BCL3 | BE2O | C2O | FEO(S) | LI(L) |
| ALCLF | BF | BE2OF2 | C3 | FEO(L) | LI |
| ALCLF2 | BF2 | BE2O2 | C3O2 | FEO | LI+ |
| ALCL2 | BF2+ | BE3O3 | C4 | FEO2H2(S) | LICL(S) |
| ALCL2+ | BF2- | BE4O4 | C5 | FEO2H2 | LICL(L) |
| ALCL2- | BF3 | BR | CL | FEO3H3(S) | LICL |
| ALCL2F | BH | BR2(L) | CL+ | FE2O3(S) | LIF(S) |
| ALCL3(S) | BHF2 | BR2 | CL- | FE3O4(S) | LIF(L) |
| ALCL3(L) | BH2 | C(S) | CLCN | H | LIF |
| ALCL3 | BH3 | C | CLF | H+ | LIF2- |
| ALF | BN(S) | C+ | CLF3 | H- | LIFO |
| ALF+ | BN | C- | CLO | HALO | LIH(S) |
| ALF2 | BO | CCL | CLO2 | HBO | LIH(L) |
| ALF2+ | BOCL | CCL2 | CL2 | HBO+ | LIH |
| ALF2- | BOF | CCL3 | CL2O | HBO2 | LIN |
| ALF3(S) | BOF2 | CCL4 | CS(S) | HCL | LIO |
| ALF3(S) | BO2 | CF | CS(L) | HCN | LIO- |
| ALF3 | BO2- | CF2 | CS | HCO | LIOH(S) |
| ALH | BS | CF3 | CS+ | HCO+ | LIOH(L) |
| ALN(S) | B2 | CF4 | CSCL(S) | HCP | LIOH |
| ALN | B2O | CH | CSCL(S) | HF | LION |
| ALO | B2O2 | CH2 | CSCL(L) | HNO | LI2 |
| ALO+ | B2O3(L) | CH2O | CSCL | HO2 | LI2CL2 |
| ALOCL | B2O3 | CH3 | CSF(S) | H2 | LI2F2 |
| ALOF | B3O3CL3 | CH4 | CSF(L) | H2O(S) | LI2O(S) |
| ALOH | B3O3F3 | CN | CSF | H2O(L) | LI2O(L) |
| ALOH+ | BE(S) | CN+ | CSO | H2O | LI2O |
| ALOH- | BE(L) | CN- | CS2 | H2O2 | LI2O2 |
| ALO2 | BE | CN2 | CS2CL2 | H2S | LI2O2H2 |
| ALO2- | BE+ | CO | CS2F2 | H3B3O6 | LI3CL3 |
| ALO2H | BEBO2 | CCCL | CS2C | HE | LI3F3 |
| AL2CL6 | BECL | CCCL2 | E | HE+ | MG(S) |
| AL2F6 | BECL+ | CCF | F | K(S) | MG(L) |
| AL2O | BECLF | COF2 | F- | K(L) | MG |
| AL2O+ | BECL2(S) | COS | FCN | K | MG+ |
| AL2O2 | BECL2(L) | CO2 | FO | K+ | MGCL |
| AL2O2+ | BECL2 | CO2- | FO2 | KCL(S) | MGCL+ |
| AL2O3(S) | BEF | CP | F2 | KCL(L) | MGCLF |
| AL2O3(L) | BEF2(S) | CS | F2O | KCL | MGCL2(S) |
| AR | BEF2(S) | CS2 | FE(S) | KF(S) | MGCL2(L) |
| AR+ | BEF2(L) | C2 | FE(S) | KF(L) | MGCL2 |
| B(S) | BEF2 | C2- | FE(S) | KF | MGF |
| B(L) | BEH | C2CL2 | FE(L) | KF2- | MGF2(S) |
| B | BEH+ | C2F2 | FE | K2F2 | MGF2(L) |
| B+ | BEN | C2F4 | FECL | KO | MGF2 |

Table 6-4. (cont'd)

| | | |
|---|---|---|
| MGH | O | SIN |
| MGN | O+ | SIO |
| MGO(S) | O- | SIO2(S) |
| MGO(L) | OH | SIO2(S) |
| MGO | OH+ | SIO2(S) |
| MGOH | OH- | SIO2(L) |
| MGOH+ | O2 | SIO2 |
| MGO2H2 | O2- | SIS |
| N | P | SI2 |
| NF | P(S) | SI2C |
| NF2 | P+ | SI2N |
| NF3 | PCL3 | SI3 |
| NH | PF3 | XE |
| NH2 | PF5 | |
| NH3 | PH | |
| NO | PH3 | |
| NO+ | PN | |
| NOCL | PO | |
| NOF | PS | |
| NOF3 | P2 | |
| NO2 | P4 | |
| NO2- | S(S) | |
| NO2CL | S(L) | |
| NO2F | S | |
| N2 | S+ | |
| N2C | SF4 | |
| N2H4 | SF6 | |
| N2O | SH | |
| N2O4 | SN | |
| NA(S) | SO | |
| NA(L) | SOF2 | |
| NA | SO2 | |
| NA+ | SO2F2 | |
| NACL(S) | SO3 | |
| NACL(L) | S2 | |
| NACL | SI(S) | |
| NAF(S) | SI(L) | |
| NAF(L) | SI | |
| NAF | SI+ | |
| NAF2- | SIC | |
| NAH | SIC2 | |
| NAO | SICL | |
| NAO- | SICL2 | |
| NAOH(S) | SICL3 | |
| NAOH(L) | SICL4 | |
| NAOH | SIF | |
| NA2 | SIF2 | |
| NA2CL2 | SIF3 | |
| NA2F2 | SIF4 | |
| NE | SIH | |
| NE+ | SIH4 | |

### 6.1.1 THERMODYNAMIC DATA BELOW 300°K.

Ordinarily this data set is not required. However, for low temperature calculations it may be necessary to extend the curve fit data in the Thermodynamic Data file (see Section 6.1). The lower temperature limit, $T_\ell$, in the Thermodynamic Data supplied with the program is 300°K.

Thermodynamic Data below the temperature, $T_\ell$, may be input by data cards as described below.

| | | |
|---|---|---|
| card 1 | LØW T CPHS | Directive for start of low temperature CPHS tables (col 1 through 10). |
| card 2 | . . . . . n | 12 character species name, left justified, followed by the integer, n, punched in column 21. The itegrer n must be such that 1<n<3 and represent the number of Thermodyanmic Data points to be input for this species. |
| card 3 | $T_1^\circ K$ $C_{P_T}^\circ$ $H_T^\circ$ $S_T^\circ$ 1 | First Thermodynamic Data point for the above species, input 4F 10.0, I5. |
| | . | |
| | . | |
| | . | |
| card n+2 | $T_n^\circ K$ $C_{P_T}$ $H_T^\circ$ $S_T^\circ$ nth (1<n<3) | nth Thermodynamic Data point for the above species, input 4F10.0, I5. |
| . . . | Repeat cards through n+2 above for each species to be input. | |
| | Temperature must be $T_1 < T_2 < T_3 < T_\ell$. | |
| (final card) | END LØW T CPHS | end directive (col 1 through 14) |

An example of this input is given in Table 6-5 which shows a card listing extending the Thermodynamic Data for an $O_2/H_2$ propellant to 100°K. Data in Table 6-5 is taken directly from the JANAF tables (Reference 23), except for Argon which is taken from NASA SP-3001.

The quantity $H_T^o$ is defined as

$$H_T^o = (H^o - H_{298}^o) + \Delta H_{f_{298}}^o \quad , \text{cal/mole}$$

and

$$C_{P_T}^o \quad , \text{cal/mole - deg K}$$

$$S_T^o \quad , \text{cal/mole - deg K}$$

---

Ref. 23. 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.

TABLE 6-5. LOW TEMPERATURE $C^{\circ}_{P_T}$, $H^{\circ}_T$, $S^{\circ}_T$ DATA FOR AN $O_2/H_2$ PROPELLANT

```
LOW T CPHS
AR                                    2
100.0        4.9681      -984.5       31.556          1
200.0        4.9681      -487.7       34.999          2
H                                     2
100.0        4.968        51118.      21.965          1
200.0        4.968        51614.      25.408          2
H2                                    2
100.0        5.393       -1265.       24.387          1
200.0        6.518       -962.0       28.520          2
H2O                                   2
100.0        7.961       -59378.9     36.396          1
200.0        7.969       -58581.9     41.916          2
N2                                    2
100.0        7.074       -1387.0      38.113          1
200.0        6.989       -684.        42.986          2
O                                     2
100.0        5.666        58479.      32.466          1
200.0        5.434        59036.      36.340          2
OH                                    2
100.0        7.567        7879.       35.852          1
200.0        7.309        8623.       41.021          2
O2                                    2
100.0        6.958       -1381.       41.395          1
200.0        6.961       -685.        46.218          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 |

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.

| Item | Description | Units | Assumed Value(s) |
|---|---|---|---|
| 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 ØDE module be run, it is necessary to input ØDE = 1. Only certain combinations of modules are allowed. These are described in Table 6-6. The module flags are:

| Item | | Description | Units | Assumed Value(s) |
|---|---|---|---|---|
| ØDE | = | Set ØDE = 1 if the ODE module is to be executed. | none | 0. |
| ØDK | = | Set ØDK = 1 if the ODK module is to be executed. | none | 0. |
| TDE | = | Set TDE = 1 if the TDE option of the MØC module is to be executed | none | 0. |
| TDK | = | Set TDK = 1 if the TDK option of the MØC module is to be executed | none | 0. |
| TDF | = | Set TDF = 1 if the TDF option of the MØC is to be executed | none | 0. |
| TDKIL | = | Set TDKIL = 1 if the TDK option of the MØC is to be executed with an initial data line input as described in Section 6.9.2. | none | 0. |
| BLM | = | Set BLM = 1 if the BLM option of the MØC module is to be executed | none | 0. |
| PFGØPT | = | Set PFGØPT = 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

| Input | Mode of Execution |
|---|---|
| ØDE=1, | ØDE is run alone. Options other than the rocket (RKT=T) option are allowed. See Section 6.4.3 and Reference 9. |
| 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. |
| 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. |
| TDKIL=1, | TDK is run with a MØC initial data line input as described in Section 6.9.2. |
| 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)

| Input | Mode of Execution |
|---|---|
| ØDE=1, ØDK=1, TDF=1, | ØDE is run. ØDK is run with ØDE providing start conditions. However, the ØDK run will have a frozen chemical composition. TDK will also be run with a frozen composition. |
| ØDE=1, ØDK=1, TDF=1, BLM=1, | As above with BLM. |
| ØDF=1, ØDK=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. |
| PFGØPT=1, | The TRANS and MØC modules are run with constant gas properties. See Section 6.9.1. |

6.3.2 Inputs for Control for the Program.

| Item | | Description | Units | Assumed Value(s) |
|---|---|---|---|---|
| IRPEAT | = | 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.<br><br>If IRPEAT = 1, the ODE and ODK module executions will be repeated with adjusted enthalpies for regen cooling, see Section 6.8.4.<br><br>If IRPEAT = 2, the ØDE and ØDK module executions will not be repeated. The system enthalpy will be unchanged. | none | 0 |
| IRSTRT | = | 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 inputing<br><br>IRSTRT = 2,<br><br>This will restart the program after the MOC calculation and before the BLM calculation. The restart handles all options involving BLM. | | |

| Item | | Description | Units | Assumed Value(s) |
|---|---|---|---|---|
| NZØNES | = | Number of zones, N, to be used in the anlysis. 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.<br><br>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.<br><br>If IØFF is input, do not input NXINØ in BLM. | | 0 |

### 5.3.3 Specification of nozzle geometry.

To eliminate redundancy, all geometry inputs that are common throughou· 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 ØDE and ØDK 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 ØDK 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 THETAI be input such that

$$\sqrt{\text{ECRAT}} > 1 + (\text{RI} + \text{RWTU})\ (1 - \cos \text{THETAI}).$$

If this condition is not met, subroutine PRES of ØDK will print the terminal error message:

INLET GEOMETRY INCOMPATIBLE WITH INITIAL CONDITIONS.

In addition, the transonic analysis requires that a value of 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 RWTD which extends from the throat point through an angle of THETA. Geometries that can be input to both the ØDK and MØC modules are described in Section 5.3.3.1.

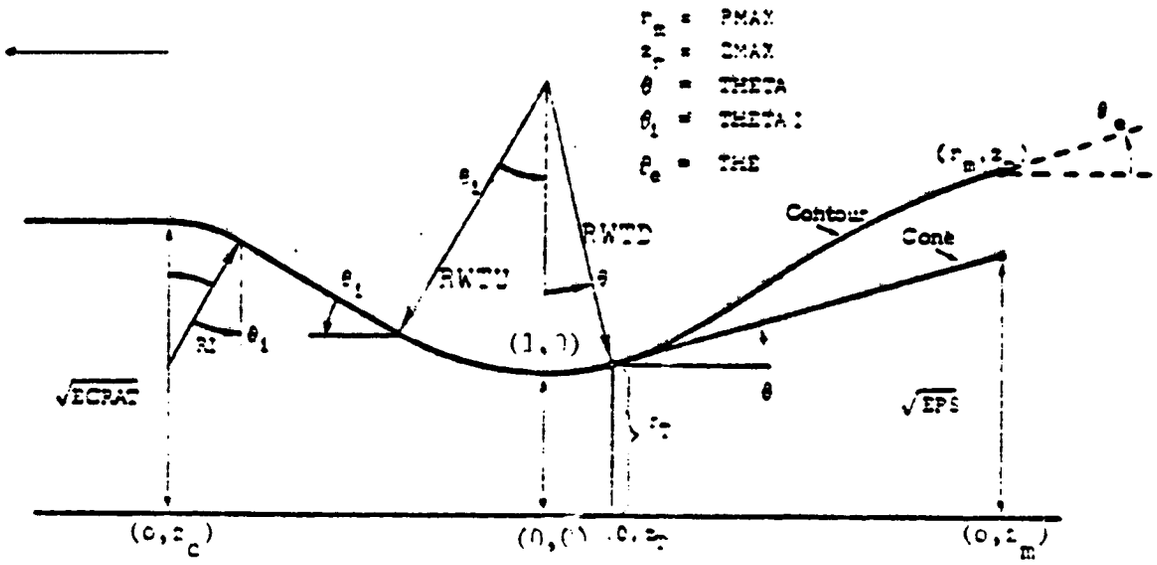


Figure 6-1: Nozzle Geometry, all coordinate values are normalized by RSI = $r_t$.

| Item | | Description | Units | Assumed Value(s) |
|---|---|---|---|---|
| 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 $\leq$ 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 $\leq$ 50. | none | 0. |
| ECRAT | = | Nozzle inlet contraction ratio for use in ØDE and ØDK calculations. | none | 0. |
| RI | = | Normalized inlet wall radius. | none* | 0. |
| THETAI | = | Nozzle inlet angle. | degrees | 0. |
| RWTU | = | Upstream normalized wall throat radius RWTU > .5 is required. | none* | 0. |
| ITYPE | = | Type of nozzle wall to be input.<br>ITYPE = 0, if the real wall contour is input.<br>ITYPE = 1, if the potential flow wall contour is input.<br>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 (ITYPE = 0), or $+\delta^*$ for the potential flow wall ( ITYPE = 1). | none | 0. |

* Normalized by the throat radius, $r_t$

6.3.3.1 Exhaust Nozzle Geometry Specification, for ØDK and the MØC Modules.

| Item | | Description | Units | Assumed Value(s) |
|---|---|---|---|---|
| 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.

| Item | | Description | Units | Assumed Value(s) |
|---|---|---|---|---|
| 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+ | 0. |
| ZS(2) | = | table of normalized axial position downstream of the nozzle tangency point (input if IWALL=4). | none+ | 0. |
| NWS | = | 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 RZNORM.

## 6.4 ØDE INPUT DATA (ALL PROBLEMS SPECIFYING ØDE)

The ØDE input data described here is exactly as defined in NASA SP-273, Reference 9, 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 9 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 9 for problem types other then 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)[a] | 5(A2, F7.5) | 1 to 45 |
| | (2) Relative weight[b] 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[a], 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) | F8.5 | 64 to 71 |
| | (7) F if fuel or O if oxidant | A1 | 72 |
| | (8) Density in g cm$^{-3}$ (optional) | F8.5 | 73 to 80 |
| Last | Blank | | |

[a]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.)

[b]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.                                          100.    0.        G298.15  F
N .7808810 .209795AR.004682                   100.    -7.202164G298.15  0


REACTANTS
N 1.     H 4.     CL1.     O 4.               72.06   -70730.   S298.15  F
C 1.     H 1.869550 .0312565 .008415          18.58   -2999.082L298.15  F
AL1.                                          9.00    +0.0      S298.15  F
MG1.     O 1.                                 .20     -143700.  S298.15  F
H 2.     O 1.                                 .16     -66317.4  L298.15  F


REACTANTS
H 2.                                  .00     100.    0.        G298.15  F
O 2.                                  .00     100.0   0.0       G298.15  0


REACTANTS
N 2.     H 8.     C 2.                        50.0    12734.8   L298.15  F  .786
N 2.     H 4.                                 50.0    12050.    L298.15  F 1.002
F 2.                                          100.    -3030.892L 85.24   0 1.54


REACTANTS
LI1.                                          100.    0.        S298.15  F
F 2.                                          100.    -3030.892L 85.24   0 1.54


REACTANTS
N 2.     H 4.                                 80.     12100.    L298.15  F 1.003
BE1.                                          20.     0.0       S298.15  F 1.85
H 2.     O 2.                                 100.    -44880.   L298.15  0 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 (ERATIØ 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 MIX array is used as described in Reference 9.

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, $NH_3(g)$ is in the set of THERMØ data but $NH_3(\ell)$ is not. Therefore, if $NH_3(g)$ is used as a reactant its enthalpy could be calculated automatically, but that of $NH_3(\ell)$ could not be.
2. The temperature T must be in the range $T_{low}/1.2 \leq T \leq T_{high} \times 1.2$ where $T_{low}$ to $T_{high}$ is the temperature range of the THERMØ data.

For cases with 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 $i^{th}$ zone the $i^{th}$ DELH entry will be added to the system

enthalpy as computed by ØDE 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 ØMIT and INSERT Cards

ØMIT 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 ØMIT (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 THERMØ data.

#### 6.4.2.1 ØMIT Cards

These cards list species to be omitted from the THERMØ data. If ØMIT cards are not used, the program will consider as possible species all those species in the THERMØ 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 ØMIT 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 descrited 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)

RKT problem. - Only one value for chamber pressure, P, is to be input for cases with NZØNES > 1 (see $DATA input, Section 6.3). The stagnation pressure used for the $i^{th}$ zone will be the value input for P multiplied by the $i^{th}$ value input in the schedule XP. If not input, all XP entries are assumed equal to one. For TDK type

problems, zone one is taken about the nozzle axis of symmetry and the last zone is bounded by the nozzle wall. Similarly, the $i^{th}$ zone will have a mixture ratio equal to the $i^{th}$ entry in the ØFSKED 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 FRØZ = F or EQL = F are input. If FRØZ = F, only equilibrium performance will be calculated. If EQL = F, only frozen performance will be calculated.

TABLE 6-9 VARIABLES IN SØDE NAMELIST

| Variable | No. of entries | Type | Value before read | Definition and comments |
|---|---|---|---|---|
| RKT | 1 | L | False | Rocket problem[a] |
| 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 | [a]Values in P array are in $N/m^2$ |
| PSIA | 1 | L | False | [a]Values in P array are in psia units |
| XP | 50 | R | 1. | Multipliers for the $i^{th}$ zone stagnation pressure (zone 1 = inner zone) |
| ØF | 1 | L | False | Oxidant to fuel weight ratios are to be input[a] |
| ERATIØ | 1 | L | False | Equivalence ratios are to be input[a] |
| FPCT | 1 | L | False | Percent fuel by weight are to be input[a] |
| FA | 1 | L | False | Fuel to air weight ratios are to be input[a] |
| ØFSKED | 50 | R | 0 | For a Rocket problem, and NZØNES ⩾ 1, ØFSKED will be used rather than MIX (see Reference 9). Relative amounts of total oxidant to total fuel are input as defined by ØF, ERATIØ, 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 $DATA, rerun the ØDE, ØDK, TDK (or TDE) analysis. Same units as DELH. |

[a]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 th entry of XP will be used for the stagnation pressure of the i th zone.

Table 6-9 (cont'd)

| Variable | No. of entries | Type | Value before read | Definition and comments |
|---|---|---|---|---|
| IØNS | 1 | L | False | Consider ionic species[a] |
| 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.[a] |
| EQL | 1 | L | True | Calculate rocket performance assuming equilibrium composition during expansion[b]. |
| FRØZ | 1 | L | True | Calculate rocket performance assuming frozen composition during expansion[b]. |
| LISTSP | 1 | L | False | List names and dates of all species residing on thermodynamic data used[a]. |
| KASE | 1 | I | 0 | Optional assigned number associated with case. |

[a]If variable is set to be true.

[b]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 b 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 wit 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 will be computed by the program and need not be input.

| Item | Description | Assumed Value(s) |
|---|---|---|
| VARMIX= | If VARMIX=.FALSE., do not use variable mixture ratio option.<br><br>If VARMIX=.TRUE., the variable mixture ratio option is to be used. The following must be input:<br>NZØNES in $DATA,<br>ØFSKED(1) in $ØDE and<br>STREAM(1) in $ØDE, below. | F |
| STREAM(1)= | If VARMIX=.TRUE., values must be input here corresponding to the O/F values input in ØFSKED(1).<br><br>The values input represent<br>$(O/F)_i$ vs $\psi_i$ i=1,...,NZØNES<br>where i represents the mass flow between streamline i and the axis, divided by the total mass flow.<br>Thus<br>$\psi = 0$ at the axis, and<br>$\psi = 1$ at the wall.<br>The ith entry of ØFSKED is $(O/F)_i$.<br>The ith entry of STREAM is $\psi_i$<br>$0 \leq \psi_i \leq 1$ i =,...,NZØNES = 50<br>and $\psi_i < \psi_{i+1}$ | - |

### 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 (see the punched card listing given at the end of the sample output, Section 7).

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 IØFF=4. The use of IØFF 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 $ØDE Namelist input:

| Item Name | | Description |
|---|---|---|
| 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 6-8). |
| IØFF | = | The first point to be punched will be numbered as IØFF+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, THETAI, 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 ØDK INPUT DATA

ØDK input data is required if ØDK =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 |
| $ ØDK | data group |

These data groups are described below in sections 6.5.1, 6.5.2, and 6.5.3, respectivly.

### 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 probelm type are discussed below.

ØDK

For ØDK problems species names and concentrations must be input, see Section 6.5.1.1.

ØDE-ØDK

For ØDE-ØDK problems the initial start conditions for the kinetic expansion are obtained from an equilibrium calculation. The species list generated by

the equilibrium calculation generally contains many more species than the 40 species for which the ØDK subprogram is dimensioned. Therefore a selection processes 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 ØDE-ØDK-TDK problems species are selected by the above rules for ØDE-ØDK problems. However, for multizone TDK cases it is necessary that each zone have the same species list. Thus the INERTS input (see Section 6.5.2.7) must be used to assure the same species are selected for each zone.

TDK with Input Initial Line Option

Species names and concentrations must be input as described in Section 6.8.2 when TDKIL =1 is input in $DATA.

### 6.5.1.1 ØDK OPTION FOR INPUT OF INITIAL SPECIES CONCENTRATIONS (APPLIES ONLY TO THE ØDK PROBLEM TYPE)

This input begins with a single card with SPECIES in columns 1 through 7 and with either MASS FRACTIØNS or MØLE FRACTIØNS 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 5-4 (condensed species, however, may not be specified in the species list.) The species symbol may not contain the characters * or =.

| Col | Function |
|---|---|
| 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 |

### 6.5.2 REACTIØNS

Chemical reactions must be input if ØDK =1 or TDK =1 in $DATA.

Up to 50 reactions with an implied third body and a total 150 reactions may by 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). A card listing for a sample reaction set is presented in Table 6-10.

The symbolic reaction set contains directive cards and reaction/data cards in groups as outlined below:

| | |
|---|---|
| REACTIØNS | Directive for start of symbolic reaction input |
| . | |
| . | Reactions with implied third body speices |
| 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 BØDY REAX RATE RATIØS | Directive for start of third body reaction rate ratios |
| . | |
| . | Third body reaction rate ratios |
| . | |
| LAST CARD | Directive for end of REACTIØNS input |

The content and format of each type of card is defined as follows:

6.5.2.1 The symbolic reaction set begins with a card containing the word REACTIØNS in columns 1 through 9. Other columns on this card can be used for comments.

6.5.2.2 Each card defining a reaction is divided into five fields, separated by commas. Each field contains:

| | | |
|---|---|---|
| field 1 | a reaction | |
| field 2 | A = followed by a value of A | rate parameters for the reaction |
| field 3 | N = followed by the value of N | |
| field 4 | B = followed by the value of B, the activation energy (Kcal/mole) | |
| field 5 | available for comments | |

The general form of a reaction is:

$$N_1 \text{*Symbol}_1 + N_2 \text{*Symbol}_2 + \ldots = N_a \text{*Symbol}_a + N_b \text{*Symbol}_b + \ldots$$

where the left hand side represents reactants and the right hand side represents products. The reaction can be either endothermic or exothermic.

The multipliers, N, must be integers and represent stoichiometric coefficients. If no stoichiometric coefficient is given, the value 1 is assumed. The dimensioning currently in the program requires that:

$$N_1 + N_2 + \ldots . \leq 10$$

and

$$N_a + N_b + \ldots . \leq 10$$

The chemical species (denoted by the word "symbol" in the above general form) can contain up to 12 characters each of which must match a species name contained in the thermodynamic data (see Table 6-2, card 3).

examples:

| Reaction | Interpretation |
|---|---|
| NA++CL-=NACL | $Na^{+} + Cl^{-} = NaCl$ |
| B+2+Ø-2=BØ | $B^{++} + Ø^{--} = BØ$ |
| BE+2+2*ØH-=BEØHØH | $Be^{++} + 2ØH^{-} = Be(ØH)_2$ |

The value assigned to A, N, B define the forward (i.e. left to right) reaction rate, k, as

$$k = A \cdot T^{-N} \cdot e^{-(1000B/\mathcal{R}T)}$$

in units of cc, °K, mole, sec.

All three reaction rate parameters must be input. The numeric value of each parameter may be specified in either I, F, or E format. If E format is used the E must appear before the exponent.

6.5.2.3 The reactions with an implied third body must precede other types of reactions, and must be followed by the directive (columns 1 through 12):

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.

H2 = H + H, . . .

END TBR REAX

defines the chemical reaction

$$H_2 + M = H + H + M$$

where M is a generalized third body. Specific third body effects may be included by inputing specific third body reaction rate ratios as outlined in 6.5.2.8. Cards encountered after the END TBR REAX directive card do not have a third body term added.

All other reactions are input next, exactly as described under 6.5.2.2.

6.5.2.4 After the last reaction has been defined, a card with LAST REAX in columns 1 through 9 is input.

6.5.2.5 Reaction rate data for 13 dissociation-recombination (implied third body) reactions and 35 binary exchange reactions are listed in Table 6-10 for propulsion systems containing elements C, Cl, F, N and O. These rates are taken from Reference 16 (two additional reactions from Reference 15 are included). Cards can be abstracted from Table 6-10 for input to the computer program. For the implied third body reactions, the third body for which the rate applies is indicated in parenthesis in the comment field (M represents a "generalized" third body, see Section 2.2 for further details).

6.5.2.6 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 written exactly as in the master Thermodynamic Data. The last comma must be followed by the word END. See Table 6-11 for an example. The species list can continue on to the next card, but a species name can not overlap onto the next card.

6.5.2.7 THIRD BODY REACTION RATE RATIOS

As described above in Section 6.5.2.2 for the $j^{th}$ reaction only one reaction rate, $k_j$, where

$$k_j = AT^{-N_j} e^{-B_j/RT} ,$$

can be input. For three body recombination reactions such as

$$H + \emptyset H + M_i = H_2\emptyset + M_i$$

the rate of reaction is in general different for each species, $M_i$, depending upon the efficiency of the species, $M_i$, as a third body collision partner. As discussed in Section 2.2 the temperature dependance of a recombination rate is approximately independant of the third body, i.e. for the $i^{th}$ third body and $j^{th}$ reaction:

$$k_{ij} \doteq A_{ij} T^{-N_j} e^{-B_j/RT}$$

The third body efficiency of the $i^{th}$ species for the $j^{th}$ reaction is then defined as

$$m_{ij} = A_{ij}/A_j$$

TABLE 6-10 REACTIONS AND RATE DATA FOR C, CL, F, H, N, AND O SYSTEMS
(FROM REFERENCE 16)

```
REACTIONS CCLFHNO    MAY 7=4 1972   JANNAF PSHG      RATE=A*T**N*EXP(-1000B/RT)
   H + OH  = H2O     , A=7.5E23 , N=2.6 , B=0.,                    (AR)  NO.  1
   O + H   = OH      , A=4.0E18 , N=1.  , B=0.,                    (AR)  NO.  2
   O + O   = O2      , A=1.2E17 , N=1.  , B=0.,                    (AR)  NO.  3
   F + F   = F2      , A=5.7E15 , N=1.  , B=0.,                    (AR)  NO.  4
   H + F   = HF      , A=2.5E18 , N=1.  , B=0.,                    (AR)  NO.  5
   H + H   = H2      , A=6.4F17 , N=1.  , B=0.,                    (AR)  NO.  6
     CO2   = O + CO  , A=2.7E32 , N=4.5 , B=127.555,               (N2)  NO.  7
   C + O   = CO      , A=3.0E16 , N=.5  , B=0.,                    (M)   NO.  8
   N + N   = N2      , A=1.0E18 , N=1.  , B=0.,                    (M)   NO.  9
   N + O   = NO      , A=6.4F16 , N=.5  , B=0.,          BAULCH    (N2)  NO. 10
  CL + F   = CLF     , A=3.0E16 , N=.5  , B=0.,                    (M)   NO. 11
   H + CL  = HCL     , A=3.0E18 , N=.5  , B=0.,                    (M)   NO. 12
  CL + CL  = CL2     , A=1.1E19 , N=1.  , B=0.,                    (M)   NO. 13
END THR REAX
   H2 + OH  = H + H2O  , A=2.18E13, N=0.  , B=5,14,          BAULCH  NO. 21
   OH + OH  = O + H2O  , A=5.75E12, N=0.  , B=.78,           BAULCH  NO. 22
   H + OH   = O + H2   , A=7.33E12, N=0.  , B=7.300,         BAULCH  NO. 23
   O + OH   = H + O2   , A=1.3F13 , N=0.  , B=0.,            BAULCH  NO. 25
   OH + CO  = H + CO2  , A=5.6E11 , N=0.  , B=1.0R0,         BAULCH  NC. 41
   O2 + CO  = O + CO2  , A=8.4SE9 , N=.65A, B=45.920,        BAULCH  NO. 42
    N + NO  = O + N2   , A=3.1F13 , N=0.  , B=.3J4,          BAULCH  NO. 48
    N + O2  = O + NO   , A=6.43E9 , N=1.  , B=6.250,         BAULCH  NO. 51
   OH + OH  = H2 + O2  , A=1.41E13, N=.015, B=49.264,                NO. 24
    H + F2  = HF + F   , A=5.3F12 , N=.5  , B=4.000,                 NO. 26
   H2 + F   = HF + H   , A=5.0E12 , N=0.  , B=5.700,                 NO. 27
   H2 + F2  = HF + HF  , A=1.79E10, N=.5  , B=39.739,                NO. 28
    H + CL2 = HCL + CL , A=3.0F14 , N=0.  , B=3.000,                 NO. 29
   H2 + CL2 = HCL + HCL, A=1.79E10, N=.5  , B=45.375                 NO. 30
   HCL + H  = H2 + CL  , A=6.2E11 , N=.5  , B=3.100,                 NO. 31
   HCL + F  = HF + CL  , A=1.9F12 , N=.68, B=.600,                   NO. 32
   CL2 + F  = CL + CLF , A=6.2E12 , N=.6A, B=.500,                   NO. 33
   CL + F2  = F + CLF  , A=7.6E12 , N=.6A, B=.300,                   NO. 34
   CLF + H  = HF + CL  , A=1.8E12 , N=.68, B=3.200,                  NO. 35
   CLF + H  = HCL + F  , A=5.6E12 , N=.68, B=1.900,                  NO. 36
   CLF + H2 = HCL + HF , A=1.8E10 , N=.5  , B=46.337,                NO. 37
   F2 + HCL = HF + CLF , A=1.6E10 , N=.5  , B=39.427,                NO. 38
   CLF + HCL = HF + CL2, A=1.8E10 , N=.5  , B=46.025,                NO. 39
   F2 + CL2 = CLF + CLF, A=1.8E10 , N=.5  , B=26.758,                NO. 40
   CO2 + C  = CO + CO  , A=1.1E11 , N=.5  , B=6.995,                 NO. 43
    C + OH  = CO + H   , A=5.3E11 , N=.5  , B=5.62A,                 NO. 44
    C + NO  = CO + N   , A=5.3E11 , N=.5  , B=A.303,                 NO. 45
   CO2 + N  = CO + NO  , A=1.1E11 , N=.5  , B=59.618,                NO. 46
    C + O2  = CO + O   , A=5.3E11 , N=.5  , B=6.552,                 NO. 47
   NO + NO  = N2 + O2  , A=1.0F13 , N=0.  , B=79.490,                NO. 49
    N + OH  = NO + H   , A=5.3F11 , N=.5  , B=5.62H,                 NO. 50
   OH + F   = HF + O   , A=2.9E12 , N=.6A, B=.200,                   NO. 52
  H2O + F   = HF + OH  , A=1.4F10 , N=.6A, B=.600,                   NO. 53
  HCL + OH  = H2O + CL , A=1.0F11 , N=.5  , B=6.0,
   OH + CL  = HCL + O  , A=5.0E11 , N=.5  , B=6.0,
LAST REAX
```

Thus $m_{ij}$ is the ratio of the reaction rate with species $M_i$ as the third body to the reaction rate input on the reaction card described in Section 6.5.2.2.

If reaction rate ratios, $m_{ij}$, are to be input for the dissociation-recombination reactions, a card with THIRD BØDY REAX RATE RATIØS 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 SPECIES cards as described below:

The $m_{ij}$, can be input using a card with the word SPECIES in columns 1 through 7. This word is followed by the name of the $i^{th}$ species followed by a comma, followed by the values $m_{ij}$ in F format, each followed by a comma. These $m_{ij}$ values can be continued onto succeeding cards. Note that the $m_{ij}$ values depend on the order of input of the reaction cards, i.e. the $j^{th}$ reaction is defined by the $j^{th}$ card input after the REACTIØNS card.

Table 6-11 gives a sample input for a Hydrogen/Oxygen system using third body reaction rate ratios. In this example the three body recombination rates are input with Argon as the third body. The rate with $H_2$ as a third body is a factor of 5 larger then with Ar as a third body for the first three reactions and a factor of 4 larger for the fourth (Hydrogen recombination) reaction.

6.5.2.9 At this point in the data input deck a card with LAST CARD in columns 1 through 9 must be input.

TABLE 6-11 LISTING OF SAMPLE REACTIONS CARDS FOR AN $O_2/H_2$ PROPELLANT

```
REACTIONS    O-H      MAY 3-4 1972  JANNAF PSWG
   H + OH  = H2O      , A=7.5E23 , N=2.6 , B=0.,        (AR) NO.
   O + H   = OH       , A=4.0E18 , N=1.  , B=0.,        (AR) NO.
   O + O   = O2       , A=1.2E17 , N=1.  , B=0.,        (AR) NO.
   H + H   = H2       , A=6.4E17 , N=1.  , B=0.,        (AR) NO.
END TBR REAX
  H2 + OH  = H + H2O  , A=2.19E13, N=0.  , B=5.15,   BAULCH NO. ;
  OH + OH  = O + H2O  , A=5.75E12, N=0.  , B=.78,    BAULCH NO. ;
   H + OH  = O + H2   , A=7.33E12, N=0.  , B=7.30,   BAULCH NO. ;
   O + OH  = H + O2   , A=1.3E13 , N=0.  , B=0.,     BAULCH NO. ;
LAST REAX
!NERTS N2,AR,END
THIRD BODY REAX RATE RATIOS
SPECIES AR,1.,1.,1.,1.,
SPECIES H2,.5,.5,.5,.4,
SPECIES H2O,20.,5.,5.,20.,
SPECIES O2,5.,5.,4.5,1.5,
SPECIES N2,4.,4.,4.,1.5,
SPECIES H,12.5,12.5,12.5,25.,
SPECIES O,12.5,12.5,12.5,25.,
SPECIES OH,12.5,12.5,12.5,25.,
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 or TDK = 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.

| Item | | Description | Units | Assumed Value(s) |
|---|---|---|---|---|
| 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

$$\left| \frac{(\rho VA)_{N+1} - (\rho VA)_N}{(\rho VA)_{N+1}} \right| < \text{CØNDEL}$$

where CØNDEL 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.

| Item | | Description | Units | Assumed Value(s) |
|---|---|---|---|---|
| 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 |

| Item | | Description | Units | Assumed Value(s) |
|---|---|---|---|---|
| TEXPLI | = | temperature below which explicit integration will start. Not recommended. | $^{o}R$ | 0 |
| CØNDEL | = | relative error criterion for continuity check for supersonic flow | none | $1x10^{-6}$ |
| JF | = 0 | all variables considered for step size control | none | 0 |
| | = 1 | only fluid dynamic variables considered for step size control, i.e., ρ,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:

| Item | | Description | Assumed Value(s) |
|---|---|---|---|
| JPRNT | = -2 | print throat and input area ratios (see ARPRNT) | -2 |
| | = -1 | print at internally set area ratios 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,...,38,40,42,...,58,60,64,...116,120,128,...,200,210, 220,...,400

If JPRNT is +1 or +2, the following must be input:

| Item | | Description | |
|---|---|---|---|
| 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:

| Item | | Description | |
|---|---|---|---|
| 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 ≤ 100. | - |

An extended print option may be selected as follows:

| Item | Value | Description | |
|---|---|---|---|
| IDYSCI | = 0 | no extended print requested | 0 |
| | = 1 | extended print option selected (not suggested) | |

### 6.5.3.4 SPECIES SELECTION AND MOLE/MASS FRACTION CHECK

In order to interface ØDE 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 (6.5.2.6).

The relative selection criterion (ØDK or 1 Zone TDK problems,) is described below:

| Item Name | | Function |
|---|---|---|
| EPSEL | = | all species which do not appear explicitly in the reaction set but whose mole fractions are greater then 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.

| Item Name | | Function |
|---|---|---|
| XMFTST | = | Input species concentrations are summed and checked versus unity using this input criterion. If $\left\| 1 - \sum \text{species concentrations} \right\| < \text{XMFTST}$ 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 ØDK PROBLEM INPUT

This input is required when PROBLEM ØDK is specified on the problem card. 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 ØDK problem requires input of those items described in sections 6.5.1 and 2.

| Item Name | | Input Quantity | Units | SI Units |
|---|---|---|---|---|
| PC | = | chamber pressure | PSIA | $N/M^2$ |
| 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:

| Item Name | | Input Quantity | Units | SI Units |
|---|---|---|---|---|
| PI | = | initial pressure | PSIA | $N/M^2$ |
| PESTAR | = | throat pressure | PSIA | $N/M^2$ |

For JPFLAG = 1 option the following must be input:

| Item Name | | Input Quantity | Units |
|---|---|---|---|
| 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

### 6.5.3.6 MASS AVERAGED ØDK ISP

A mass averaged ØDK ISP summary page may be obtained at the end of the ØDK calculations as described below:

| Item Name | | Description |
|---|---|---|
| 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 MØC problem has been specified, the input data set $TRANS is required for the transonic calculation.

| Item | | Description | Assumed Value(s) |
|---|---|---|---|
| $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 $ØDK). | 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 (RWTD = 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:

| Item | Description | Assumed Value(s) |
|---|---|---|
| MP | Number of points to be placed on the initial line. MP 275. A sinusiodal distribution of the following form is used: $r_i = [r_w \sin(\frac{i}{N}\frac{\pi}{2})]^{\varepsilon_1}$ $i = 0,1,2....N$ where N = MP and $\varepsilon_1$ is EXP1 described below. Editing is done to control the spacing, see DRMIN. | 50 |

| Item | | Description | Assumed Value(s) |
|---|---|---|---|
| EXP1 | = | $\varepsilon_1$ 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<br><br>$r_w - r_1 > \min [DRMIN * RWTD, .025]$<br><br>If a value of DRMIN is to be input in \$INC, then set DRMIN=.01 | .01 |
| DRMIN1 | = | Editing criteria for sinusoidal distribution. Points on the initial line will be spaced such that<br><br>$r_n - r_{n-1} > DRMIN1$ | $5*10^{-4}$ |
| \$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 Inputs from SDER
6.7.3 Print Control
6.7.4 Exit Plane Option

Often no $MOC input is necessary since the default values are usually sufficient.

6.7.1 Characteristics Mesh Control

| Item Name | | Input Quantity | Units | Assumed Values |
|---|---|---|---|---|
| SMOC | = | 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. | none | .15 |
| DWWI | = | insertion control parameter $\Delta\theta_\omega$ described in Section 5.9.2. | degrees | 2. |
| EPW | = | the program will insert such that the wall end point is located within a tolerance EPW. | none | .01 |
| IMAX | = | the maximum number of interations to be allowed while attempting to achieve a relative convergence for the flow variables of $5*10^{-5}$. | none | 10 |
| IMAXF = 1 | | the program will terminate the case if a printed point requires maximum iterations for convergence. | none | 0 |
| or | | | | |
| IMAXF = 0 | | program will continue the case after IMAX iterations per point have occurred | | |
| TEXPLI | = | input temperature below which explicit integration for the species concentrations will be used. | °R, °K if SI Units | |
| ETHI | = | $\epsilon_\theta$ for point editing as described in Section 5.9.2, CNTRL. | degrees | .25 |
| ES | = | $\epsilon_s$ for point editing as described in Section 5.9.2, CNTRL. | none | .005 |
| DTWI | = | $\Delta\theta_{t\omega}$ criterion for insertion in subroutines INPT, DSPT as described in Section 5.9.2, CNTRL. | degrees | 2. |

### 7.1.1 MOC Shock Option

If the MOC shock option is requested (SHØCK=1), then the mesh construction begins at the intersection of the initial data line and the nozzle wall. RRC's are constructed. Successive RRC's emanating from the wall 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.

| ITEM NAME | INPUT QUANTITY | ASSUMED VALUE |
|---|---|---|
| SHØCK= | If SHØCK=0, shocks will be ignored and the MOC flow field will use LRC construction.<br>If SHØCK=1, a shock will be inserted, and traced as described above. | 0 |
| ISHCK= | If ISHCK=1, no special action taken<br>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. | 1 |
| A= | Axial coordinate position on wall discussed under ISHCK, above. | 0 |

### 6.7.2 Print Control

| Item Name | | Input Quantity | Units | Assumed Values |
|---|---|---|---|---|
| N1 | = | flow parameters will be printed for every N1$^{th}$ interior point along characteristics selected for print | none | 1000 |
| N2 | = | every N2$^{th}$ 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-$^{o}$R), and enthalpy ($ft^2/sec^2$) 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<br>MASSFL = 0 then no mass flow printed<br>MASSFL = 1 then total mass flow and the number of points on the LRC are printed for each LRC<br>MASSFL = 2 then mass flow for each point along LRC is printed<br>MASSFL = 3 Same as MASSFL = 2 with the addition of execution time at the end of each LRC<br>see Section 5.8.1, CHAR | none | 1 |
| NDS | = | for NDS = 1 Dividing Streamline Points will be printed. (Nominal)<br>for NDS = 0 Dividing Streamline Points will be suppressed. | none | 1 |

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6.7.3 Inputs from DER, Reference 10.

| Item Name | | Input Quantity | Units |
|---|---|---|---|
| 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) |

### 6.7.4 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.

| Item | | Description | Assumed Value(s) |
|---|---|---|---|
| EXITPL | = | Exit plane calculation requested if set .TRUE. not operational for shock option.<br><br>For the case when two TDK runs are to be made, i.e., when<br><br>IRPEAT = 1, or 2 in $DATA<br><br>then the exit plane will be computed for the second TDK run, but not for the first TDK run. | .FALSE. |

### 6.7.5 Punch Initial Line

During any calculation generating an initial line, the initial line may be punched in a form suitable for running an input initial line option. The following input is required.

| Item | | Description | Assumed Value(s) |
|---|---|---|---|
| ILPUCH | = | Requests Punching of Initial Line if set .TRUE. | .FALSE. |
| IPUNIT | = | The Fortran unit number assigned to the PUNCH. (e.g., on Univac 1108 INPUNIT = -3, on the other machines it may be 7, 8, etc.) | |

IMPORTANT NOTE

If IPTAB = 1 option is selected, i.e., the boundary layer edge conditions punched for TBL input, the initial line punched cards will be interspersed with the TBL edge conditions punched cards.

$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 ØDE and/or MØC 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.

| Item | | Description | Units | Assumed Value(s) |
|---|---|---|---|---|
| $BLM | = | Namelist name, read in Subroutine INPUTB | | |
| ITYPE | = | flag to specify the type of body geometry | | 1 |
| | = 1, | for an axisymmetric nozzle, required by TDK | | |
| | = 2, | for an axisymmetric external flow | | |
| | = 3, | for a two-dimensional external flow starting at a stagnation point. | | |
| WDØT2D | = | $\dot{w}_{2D}$, 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. |

### 6.8.1 BLM Gas Properties

Gas properties that are required by the BLM are $\gamma$, $C_p$, and $\mu$ versus T, and a value for the Prandtl number, $P_r$.

If tables for $C_p$ and $\gamma$ are not input (see CPO, CKO, and TO, below) then the program will prepare these tables using the ØDE module. The tables are prepared using a series of (T,S) equilibrium calculations, where T varies from 600°R to 7000°R at 200°R increments. The chamber entropy value is used for S. Values at 100°R are then extrapolated and added to the table. The table is printed with the BLM output.

If constants defining the gas viscosity, $\mu$, and if the Prandtl number, $P_r$, are not input, then they will be transmitted from the ODE module.

If the TD2P and ØDE modules have not been run, then the data listed below must be input.

| Item | | Description | Units | Assumed Value(s) |
|---|---|---|---|---|
| CKO(1) | = | table of ratio of specific heats, $\gamma$, versus T. | none | 101*1.4 |
| CPO(1) | = | table of specific heat at constant pressure, $C_p$, versus T | ft/sec-R | 101*6006 |
| TO(1) | = | temperatures corresponding to the entries in CKO and CPO arrays, above | °R | 300,...,7000 |

| Item | | Description | Units | Assumed Value(s)* |
|---|---|---|---|---|
| NTAB | = | number of values entered in CKO, the CPO, and TO arrays. $3 \leq$ NTAB. $\leq 101$. | - | 24 |
| RMUI | = | Reference viscosity, $\mu_o$, where viscosity is expressed as $\mu = \mu_o(T/T_o)^{\omega}$ | lbm/ft-sec | .25*10$^{-4}$ |
| TI | = | reference temperature, $T_o$, for viscosity. See RMUI, above. | $^oR$ | 1500. |
| ØMEGA | = | Viscosity exponant, $\omega$. See RMUI, above. | - | |
| PR | = | Molecular Prandtl number, $P_r$ | - | .72 |

* The assumed values for RMUI, TI, ØMEGA, PR, CPO, and CKO 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 specifed 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 201 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 $y, U_e, T_e, P_e, T_w$ (or $c_w$), and $(\rho V)_w$ are interpolated at the new x-stations and used in the boundary-layer calculations.

Values of RINO versus XINO 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.

| Item | | Description | Units | Assumed Value(s) |
|---|---|---|---|---|
| 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 | $^oR$ | - |
| PEØ(1) | = | $P_e$, gas pressure at the inviscid edge | psi | - |
| NXINØ | = | number of items in the XINØ, RINØ, UEØ, TEØ, and PEØ tables. $3 \leq NXINO \leq 201$ | | |

| Item | | Description | Units | Assumed Value(s) |
|---|---|---|---|---|
| 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.<br>IHFLAG = 0, for temperature<br>IHFLAG = 1, for heat flux* | - | 1 |
| TQW(1) | = | $T_w$, wall temperature or $\dot{q}_w$, wall heat flux, depending in IHFLAG.<br>For an adiabatic wall, set IHFLAG = 1 and all TQW(1) = 0.<br>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 negative. | $^{o}R$ or $\frac{BTU}{in^2\text{-sec}}$ | 201*0. |
| CQW(1) | = | $(\rho V)_w$, mass transfer parameter at the wall | $lbm/ft^2$-sec | 201*0 |
| NTQW | = | Number of axial stations, $X_w$. Each of the above tables must have this number of entries.<br>$3 \leq NTQW \leq 201$. | - | 3 |

* Default values are set for an adiabatic wall, i.e., IHFLAG = 1, and TQW(1) = 201*0.

6.8.3 Integration Step Size Control.

| Item | | Description | Units | Assumed Value(s) |
|---|---|---|---|---|
| NSEGS | = | Number of Segments, $1 \leq NSEGS \leq 10$ 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: $XSEG(i) = z_c + (z_m - z_c)\,(i-1)/NSEGS \quad i=1,2,\ldots NSEGS+1$ 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 on page 6-20. If the boundary layer is to be extended upstream of $z_c$, the usual procedure is to input XSEG(1) = XINØ(1) and XINØ(1) through XINØ(IOFF), etc., of $BLM are input by the user as described in $DATA under input item IØFF. | 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. NTR > $\sum$ NISPS(I). | none | 3 |

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, $h_w$(BTU/ft -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

$$\Delta H = \frac{1}{\dot{m}_T} \eta \int_{x_o}^{x_e} h_w dA \qquad \text{(BTU/lbm)}$$

where

$\dot{m}_T$ is the total engine mass flow rate

dA is the nozzle surface area differential, $2\pi r dx$

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.

DELH1(1) = $\Delta H$, $\Delta H$, .... 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.

| Item | | Description | Assumed Value(s) |
|---|---|---|---|
| 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:<br>ØFC(I) = 0. if there is no ith circuit<br>ØFC(I) = 1. if the Ith circuit is oxidizer<br>ØFC(I) = 2. if the Ith circuit is fuel<br>I $\leq$ 3 | 3*0 |
| DISTRB(1) | = | Flag for method of distributing ΔH increments<br>DISTRB(I) = 0. for equal distribution of heat to chamber<br>DISTRB(I) = 1. for distribution of ox heat to ox in chamber, and fuel heat to fuel in chamber.<br>The Ith entry is for the Ith circuit. | 3*1. |

* 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.

| Item | | Description | Assumed Value(s) |
|---|---|---|---|
| IPRØF | = | If IPRØF = 0, then supersonic area ratios are input in APRØF.<br><br>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

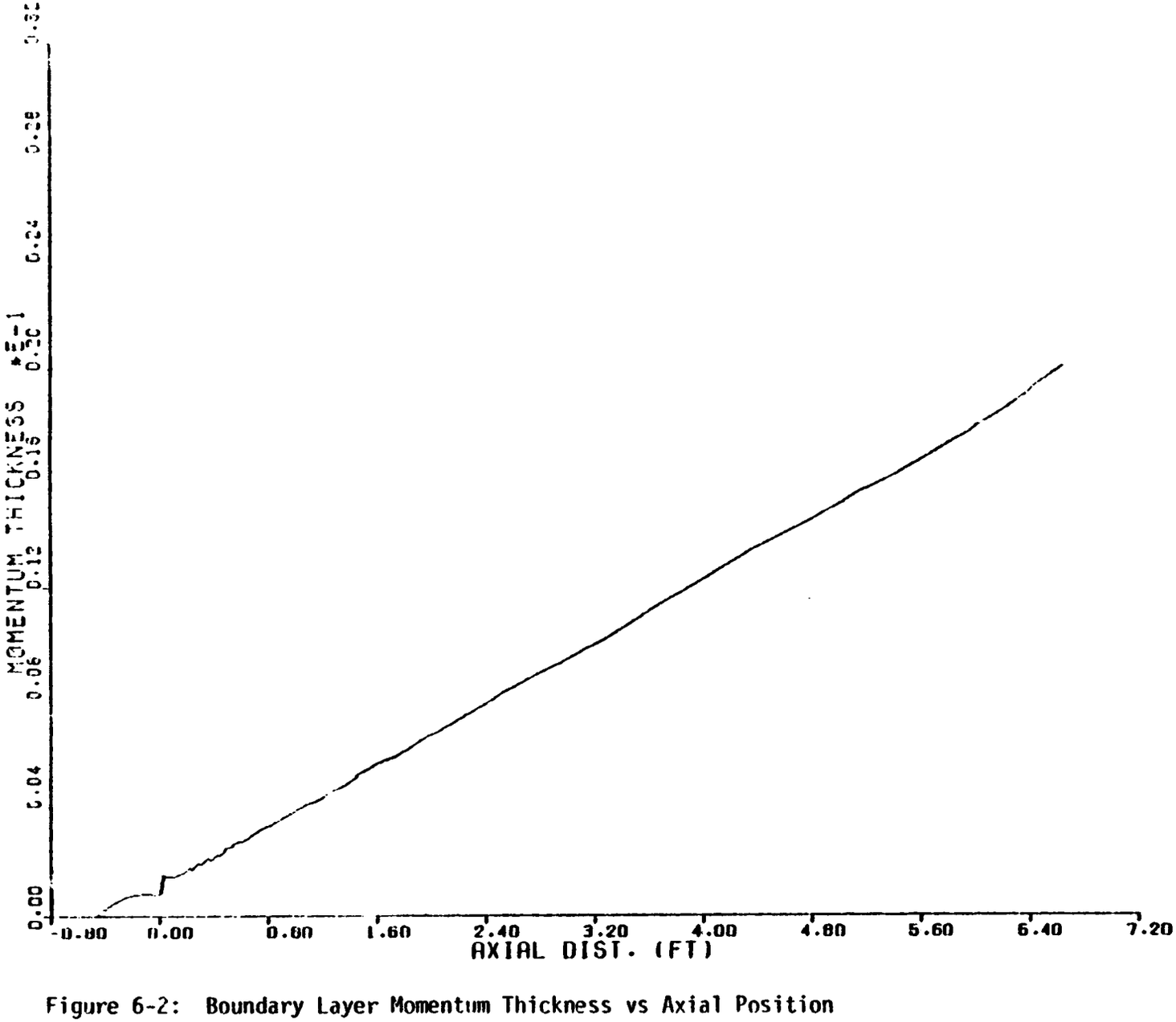


Figure 6-2: Boundary Layer Momentum Thickness vs Axial Position

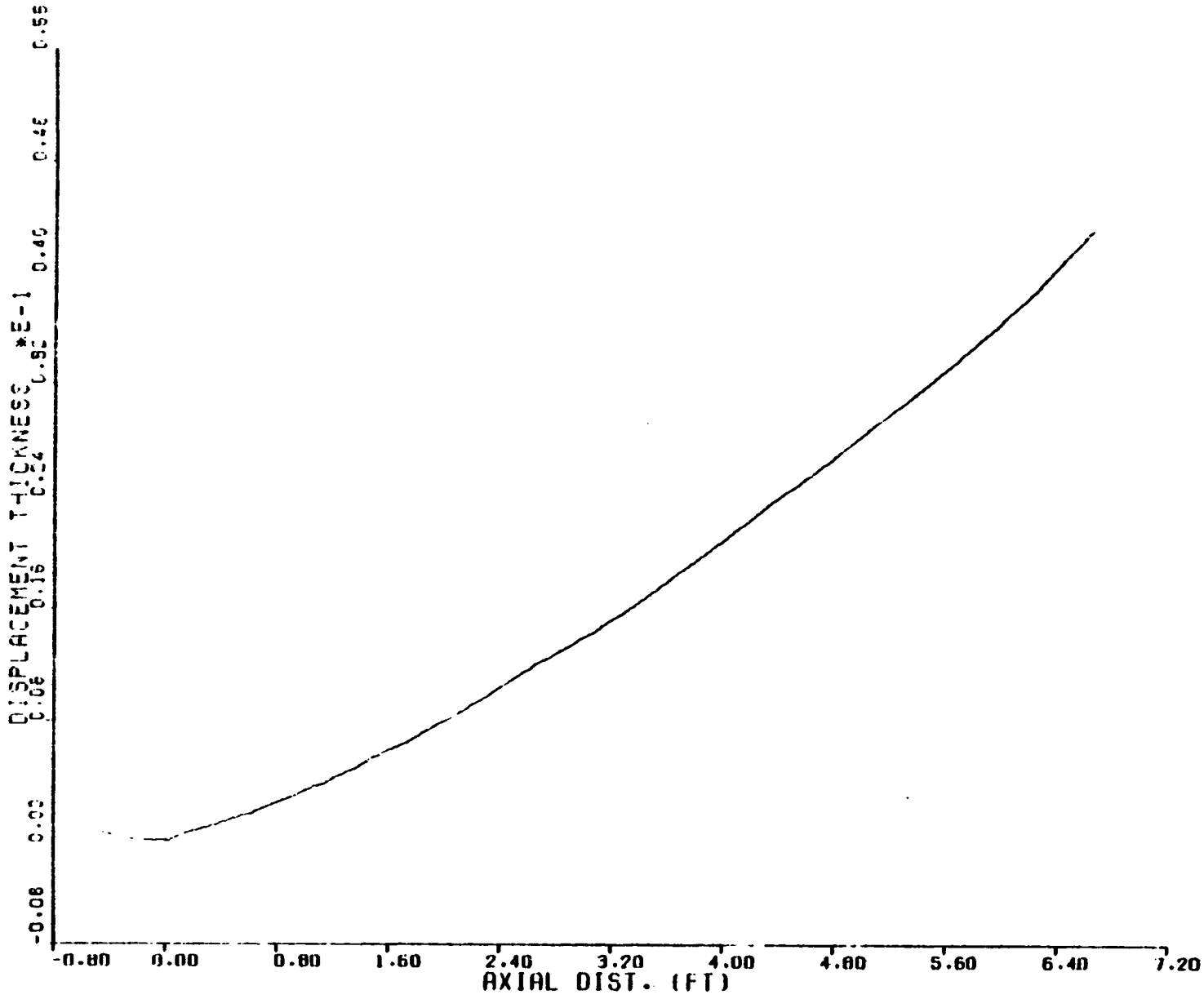


Figure 6-3: Boundary Layer Displacement Thickness vs Axial Position

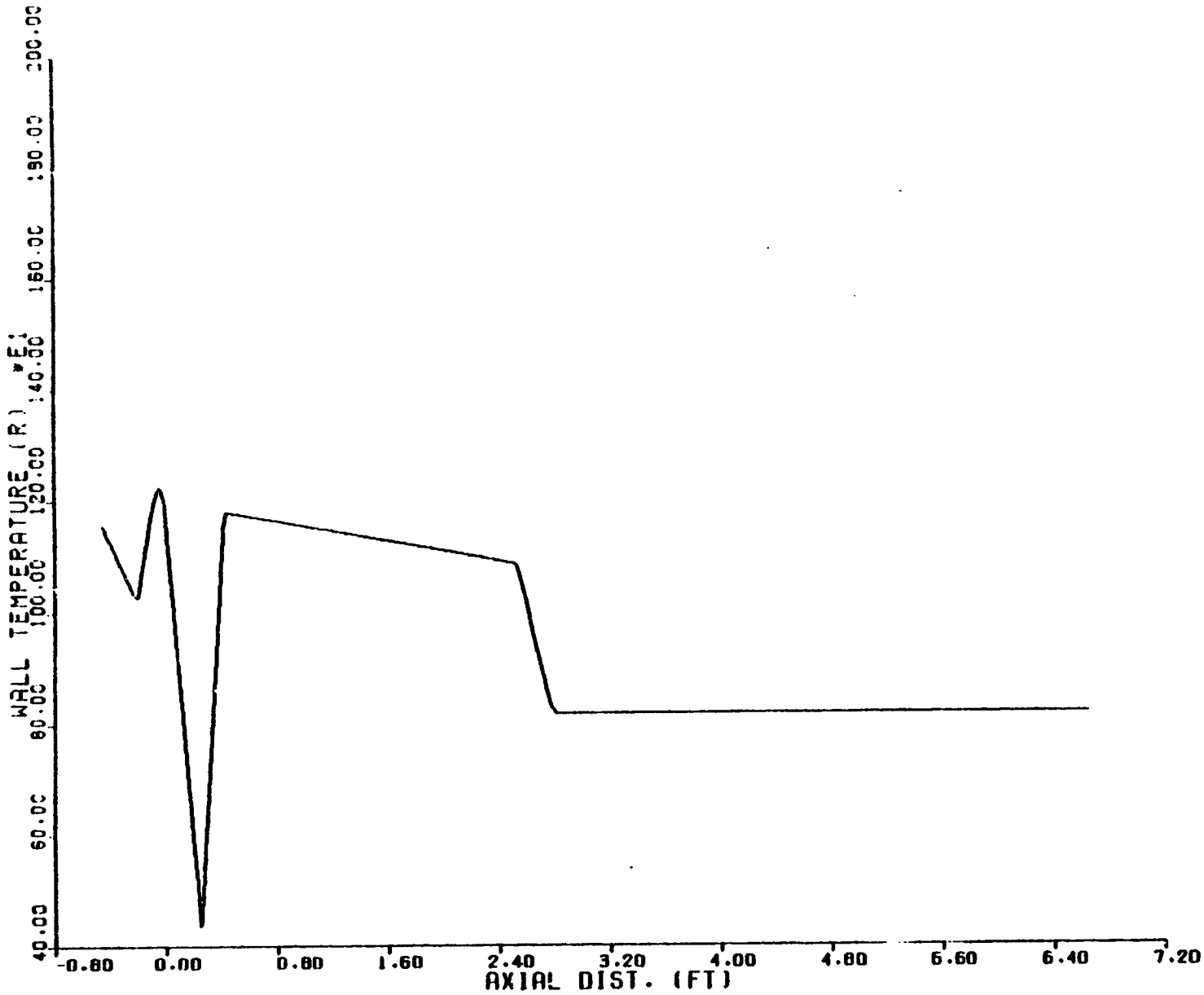


Figure 6-4: Wall Temperature (Input) vs Axial Position

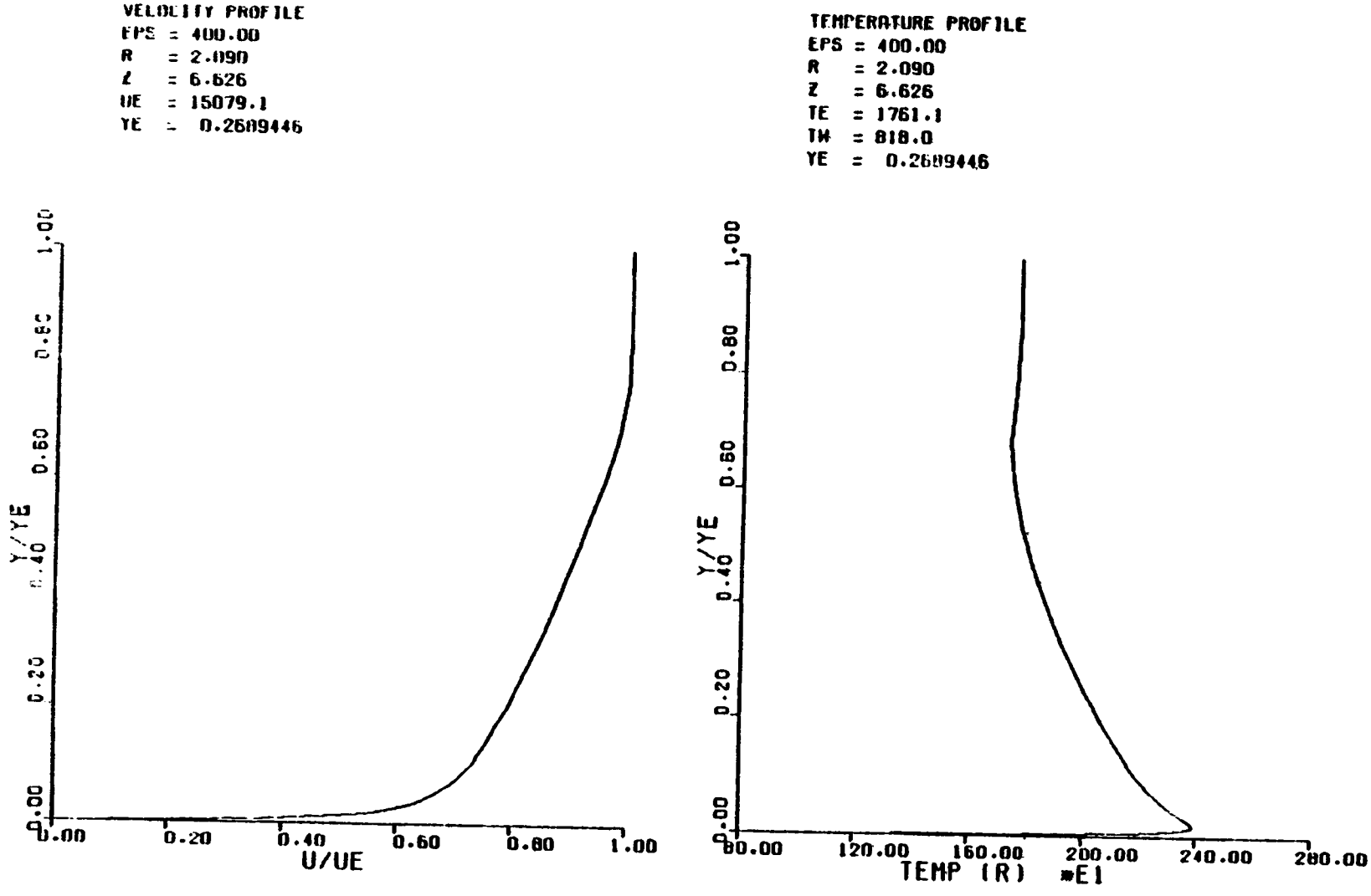


Figure 6-5: Velocity and Temperature Profiles at a Given Area Ratio

## 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 PFGØPT = 1 in $DATA. Sample input data for the constant properties gas option is listed in Table 6-12.

Only the $DATA, $TRAN and $MØC 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$^2$. (N/m$^2$ if SI units)

XP(1) = (From Table 6-9) All assumed = 1, if not input.

TC(1) = Chamber temperature, $^oR$, for each zone, inner to outer. ($^oK$ if SI units)

RGC(1) = Real gas constant, ft$^2$/sec$^2$ $^oR$, (i.e., $49721/M_w$ = g*J*1.986/$M_w$) for each zone, inner to outer. (m$^2$/sec$^2$ $^oK$ if SI unts)

WMW(1) = Gas Molecular Weight. If input then RGC(1) need not be input.

Table 6-12: Sample Case for the Constant Properties Gas Option.

```
TITLE SAMPLE CASE ONC
DATA
 $DATA
 PFSOPT=1,
 NZONES=1,
 RSI=2,
 RWTU=2, RATO=.5,
 THETA=35.8738,
 IWALL=4,
 NWS=11,
 RS(2)= 1.10343,1.26475,1.47910,1.73375,2.04940,2.45930,
        3.66220,4.84772,5.79198,6.32481,
 ZS(2)=  .30575, .53008, .82905,1.19473,1.66923,2.32795,
        4.68717,7.58599,10.9601,13.3114,
 THE=11.5813,
 $END
 $TRANS
 G=1.23,
 PSA=100,
 TC=5500,
 XMA=20,
 XM=1,
 ALI=0,
 $END
 $MOC
 $END
```

## 6.10 INITIAL VALUES FOR THE $ØDK, $TRANS, AND $TDK 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. |
| ECRAT | = | 0. |
| EQL | = | .TRUE. |
| EQTHST | = | .FALSE. |
| ERATIØ | = | .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(I) | = | 0. |
| XMFTST | = | 1.0E-3 |

$TRANS, set in subroutine TRAN

| | | |
|---|---|---|
| ALI | = | 0. |
| IBUG | = | 0 |
| MP | = | 50 |
| PMCRIT | = | 1. |
| PMDEG | = | 1. |
| XM(I) | = | 0. |

$TDK, set in subroutine CHAR

| | | |
|---|---|---|
| DRPISP | = | 0. |
| DS | = | .15 |
| DTWI | = | 2. |
| DWWI | = | 3. |
| EPW | = | .01 |
| ES | = | .005 |

$TDK (cont'd)

| | | |
|---|---|---|
| ETABAR | = | 1. |
| ETHI | = | .25 |
| IMAX | = | 10 |
| IMAXF | = | 0 |
| MASSFL | = | 1 |
| NC | = | 0 |
| NDS | = | 1 |
| N1 | = | 1000 |
| N2 | = | 1000 |