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FINAL REPORT

IMPROVED

TWO-DIMENSIONAL KINETICS (TDK)

Computer Program

Contract Number NAS8-35046

October 1983

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Prepared For
George C. Marshall Space Flight Center
Marshall Space Flight Center, Alabama 35812

Prepared by
Gary R. Nickerson
Lanh D. Dang
Software and Engineering Associates, Inc.
1560 Brookhollow Drive, Suite 203
Santa Ana, CA 92705

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FORWARD

This report describes work performed by Software and Engineering Associates, Inc. (SEA) under NASA contract NAS8-35046, titled 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. Improvements to the TDK computer program are necessary if it is to be applied engines of the OTV type. This study represents a first step in extending the TDK computer program so that it can be used for these operating regimes.

The method of approach used in this study has been to transfer technology from the Solid Performance Program (SPP) to the TDK computer program. The SPP was developed by SEA for the Air Force under contract F04611-77-C-0046. In this manner, the TDK computer program has been equipped with a boundary layer analysis, and a limited capability for treating two-phase flow. In addition, a method has been added that will automatically calculate the effects of regnerative cooling on thrust chamber performance.

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. Krebsbach.

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ABBREVIATIONS

BLIMP	Boundary Layer Integral Matrix Procedure, JANNAF computer program.
BLM	Boundary Layer Module, computer program
JANNAF	Joint Army-Navy-NASA-Air Force
MØC	Method of Characteristics, module of SPP and TDK
ØDE	One-Dimensional Equilibrium, module of SPP and TDK
ODK	One-Dimensional Kinetics, module of SPP and TDK
PSS	Performance Standardization Subcommittee of JANNAF
SEA	Software and Engineering Associates, Inc.
SPP	Solid Performance Program, JANNAF computer program
TDE	Two-Dimensional Equilitrium, 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 designs, has required an extension of the analytical methods used by the TDK computer program. The study reported here is a first attempt in extending TDK so that it is applicable to the operating conditions imposed by these high performance OTV designs.

High performance can be obtained with large area ratio thrust chambers using oxygen with either hydrogen or hydrocarbon fuels. Due to the large area ratios, the combustion products are expanded to low pressures such that condensed phases of water may form in addition to soot particles with hydrocarbon fuel application. The existing TDK analytical nozzle flow model for liquid rocket engines did not possess the capability of particle flow simulation. However, a recently developed Solid motor

Ref. 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.

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

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Performance Program (SPP) does contain the simulation of particle flow[3]. This capability, which assumes gas-particle equilibrium, has been transferred from the SPP to the TDK computer program.

The engine specific impulse value includes boundary layer losses. At present, this loss is identified by feeding results from the TDK program solution to a boundary layer code which calculates friction losses along the wall and heat energy transferred through the wall. In a regeneratively cooled engine, most of the heat energy transferred to the wall is returned to the main combustion chamber in the form of increased propellant enthalpy. In addition, the friction effect requires a displacement of the wall contour in order to conserve mass flow through the nozzle. Both phenomena necessitate the recalculation of the two-dimensional flow field at least one time to achieve a mass flow and energy balance. At present, this process is conducted by iterating using two computer programs, the two-dimensional kinetics (TDK) and the Boundary Layer Integral Matrix Procedure (BLIMP) program[4]. Both of these programs are quite complex, especially the boundary layer code, and they must be run in series.

For study purposes, a simplified approach is very useful, especially when many computer runs are required with only one or a few input parameters to be changed at a time. The

Ref. 3. Nickerson, G.&R., Coats, D. E., Hermsen, R. W., "A Computer Program for the Prediction of Solid Propellant Rocket Motor Performance", Volumes I, II, III, Interim Technical Report, for Air Force Rocket Propulsion Laboratory, AFRPL-TR-80-34, April 1981.

Ref. 4. Evans, R., "Boundary Layer Integral Matrix Procedure", BLIMP-J User's Manual, Aerotherm Division/Acurex Corporation, Prepared for NASA George C. Marshall Space Flight Center under Contract NAS8-30930, July 1975.

One-Dimensional Equilibrium (ODE) module, the One-Dimensional Kinetics (ODK) module, and the Two-Dimensional Equilibrium (TDE) module are such simplified options within the TDK computer program. The boundary layer program (BLIMP) also contains various simplified options. However, the program has a large computer core demand, needs long execution times, and the input is rather difficult to prepare.

Recently, a new Boundary Layer Module (BLM) was developed for solid motor nozzles. This program holds all the essential analytical and operating features to produce an efficient coupling with the TDK program. As part of the study reported here, the BLM was taken from the SPF and coupled to the TDK program. The capability of treating regeneratively cooled nozzle walls was added to both BLM and TDK.

The work carried out in this study is summarized below.

a) The current method of condensed phase flow treatment in the ODE and ODK modules of the SPP program have been incorporated in the TDK program with appropriate changes. Specific attention has been given to the presence of water droplets and ice crystals and of solid carbon particulates.

b) Using subroutines existing in the SPP, the ODE module of TDK has been modified so that it will compute transport properties for the nozzle exhaust composition. This information is required by the BLM. Numerous other features contained in the SPP, such as wall contour options, have also been transferred to TDK.

c) The ODE module of TDK has been modified so that it will provide tables of gas properties versus temperature for the stream tube mixture ratio adjacent to the nozzle wall. This information is required by the BLM.

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d) The Boundary Layer Module (BLM) of the SPP has been coupled with the TDK program such that it will automatically calculate the wall boundary layer after execution of the TDE or TDK modules, if so desired. The resulting wall displacement and the heat transferred through the wall increasing the energy level of the cooling propellant are used to repeat a TDE or TDK calculation once with the appropriate parameters (wall contour and propellant enthalpy) updated.

e) The boundary layer module has been equipped with a feature to account for the heat transfer along wall contour sections where regenerate cooling takes place. The wall heat flux, as determined by the BLM, is integrated and the result (multipled by an input efficiency factor) is returned to the main combustion chamber in the form of increased propellant enthalpy.

f) Two proof cases have been run on the revised program for the purpose of verification. The first case is a Pratt & Whitney RL-10 engine configured to operate at an expansion ratio of 205. The second case is a Rocketdyne Advanced Space Engine (ASE) configured to operate at an expansion ratio of 400. Performance measurements exist for both of these engines.

g) A User's Manual has been prepared for the improved TDK program. This has been done by revising Section 6 of Reference 1. A copy of this User's Manual is attached as Appendix A.

h) The Improved TDK computer program has been delivered to NASA-MSFC for use on the UNIVAC 1100/82 computer. The program is also operational at SEA on the DEC VAX/780 computer.

Technical details of the above work items are reported in Sections 2 and 3.

2. METHOD OF APPROACH.

Prior to the work performed during this contract, two versions of the TDK program have been generally available. The first of these is the version documented in Reference 1. A number of improvements have been made to this program by SEA, such as those described in Reference 5. However, the basic program is as presented in Reference 1. A second version of the TDK program has been developed by NASA-MSFC and has been distributed by them. This version of TDK contains many programming modifications. For the most part, these modifications are improvements to the internal structure of the program and its input and output features. The basic analytical models have not been changed. The program is undocumented.

For this contract it was necessary to combine the best features of both of the above programs, forming a "baseline" computer program, and to then transfer advanced features contained in SPP to this baseline program. Most of the features of interest are contained in the ODE and ODK modules of SPP and concern fluid chemistry.

Features of SPP other than the fluid chemistry were also transferred to TDK. In particular, the wall geometry options in SPP were installed into TDK. First, all of the wall geometry options were moved forward in the code and unified in one

Ref. 5. Nickerson, G. R., "Modification to the Two-Di...ensional Kinetics (TDK) Computer Program", Software and Engineering Associates, Inc., prepared for NASA George C. Marshall Space Flight Center, under Contract No. NAS8-31988, October 1976.

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Namelist input data set, called $DATA. Next, the spline fit option for ODK was modified so that the ODK printout could be requested at input values of area ratio. The option for a cone with specified end point was added to ODK. An option for a wall defined by a skewed-parabola was transferred from SPP and added to both ODK and TDK. These geometry options are described in the revised User's Manual, Section 6.3.3 (see Appendix A).

The "problem card" feature of TDK was replaced with a "module selection" feature of the type used by SPP, i.e., module selection by using input flags. This method allows greater flexibility than the "problem card" method, and is described in the revised User's Manual, Section 6.3.1.

With the completion of the transfer of technology from SPP, the condensed flow capability and the transport property calculations items 1.a and 1.b) were essentially complete. A discussion of the gas-particle properties now used in TDK is presented in Section 3.1.

The requirements for coupling BLM with TDK go well beyond the usage of BLM in SPP. SPP does not require a second pass through the Method of Characteristics (MOC) solution, and there is no regen cooling to consider. These two topics, BLM and regen cooling, are discussed in Section 3.2 and 3.3.

Further work is being carried out on TDK by SEA under contract NAS8-34974. The work being done is primarily concerned with adding a shock-wave capability to TDK. Work is being coordinated between the two contracts so that one final computer program will result.

3. TECHNICAL DISCUSSION.

The technical effort is discussed under the three topics given below.

> Fluid Properties,
> The Boundary Layer Module, and
> Regenerative Cooling.

3.1 Fluid Properties.

In order to expand the fluid property capabilities of TDK, changes of three basic types were made to the program, as follows:

a) The calculation of transport properties (gas viscosity, conductivity, and Prandtl number);

b) The calculation of gas properties adjacent to the nozzle wall, and

c) Core flow gas-particle equilibrium chemistry for the ODK, TDE, and TDK modules.

Each of these items is discussed in the following subsections.

3.1a   Near Wall Gas Transport Properties.

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

The viscosity and thermal conductivity of the individual gaseous species are calculated from formulas given in Reference 6 as follows:

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

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

The required Lennard Jones parameters, (σ_i, Ω_i) are internally stored in the computer program for 206 gas phase species. (See Subroutine MUK, Volume II, of Reference 3, for a list of the species.) The viscosity of the mixture is calculated from Wilke's semi-empirical formula[7].

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

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

Ref. 6.   Svehla, R. A., "Estimated Viscosities and Thermal Conductivities of Gases at High Temperatures," NASA TR-132, 1962.

Ref. 7.   Bird, R. B., Stewart, U. E., and Lightfoot, E. N., Transport Phenomena, John Wiley & Sons, 1960.

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

The thermal conductivity, κ, is based on the equation given by Mason and Saxena[8] which is a slight modification of Eucken's relation,

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

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

The viscosity at the nozzle throat, μ^*, and the corresponding temperature, T^*, are calculated. Using these values, an exponant, ω, is computed such that the expression

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

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

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

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

Ref. 8. Mason, E. A., and Saxena, S. C., Physics of Fluids, Vol. 1, No. 5, pp. 361-369, 1958.

3.1b   Near Wall Gas-Particle Mixture Properties .

Values of specific heat at constant pressure, C_p, and ratio of specific heats, γ, static enthalpy, h, and the gas constant R, are required by BLM. These properties are evaluated along the wall streamline as a function of temperature using the ODE module. The tables are prepared using a series of (T,S) equilibrium calculations, where T varies from 600°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. An example of this output is presented in Figure 1.

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

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

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

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

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

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

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Figure 1: Tables of h, μ, k, C_p, γ, and R versus $T^{\circ}R$ for use by the BLM

GAS PROPERTIES TABLES

I	T	HS	MU	K	CP	GAMMA	RGAS
1	1.0000E+02	-1.4270E+08	2.0013E-06	5.8598E-02	1.5750E+04	1.3507E+00	1.2710E+02
2	6.0000E+02	-1.3482E+08	8.9624E-06	2.4565E-01	1.5750E+04	1.3507E+00	1.2710E+02
3	8.0000E+02	-1.3164E+08	1.1402E-05	3.1881E-01	1.6068E+04	1.3414E+00	1.2710E+02
4	1.0000E+03	-1.2839E+08	1.3742E-05	3.9309E-01	1.6437E+04	1.3312E+00	1.2710E+02
5	1.2000E+03	-1.2507E+08	1.6007E-05	4.6946E-01	1.6853E+04	1.3204E+00	1.2710E+02
6	1.4000E+03	-1.2165E+08	1.8211E-05	5.4850E-01	1.7308E+04	1.3094E+00	1.2710E+02
7	1.6000E+03	-1.1814E+08	2.0363E-05	6.3046E-01	1.7791E+04	1.2984E+00	1.2710E+02
8	1.8000E+03	-1.1453E+08	2.2473E-05	7.1531E-01	1.8291E+04	1.2879E+00	1.2710E+02
9	2.0000E+03	-1.1082E+08	2.4544E-05	8.0429E-01	1.8831E+04	1.2778E+00	1.2710E+02
10	2.2000E+03	-1.0700E+08	2.6581E-05	8.9455E-01	1.9336E+04	1.2682E+00	1.2710E+02
11	2.4000E+03	-1.0309E+08	2.8589E-05	9.8597E-01	1.9810E+04	1.2600E+00	1.2710E+02
12	2.6000E+03	-9.9076E+07	3.0569E-05	1.0787E+00	2.0276E+04	1.2527E+00	1.2713E+02
13	2.8000E+03	-9.4974E+07	3.2524E-05	1.1735E+00	2.0734E+04	1.2459E+00	1.2726E+02
14	3.0000E+03	-9.0785E+07	3.4457E-05	1.2719E+00	2.1211E+04	1.2399E+00	1.2736E+02
15	3.2000E+03	-8.6498E+07	3.6369E-05	1.3762E+00	2.1745E+04	1.2330E+00	1.2770E+02
16	3.4000E+03	-8.2104E+07	3.8262E-05	1.4905E+00	2.2385E+04	1.2261E+00	1.2831E+02
17	3.6000E+03	-7.7582E+07	4.0136E-05	1.6196E+00	2.3188E+04	1.2188E+00	1.2936E+02
18	3.8000E+03	-7.2906E+07	4.1994E-05	1.7696E+00	2.4215E+04	1.2108E+00	1.3102E+02
19	4.0000E+03	-6.8040E+07	4.3835E-05	1.9475E+00	2.5530E+04	1.2022E+00	1.3347E+02
20	4.2000E+03	-6.2947E+07	4.5662E-05	2.1600E+00	2.7183E+04	1.1934E+00	1.3689E+02
21	4.4000E+03	-5.7587E+07	4.7474E-05	2.4131E+00	2.9209E+04	1.1846E+00	1.4146E+02
22	4.6000E+03	-5.1923E+07	4.9273E-05	2.7115E+00	3.1623E+04	1.1763E+00	1.4729E+02
23	4.8000E+03	-4.5930E+07	5.1059E-05	3.0577E+00	3.4412E+04	1.1688E+00	1.5445E+02
24	5.0000E+03	-3.9590E+07	5.2834E-05	3.4512E+00	3.7536E+04	1.1623E+00	1.6292E+02
25	5.2000E+03	-3.2904E+07	5.4596E-05	3.8882E+00	4.0924E+04	1.1570E+00	1.7259E+02
26	5.4000E+03	-2.5842E+07	5.6348E-05	4.3622E+00	4.4486E+04	1.1528E+00	1.8329E+02
27	5.6000E+03	-1.8551E+07	5.8089E-05	4.8640E+00	4.8116E+04	1.1497E+00	1.9478E+02
28	5.8000E+03	-1.0950E+07	5.9820E-05	5.3800E+00	5.1681E+04	1.1477E+00	2.0668E+02
29	6.0000E+03	-3.1253E+06	6.1541E-05	5.9035E+00	5.5123E+04	1.1464E+00	2.1884E+02
30	6.2000E+03	4.9006E+06	6.3253E-05	6.4223E+00	5.8345E+04	1.1459E+00	2.3092E+02
31	6.4000E+03	1.3076E+07	6.4956E-05	6.9280E+00	6.1289E+04	1.1460E+00	2.4269E+02
32	6.6000E+03	2.1370E+07	6.6650E-05	7.4135E+00	6.3917E+04	1.1466E+00	2.5394E+02
33	6.8000E+03	2.9743E+07	6.8336E-05	7.8742E+00	6.6214E+04	1.1475E+00	2.6455E+02
34	7.0000E+03	3.6172E+07	7.0013E-05	8.3076E+00	6.8185E+04	1.1488E+00	2.7447E+02

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

The fluid properties shown in Table 1 are h, μ, κ, C_p, γ, and R versus $T^O R$. The values of μ and κ are prepared as described in Section 3.1a. The values for h, C_p, γ, and R are prepared as described above, i.e., they are equilibrium properties including condensed phases (no gas particle lag).

3.1c   Core Flow Gas-Particle Equilibrium Chemistry.

The TDK program described in Reference 1 contains only the most rudimentary capability to compute the effects of two-phase flow (gas plus condensed phases) on nozzle performance. In that program only the ODE module is capable of considering the existence of different phases. This is done by treating the entire chemical system as if it were in chemical equilibrium and the particulate and gas phases as if they were in dynamic and thermal equilibrium. For high pressure systems and where the characteristic particle sizes are small, the above assumptions are quite reasonable. For systems where there is a significant departure from either of the above assumptions, then the TDK code described in Reference 1 does not have the capability to even assess the importance of these effects, let alone to quantitatively predict the magnitude of them. Systems where two-phase flow phenomena could be of importance are those with soot formation using hydrocarbon propellants, and with the formation of water droplets and ice in low pressure, high expansion ratio H_2/O_2 systems.

In order to improve the capability of TDK with respect to two-phase flow, the ODK module of SPP was installed in TDK. The chemistry subroutines of ODK also serve the same function for TDK, so that TDK has been given the same two-phase flow (no lag) capability as ODK. Unlike TDK, the SPP has no two-dimensional kinetics capability.

The Two-Dimensional Equilibrium (TDE) option has been updated to consider two-phase flow in the same manner as the ODE module, but for a two-dimensional calculation. Source flow calculations were carried out to verify the program. Under this assumption TDE was shown to calculate the same results as ODE for all streamlines. The TDE capability allows the user to assess the effect of particles on specific impulse, and also to indicate the possibility of the onset of condensation. Further development along these lines would require the generation of

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kinetic models to predict both condensation and mass transfer between phases and is beyond the scope of this study. Implicit in the above is the assumption that gas-particle lag effects are small. If this assumption is violated then the SPP code should be used to estimate the performance loss because the two-phase flow loss becomes the major thrust loss in the system.

3.2   The Boundary Layer Module (BLM)

The BLM was developed for SEA by CBC Enterprises. Documentation for the BLM as delivered to SEA is presented in Reference 9. The purpose of the BLM is to compute compressible laminar and turbulent flows in axisymmetric nozzles. It can also be used to calculate two-dimensional and axisymmetric external flows. The method utilizes an efficient two-point finite difference method developed by Keller and Cebeci[10]. Turbulence modeling is achieved through the use of the Cebeci-Smith eddy-viscosity formulation[11] which has been tested for a large class of flows with various boundary conditions.

The BLM has been modified by SEA to interface automatically with the SPP and with the TDK programs. TDK supplies all of the inputs required by BLM.

In order to be able to use BLM for large expansion ratio nozzles, the boundary layer calculation was divided into adjacent axial segments, and the calculation restarted automatically at each segment. This feature is also useful when nozzles with regen cooling are being analyzed. A segment can be placed at the start (or end) of the cooling circuit where there is a discontinuity in the wall temperature (or heat flux), and the calculations can be restarted with an integration step size change.

Ref. 9. Cebeci, T., "Boundary Layer Analysis Module", prepared for Software Engineering Associates, Inc., January 1982.

Ref. 10. Keller, H. B., and Cebeci, T., "Accurate Numerical Methods for Boundary Layer Flows, Part 2, Two-Dimensional Turbulent Flows", AIAA J., 10, 1972, p. 1193.

Ref. 11. Cebeci, T., and Smith, A. M. O., Analysis of Turbulent Boundary Layers, Academic Press, N.Y., 1974.

At high expansion ratio , it is possible for the gas density in the boundary layer to become very low. If the mean free path in the boundary layer approximates the wall roughness height, the non-slip condition at the wall can break down. To aid in the assessment of this condition, the mean free path, λ , at the edge of the boundary layer is calculated and printed, where

$$\lambda = 1.26 \, \mu / (\, \rho \sqrt{RT} \,) \qquad\qquad (ft)$$

At the end of the nozzle, the Knudsen number, Kn, based on displacement thickness, δ^*, is printed so that the approach to rarified flow can be monitored, where

$$Kn = \lambda / \delta_e^*$$

The following options for plotted output have been added to the BLM by SEA:

1) Momentum thickness, θ , versus axial position.
2) Displacement thickness, δ^*, versus axial position.
3) Wall temperature, T_w, versus axial position
4) Velocity profiles at specified are ratios, or at specified axial locations.
5) Temperature profiles at specified area ratios, or at specified axial locations.

The analysis used by the BLM is described in Reference 9. Usage of the program within TDK is described in Section 6.8 of the User's Manual (see Appendix A), as follows:

6.8.1   BLM Gas Properties
6.8.2   Boundary Layer Edge Conditions
6.8.3   Integration Step Size Control
6.8.4   Regenerative Cooling Heat Transfer
6.8.5   BLM Plotted Output

3.3   Regenerative Cooling

When an engine is cooled using a regenerative device, propellant (usually fuel) is routed around the nozzle so that heat is transmitted from the boundary layer to the coolant[*]. This heat is then returned to the combustion chamber in the form of increased propellant enthalpy. When the nozzle wall temperatures are assumed known (IHFLAG = 0 option), the BLM will calculate the heat flux from the boundary layer to the wall, $\dot{h}_w$ (BTU/ft -sec). These values can also be input directly (IHFLAG = 1 option). If the coolant circuit extends from position x_o to position x_e and operates at an efficiency, η, then the propellant enthalpy entering the chamber will be increased by

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

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

---

[*]   Heat can be extracted from the boundary layer as a function of length (BLM analysis). The core flow (TDK analysis) does not include heat transfer effects other than to modify the initial value for chamber enthalpy used by TDK'.

$$\Delta H_{\underline{2}} \quad = \quad \Delta H$$

i.e.

$$DELH1(1) = \Delta H, \Delta H, \ldots \text{ etc.}$$

The second method is to assume that a fuel circuit adds enthalpy only to fuel, and an ox circuit adds enthalpy only to ox. It follows that

for a fuel circuit

$$\Delta H_i = (\frac{r+1}{r_i+1}) \Delta H$$

and for an ox circuit

$$\Delta H_i = (\frac{r+1}{r_i+1}) \frac{r_i}{r} \Delta H$$

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.

A second pass can be made without adjusting the enthalpy by setting IRPEAT = 2. In this case neither the ODE nor ODK runs will be repeated. The nozzle wall, however, will be displaced for TDK (or TDE). This option is useful if an adiabatic wall (zero heat flux) case is run.

The boundary layer calculations are automatically started at the downstream end of the combustion chamber (position ECRAT of Figure 6-1, Appendix A). However, an option has been provided that allows the user to input values for the upstream boundary layer edge conditions and then start the boundary layer further upstream (see item IOFF, Section 6.3.2, Appendix A). This option can be important when calculating heat transfer for the chamber-throat wall assembly.

4. CONCLUSIONS.

Work items a) through h) described in Section 1 of this report have been completed. This has resulted in the technical improvements to the TDK computer program that are discussed below.

TDK has been equipped with a limited capability (zero velocity and thermal lag) for treating rocket nozzle exhaust flow containing condensed phase species. This has been accomplished by a transfer of technology from the SPP[3] to TDK.

A boundary layer program, known as BLM[9], has been installed in TDK as a module. The BLM was developed for SPP in response to requirements set forth by experts in the field at the 2nd SPP Workshop[12]. Further development of this module has been carried out by SEA to make it applicable to high area ratio liquid rocket engines with regen cooling.

TDK has been modified to incorporate a capability for calculating the effect of regen cooling on engine performance. The nozzle wall temperature (or heat flux) profile must be specified by the user. The engine cycle balance must also be performed external to the program.

The CPIA 246 standard procedure for computing engine performance[2] has been automated within TDK; but with BLM[9] substituted for BLIMP[4]. A complete TDK-BLM-TDK calculation can be carried out in one computer run with a minimum of user input.

Two sample cases were run for the purpose of demonstrating the program. These are 1) the Pratt and Whitney RL10 engine operating at an area ratio of 205.03:1 and 2) the Rocketdyne

Advanced Space Engine (ASE), operating at an area ratio of
400.71:1. Results of these computer runs have been sent to
NASA-MSFC for evaluation.

The improved TDK program has been delivered to NASA-MSFC
converted for use on the Univac 1100/80 computer using the FTN
compiler. The program is available from SEA for the DEC VAX 780
computer.

A User's Manual for these programs are presented in Appendix
A.

5.   RECOMMENDATIONS.

Recommendations concerning the following topics are discussed below: chemistry, low density, flow effects, test cases, input/output, and documentation.   No recommendations are made here regarding shock waves since TDK is currently undergoing modification for this purpose under Contract NAS8-34974.

5.1   Chemistry.

The TDK program contains two chemistry modules, which are 1) the chemical equilibrium solution subroutines of ODE, and 2) the streamline chemical kinetics subroutines of ODK.   These latter subroutines are also used in a modified form to compute kinetics in a TDK calculation.   No improvements to the ODE chemistry are recommended.   However,   several   important   improvements   are recommended for the ODK (and TDK) chemistry.

ODK   should   be modified to include input of "global" reactions and "hetrogeneous" reactions.   For   example, hydrocarbon decomposition can be characterized by reactions such as:

$$(C_nH_m) \longrightarrow CH_4, H_2, \text{ other fragments.}$$
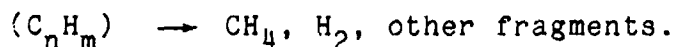
In order to effectively model the chemistry of propellants   such as   LOX/RP-1, it is often necessary to include reactions of this type.   Further examples are the condensation of water, and also the   kinetics   of   soot   formation.   These   processes   can   be important in rocket engines.   Further work is needed which will allow   ODK to be used to assess the effects of these   proceesses on rocket engine performance.

A   more advanced reaction rate processor is available in the GKAP computer program.   It is recommended that this processor be installed   in ODK.   This will add the following capabilities   to ODK:

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a) Improved treatment of third body type reactions (rate ratios assigned with each reaction).

b) Input of reaction rates of the Landau-Teller form (necessary for most T-V and V-V reactions).

c) radiative reactions, such as

$$HF(1) \longrightarrow HF(0) + PH\emptyset T\emptyset N$$

The new rate processor will provide a firm basis for expanding the chemical kinetics capability of ODK.

Other recommendations in the chemistry area are: 1) providing thermodynamic data for the temperatures below $100^{O}K$, 2) replacing the thermodynamic data library with the latest data available from the NASA LRC, 3) updating of the kinetic rate data for reactions in the CFHNO systems that are important in rocket performance calculations. These items should be done on a "first cut" basis and then reviewed by the JANNAF membership.

5.2   Low Density Flow Effects.

Exhaust nozzle designs for future space engines may   operate at expansion ratios so high   that   low density flow effects must be considered.   If so, the following questions must be examined:

a)   At what conditions do low density effects at the nozzle wall require that a slip condition be imposed?

b)   Where does transition to   free   molecular   flow cause a breakdown of the continuum flow assumption?

c)   Is   the boundary layer interaction with the   core   flow sufficiently weak so that   the JANNAF procedures can be used with confidence?

Questions a) and b) above, can   be   answered in part by examining the   mean   free path based on   the   average   gas   molecular weight.   This item has been added to the BLM output   along   the boundary layer edge.   For the boundary layer, question b) can be answered   in   part   by   examining the Knudsen   number   based   on displacement thickness.   This   item   has   also been added to the BLM output.

Question   c)   is   more   difficult in   that   it   requires   an analysis of the   boundary   layer-core   flow   interaction.   It is recommended that an analysis of this interaction be conducted.

5.3   Test Cases.

The JANNAF standard performance prediction procedure was applied to two engines (the RL10 and the ASE) using the improved TDK program. The BLM was used rather than BLIMP-J[4]. Input data for the cases, including data on the engine cycle balance, was provided by NASA/MSFC.

It is recommended that further cases be run for the purpose of obtaining estimates of the accuracy of ODK, TDK, and BLM as a function of items that control the numerical methods. Cases should be run to determine if all of the program options work properly.

Cases should also be run for the purpose of determining the role of the boundary layer in performance prediction. The following questions need to be addressed:

1)   How do the BLM predictions compare with BLIMP-J?
2)   How do BLM calculations with regen cooling compare with adiabatic wall calculations?
3)   What is the magnitude of performance gains due to "enthalpy pumping" in regen cooled engines?

5.4   Input and Output for TDK.

The following recommendations are made with respect to input and output for TDK and its modules.

a) A summary page should be added at the end of the output which lists in a clear format all of the key performance results. This page would correspond to the summary page listed by the SPP.

b) Some, or all, of the following computer plots should be added to the program:

I_{sp} versus X_{wall} and ε

θ_{wall}, r_{wall} versus X_{wall}

P,V,M, versus X_{wall} and X_{axis}

P and M contour plots

P,V,M, versus r at X_{exit}

MOC plots for a window

c) The linkage data files of SPP have been installed in TDK (see Reference 3, Volume III, Section 2.9). This capability allows a module of TDK to be run from a file

generated on a previous run. To be completely effective the file structure and programming must be modified specifically for TDK, and documented. This is recommended.

d) The BLM output should be reviewed for the purpose of improving the format and to determine which quantities should be added, or deleted.

5.5   Documentation.

A complete set of manuals for TDK should be written which discuss the following topics:

1) Methods of analysis (all modules).
2) Program structure and subroutine write-ups.
3) User's Manual.

The documents should be written so that new users of the computer program can be systematically guided through the principles involved in the analysis. The analytical procedures should be related to the thrust chamber performance prediction methodology defined in CPIA 246, Reference 2. Test cases should be included that demonstrate the differen. problem types solved by the program. Text should be included describing each test case; its purpose, the engine type and caracteristics, unique features, interpretation of output results, etc.

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APPENDIX A

Section 6
Engineering and Programming Manual

TDK

Two-Dimensional Kinetic Reference
Computer Program

By
G. R. Nickerson
D. E. Coats
L. D. Dang

Software and Engineering Associates, Inc.
1560 Brookhollow Drive, Suite 203
Santa Ana, California 92705

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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:

$$\frac{C^o_{p_T}}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\frac{H^o_T}{RT} = a_1 + \frac{a_2 T}{2} + \frac{a_3 T^2}{3} + \frac{a_4 T^3}{4} + \frac{a_5 T^4}{5} + \frac{a_6}{T}$$

$$\frac{S^o_T}{R} = a_1 \ln T + a_2 T + \frac{a_3 T^2}{2} + \frac{a_4 T^3}{3} + \frac{a_5 T^4}{4} + a_7$$

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^oK and the upper temperature interval is 1000^oK to 5000^oK.

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 pr gram. 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)	5(E15.8)	1 to 75
	(for upper temperature interval)		
	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 6/62O   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 3/66O   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 9/65O   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 calcu-
lations it may be necessary to extend the curve fit data in the Thermodynamic Data
file (see Section 6.1). The lower temperature limit, T_ℓ, in the Thermodynamic Data
supplied with the program is 300°K.

Thermodynamic Data below the temperature, T_ℓ, may be input by data cards as
described 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	$T_1K \ C_{P_T}^{o} \ H_T^{o} \ S_T^{o} \ 1$	First Thermodynamic Data point for the above species, input 4F 10.0, I5.
card n+2	$T_n^{o}K \ C_{P_T}^{o} \ H_T^{o} \ S_T^{o}$ 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 $100^{O}K$. 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

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

and

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

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

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 $C^o_{P_T}$, H^o_T, S^o_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 cont-
rols 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 i. 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)

<u>Input</u>   <u>Mode of Execution</u>

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.

ØDE=1, ØDK=1, TDF=1, BLM=1,   As above with TDF repeated.
IRPEAT=1 or 2,

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. If IRPEAT = 1, the ØDE and ØDK module executions will be repeated with adjusted enthalpies for regen cooling, see Section 6.8.4. If REPEAT = 2, the ØDE and ØDK module executions will not be repeated. The system enthalpy will be unchanged.	none	0
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 IOFF is not input, then these values are stored starting with the first entry in each array. If IØFF is input then these values are stored starting in the IØFF + 1 entry of each array. Values must then be input into entries 1 through IØFF. The boundary layer calculations will start at position XINØ(1) of these arrays using the $BLM input. This input allows the user to account for the development of the boundary layer in the nozzle chamber, upstream of ECRAT. IØFF < 100. If IØFF is input, do not input NXINØ in BLM.		0

6.3.3 Specification of nozzle geometry.

To eliminate redundancy, all geometry inputs that are common throughout the modules are input here. Note that the center of the nozzle geometry coordinate system is at the centerline at the throat plane, and that all coordinates are normalized by the nozzle throat radius, r_t. Hence, axial positions upstream of the throat are always negative numbers. In the figures describing the geometry, positive angles are shown as counter-clockwise, and negative angles are shown as clockwise.

Geometric area ratios at which 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

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

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 6.3.3.1.
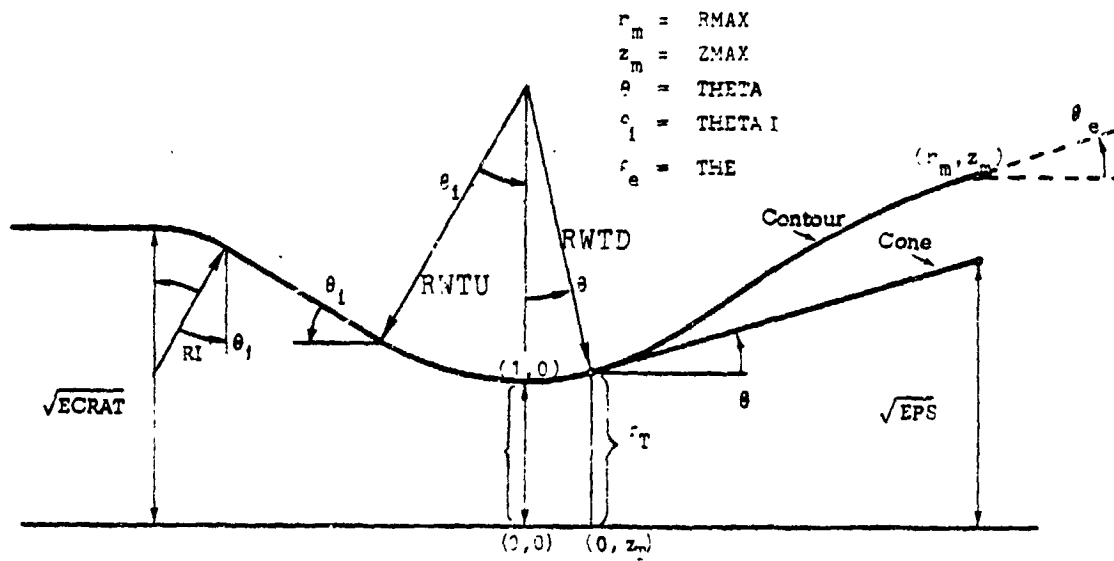
Figure 6-1:   Nozzle Geometry, all coordinate
values are normalized by RSI = r_t.

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 ≤ 50.	none	0.
ASUP(1)	=	Supersonic area ratios at which information will be printed. For the TDE option, ASUP must contain an entry $\geq$ the nozzle expansion ratio.	none	0.
NASUP	=	Number of entries in the ASUP array ≤ 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. ITYPE = 0, if the real wall contour is input. ITYPE = 1, if the potential flow wall contour is input. If IRPEAT = 1 or 2, then the nozzle wall will be displaced by $+\bar{\delta}^*$ 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:

Item		Description	Units	Assumed Value(s)
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 T ZS(1)=z_T in Figure 6-2. The T 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 RZNØRM.

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.004662                  100.    -7,2021646298,15  O


REACTANTS
N 1.      H 4.      CL1.      O 4.           72.06   -70730.  S298.15  F
C 1.      H 1.869550 .031256S .008415        18.58   -2999.082L298,15  F
AL1.                                          9,00   +C.0      S298.15  F
MG1.      O 1.                                 .20   -143700.  S298.15  F
H 2.      O 1.                                 .16   -68317.4  L298.15  F


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


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 1.003
F 2.                                         100.   -3030.892L 85,24  O 1.54


REACTANTS
LI1.                                         100.    0.        S298.15  F
F 2.                                         100.   -3030.892L 85,24  O 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  O 1.407
```

*Listed above are six examples. Each example must end with a blank card.

given on the REACTANTS cards are relative to total fuel or total oxidant rather than total reactant.

There are four options in the $ØDE namelist for indicating relative amounts of total fuel to total oxidant as follows:
1. Oxidant to fuel weight ratio (ØF is true)
2. Equivalence ratio (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 $T_{low}/1.2 \le T \le T_{high} \times 1.2$ 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 ith zone the ith 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 ass'gned points the inclusion of condensed species is handled automatically by the program.

6.4.3 $ØDE NAMELIST INPUT

The ØDE subprogram contains namelist input sections $ØDE
and $SHKINP. The Namelist $ØDE must be preceded by a card with NAMELISTS
punched in card columns 1-9.

The $ØDE Namelist is required if ØDE =1. or TDK =1, in $DATA as
described in section 6.3.

For the ØDE problem type any of nine (9) different equilibrium problems can be
solved. These are TP, HP, SP, TV, UV, SV, RKT, DETN, and SHØCK. For the ØDE-
ØDK, ØDE-ØDK-TDK, or TDE problem type, only the RKT problem can be
solved. In this section only the RKT input option is discussed. Reference 9 is
to be used to prepare input for the other equilibrium problems.

The variables input by the $ØDE namelist are listed in Table 6-9.
Additional information about some of these variables follows:

Pressure units. - The program assumes the pressure in the P schedule to be in
units of atmospheres unless either PSIA = true, or SI = true.

Relative amounts of fuel(s) and oxidizer(s). - These quantities may be specified by
assigning 1 to 15 values for either o/f, %F, f/a, or r. If no value is assigned
for any of these, the program assumes the relative amounts of fuel(s) and oxidizer(s)
to be those specified on the REACTANTS cards. (See discussion in REACTANTS
Cards, Section 6.4.1)

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 ith zone will be the value input for P multiplied by the ith 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 ith zone will have a mixture ratio equal to the ith entry in the OFSKED schedule.

Print out will be given for the chamber pressure condition (i.e. stagnation) and the throat condition. Print out may be requested at other conditions by use of the PCP schedule and the SUBAR and SUPAR schedules.

The program will calculate both equilibrium and frozen performance unless 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 $ØDE 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 pressures 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 ith 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 $BLM). 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.

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 $\neq$ 1.)
SUPAR	50	R	0	Compute and print solutions at these values of supersonic area ratio (entries must $\neq$ 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 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 ρ, 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   ODK 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 6-4 (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 reactions
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:

$$N_1 \, {}^*Symbol_1 + N_2 \, {}^*Symbol_2 + \ldots = N_a \, {}^*Symbol_a + N_b \, {}^*Symbol_b + \ldots$$
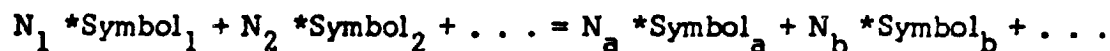
where the left hand side represents reactants and the right hand side represents products. The reaction can be either endothermic or exothermic.

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

$$N_1 + N_2 + \ldots \le 10$$

and

$$N_a + N_b + \ldots \le 10$$

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).

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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

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

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

$$H_2 + M = H + H + M$$
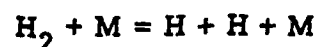
where M is a generalized third body. Specific third body effects may be included by inputing specific third body reaction rate ratios as outlined in 6.5.2.8. Cards encountered after the END TBR REAX directive card do not have a third body term added.

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 jth reaction only one reaction rate, k_j, where

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

can be input. For three body recombination reactions such as

$$H + \emptyset H + M_i = H_2\emptyset + M_i$$
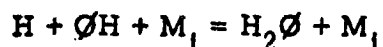
the rate of reaction is in general different for each species, M_i, depending upon the efficiency of the species, M_i, as a third body collision partner. As discussed in Section 2.2 the temperature dependance of a recombination rate is approximately independant of the third body, i.e. for the ith third body and j^{th} reaction:

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

The third body efficiency of the ith species for the jth reaction is then defined as

$$m_{ij} \equiv A_{ij}/A_j$$

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

```
REACTIONS CCLFHNO    MAY 3-4 1972   JANNAF PSWG    K=AT**-N EXP(-1000B/RT)
      H + OH   = H2O      . A=7.5E23 . N=2.6 . B=0.,              (AR) NO.  1
      O + H    = OH       . A=6.0E18 . N=1.  . B=0.,              (AR) NO.  2
      O + O    = O2       . A=1.2F17 . 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.,              (AP) 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 RFAX
     H2 + OH   = H + H2O  . A=2.19E13. N=0.  . B=5.15,         BAULCH NO. 21
     OH + OH   = O + H2O  . A=5.75E12. N=0.  . B=.780,         RAULCH 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=1.080,        BAULCH NO. 41
     O2 + CO   = O + CO2  . A=8.85E9 . N=-.656.B=45.920,       BAULCH NO. 42
      N + NO   = O + N2   . A=3.1F13 . N=0.  . B=.334,         RAULCH 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=1.75E10. N=-.5 . B=39.739,             NO. 28
      H + CL2  = HCL+CL   . A=3.0E14 . N=0.  . B=3.000,               NO. 29
     H2 + CL2  = HCL+HCL  . A=1.75E10. 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=-.68. B=.500,               NO. 33
     CL + F2   = F +CLF   . A=7.6E12 . N=-.68. 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=1.8E10 . 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=5.678,              NO. 44
      C + NO   = CO+ N    . A=5.3E11 . N=-.5 . B=8.303,              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=5.3E11 . N=-.5 . B=5.678,             NO. 50
     OH + F    = HF+ O    . A=2.9E12 . N=-.68. B=.200,              NO. 52
     H2O+ F    = HF+OH    . A=1.4F10 . N=-.68. B=.600,             NO. 53
     HCL + OH  = H2O+CL   . A=1.0E11 . N=-.5 . B=6.0,
     OH + CL   = HCL+O    . A=5.0E11 . N=-.5 . B=6.0,
LAST RFAX
```

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 ith 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 jth reaction is defined by the jth 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. 2
   OH + OH  = O + H2O  , A=5.75E12, N=0. , B=.780,       BAULCH NO. 2
   H + OH   = O + H2   , A=7.33E12, N=0. , B=7.300,      BAULCH NO. 2
   O + OH   = H + O2   , A=1.3E13 , N=0. , B=0.,,        BAULCH NO. 2
LAST REAX
INERTS 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 calcula-
tion. The input is read in subroutine ,ÖDKINP 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 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

$$\left| \frac{(\rho VA)_{N+1} - (\rho VA)_N}{(\rho VA)_{N+1}} \right| \quad < \quad C\emptyset NDEL$$

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)
$ODK		namelist, read in subroutine ODKINP.		
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 super-sonic flow	none	1×10^{-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 $SPP. For other contours (IWALL=2 or 3), print out will occur at 20 equally spaced axial locations along the nozzle.	
	= 0	print at every integration step	
	= +1	print every ND3rd step up to the throat and then nominal area ratios	
	= +2	print every ND3rd step over entire nozzle	

---

*For JPRNT = -1 and a conical nozzle (i.e. IWALL = 1), the internally set area ratios are:
ARPRNT(1) = 2,3,4,.. 39,40,42, ..,58,60,64,...116,120,128 ...,200,210, 220,. .400

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

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 $SPP.
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 select·· ed 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   ODK 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 ∅DK ISP

A mass averaged ∅DK ISP summary page may be obtained at the end of the ∅DK 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)
$TRAN	=	Namelist, read in subroutine TRAN	50*0
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).	
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. For RWTD < PMCRIT the number of points placed on the initial line will be incremented by the largest integer of theta, the downstream tangent angle.	50
PMCRIT	For RWTD > PMCRIT a sinusiodal distribution is requested; i.e. $$r_i = [r_w \sin (\frac{i}{N} \frac{\pi}{2})]^{\varepsilon_1} \quad i = 0,1,2....N$$ where N = MP and ε_1 is EXP1 described below. Editing is done to control the spacing. If RWTD < PMCRIT an initial line distribution will result such that the first left running characteristic intersects the wall at a wall angle of PMDEG degrees.	1.

Item		Description	Assumed Value(s)
PMDEG	=	Intersection angle, in degrees, for the first left running characteristic if RWTD $\leq$ PMCRIT.	1.
EXP1	=	ε_1 for sinusoidal distribution.	1.2

$END

6.7 $MOC NAMELIST INPUT.

This data set contains the input items for the supersonic Method of Character-
istics (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 suf-
ficient.

6.7.1 Characteristics Mesh Control

Item Name		Input Quantity	Units
$MOC	=	Namelist name, read by subroutine CHAR	
DS	=	insertions will be made such that successive points along streamlines will not be separated by more than DS.	none
DWWI	=	insertion control parameter $\Delta\theta_\omega$ described in Section 5.9.2.	degrees
EPW	=	the program will insert such that the wall end point is located within a tolerance EPW.	none
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
IMAXF = 1		the program will terminate the case if a printed point requires maximum iterations for convergence.	none
or			
IMAXF = 0		program will continue the case after IMAX iterations per point have occurred	none
TEXPLI	=	input temperature below which explicit integration for the species concentrations will be used.	$^\circ R$, $^\circ K$ if SI Units
ETHI	=	ϵ_θ for point editing as described in Section 5.9.2, CNTRL.	degrees
ES	=	ϵ_s for point editing as described in Section 5.9.2, CNTRL.	none
DTWI	=	$\Delta\theta_{t\omega}$ criterion for insertion in subroutines INPT, DSPT as described in Section 5.9.2, CNTRL.	degrees

6.7.2 Print Control

Item Name		Input Quantity	Units
N1	=	flow parameters will be printed for every N1th interior point a-long characteristics selected for print	none
N2	=	every N2th characteristic will be selected for print	none
NC	=	for NC $\neq$ 0 species concentrations (partial densities) will be printed with the flow parameters. If NC=1 the quantities A,B,γ, heat capacity (BTU/Lb-$^{\circ}$R), and enthalpy (ft^2/sec^2) will be appended to the species concentration print.	none
MASSFL	=	at the completion of each left running characteristic (LRC) the massflow is integrated. If	none
		MASSFL = 0 then no mass flow printed	
		MASSFL = 1 then total mass flow and the number of points on the LRC are printed for each LRC	
		MASSFL = 2 then mass flow for each point along LRC is printed	
		MASSFL = 3 Same as MASSFL = 2 with the addition of execution time at the end of each LRC	
		see Section 5.8.1, CHAR	
NDS	=	for NDS = 1 Dividing Streamline Points will be printed. (Nominal)	none
		for NDS = 0 Dividing Streamline Points will be suppressed.	

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 Name	Input Quantity	Function
EXITPL =	.TRUE.	Exit plane calculation requested.

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.

Input Quantity	Function
ILPCH = .TRUE.	Requests Punching of Initial Line
IPUNIT =	The Fortran unit number assigned to the PUNCH. (e.g. on Univac 1108 IPUNIT = -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 SPP		
	=	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 TD2P module was not executed, a value can be input here so that a boundary layer ISP decrement can be computed	lb/sec	0.

6.8.1   BLM Gas Properties

Gas properties that are required by the BLM are γ, C_p, and μ versus T, and a value for the Prandtl number, P_r.

If tables for C_p and γ 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 $600^{\circ}R$ to $7000^{\circ}R$ at $200^{\circ}R$ increments. The chamber entropy value is used for S. Values at $100^{\circ}R$ are then extrapolated and added to the table. The table is printed with the BLM output.

If constants defining the gas viscosity, μ, 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, γ, 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	$^{\circ}R$	300,...,7000

Item		Description	Units	Assumed Value(s)
NTAB	=	number of values entered in CKO, the CPO, and TO arrays. $3 \leq 101. \leq$ NTAB	–	24
RMUI	=	Reference viscosity, μ_o, where viscosity is expressed as $$\mu = \mu_o (T/T_o)^\omega$$	lbm/ft-sec	$.605934*10^{-4}$
TI	=	reference temperature, T_o, for viscosity. See RMUI, above.	^oR	6032
ØMEGA	=	Viscosity exponant, ω. See RMUI, above.	–	.66843
PR	=	Molecular Prandtl number, P_r	–	.4385

$C - 2$

6.8.2 Boundary Layer Edge Conditions

The coordinates for the boundary layer are specified in the RINØ versus XINØ table. Conditions at the invisid 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 q_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 invisid edge of the boundary layer will be automatically transmitted from the TD2P 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 invisid edge	ft/sec	-
TEØ(1)	=	T_e, gas static temperature at the invisid edge	^{o}	-
PEØ(1)	=	P_e, gas pressure at the invisid edge	psi	-
NXINØ	=	number of items in the XINØ, RINØ, UEØ, TEØ, and PEØ tables. NXIN < 201.		

Item		Description	Units	Assumed Value(s)
XTQW(1)	=	X , axial coordinate for the TQW and CQW tables.	-	-
IHFLAG	=	Flag specifying wall boundary condition input through TQW array. IHFLAG = 0, for temperature IHFLAG = 1, for heat flux	-	1
TQW(1)	=	T_w, wall temperature or $\dot{q}_w$, wall heat flux, depending in IHFLAG. For an adiabatic wall, set IHFLAG = 1 and all TQW(1) = 0. To convert $(BTU/hr\text{-}ft^2)$ to (lbm/sec^3) multiply by 6.9547, which is $Jg/3600$.	^{o}R or 3 lbm/sec	-
CQW(1)	=	$(\rho V)_w$, mass transfer parameter at the wall	$lbm/ft^2\text{-}sec$	101*0
NTQW	=	Number of axial stations, X_w. Each of the above tables must have this number of entries. NTQW $\leq$ 101.	-	-

6.8.3 Integration Step Size Control.

Item		Description	Units	Assumed Value(s)
NSEGS	=	Number of Segments, $1 \le$ NSEGS ≤ 10	none	1
NISPS(1)	=	Number of Integration Steps per Segment, ≤ 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 and is defaulted to the starting and ending values of the wall table supplied by the TD2P module. (The variable XITBL is used to define the starting axial location for the boundary layer edge table in the $TD2 namelist. The ending points for the edge table is taken as the nozzle lip.)	ft	-
NTR	=	Station at which transition to turbulent flow is allowed. The program starts with an assummed 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, e.g. NTR $> \Sigma$ 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, $\dot{h}_w$(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, η, then the propellant enthalpy entering the chamber will be increased by

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

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) = ΔH, ΔH, ... 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)
XO(1)	=	the Ith entry is the starting position for the Ith cooling circuit*.	3*0
XE(1)	=	the Ith entry is the ending position for the Ith cooling circuit*.	3*0
ETA(1)	=	the Ith entry is the efficiency for the Ith cooling circuit.	3*1
ØFC(1)	=	Type of coolant for the cooling circuit:	3*0

$ØFC(I) = 0.$ if there is no ith circuit
$ØFC(I) = 1.$ if the Ith circuit is oxidizer
$ØFC(I) = 2.$ if the Ith circuit is fuel
$I \leq 3$

| DISTRB(1) | = | Flag for method of distributing ΔH increments | 3*0 |

$DISTRB(I) = 0.$ for equal distribution of heat to chamber

$DISTRB(I) = 1.$ for distribution of ox heat to ox in chamber, and fuel heat to fuel in chamber.

The Ith entry is for the Ith circuit.

---

* Normalized by the throat radius, r_t.

6.8.5 BLM Plotted Output.

The input described below is used to control plotted output from the BLM. The plot options available from BLM are:

1) Momentum thickness, θ, vs. axial position.
2) Displacement thickness, δ^*, 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. If IPRØF = 1, then axial locations, x/r_t, are input in APRØF	0
APROF(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
NPROF	=	Number of area ratios (or axial locations) requested in APROF. NPROF $\leq$ 20.	0
KDIPLT	=	If KDIPLT = 1, then displacement thickness, δ^*, vs. axial location, x, will be plotted.	0
KMTPLT	=	If KMTPLT = 1, then momentum thickness, θ, vs. axial location, x, will be plotted.	0
KTWTPLT	=	If KTWPLT = 1, then wall temperature, T_w, vs. axial location will be plotted.	0

$END

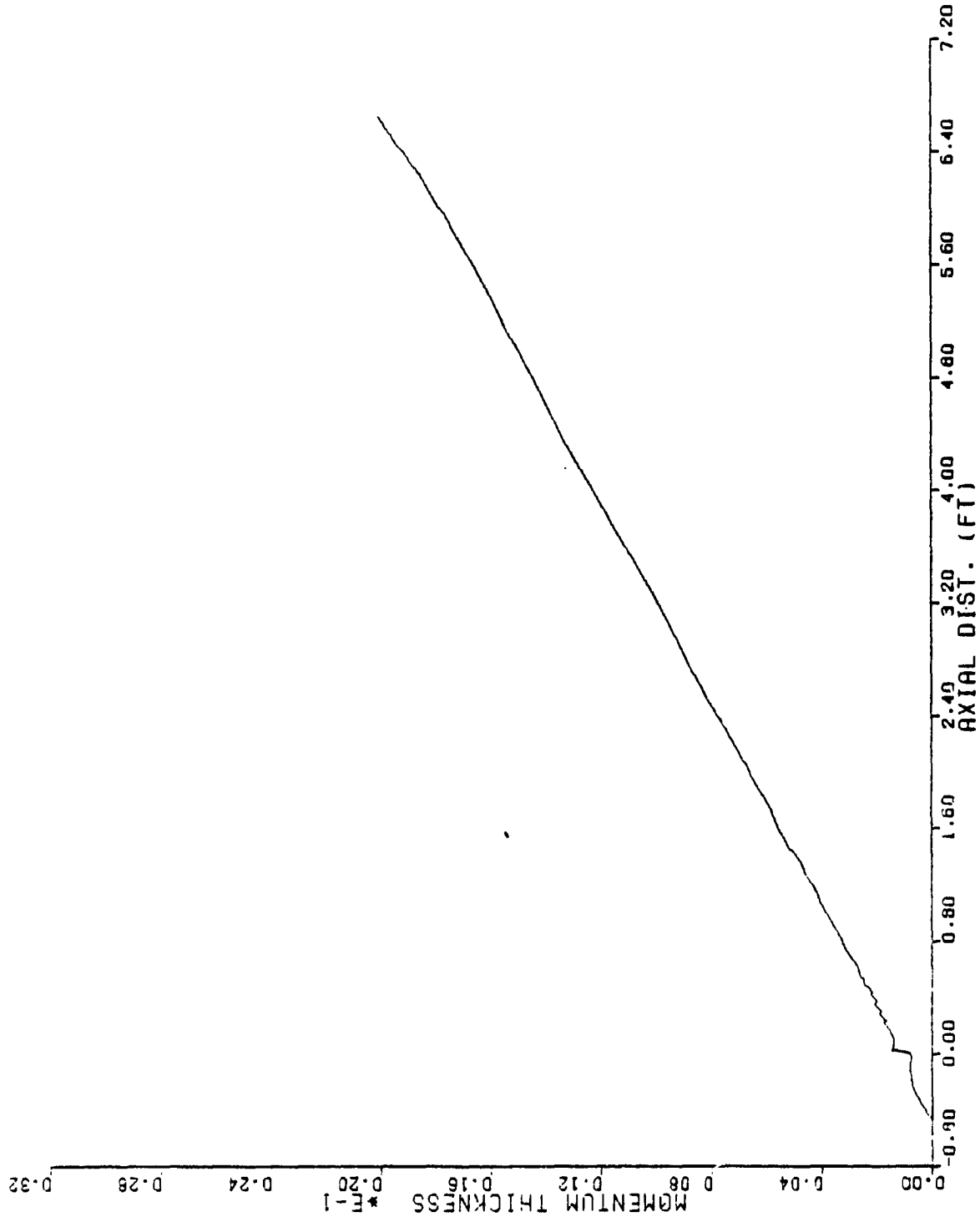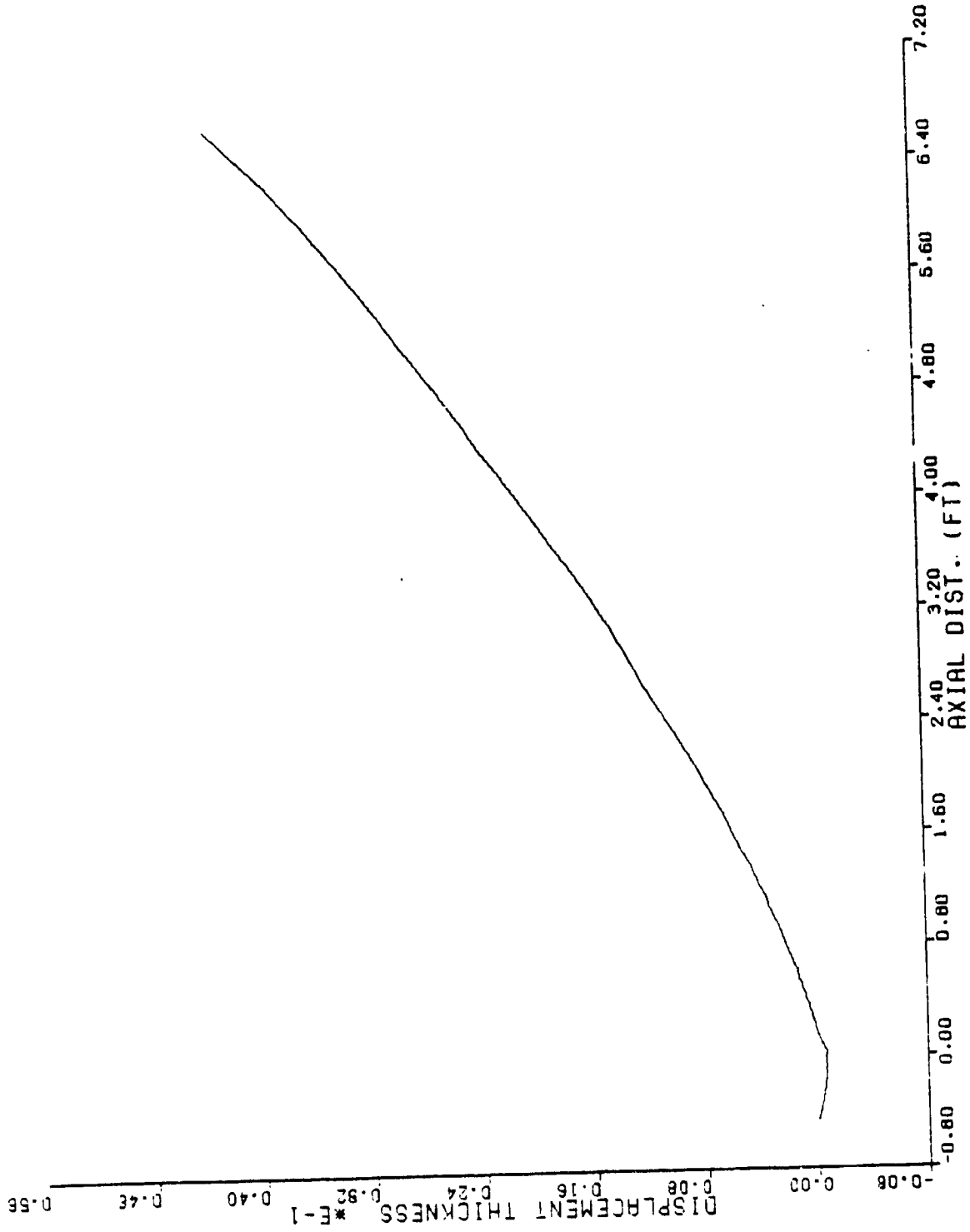Figure 6-2: Boundary Layer Momentum Thickness vs Axial Position
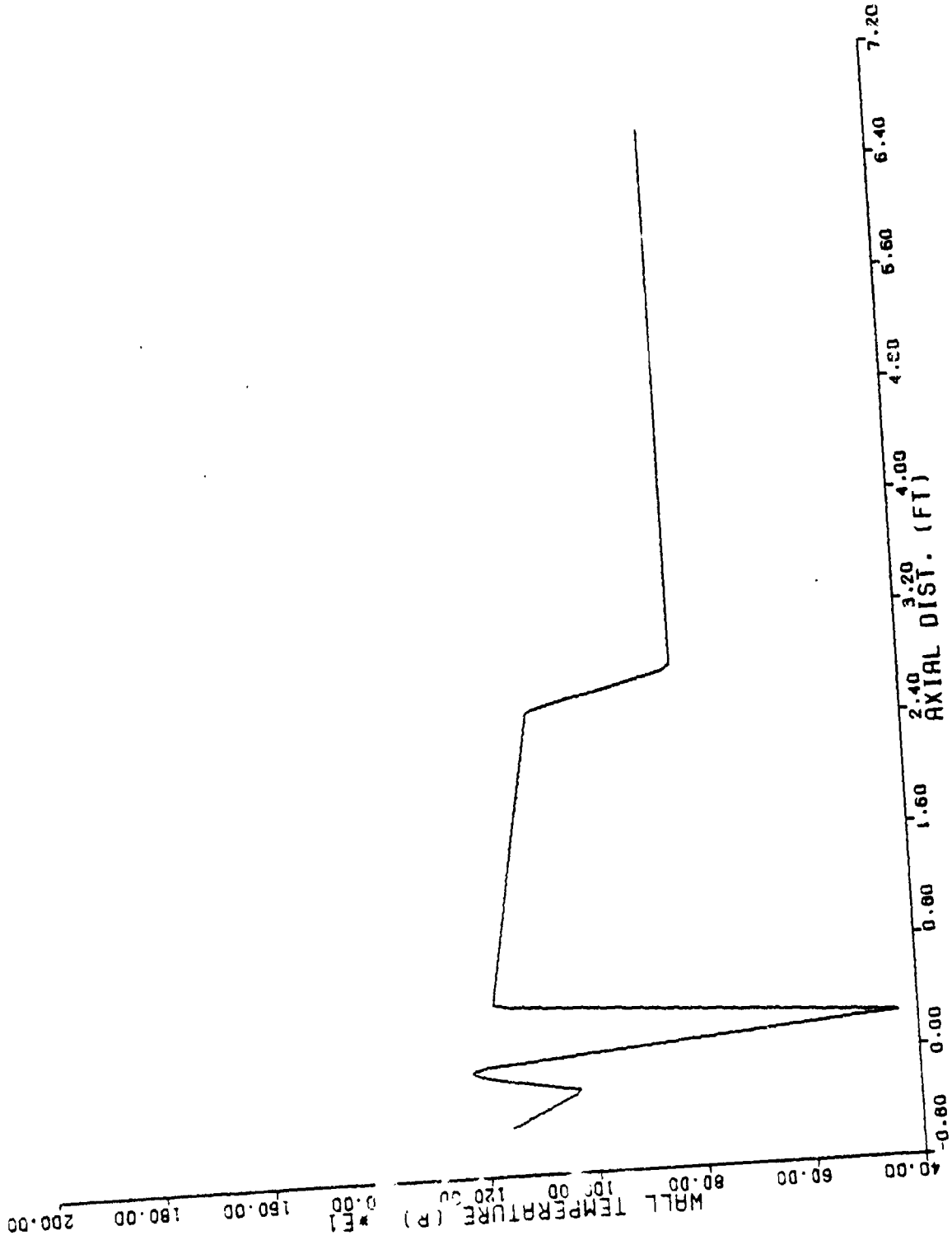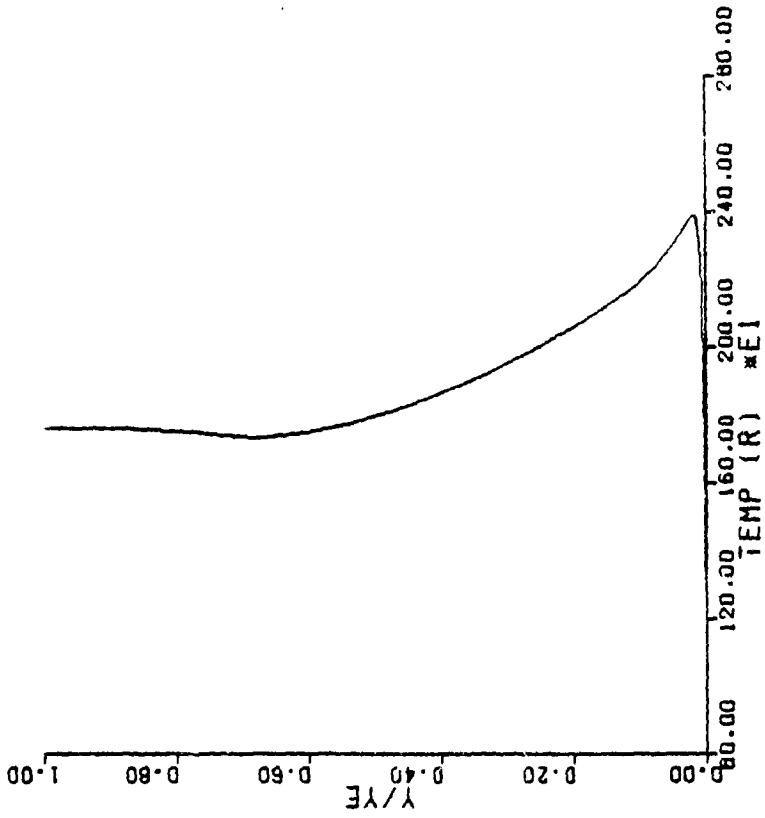
Figure 6-3: Boundary Layer Displacement Thickness vs Axial Position

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

TEMPERATURE PROFILE
EPS = 400.00
R   = 2.090
L   = 6.626
TE   = 1761.1
TW   = 818.0
YE   = 0.2689446

VELOCITY PROFILE
EPS = 400.00
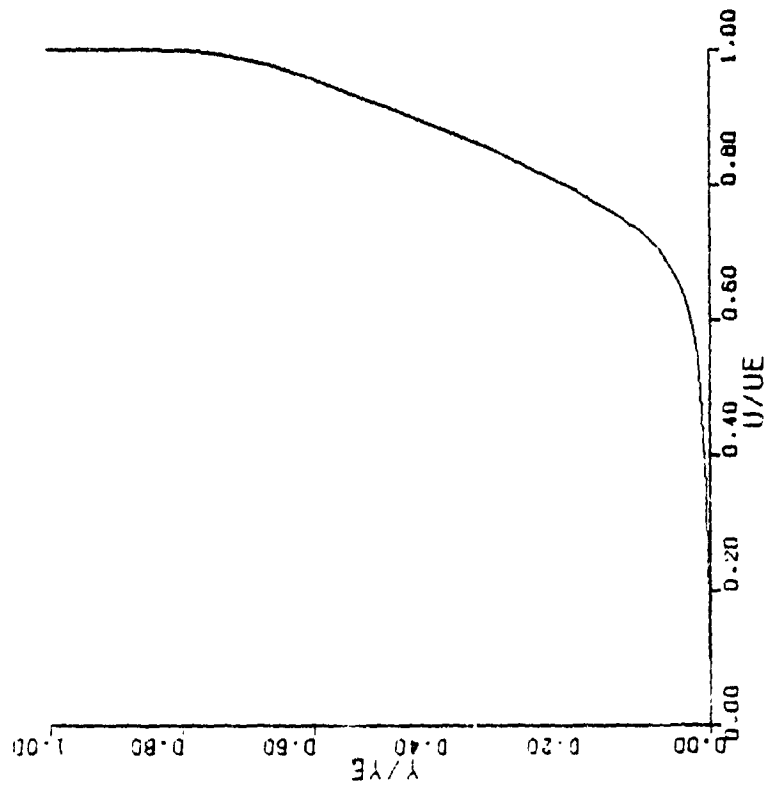R   = 2.090
L   = 6.626
UE   = 15079.1
YE   = 0.2689446

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

6.9   SPECIAL OPTIONS.

6.9.1   Constant Properties Gas Option.

The TDK program contains a useful option by which the real gas chemistry can be replaced by constant properties chemistry. Multiple zones can be calculated. The output includes the nozzle divergence efficiency, η_{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, γ, 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, ^{O}R, for each zone, inner to outer. (^{O}K in SI units)

RGC(1)   =   Real gas constant, ft^2/sec^2 ^{O}R, (i.e., $49721/M_w = g*J*1.986/M_w$) for each zone, inner to outer. (m^2/sec^2 ^{O}K if SI units)

XMW(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
 PFGOPT=1,
 NZONES=1,
 RSI=2,
 RWTU=2, RWTO=.5,
 THETA=35.6738,
 IWALL=4,
 NWS=11,
 RS(2)= 1.16843,1.26475,1.47910,1.73375,2.04940,2.45930,
        3.68226,4.94772,5.79198,6.32451,
 ZS(2)=  .39575, .53008, .87705,1.19473,1.66923,2.32795,
        4.68717,7.68599,10.9601,13.3114,
 THE=11.5813,
 $END
 $TRANS
 G=1.23,
 PSA=100,
 TC=5500,
 XMW=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.
REI.ERR	=	.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