PACKAGE (Plasma Analysis, Chemical Kinetics, And
Generator Efficiency): A computer program
for the calculation of partial chemical
equilibrium/partial chemical rate controlled
composition of multiphased mixtures under one
dimensional steady flow

By

V. Yousefian, M.H. Weinberg, and R. Haimes

Aerodyne Research, Inc.
Bedford Research Park, Crosby Drive
Bedford, Massachusetts 01730

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PREFACE

The prediction of multiphase combustion product parameters, such as mixture composition and temperature, is very important for designing such systems as rocket engines and coal fired energy conversion systems. The presence of a multitude of species, some in several phases, requires numerical methods for the prediction of the mixture properties. One such method in general use is the NASA CEC Code developed by Gordon and McBride.⁽¹⁾ For a given mixture the NASA CEC Code assumes chemical equilibrium to calculate the mixture composition given a selected pair of thermodynamic variables (e.g., pressure and temperature). For certain problems, however, the mixture residence time may be short, and in such cases, the assumption of chemical equilibrium is not, in general, valid. Therefore, the NASA CEC Code cannot be used. In addition, for mixtures where several liquid species can form, the NASA CEC assumption of pure condensed phases may also be invalid. To account for these effects, the PACKAGE Code which stands for 'Plasma Analysis Chemical Kinetics, And Generator Efficiency!' was developed.

Detailed discussions of formulation and input/output information used in the PACKAGE Code are given in Sections 1 and 2. Combined with the sample problems of Section 3, this Preface is intended to familiarize the user with the capabilities of the code and to help indicate if it can be adapted to his/her needs without detailed understanding of Sections 1 and 2. The following topics will be discussed in this Preface:

- a) PACKAGE Code Development,
- b) PACKAGE Code Description, and
- c) Current Programming Constraints.

a) PACKAGE Code Development

The NASA CEC Code was the starting point for PACKAGE Code development. During this development, several of the NASA CEC subroutines were greatly modified, six new subroutines were added and three were eliminated.

The modified subroutines are: MAIN, SRCHCC (same as SEARCH), ROCKET, OUT1, OUT2, OUT3, EQLBRM, REACT, and MATRIX. Subroutines with minor or no modifications are: CPHS, SAVE, BLOCKD, HCALC, NEWOF, GAUSS, VARFMT, EFMT, and THERMP. Subroutines which are eliminated are: FROZEN, SHCK, and DETON. Added subroutines are: MHD, DIFFUN, DIFSUB, CONDUCT, SETEQU, and function INTERP.

A description of these subroutines is given in Section 2. To describe these subroutines full advantage is taken of the NASA CEC manual. When possible the descriptions are kept identical to that of the NASA CEC. This has two advantages. First, it makes the PACKAGE Code manual self-contained and eliminates constant referencing of the NASA CEC Code. Second, it makes the utilization of the PACKAGE Code much easier for those who are familiar with the NASA CEC Code.

The modification of the NASA CEC subroutines and the addition of the new subroutines give the PACKAGE Code several new computational capabilities. These are described below.

b) PACKAGE Code Description

The following is a list of options available in the PACKAGE Code:

- Flow Model

- 1) One-dimensional steady channel flow with either area, pressure, or velocity specified along the channel,
- 2) Full MHD interaction model with variable Hall parameter,
- 3) Complete calculation of plasma conductivity, and
- 4) Inclusion of arbitrary force and heat terms in the momentum and energy equation.

- Chemical Model Options

- 1) Complete chemical equilibrium with ideal liquid solution or pure condensed phases only,
- 2) Partial chemical equilibrium - partial finite rate, and
- 3) Fully chemically finite rate

- Two-Stage/Single-Stage Combustor Option

- 1) Arbitrary fraction of reactants injected in the first- or second-stage and
- 2) Rejection of any fraction of condensed species from the first stage.

The six new subroutines and the modified NASA CEC subroutines enable the PACKAGE Code to integrate the one dimensional conservation equations under the different chemical options. The following is a brief description of the method used.

Under full or partial chemical equilibrium option the minimization of Gibbs free energy is used to evaluate the concentration of species which are not rate controlled, temperature, and other thermodynamic parameters. The Gibbs free energy is minimized given the concentration of rate controlled species, pressure, enthalpy, and subject to the conservation of chemical elements comprising the mixture. At each integration point, pressure, enthalpy, and rate controlled species concentration are determined from the solution of the conservation equations. When the fully rate controlled chemical model is used, the minimization of Gibbs free energy is no longer required. Given the species concentration and mixture enthalpy an iterative method is used to calculate the mixture temperature. The following list shows the solution procedure used in this code:

- Given all the flow parameters at the initial station $x = x_0$, the conservation equations are solved to obtain the mixture enthalpy, the concentration of rate controlled species, and either pressure and channel area (when velocity is specified), pressure and velocity (when area is specified), or area and velocity (when pressure is specified) at $x = x_0 + \Delta x$, subject to the conservation of chemical elements to get the concentration of the species which are not rate controlled, temperature, and other thermodynamic variables at $x = x_0 + \Delta x$.
- The Gibbs free energy is minimized given pressure, enthalpy, and rate controlled species concentration at $x = x_0 + \Delta x$ subject to the conservation of chemical elements to get the concentration of the nonrate controlled species, temperature, and other thermodynamic variables at $x = x_0 + \Delta x$.
- The first two steps are repeated to give the mixture properties at other x stations.

For all channel flow problems, the initial station $x_0 = 0$ defines the channel entrance. If the channel is attached to a combustor-nozzle unit, equilibrium chemistry is assumed in the combustor and in the throat. For subsonic entrance velocities, the rate controlled chemistry can be initiated at the channel entrance. For supersonic channel flow, rate controlled chemistry can be initiated either from the throat or the channel entrance. The entrance conditions are calculated by assigning either a channel entrance pressure ratio, subsonic area ratio, or supersonic area ratio. When rate controlled chemistry begins at the throat, a linear pressure drop is assumed from the throat to the channel entrance. In this case, the entrance pressure ratio must be specified. Downstream of the channel entrance, however, either velocity, pressure, or area ratio can be specified. When the two-stage combustor option is used, equilibrium chemistry is assumed in both stages. Downstream of the second stage, the problem is treated as if the first-stage did not exist. To account for combustor heat loss, the user has the option of reducing the combustor enthalpy by any desired amount.

If nonequilibrium chemistry is desired in the combustor, the channel entrance becomes the combustor entrance. Special input parameters are required for evaluating the initial conditions of such a flow. It is assumed here, that the reactants are well mixed before the reactions begin.

To account for interaction between the fluid and its surroundings (e.g., channel wall friction forces, radiative and conductive heat loss), the Subroutine SETEQU is added to the code. The user can define his/her own set of force and energy terms in this subroutine. A simple channel heat loss model and MHD interaction model are the integral part of the code and need not be set in the SETEQU subroutine. Under their default mode, however, these interactions are not considered. If additional interactions are required (e.g., MHD interaction in the presence of channel wall friction), the additional terms must be set in this subroutine.

In addition to the options described above, the PACKAGE Code can be used to evaluate the properties of a mixture in thermodynamic equilibrium given the mixture pressure and either temperature, enthalpy, or entropy. Under

these conditions, the predictions of the PACKAGE and NASA CEC Codes become identical unless the ideal liquid solution option is used.

A detailed description of the options listed above is given in Section 1. Again, when possible, the description is kept similar to that given in the NASA CEC manual (e.g., Subsections 1.6.1.1 - 1.6.1.6).

In order to show the input commands required to execute the many options considered above, 12 sample problems are included in Section 3. Input/output formats for each sample problem are fully described. The following contains a brief description of these sample problems and the physical models they can represent. Note that these are illustrative and do not necessarily represent practical problems

- Sample Problems 1, 2, and 3 - These examples show how to execute pressure-temperature, pressure-enthalpy and pressure-entropy assigned problems. These represent combustor composition calculations under chemical equilibrium using the ideal liquid solution model.
- Sample Problems 4, 5, and 6 - These examples represent channel flow problems assuming equilibrium chemistry. In problems 4 and 5 channel pressure and area ratio are specified, respectively. In problem 6, the two-stage combustor model is used with channel velocity specified. In all these problems MHD interaction terms are used. In the absence of any interaction (for example by setting the magnetic field equal to zero in the input), these channel flows become isentropic and can represent nozzle flows of the type considered in the NASA CEC Code. With the addition of proper force and energy terms in the SETERU subroutine these flows can represent a variety of channel flows, such as flows in smokestacks, conventional entrained combustion, advance concepts such as fluidized bed combustion or gasification, and others.
- Sample Problems 7, 8, 9, and 10 - These examples represent channel flow problems assuming partial equilibrium/partial rate controlled chemistry. In the first three problems rate controlled chemistry begins at the channel entrance with channel area ratio, velocity, and

pressure specified, respectively. In the fourth rate controlled chemistry begins from the throat with channel area ratio given. Here again, MHD interactions are considered. With the proper force and energy terms included, these type of problems can represent channel flows where it is known that chemical kinetic bottlenecks exist. These can happen in the type of flows discussed with the previous sample problems.

- Sample Problems 11 and 12 - These examples are models for channel flows with fully rate controlled chemistry where the reactions begin at the channel entrance. An example is the combustion of premixed reactants in a flow tube. Both samples represent the same flow with a constant channel area specified. In the second, a simple heat loss model is also used.

It is hoped that familiarity with these sample problems will give the user the experience necessary to use the Code for other kinds of problems.

As with most computer programs there are certain constraints associated with the PACKAGE Code. These are described below.

c) Current Programming Constraints

There are three categories of constraints associated with this program. The first category includes constraints on certain variables which are related to storage and can be readily changed by the programmer. These variables are:

- Maximum number of species, 600
- Maximum number of condensed species, 175
- Maximum number of rate controlled species, 29
for area specified channel flows, 30 otherwise
- Maximum number liquid species in the ideal liquid solution, 16
- Maximum number of discrete assigned values for either
channel pressure, velocity, or area ratio, 90.

The second category contains constraints related to convergence failures.

These are:

- Convergence problems associated with solving a set of stiff differential equations (Subroutine DIFSUB)
- Convergence problems associated with a singular matrix (Subroutine GAUSS)
- Convergence problems associated with assigned convergence tests (Subroutine EQLBRM)
- Round-off errors due to machine precision.

By gaining experience with the workings of the subroutines listed above all of the problems have been recognized and the majority have been solved.

The third category of current programming constraints is related to the ideal liquid solution model. The program does not allow the existence of the solid phase of a species whose liquid phase is in the liquid solution. A liquid species is allowed to freeze out of the liquid solution when the temperature is below the species melting temperature. For temperature-pressure assigned problems the freeze-out occurs when the temperature is 50 K below the melting point. For other options it occurs when the temperature is 150 K below the melting point. These temperature differences are arbitrary and may be changed by the user. Once a liquid is removed from the solution, its solid phase is allowed to form. For high temperature flows where formation of solid species is less likely, this model is adequate. The code will be updated to consider the presence of solids whose liquid phase is in the solution.

In closing this Preface, it should be noted that a computer code may become a valuable research tool when it can be successfully applied to all the problems it is intended for. Due to the nature of programming, most of the programming errors surface only during its use.

It is therefore encouraged, that any such problem be brought to the attention of the authors.

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1. FORMULATION AND ANALYSIS

The main function of the PACKAGE code is to evaluate the composition of a multiphase mixture under the following chemical conditions:

- Total equilibrium with pure condensed species,
- Total equilibrium with ideal liquid solution,
- Partial equilibrium/partial finite rate chemistry, and
- Fully finite rate chemistry.

The first condition is considered by the NASA CEC code.⁽¹⁾ The remaining conditions were developed to treat the evolution of complex mixtures, such as coal combustion products, where the assumption of total chemical equilibrium and pure condensed species may not, in general, be valid. Under total (or partial) chemical equilibrium, the total (or partial) mixture composition is determined by the minimization of total (or partial) Gibbs free energy of the system. The minimization can be accomplished given any two thermodynamic variables and the concentration of rate controlled species, subject to the conservation of the chemical elements comprising the mixture.

The pairs of thermodynamic variables considered here are either pressure and enthalpy, pressure and entropy, or pressure and temperature. In fluid flow problems, the conservation equations are generally solved for pressure and enthalpy; therefore, it is natural to use these two variables to minimize Gibbs free energy. For isentropic (i.e. constant entropy) flows, however, it is more convenient to use pressure and entropy. The pressure and temperature option is used for other applications, such as calculation of thermodynamic variables in a combustor when pressure and temperature are assigned or construction of Mollier diagrams.

In the following subsections, we first describe the equations required for the minimization of Gibbs free energy. This is followed by a description of relations which yield thermodynamic variables such as specific heat ratio, speed of sound, etc. Procedures for obtaining equilibrium composition are considered next. A description

of tests required for including condensed species in the system, the singularities that may occur during the Gibbs free energy minimization, and the format of thermodynamic data used, are then described. The section concludes with the treatment of the types of channel flows which are programmed in the code.

1.1 Channel Flow Conservation Equations

In this report, we only consider one-dimensional, steady-channel flows. The conservation equations describing such flows are mass, species, momentum, and energy. These are as follows:

mass,

$$\rho u A = \text{const} \quad , \quad (1)$$

species,

$$\rho u \frac{dn_i}{dx} = \dot{w}_i \quad , \quad (2)$$

$$(i = 1, \dots, NT)$$

momentum,

$$\rho u \frac{du}{dx} + \frac{dp}{dx} = F \quad , \quad (3)$$

and energy,

$$\rho u \frac{dh}{dx} + \rho u^2 \frac{du}{dx} = q \quad . \quad (4)$$

Here, ρ is the density (kg/m^3), u is the velocity (m/sec), n_i is the i -th species concentration in moles per kilogram of mixture, p is the pressure (N/m^2), and h is the enthalpy (J/kg). The source terms $\dot{w}_i$ and F are the i -th species net production rate ($\text{moles}/\text{m}^3\text{-sec}$) and force per unit volume (N/m^3), respectively. The source term q is the rate of added energy (heat plus work done by all external forces) per unit volume ($\text{J}/\text{m}^3\text{-sec}$). Also, A is the channel area (m^2), x is the axial coordinate (m), and NT is the total number of species in the mixture. Including two equations of state,

$$h = \sum_{i=1}^{NT} n_i (H_T^0)_i \quad , \quad (5)$$

and

$$\frac{p}{\rho} = n_g RT \quad , \quad (6)$$

(NT+5) equations are obtained for (NT+6) unknowns, namely, ρ , u , p , A , n_i ($i=1, \dots, NT$), h , and T ; therefore, one of the parameters must be specified. In Eqs. (5) and (6), $(H_T^0)_i$ is the i -th species enthalpy (J/mole), n_g is the total number of moles of gaseous species per kilogram of mixture, R is the universal gas constant (8314.3 J/kg-mole-K), and T is the temperature (K).

Equations (1) through (6) can, in principle, be solved to get the mixture composition under all chemical conditions. This, however, requires a knowledge of $\dot{w}_i$, the species production rate, for all $i = 1, \dots, NT$. To determine $\dot{w}_i$ all elementary chemical reactions and their rate constants leading to the net production of i -th species must be known. This may be impossible for multiphase mixtures like coal combustion products, which contain hundreds of species. In such cases, we make the practical assumption that the mixture is in total or partial thermochemical equilibrium. By partial equilibrium, we imply the following:

- The history of certain species are known to be kinetically controlled with all relevant reactions and rate constants known,
- The remaining species are at chemical equilibrium.

In such a case, the number of species conservation equations is reduced from NT to a number equal to that of the rate controlled species. Equations (1) through (6), then, yield the concentration of rate controlled species, pressure, and enthalpy. These are then used to minimize the Gibbs free energy in order to obtain the concentration of species which are at chemical equilibrium. As will be shown below, the minimization also yields the mixture temperature.

1.2 Minimization of Gibbs Free Energy

At the beginning of this section, four chemical conditions were listed for consideration. For each case, the minimization of Gibbs free energy results in a different type of equation. However, since fully equilibrium and fully rate-controlled chemistry are special cases of partial equilibrium/partial rate controlled chemistry, only the minimization of partial equilibrium case will be discussed in detail below.

Let the equilibrium and rate controlled species be indexed as shown below.

Indexing of Species in the Mixture

$i=1, \dots, MG$	$i=MG+1, \dots, MS$	$i=MS+1, \dots, ME$	$i=ME+1, \dots, NG$	$i=NG+1, \dots, NT$
species in gas phase	species in pure condensed phase	liquid species in ideal solution	species in gas phase	species in pure condensed phase
← Equilibrium controlled species →			← Rate controlled species →	

For this system, the concentration of the first ME species (with $i=1, \dots, ME$) is determined from the minimization of the partial Gibbs free energy of the system which is composed of the contributions from these species. Note that the concentration of the remaining $(NT-ME)$ species (with $i > ME$) are evaluated from the species conservation equations.

If g is the partial Gibbs free energy to be minimized, then,

$$g = \sum_{j=1}^{ME} \mu_j n_j \quad , \quad (7)$$

where the chemical potential per kilogram-mole of species j is given by

$$\mu_j = \left(\frac{\partial g}{\partial n_j} \right)_{T, P, n_{i \neq j}} \quad (8)$$

The minimization is subject to the constraint that the number of moles of chemical elements per kilogram of mixture are conserved. This constraint may be represented by:

$$\sum_{j=1}^{ME} a_{ij} n_j - \left(b_i^0 - \sum_{j=ME+1}^{NT} a_{ij} n_j \right) = 0 \quad (i=1, \dots, \ell) \quad (9)$$

Here, the stoichiometric coefficients a_{ij} are the number of kilogram-atoms of element i per kilogram-mole of species j , and b_i^0 is the assigned number of kilogram-atoms of element i per kilogram of mixture. Since no elements are destroyed or created during chemical reactions of the type considered here, b_i^0 is a constant and equal to the number of kilogram moles of the i -th element per kilogram of total reactants. Since, during the minimization process, all n_j with $j > ME$ are known and remain unchanged, Eq. (9) can also be written as:

$$b_i - b_i^0 = 0 \quad (i=1, \dots, \ell) \quad (10)$$

where

$$b_i = \sum_{j=1}^{NT} a_{ij} n_j \quad (11)$$

Defining G to be

$$G = g + \sum_{i=1}^{\ell} \lambda_i (b_i - b_i^0) \quad (12)$$

where λ_i are Lagrangian multipliers, the condition for equilibrium becomes

$$\delta G = \sum_{j=1}^{ME} \left(\mu_j + \sum_{i=1}^{\ell} \lambda_i a_{ij} \right) \delta n_j + \sum_{i=1}^{\ell} (b_i - b_i^0) \delta \lambda_i = 0 \quad (13)$$

Treating the variations δn_j and $\delta \lambda_i$ as independent yields

$$\mu_j + \sum_{i=1}^{\ell} \lambda_i a_{ij} = 0 \quad (j = 1, \dots, ME) \quad (14)$$

and Eq. (10).

The chemical potential may be written as:

$$\mu_j = \begin{cases} \mu_j^0 + RT \ln \left(\frac{n_j}{n_g} \right) + RT \ln p_{\text{atm}} & \text{for gaseous species} \\ \mu_j^0 & \text{for pure condensed species} \\ \mu_j^0 + RT \ln \left(\frac{n_j}{n_c} \right) & \text{for species in ideal liquid solution} \end{cases} \quad (15)$$

$\mu_i^0(T)$, which are functions of temperature alone, are the standard state chemical potentials, p_{atm} is the total pressure in atmospheres, and n_c is the total number of moles of condensed species in the ideal solution per kilogram of mixture.

It is readily seen that

$$n_g = \sum_{i=1}^{MG} n_i + \sum_{i=ME+1}^{NG} n_i \quad (16a)$$

and

$$n_c = \sum_{i=MS+1}^{ME} n_i \quad (16b)$$

Note, that in this model, no rate controlled condensed species are contained in the solution.

Equations (9) and (14) permit the determination of equilibrium compositions for thermodynamic states specified by an assigned enthalpy, h_0 , pressure, p_0 , and n_{0i} ($i > ME$). That is, in addition to Eqs. (9) and (14), we have the trivial equations

$$h = h_0 \quad (17a)$$

$$p = p_0 \quad (17b)$$

$$n_i = n_{0i} \quad (i > ME) \quad (17c)$$

where h is given by Eq. (5). In this model, assigned variables generally refer to the values of these variables attained from the solution of the conservation equations [cf. Eqs. (1-4)].

The equilibrium composition can also be determined if temperature T_0 or entropy s_0 is assigned instead of enthalpy. In such cases, Eq. (17a) is replaced by either

$$T = T_0 \quad , \quad (18)$$

if temperature is specified, or by

$$s = s_0 \quad , \quad (19)$$

if entropy is specified. The mixture entropy is given by

$$s = \sum_{j=1}^{NT} n_j S_j \quad , \quad (20)$$

where

$$S_j = \begin{cases} \left(S_T^0 \right)_j - R \ln \left(\frac{n_j}{n_g} \right) - R \ln p_{atm} & \text{for gaseous species} \\ \left(S_T^0 \right)_j & \text{for pure condensed species} \\ \left(S_T^0 \right)_j - R \ln \left(\frac{n_j}{n_c} \right) & \text{for condensed species in liquid solution} \end{cases} \quad (21)$$

with $\left(S_T^0 \right)$ as the standard state entropy for j -th species.

The equations required to obtain the composition are not all linear in the composition variables, therefore, an iteration procedure is generally required.

1.2.1 Gibbs Iteration Equations

A descent Newton-Raphson method is used to solve for corrections to initial estimates of compositions, n_j ($j \leq ME$), Lagrangian multipliers, λ_i , total moles, N (the total number of moles of gaseous species per kilogram of mixture which are in the equilibrium pool, see Eq. (22) below), total moles in the liquid solution, n_c , and, when required, temperature, T . This method involves a Taylor series expansion of the appropriate equations, truncated for derivatives higher than the first. The correction variables used are $\Delta \ln n_j$ ($j = 1, \dots, MG$), Δn_j ($j = MG + 1, \dots, MS$), $\Delta \ln n_j$ ($j = MS + 1, \dots, ME$), $\Delta \ln N$, $\Delta \ln n_c$, $\pi_i = -\lambda_i/RT$ and $\Delta \ln T$. It is no restriction to start each iteration with the estimate for the Lagrangian multipliers equal to zero, since they appear linearly in Eq. (14). After making those equations which contain thermodynamic functions dimensionless, the Newton-Raphson equations obtained from the proper combination of Eqs. (9), (14), (16b), (17a), (19), and

$$N = \sum_{j=1}^{MG} n_j \quad , \quad (22)$$

are

$$\Delta \ln n_j - \frac{N}{N+M} \Delta \ln N - \sum_{i=1}^{\ell} a_{ij} \pi_i - \left[\frac{(H_T^0)_j}{RT} \right] \Delta \ln T = -\frac{\mu_j}{RT} \quad (j = 1, \dots, MG) \quad , \quad (23)$$

$$\sum_{j=1}^{\ell} a_{ij} \pi_j + \frac{(H_T^0)_j}{RT} \Delta \ln T = \frac{\mu_j}{RT} \quad (j = MG + 1, \dots, MS) \quad , \quad (24)$$

$$\Delta \ln n_j - \sum_{j=1}^{\ell} a_{ij} \pi_j - \Delta \ln n_c - \frac{(H_T^0)_j}{RT} \Delta \ln T = -\frac{\mu_j}{RT} \quad (j = MS + 1, \dots, ME) \quad , \quad (25)$$

$$\begin{aligned}
& \sum_{j=1}^{MG} a_{ij} n_j \Delta \ln n_j + \sum_{j=MS+1}^{ME} a_{ij} n_j \Delta \ln n_j \\
& + \sum_{j=MG+1}^{MS} a_{ij} \Delta n_j = b_i^0 - b_i \quad (i = 1, \dots, \ell) , \quad (26)
\end{aligned}$$

$$\sum_{j=1}^{MG} n_j \Delta \ln n_j - N \Delta \ln N = N - \sum_{j=1}^{MG} n_j , \quad (27)$$

$$\sum_{j=MS+1}^{ME} n_j \Delta \ln n_j - n_c \Delta \ln n_c = n_c - \sum_{j=MS+1}^{ME} n_j , \quad (28)$$

$$\begin{aligned}
& \sum_{j=1}^{MG} n_j \frac{(H_T^0)_j}{RT} \Delta \ln n_j + \sum_{j=MS+1}^{ME} n_j \frac{(H_T^0)_j}{RT} \Delta \ln n_j + \sum_{j=MG+1}^{MS} \frac{(H_T^0)_j}{RT} \Delta n_j \\
& + \left[\sum_{j=1}^{NT} n_j \frac{(C_p^0)_j}{R} \right] \Delta \ln T = \frac{h_0 - h}{RT} , \quad (29)
\end{aligned}$$

$$\begin{aligned}
& \sum_{j=1}^{MG} \left(\frac{n_j S_j}{R} \right) \Delta \ln n_j + \sum_{j=MS+1}^{ME} \left(\frac{n_j S_j}{R} \right) \Delta \ln n_j + \sum_{j=ME+1}^{MS} \left[\frac{(S_T^0)_j}{R} \right] \Delta n_j \\
& + \left[\sum_{j=1}^{NT} \frac{n_j (C_p^0)_j}{R} \right] \Delta \ln T = \frac{s_0 - s}{R} + N - \sum_{j=1}^{ME} n_j + n_c - \sum_{j=MS+1}^{ME} n_j
\end{aligned}$$

with M, the number of kilogram-moles of rate controlled gaseous species per kilogram of mixture, given by:

$$M \equiv \sum_{j=ME+1}^{NG} n_j \quad . \quad (31)$$

Therefore, $n_g = N + M$. In Eq. (29), $(C_p^0)_j$ is the specific heat of the j-th species at constant pressure (J/kg-mole-K).

In the absence of rate controlled chemistry and condensed solution, when $M = n_c = 0$, $N = n_g$, and $MS = NT$, the terms which are summed over species indexed from $(MS+1)$ to ME are eliminated from Eqs. (26), (29), and (30). Eqs. (25) and (28) are eliminated altogether. The remaining equations become identical to their counterparts given on pages 9 and 10 of the NASA CEC⁽¹⁾ manual. When condensed ideal solution is included in the equilibrium mixture, we have, in the absence of rate controlled chemistry, $M = 0$, $N = n_g$, and Eqs. (23) through (30) reduce to their form applicable to such a system. In the limit of fully rate controlled chemistry, we have $N = MG = MS = ME = n_c = 0$ and $M = n_g$ with Eqs. (23) through (28) eliminated. Eqs. (29) and (30) reduce to

$$\sum_{j=1}^{NT} n_j \frac{(C_p^0)_j}{R} \Delta \ln T = \frac{h_0 - h}{RT} \quad , \quad (32)$$

and

$$\sum_{j=1}^{NT} n_j \frac{(C_p^0)_j}{R} \Delta \ln T = \frac{s_0 - s}{R} \quad . \quad (33)$$

With all the n_i calculated from the species conservation equations, the mixture temperature can be evaluated using Eq. (32), when h_0 is specified, or Eq. (33) when s_0 is specified. We conclude, therefore, that in their proper limits, Eqs. (23) through (31) effectively describe all the chemical conditions listed on page 1-1.

1.2.2 Reduced Gibbs Iteration Equations

Equations (23) through (28) and Eq. (29) or (30) represent a total of $ME + \ell + 3$ equations. By properly combining Eqs. (23) through (30), the total number of equations to be solved can be reduced to $(MS - MG + \ell + 3)$. After considerable algebra, it can be shown that the reduced equations are given by:

$$\begin{aligned}
 & \sum_{i=1}^{\ell} \left(\sum_{j=1}^{MG} a_{kj} a_{ij} n_j + \sum_{j=MS+1}^{ME} a_{kj} a_{ij} n_j \right) \pi_i \\
 & + \sum_{j=MG+1}^{MS} a_{kj} \Delta n_j + \frac{N}{N+M} \sum_{j=1}^{MG} a_{kj} n_j \Delta \ln N \\
 & + \sum_{j=MS+1}^{ME} a_{kj} n_j \Delta \ln n_c + \left[\sum_{j=1}^{MG} a_{kj} n_j \frac{(H_T^0)_j}{RT} \right. \\
 & \quad \left. + \sum_{j=MS+1}^{ME} a_{kj} n_j \frac{(H_T^0)_j}{RT} \right] \Delta \ln T \\
 & = b_k^0 - b_k + \sum_{j=1}^{MG} a_{kj} n_j \frac{\mu_j}{RT} \\
 & + \sum_{j=MS+1}^{ME} a_{kj} n_j \frac{\mu_j}{RT} \quad (k = 1, \dots, \ell) \quad , \quad (34)
 \end{aligned}$$

$$\sum_{i=1}^{\ell} a_{ij} \pi_i + \left[\frac{(H_T^0)_j}{RT} \right] \Delta \ln T = \frac{\mu_j}{RT} \quad (j = MG + 1, \dots, MS), \quad (35)$$

$$\begin{aligned} \sum_{i=1}^{\ell} \sum_{j=1}^{MG} a_{ij} n_j \pi_i + \left(\frac{N}{N+M} \sum_{j=1}^{MG} n_j - N \right) \Delta \ln N \\ + \left[\sum_{j=1}^{MG} \frac{n_j (H_T^0)_j}{RT} \right] \Delta \ln T \\ = N - \sum_{j=1}^{MG} n_j + \sum_{j=1}^{MG} \frac{n_j \mu_j}{RT}, \quad (36) \end{aligned}$$

$$\begin{aligned} \sum_{i=1}^{\ell} \sum_{j=MS+1}^{ME} a_{ij} n_j \pi_i + \left(\sum_{j=MS+1}^{ME} n_j - n_c \right) \Delta \ln n_c \\ + \left[\sum_{j=MS+1}^{ME} \frac{n_j (H_T^0)_j}{RT} \right] \Delta \ln T \\ = n_c - \sum_{j=MS+1}^{ME} n_j + \sum_{j=MS+1}^{ME} \frac{n_j \mu_j}{RT}, \quad (37) \end{aligned}$$

$$\begin{aligned}
& \sum_{i=1}^l \left[\sum_{j=1}^{MG} a_{ij} n_j \frac{(H_T^0)_i}{RT} + \sum_{j=MS+1}^{ME} a_{ij} n_j \frac{(H_T^0)_i}{RT} \right] \pi_i + \sum_{j=MG+1}^{MS} \frac{(H_T^0)_i}{RT} \Delta n_j \\
& + \frac{N}{N+M} \sum_{j=1}^{MG} n_j \frac{(H_T^0)_i}{RT} \Delta \ln N + \sum_{j=MS+1}^{ME} n_j \frac{(H_T^0)_i}{RT} \Delta \ln n_c \\
& + \left[\sum_{j=1}^{NT} n_j \frac{(C_p^0)_i}{R} + \sum_{j=1}^{MG} n_j \frac{(H_T^0)_i^2}{R^2 T^2} \right. \\
& \quad \left. + \sum_{j=MS+1}^{ME} n_j \frac{(H_T^0)_i^2}{R^2 T^2} \right] \Delta \ln T \\
& = \frac{h_0 - h}{RT} + \sum_{j=1}^{MG} n_j \frac{\mu_j (H_T^0)_i}{R^2 T^2} + \sum_{j=MS+1}^{ME} n_j \frac{\mu_j (H_T^0)_i}{R^2 T^2} ,
\end{aligned}$$

(38)

$$\begin{aligned}
& \sum_{i=1}^{\ell} \left(\sum_{j=1}^{MG} a_{ij} n_j \frac{s_j}{R} + \sum_{j=MS+1}^{ME} a_{ij} n_j \frac{s_j}{R} \right) \pi_i + \sum_{j=MG+1}^{MS} \frac{s_j}{R} \Delta n_j \\
& + \frac{N}{N+M} \left(\sum_{j=1}^{MG} n_j \frac{s_j}{R} \right) \Delta \ln N + \left(\sum_{j=MS+1}^{ME} n_j \frac{s_j}{R} \right) \Delta \ln n_c \\
& + \left[\sum_{j=1}^{NT} n_j \frac{(C_p^0)_j}{R} + \sum_{j=1}^{MG} n_j \frac{(H_T^0)_j}{R^2 T} s_j \right. \\
& \quad \left. + \sum_{j=MS+1}^{ME} n_j \frac{(H_T^0)_j}{R^2 T} s_j \right] \Delta \ln T \\
& = \frac{s_0 - s}{R} + \left(N - \sum_{j=1}^{MG} n_j \right) + \left(n_c - \sum_{j=MS+1}^{ME} n_j \right) \\
& + \sum_{j=1}^{MG} \frac{n_j S_j \mu_j}{R^2 T} + \sum_{j=MS+1}^{ME} \frac{n_j S_j \mu_j}{R^2 T}
\end{aligned} \tag{39}$$

Given p , h_0 , n_i ($i > ME$) and b_0^i the procedure for obtaining the equilibrium species composition n_i ($i \leq ME$) and temperature is as follows:

- Estimate n_i ($i \leq ME$), T , N , and n_c ,
- Solve Eqs. (34) through (38) to evaluate corrections to these estimates, and
- If the correction terms are greater than a specified value, repeat the above two steps to get new estimates, otherwise the estimated values are the solution.

More details of this procedure are given in Subsection 1.4.

In the PACKAGE code, the coefficients of the unknowns given by Eqs. (34) through (38) or (39) are set in subroutine MATRIX while the equations are solved in subroutine GAUSS. The new estimates are calculated in subroutine EQLBRM.

1.3 Thermodynamic Derivatives From Matrix Solutions

To evaluate thermodynamic variables such as the specific heats and speed of sound it is required to determine certain thermodynamic derivatives. In this subsection, a description of these derivatives and the methods for evaluating them is given.

All thermodynamic first derivatives can be expressed in terms of any three independent first derivatives. Here, as in the NASA CEC code, we will express first derivatives in terms of $(\partial V/\partial T)_{p, NE}$, $(\partial V/\partial p)_{T, NE}$, and $(\partial h/\partial T)_{p, NE} \equiv C_{p, NE}$, where subscript NE implies that concentrations of all rate controlled species are kept constant during differentiation. Therefore, $C_{p, NE}$ means specific heat with constant pressure and constant n_i ($i > ME$). We will use the logarithmic form of the volume derivatives since in that form they give an indication of the extent of equilibrium chemistry occurring among the equilibrium reaction species. From Eq. (5)

$$\begin{aligned}
 C_{p, NE} \equiv \left(\frac{\partial h}{\partial T} \right)_{p, NE} = & \sum_{j=1}^{NT} n_j (C_p^0)_j + \sum_{j=1}^{MG} n_j \frac{(H_T^0)_j}{T} \left(\frac{\partial \ln n_j}{\partial \ln T} \right)_{p, NE} \\
 & + \sum_{j=MG+1}^{MS} \frac{(H_T^0)_j}{T} \left(\frac{\partial n_j}{\partial \ln T} \right)_{p, NE} \\
 & + \sum_{j=MS+1}^{ME} n_j \frac{(H_T^0)_j}{T} \left(\frac{\partial \ln n_j}{\partial \ln T} \right)_{p, NE} . \quad (40)
 \end{aligned}$$

From Eq. (6) and with $\rho = 1/V$ and $n_g = N+M$, we find

$$\left(\frac{\partial \ln V}{\partial \ln T}\right)_{p, NE} = 1 + \frac{N}{N+M} \left(\frac{\partial \ln N}{\partial \ln T}\right)_{p, NE} \quad (41)$$

$$\left(\frac{\partial \ln V}{\partial \ln p}\right)_{T, NE} = -1 + \frac{N}{N+M} \left(\frac{\partial \ln N}{\partial \ln p}\right)_{T, NE} \quad (42)$$

1.3.1 Derivative With Respect to Temperature

The derivatives of n_j and N with respect to temperature are needed to evaluate Eqs. (40) and (41). These derivatives may be obtained from differentiation of Eqs. (14), (19), (22), and (16b) yielding

$$\begin{aligned} \left(\frac{\partial \ln n_j}{\partial \ln T}\right)_{p, NE} - \sum_{i=1}^{\ell} a_{ij} \left(\frac{\partial \pi_i}{\partial \ln T}\right)_{p, NE} - \frac{N}{N+M} \left(\frac{\partial \ln N}{\partial \ln T}\right)_{p, NE} \\ = \frac{(H_T^0)_j}{RT} \quad (j = 1, \dots, MG) \end{aligned} \quad (43)$$

$$- \sum_{i=1}^{\ell} a_{ij} \left(\frac{\partial \pi_i}{\partial \ln T}\right)_{p, NE} = \frac{(H_T^0)_j}{RT} \quad (j = MG+1, \dots, MS) \quad (44)$$

$$\begin{aligned} \left(\frac{\partial \ln n_j}{\partial \ln T}\right)_{p, NE} - \sum_{i=1}^{\ell} a_{ij} \left(\frac{\partial \pi_i}{\partial \ln T}\right)_{p, NE} - \left(\frac{\partial \ln n_c}{\partial \ln T}\right)_{p, NE} \\ = \frac{(H_T^0)_j}{RT} \quad (j = MS+1, \dots, ME) \end{aligned} \quad (45)$$

$$\begin{aligned}
\sum_{j=1}^{MG} a_{ij} n_j \left(\frac{\partial \ln n_j}{\partial \ln T} \right)_{p, NE} + \sum_{j=MG+1}^{MS} a_{ij} \left(\frac{\partial n_j}{\partial \ln T} \right)_{p, NE} \\
+ \sum_{j=MS+1}^{ME} a_{ij} n_j \left(\frac{\partial \ln n_j}{\partial \ln T} \right)_{p, NE} = 0 \quad (i = 1, \dots, \ell) \quad (46)
\end{aligned}$$

$$\sum_{j=1}^{MG} n_j \left(\frac{\partial \ln n_j}{\partial \ln T} \right)_{p, NE} - N \left(\frac{\partial \ln N}{\partial \ln T} \right)_{p, NE} = 0 \quad (47)$$

$$\sum_{j=MS+1}^{ME} n_j \left(\frac{\partial \ln n_j}{\partial \ln T} \right)_{p, NE} - n_c \left(\frac{\partial \ln n_c}{\partial \ln T} \right)_{p, NE} = 0 \quad (48)$$

Combining Eqs. (43) through (48), a much smaller number of simultaneous equations is obtained, namely,

$$\begin{aligned}
\sum_{i=1}^{\ell} \left(\sum_{j=1}^{MG} a_{kj} a_{ij} n_j + \sum_{j=MS+1}^{ME} a_{kj} a_{ij} n_j \right) \left(\frac{\partial \pi_i}{\partial \ln T} \right)_{p, NE} + \sum_{j=MG+1}^{MS} a_{kj} \left(\frac{\partial n_j}{\partial \ln T} \right)_{p, NE} \\
+ \frac{N}{N+M} \sum_{j=1}^{MG} a_{kj} n_j \left(\frac{\partial \ln N}{\partial \ln T} \right)_{p, NE} + \sum_{j=MS+1}^{ME} a_{kj} n_j \left(\frac{\partial \ln n_c}{\partial \ln T} \right)_{p, NE} = - \sum_{j=1}^{MG} a_{kj} n_j \frac{(H_T^0)_j}{RT} \\
- \sum_{j=MS+1}^{ME} a_{kj} n_j \frac{(H_T^0)_j}{RT} \quad (k = 1, \dots, \ell) \quad (49)
\end{aligned}$$

$$\sum_{i=1}^{\ell} a_{ij} \left(\frac{\partial \pi_i}{\partial \ln T} \right)_{p, NE} = - \frac{(H_T^0)_j}{RT} \quad (j = MG+1, \dots, MS) \quad (50)$$

$$\sum_{i=1}^{\ell} \sum_{j=1}^{MG} a_{ij} n_j \left(\frac{\partial \pi_i}{\partial \ln T} \right)_{p, NE} - \left(\frac{NM}{N+M} \right) \left(\frac{\partial \ln N}{\partial \ln T} \right)_{p, NE} = - \sum_{j=1}^{MG} n_j \frac{(H_T^0)_j}{RT} \quad (51)$$

$$\sum_{i=1}^{\ell} \sum_{j=MS+1}^{MG} a_{ij} n_j \left(\frac{\partial \pi_i}{\partial \ln T} \right)_{p, NE} = - \sum_{j=MS+1}^{ME} n_j \frac{(H_T^0)_j}{RT} \quad (52)$$

The values of the derivatives obtained from Eqs. (49) to (52) can be used in Eqs. (43) and (45) to obtain the derivatives of gaseous species and species in solution $(\partial \ln n_j / \partial \ln T)_{p, NE}$ ($j=1, \dots, MG$, and $j=MS+1, \dots, ME$). These derivatives can then be used to evaluate $C_{p, NE}$ from Eq. (40). A simple way of obtaining $C_{p, NE}$ is to combine Eqs. (40), (43), and (45) to eliminate $(\partial \ln n_j / \partial \ln T)_{p, NE}$. The result yields

$$\begin{aligned}
\frac{C_{p, NE}}{R} = & \sum_{i=1}^{\ell} \left[\sum_{j=1}^{MG} a_{ij} n_j \frac{(H_T^0)_j}{RT} + \sum_{j=MS+1}^{ME} a_{ij} n_j \frac{(H_T^0)_j}{RT} \right] \left(\frac{\partial \pi_i}{\partial \ln T} \right)_{p, NE} \\
& + \sum_{j=MG+1}^{MS} \left[\frac{(H_T^0)_j}{RT} \right] \left(\frac{\partial n_j}{\partial \ln T} \right)_{p, NE} + \left[\sum_{j=MS+1}^{ME} n_j \frac{(H_T^0)_j}{RT} \right] \left(\frac{\partial \ln n_c}{\partial \ln T} \right)_{p, NE} \\
& + \frac{N}{N+M} \left[\sum_{j=1}^{MG} n_j \frac{(H_T^0)_j}{RT} \right] \left(\frac{\partial \ln N}{\partial \ln T} \right)_{p, NE} + \sum_{j=1}^{NT} n_j \frac{(C_P^0)_j}{R} + \sum_{j=1}^{MG} n_j \frac{(H_T^0)_j^2}{R^2 T^2} \\
& + \sum_{j=MS+1}^{ME} n_j \frac{(H_T^0)_j^2}{R^2 T^2} .
\end{aligned} \tag{53}$$

In Eq. (53), only the temperature derivatives obtained directly from solution of Eqs. (49) to (52) are required. Furthermore, all the coefficients in Eq. (55) are exactly the coefficients appearing in the reduced enthalpy equation [cf. Eq. (38)].

1.3.2 Derivatives With Respect to Pressure

The derivative $(\partial \ln N / \partial \ln p)_{T, NE}$ can be obtained in a manner similar to that described in the previous section. Differentiation of Eqs. (14), (9), (22), and (16b) yields

$$\left(\frac{\partial \ln n_j}{\partial \ln p} \right)_{T, NE} - \sum_{i=1}^{\ell} a_{ij} \left(\frac{\partial \pi_i}{\partial \ln p} \right)_{T, NE} - \frac{N}{N+M} \left(\frac{\partial \ln N}{\partial \ln p} \right)_{T, NE} = -1 \quad (j=1, \dots, MG) \tag{54}$$

$$\sum_{i=1}^{\ell} a_{ij} \left(\frac{\partial \pi_i}{\partial \ln p} \right)_{T, NE} = 0 \quad (j=MG+1, \dots, MS) \quad (55)$$

$$\left(\frac{\partial \ln n_j}{\partial \ln p} \right)_{T, NE} - \sum_{i=1}^{\ell} a_{ij} \left(\frac{\partial \pi_i}{\partial \ln p} \right)_{T, NE} - \left(\frac{\partial \ln n_c}{\partial \ln p} \right)_{T, NE} = 0$$

(j=MS+1, \dots, ME) \quad (56)

$$\sum_{j=1}^{MG} a_{ij} n_j \left(\frac{\partial \ln n_j}{\partial \ln p} \right)_{T, NE} + \sum_{j=MG+1}^{MS} a_{ij} \left(\frac{\partial n_j}{\partial \ln p} \right)_{T, NE}$$

$$+ \sum_{j=MS+1}^{ME} a_{ij} n_j \left(\frac{\partial \ln n_j}{\partial \ln p} \right)_{T, NE} = 0 \quad (i=1, \dots, \ell) \quad (57)$$

$$\sum_{j=1}^{MS} n_j \left(\frac{\partial \ln n_j}{\partial \ln p} \right)_{T, NE} - N \left(\frac{\partial \ln N}{\partial \ln p} \right)_{T, NE} = 0 \quad (58)$$

$$\sum_{j=MS+1}^{ME} n_j \left(\frac{\partial \ln n_j}{\partial \ln p} \right)_{T, NE} - n_c \left(\frac{\partial \ln n_c}{\partial \ln p} \right)_{T, NE} = 0 \quad (59)$$

Equations (54) to (59) can be combined to eliminate $(\partial \ln n_j / \partial \ln p)_{T, NE}$ producing the reduced set of equations given below:

$$\begin{aligned}
 \sum_{i=1}^{\ell} \left(\sum_{j=1}^{MG} a_{kj} a_{ij} n_j + \sum_{j=MS+1}^{ME} a_{kj} a_{ij} n_j \right) \left(\frac{\partial \pi_i}{\partial \ln p} \right)_{T, NE} + \sum_{j=MG+1}^{MS} a_{kj} \left(\frac{\partial n_j}{\partial \ln p} \right)_{T, NE} \\
 + \frac{N}{N+M} \sum_{j=1}^{MG} a_{kj} n_j \left(\frac{\partial \ln N}{\partial \ln p} \right)_{T, NE} + \sum_{j=MS+1}^{ME} a_{kj} n_j \left(\frac{\partial \ln n_c}{\partial \ln p} \right)_{T, NE} \\
 = \sum_{j=1}^{MG} a_{kj} n_j \quad (k=1, \dots, \ell)
 \end{aligned} \tag{60}$$

$$\sum_{j=1}^{\ell} a_{ij} \left(\frac{\partial \pi_i}{\partial \ln p} \right)_{T, NE} = 0 \quad (j=MG+1, \dots, MS) \tag{61}$$

$$\sum_{j=1}^{\ell} \sum_{j=1}^{MG} a_{ij} n_j \left(\frac{\partial \pi_i}{\partial \ln p} \right)_{T, NE} - \frac{NM}{N+M} \left(\frac{\partial \ln N}{\partial \ln p} \right)_{T, NE} = \sum_{j=1}^{MG} n_j \tag{62}$$

$$\sum_{j=1}^{\ell} \sum_{j=MS+1}^{ME} a_{ij} n_j \left(\frac{\partial \pi_i}{\partial \ln p} \right)_{T, NE} = 0 \tag{63}$$

Equations (60) to (63) can be solved to get $(\partial \ln N / \partial \ln p)_{T, NE}$ which is used in Eq. (42).

1.3.3 Other Thermodynamic Derivatives

As stated previously, all thermodynamic first derivatives can be expressed in terms of three thermodynamic first derivatives which are $C_{p, NE}$, $(\partial \ln V / \partial \ln T)_{p, NE}$, and $(\partial \ln V / \partial \ln p)_{T, NE}$. The velocity of sound, a , is a frequently used parameter defined by

$$a^2 = \left(\frac{\partial p}{\partial \rho} \right)_{S, NE} = \frac{p}{\rho} \left(\frac{\partial \ln p}{\partial \ln \rho} \right)_{S, NE} = - \frac{p}{\rho} \left(\frac{\partial \ln p}{\partial \ln V} \right)_{S, NE} \quad (64)$$

Using methods of manipulating thermodynamic derivatives as described by Callen,⁽²⁾ we can show that

$$\left(\frac{\partial \ln p}{\partial \ln V} \right)_{S, NE} = \frac{C_{p, NE}}{C_{p, NE} (\partial \ln V / \partial \ln p)_{T, NE} + (pV/T) (\partial \ln V / \partial \ln T)_{p, NE}^2} \quad (65)$$

This may be written as

$$\left(\frac{\partial \ln p}{\partial \ln V} \right)_{S, NE} = \frac{C_{p, NE}}{C_{V, NE} (\partial \ln V / \partial \ln p)_{T, NE}} \quad (66)$$

where

$$C_{V, NE} \equiv C_{p, NE} + \frac{(pV/T) (\partial \ln V / \partial \ln T)_{p, NE}^2}{(\partial \ln V / \partial \ln p)_{T, NE}} \quad (67)$$

Using the symbols

$$\gamma_{S, NE} \equiv \left(\frac{\partial \ln p}{\partial \ln \rho} \right)_{S, NE} \quad (68)$$

and

$$\gamma \equiv \frac{C_{p, NE}}{C_{v, NE}} \quad , \quad (69)$$

Eq. (67) becomes

$$\gamma_{S, NE} = - \frac{\gamma}{(\partial \ln V / \partial \ln p)_{T, NE}} \quad . \quad (70)$$

Using the equation of state [cf. Eq. (6)] in Eq. (64) we get

$$a = \sqrt{n_g R T \gamma_{S, NE}} \quad . \quad (71)$$

It should be noted that $\gamma_{S, NE}$ defined by Eq. (70) is required in Eq. (71) and not the specific heat ratio γ defined in Eq. (69).

An additional derivative, which will be used in Subsection 1.6, is given below

$$\left(\frac{\partial \ln p}{\partial \ln T} \right)_{S, NE} = \frac{C_{p, NE}}{n_g R (\partial \ln V / \partial \ln T)_{p, NE}} \quad . \quad (72)$$

1.4 Procedure for Obtaining Equilibrium Compositions

In principle, obtaining equilibrium composition of species in the equilibrium pool by means of the Newton-Raphson iteration procedure should offer no difficulties. However, there are a number of practical items which require detailed attention in order to avoid numerical difficulties. These items include initial estimates, tests for condensed phases, phase transitions and triple points, convergence, accidental singularities, special handling of ions, and consideration of trace species.

1.4.1 Initial Estimates

An extremely simple procedure is used to assign initial estimates for n_i ($i \leq ME$). For the first iteration of the first point, we assign N in Eq. (22) to be 0.1. Then the number of kilogram-moles of each gaseous species per kilogram of mixture is set equal to $0.1/MG$ where MG is the number of gaseous species in the equilibrium pool. The number of moles of each condensed species in the equilibrium pool is set equal to zero. For HP (i.e., enthalpy and pressure assigned) and SP (i.e., entropy and pressure assigned) problems, an arbitrary initial estimate of $T = 3000$ K is used by the program unless a different estimate is included with other input.

Admittedly, this simple procedure will often give poor initial estimates, which require many iterations before a solution is obtained. However, for a general chemistry program, we find this technique preferable to the alternate of devising numerous special routines for obtaining good estimates for numerous possible chemical systems. Furthermore, except for temperature-pressure assigned (or TP) problems, the estimating technique is used for only the first point in any schedule of points. For all points after the first, the results of preceding point serve as initial estimates. For TP problems, where a random schedule of temperatures may be assigned, the simple estimating procedure is repeated for all assigned points.

Because no attempt is made to obtain good initial estimates, the question arises whether convergence can be "guaranteed". This is discussed in the next section.

1.4.2 Convergence

Iteration equations sometimes give large corrections, which, if used directly, could lead to divergence. Two situations can cause large corrections. The first situation occurs in the early stages of the calculation and is due to poor estimates. The second may occur at later stages of the calculation when the iteration process sometimes attempts to make extremely large increases in moles of species that are present in trace amounts. In both of these cases, a control factor λ is used to restrict the size of the corrections to $\ln n_j$ ($j = 1, \dots, \text{MG}$; and $j = \text{MS}+1, \dots, \text{ME}$) and n_j ($j = \text{MG}+1, \dots, \text{MS}$) as well as to $\ln N$, $\ln T$, and $\ln n_c$ obtained from solution of Eqs. (34) through (39).

The numerical value of λ is determined on the basis of two empirical rules which experience has shown to be satisfactory. For T , N , and n_j for those gaseous species and species in liquid solution for which $n_j/(n_g + n_c) > 10^{-8}$ (or $\ln (n_j/(n_g + n_c)) > -18.420681$), see Eq. 16a,b for the definition of n_g and n_c , and for which $\Delta \ln n_j > 0$, a number λ_1 is defined as:

$$\lambda_1 = \frac{2}{\max(|\Delta \ln T|, |\Delta \ln N|, |\Delta \ln n_j|, |\Delta \ln n_c|)} \quad (j = 1, 2, \dots, \text{MG}) \text{ and} \\ (j = \text{MS} + 1, \dots, \text{ME}) \quad (73)$$

This limits the change in T , N , and n_c and the increase in n_j , for those gaseous species and species in liquid solution whose mole fraction exceeds 10^{-8} , to a factor $e^2 = 7.3891$.

For those gaseous species and species in liquid solution for which $\ln (n_j/(n_g + n_c)) \leq -18.420681$ and $\Delta \ln n_j > 0$, a number λ_2 is defined as:

$$\lambda_2 = \min \left| \frac{-\ln (n_j/(n_g + n_c)) - 9.2103404}{\Delta \ln n_j - (N \Delta \ln N + n_c \Delta \ln n_c)/(n_g + n_c)} \right| \quad (j = 1, \dots, \text{MG}) \text{ and} \\ (j = \text{MS} + 1, \dots, \text{ME}) \quad (74)$$

This prevents a gaseous species or a liquid species in solution with a mole fraction less than 10^{-8} from increasing to more than 10^{-4} . The control factor λ to be used in Eq. (76) below, is defined in terms of λ_1 and λ_2 as:

$$\lambda = \min (1, \lambda_1, \lambda_2) \quad . \quad (75)$$

A value for λ is determined for each iteration. Whenever current estimates of composition and/or temperature are far from their equilibrium values, λ will be less than 1. Whenever they are close to their equilibrium values, λ will equal 1. New estimates for composition and temperature are then obtained from the following correction equations:

$$\left. \begin{aligned} \ln n_j^{(i+1)} &= \ln n_j^{(i)} + \lambda^{(i)} (\Delta \ln n_j)^{(i)} & (j = 1, \dots, MG) \\ n_j^{(i+1)} &= n_j^{(i)} + \lambda^{(i)} (\Delta n_j)^{(i)} & (j = MG+1, \dots, MS) \\ \ln n_j^{(i+1)} &= \ln n_j^{(i)} + \lambda^{(i)} (\Delta \ln n_j)^{(i)} & (j = MS+1, \dots, ME) \\ \ln N^{(i+1)} &= \ln N^{(i)} + \lambda^{(i)} (\Delta \ln N)^{(i)} \\ \ln n_c^{(i+1)} &= \ln n_c^{(i)} + \lambda^{(i)} (\Delta \ln n_c)^{(i)} \\ \ln T^{(i+1)} &= \ln T^{(i)} + \lambda^{(i)} (\Delta \ln T)^{(i)} \end{aligned} \right\} \quad (76)$$

where the superscript i represents the i^{th} estimate.

The iteration procedure is continued until corrections to compositions satisfy the following criteria:

$$\left. \begin{aligned}
 & \frac{\sum_{j=MS+1}^{ME} n_j + \sum_{j=1}^{MG} n_{j+M}}{n_j} \frac{|\Delta \ln n_j|}{n_j} \leq 0.5 \times 10^{-5} \quad \left(\begin{array}{l} j = 1, \dots, MG, \text{ and} \\ j = MS+1, \dots, ME \end{array} \right) \\
 & \frac{\sum_{j=MS+1}^{ME} n_{j+M} + \sum_{j=1}^{MG} n_j}{n_j} \frac{|\Delta n_j|}{n_j} \leq 0.5 \times 10^{-5} \quad (j = MG+1, \dots, MS) \\
 & \frac{N}{n_c + N+M} |\Delta \ln N| \leq 0.5 \times 10^{-5} \\
 & \frac{n_c}{n_c + N+M} |\Delta \ln n_c| \leq 0.5 \times 10^{-5}
 \end{aligned} \right\} \quad (77)$$

For an entropy specified problem, the following convergence test on entropy is also required:

$$\left| \frac{s_0 - s}{R} \right| \leq 0.5 \times 10^{-4} \quad (78)$$

The convergence tests in Eqs. (77) and (78) ensure accuracy to five places in composition when expressed as mole fractions.

1.4.3 Tests for Condensed Phases

For the first iteration at the first input unless INSERT cards are used (see Subsection 2.1.3.2), the program considers only gaseous species during iteration to convergence. For each point after the first, the program

uses the results of a previous point for its initial estimate. After every convergence, the program automatically checks for the inclusion or elimination of condensed species.

The test is based on the minimization of free energy. At equilibrium, the relation $\delta G = 0$ is satisfied. The requirement for a pure condensed species j ($MG < j \leq MS$), or the ideal liquid solution comprised of species j ($MS < j \leq ME$), which were not previously included as a possible species, to now be included is that their inclusion will decrease free energy. For pure condensed species, this implies:

$$\frac{\partial G}{\partial n_j} = \left(\frac{\mu_j^0}{RT} \right)_c - \sum_{i=1}^{\ell} \pi_i a_{ij} < 0 \quad , \quad (79)$$

where the subscript c refers to condensed species. For the ideal liquid solution, this criterion becomes:

$$\frac{\partial G}{\partial n_j} = \left(\frac{\mu_j^0}{RT} \right)_c + \ln x_j - \sum_{i=1}^{\ell} \pi_i a_{ij} < 0 \quad , \quad (80)$$

where x_j is the mole fraction of j -th liquid species in the liquid solution. In order to guarantee that the addition of liquid solution will lower the Gibbs free energy, we require Eq. (80) to hold simultaneously for all species ($MS < j \leq ME$). Since the sum of x_j is equal to unity, Eq. (80) can be reduced to:

$$\sum_{j=MS+1}^{ME} \exp \left[\sum_{i=1}^{\ell} \pi_i a_{ij} - \left(\frac{\mu_j^0}{RT} \right)_c \right] > 1 \quad . \quad (81)$$

When the relation given by Eq. (81) is satisfied, the liquid solution is included in the mixture. Equations (79) and (80) are identical to the vapor pressure test when data for the gas phase, as well as condensed phase, are available. For pure condensed species, the vapor pressure test is:

$$\left(\frac{\mu_j^0}{RT}\right)_c - \left[\frac{\mu_j^0}{RT} + \ln\left(\frac{n_j P_{atm}}{n}\right)\right]_g < 0 \quad . \quad (82)$$

In Eq. (82), the subscript g refers to the gas phase of the same species as the solid phase referred to by the subscript c. The following discussion shows that Eqs. (79) and (82) are equivalent. Their term

$$\sum_{i=1}^{\ell} \pi_i a_{ij}$$

in Eq. (79) is identical for the gas and condensed phases of the same species. From Eq. (14), this term for the gas phase equals $(\mu_j/RT)_g$ which, using the definition of μ_j in Eq. (15), leads directly to Eq. (82). The same argument holds for each liquid species in the solution. The advantage of Eq. (79) over (82) is that Eq. (82) can be used only when the gas phase of the species corresponding to the condensed phase to be tested is present, whereas Eq. (79) can always be used. For example, the use of Eq. (79) eliminates the need for the extensive programming required to accommodate $Al_2O_3(S,l)$ for which gas phase data are not available.

At most, only one new pure condensed species is included after each convergence. In the event that several pure condensed species pass the test required by Eq. (79), only that species giving the largest negative change to free energy is included as a possible species and convergence to a new equilibrium composition is obtained. This process is repeated until all pure condensed species required by Eq. (79) are included.

If, after convergence, the concentration of a pure condensed species is negative, the species is removed from the list of currently considered species and convergence to a new equilibrium composition is obtained.

After the condensed solution satisfies the test required by Eq. (81), it is included in the calculation only when its negative contribution to the free energy is lower than that of any pure condensed species. To estimate the free energy reduction,

we first note that species which comprise the bulk of the liquid solution have mole fractions, x_j , which are of order unity. For these species, the relations (79) and (80) become effectively identical. This implies that the bulk of the solution is composed of those liquid species which would have existed in the pure condensed phase under the same thermodynamic conditions. The negative change in free energy per unit change in moles of solution now becomes, approximately:

$$\frac{\partial G}{\partial n_c} \approx \sum_{j=MS+1}^{ML} \left[\left(\frac{\mu_j^0}{RT} \right) - \sum_{i=1}^{\ell} \pi_i a_{ij} \right] , \quad (83)$$

where n_c is the total number of moles in the solution per kilogram of mixture. The summation is over species, indexed from $j=MS+1$ to $j=ML$, for which Eq. (80) is satisfied without contributions from $\ln x_j$. The solution is added to the mixture when $(\partial G/\partial n_c)$ is less than $(\partial G/\partial n_j)$ for all $j(MG < j \leq MS)$. Convergence to a new equilibrium is then obtained. Rare occasions may exist when Eq. (81) is satisfied while $(\partial G/\partial n_c)$, given by Eq. (83), is positive. In such a case, a small negative value of (-10^{-5}) is assigned to $(\partial G/\partial n_c)$. This will ensure that the solution will be added to the system.

To prevent certain convergence problems, the solution is removed from the mixture when n_c is less than 10^{-10} . Convergence to a new equilibrium composition is obtained. The inclusion of the solution is reconsidered for other points.

1.4.3.1 Initial estimates of species in the solution

Once the solution is admitted to the mixture, the initial values of n_c and n_j ($MS < j \leq ME$) must be estimated in order to solve the iteration equations. Numerous examples have shown that, for coal combustion products, n_j , for the condensed species, is at the order of 10^{-6} to 10^{-3} . Therefore, an initial estimate of 10^{-4} is selected for n_c . In order to estimate $n_j(MS < j \leq ME)$, we first define the two variables given below:

$$\left. \begin{aligned} \text{NSOL} &= \text{Number of condensed species in the solution} \\ A_j &\equiv \left(\frac{\mu_j}{RT} \right)_c - \sum_{i=1}^{\ell} \pi_i a_{ij} \end{aligned} \right\} \quad (84)$$

For all species j ($ML < j \leq ME$) with $A_j > 0$, we let

$$n_j = 10^{-4} \text{Exp}(-A_j) \quad (85)$$

This value of n_j makes $(\partial G / \partial n_j)$, given by Eq. (80), equal to zero. However, to control the size of the initial estimates, we either let $n_j = 10^{-12}$, when its value given by Eq. (85) is less than 10^{-12} , or let $n_j = (10^{-4} / \text{NSOL})$, when its value given by Eq. (85) is greater than $(10^{-4} / \text{NSOL})$. The lower limit is chosen to guard against computational difficulties that may occur when n_j is too small. The higher limit is chosen to make sure that the sum of n_j never exceeds n_c .

For all species, j ($MS < j \leq ML$) in the solution with $A_j \leq 0$, we let

$$n_j = \frac{10^{-4} - \sum_{j=ML+1}^{ME} n_j}{(ML - MS)} \quad (86)$$

where $(ML - MS)$ is the number of solution species with $A_j \leq 0$. Since these condensed species will be most stable under the given thermodynamic state, their concentrations are chosen to be equal to the highest estimate available. Note that for problems where n_c is of the order of 10^{-1} the initial estimate of 10^{-4} will only result in a higher number of iterations.

For other points in the calculation, the initial estimates of the above variables are set equal to the values they had at the previous point. If the solution was removed from the previous point and is being considered at the current point, the initial estimates are evaluated according to the procedure described by Eqs. (85) and (86).

1.4.4 Phase Transitions and Special Derivatives

In the case of condensed phases, the possibility exists of encountering a phase transition between solid and liquid (melting points) or between two stable solid phases. Under the working assumptions of this program, such transitions constitute triple points, since three phases of the same species coexist, one gaseous and two condensed. Such triple points are characterized by a definite vapor pressure and temperature, independent of the relative proportions of each phase. This is shown by the fact that the iteration equations (i.e., Eqs. (34) to (39)) become singular for an assigned temperature and pressure and the inclusion of two condensed phases of the same species. At a triple point, for a specified system pressure, the relative amounts of the phase can be determined only if either the enthalpy or the entropy is assigned.

The program can obtain equilibrium compositions containing either one or two condensed phases of a species with or without the corresponding gas phase. When temperature is assigned, no problems arise as to which one of two or more condensed phases is to be considered. However, when temperature is a variable, such as, in HP (enthalpy and pressure assigned), SP (entropy and pressure assigned) or RKT (i.e., channel problems), then several possibilities exist which need to be considered. For example, if a liquid phase is being considered by the program and the temperature at convergence is below the melting point, two possibilities exist. First, the solid phase might be substituted for the liquid phase and a new convergence obtained, or, secondly, both liquid and solid might be considered simultaneously and a new convergence obtained. Similar possibilities exist when convergence is obtained with a solid phase above the melting point. In brief, the following criteria are used by the program to determine whether or not to switch one condensed phase of a species to another or whether to consider both simultaneously. Liquid present at temperature $T < T_m$:

If $T_m - T > 150\text{K}$, switch solid for liquid, and

If $T_m - T \leq 150\text{K}$, include solid and liquid.

Solid present at temperature $T > T_m$:

If $T - T_m > 150\text{K}$, switch liquid for solid, and

If $T - T_m \leq 150\text{K}$, include liquid with solid.

Similar tests apply for two solid phases of a species. The programming details of switching species are given in Fig. 4 (subroutine EQLBRM).

In the present code, we do not allow the coexistence of solid and liquid phases of the same species if the liquid phase is in the solution. We do, however, let a liquid species freeze out of the solution. For problems where temperature and pressure are assigned, the freezing-out is done when $T - T_m < 50$ K. For other problems, it is done when $T - T_m < 150$ K. The values of 50 and 150 K temperature difference can be altered by the user (see Subsection 2.5.5). The inclusion of both solid and liquid phases of a species whose liquid phase is in the ideal solution will be considered as the code is further modified. Once a species is removed from the solution, it will not be introduced into the solution unless the program is restarted. If all the liquid species except one freeze out of the solution, the program continues to operate as if the solution did not exist.

The situation of constant temperature during an isentropic compression or expansion process can occur when two phases of the same species coexist. The transition temperature remains constant while one phase is being converted to the other. Under this circumstance, derivatives with respect to temperature are not defined. Thus, several of the derivatives previously discussed, $C_{p, NE}$, $C_{V, NE}$, and $(\partial \ln V / \partial \ln T)_{p, NE}$ cannot be obtained in this case. As a consequence, Eq. (71) cannot be used to obtain $\gamma_{S, NE}$.

Using the method of Ref. (2), the following expression can be derived for constant temperature and entropy:

$$\gamma_{S, T, NE} \equiv \left(\frac{\partial \ln p}{\partial \ln \rho} \right)_{S, T, NE} = - \frac{1}{(\partial \ln V / \partial \ln p)_{T, NE}} \quad (87)$$

The velocity of sound for this situation is no longer given by Eq. (72), but rather by:

$$a = \sqrt{n_g R T \gamma_{S, T, NE}} \quad (88)$$

These expressions will be used in connection with discontinuities in a rocket throat.

1.4.5 Ions

The program is capable of calculating equilibrium properties of plasmas (mixtures containing ionized species) if the plasma is considered ideal. Ideal is

meant to imply that no coulombic interactions are considered. Therefore, the results of the plasma calculations made with this program will be valid only for those conditions where the ionic density is small so that the coulombic effects are unimportant.

In order for ions to be considered, a charge balance equation is required:

$$\sum_{j=1}^{MG} a_{ij} n_j + \sum_{j=ME+1}^{NG} a_{ij} n_j = 0 \quad , \quad (89)$$

where a_{ij} indicates the excess or deficiency of electrons in the ion relative to the neutral species. For example, in a mole of an ionized species, $a_{ij} = -3$ for Ar^{+++} and $+1$ for O_2^- .

Subsection 2.1.4.1 contains instructions required by the program to consider ions.

In order to prevent difficulties in matrix solutions, the program automatically removes the charge balance equation when the mole fraction of every ion being considered is less than 10^{-8} .

1.4.6 Singularities

The iteration method used in this report has successfully handled numerous chemical systems under a wide variety of thermodynamic conditions. Nevertheless, special procedures are required to take care of situations which would otherwise cause the iteration method to fail.

One such situation is a singularity which occurs when two rows of the coefficient matrix are identical. This happens when the ratio of the assigned elements in these two rows is equal to the ratio of the stoichiometric coefficients of these two elements in every gaseous species for which $(n_j/n_g) > 10^{-8}$ and which contains both elements. That is,

$$\frac{a_{ij}}{a_{kj}} = \frac{b_i^0}{b_k^0} \quad (j=1, \dots, MG), \quad \left(\frac{n_j}{n_g} > 10^{-8} \right) \quad . \quad (90)$$

For example, for stoichiometric hydrogen and oxygen at 300 K and $p = 1000$ Newtons per square meter, the only species with $n_j/n_g > 10^{-8}$ is $H_2O(g)$ and Eq. (90) applies. Another example is stoichiometric lithium and fluorine at 500 K and $p = 101,325$ Newtons per square meter.

A procedure which usually takes care of this difficulty is to assign values in the input that will make the b_i^0/b_k^0 ratio in Eq. (90) differ from the left side in the 6 or 7th figure. The program does this automatically if an equivalence ratio $r = 1.0$ is read in by reassigning $r = 1.000005$. Both of the previous examples are taken care of by this procedure.

However, even if the b_i^0/b_k^0 ratio in Eq. (90) is made to differ from the left side in the 6 or 7th figure, there may be a temporary singularity. This can occur when the iteration procedure temporarily removes some species for which $(n_j/n_g) < 10^{-8}$ leading temporarily to two identical coefficient rows in the correction matrix. This difficulty is usually remedied by an automatic restart feature in the program. Whenever a singular matrix occurs, the program automatically reinserts the species with $n_j/n_g < 10^{-8}$ and reassigns them values of $n_j = 10^{-6}$. If, after restart, the iteration procedure still leads to a singular matrix, a message is printed and a test is made for another possible cause of singularity.

This singularity occurs if the program is considering several condensed species whose determinant of stoichiometric coefficients is zero. In this case, if two or more of the condensed species are composed of the same chemical elements, the program will remove all of these species except the one with the most negative contribution to the free energy of the mixture based on the test of Eq. (79). If, after restart, a singular matrix again occurs, a message is printed, any results up to this point are printed, and the program stops.

1.5 Thermodynamic Data

Thermodynamic data are included with the program for 62 reactants and numerous reaction species (solid, liquid, and gas phases of a species are counted as separate species). With few exceptions, data are taken from JANAF⁽³⁾ tables. Data for the reaction species are reduced to functional form by means of the PAC⁽⁴⁾ program.

1.5.1 Assigned Enthalpies

For each species, heats of formation (and, when applicable, heats of transition) were combined with sensible heats to give assigned enthalpies H_T^0 . By definition,

$$H_T^0 = H_{298.15}^0 + (H_T^0 - H_{298.15}^0) \quad (91)$$

We have arbitrarily assumed $H_{298.15}^0 = (\Delta H_f^0)_{298.15}$. Equation (91) then becomes

$$H_T^0 = (\Delta H_f^0)_{298.15} + (H_T^0 - H_{298.15}^0) \quad (92)$$

In general, $H_T^0 \neq (\Delta H_f^0)_T$ for $T = 298.15$ K. For reference elements, $(\Delta H_f^0)_{298.15} = H_{298.15}^0 = 0$. For the species included with the program, these reference elements are Al(s), Ar(g), B(s) (beta), Be(s), Br₂(l), C(s) (graphite), Cl₂(g), Cs(s), F₂(g), Fe(s), H₂(g), He(g), K(s), Li(s), Mg(s), N₂(g), Na(s), Ne(g), O₂(g), P(s) (red, V), S(s) (rhombic), Si(s), and Xe(g).

For cryogenic liquids, assigned enthalpies are given at their boiling points. These are usually obtained by subtracting the following quantities from the heat of formation of the gas phase at 298.15 K: sensible heat between 298.15 K and the boiling point, difference in enthalpy between ideal gas and real gas at the boiling point, and heat of vaporization at the boiling point.

1.5.2 Least Squares Coefficients

For each reaction species, the thermodynamic functions specific heat, enthalpy, and entropy are given as functions of temperature in the form of least squares fits as follows:

$$\frac{C_p^0}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \quad (93)$$

$$\frac{H_T^0}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T} \quad (94)$$

$$\frac{S_T^0}{R} = a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + a_7 \quad (95)$$

For gases, the PAC program first calculates thermodynamic functions from molecular constant data given in Ref. (3), and then fits these functions to the above polynomials. The final output yields the seven coefficients a_i ($i = 1, \dots, 7$). For condensed species, the thermodynamic functions are taken directly from Ref. (3) for reduction to polynomial form. However, for condensed species, we first calculate and include data at the transition points inasmuch as these data are not given in the Ref. (3) tables. For each species, two sets of coefficients are included for two adjacent temperature intervals, 300 to 1000 K and 1000 to 5000 K. The polynomial fits have been constrained to be equal at 1000 K. Details on the use of cards or files containing the coefficient data are given in the section on THERMO Data. The format and listing of coefficient data are given in Appendix D.

1.6 Channel Flows

In this subsection, we consider special applications to channel flows described by the conservation Eqs. 1 - 4. These equations are general in the sense that the source terms $\dot{w}_i$ ($i=ME+1, \dots, NT$), F , and q are not specified. The three special cases that are programmed in the code are: rocket performance with chemical equilibrium and isentropic flow, magnetohydrodynamic (MHD) channel performance with partial equilibrium/partial rate controlled chemistry, and channel flow with fully rate controlled chemistry. The user, however, can readily manipulate the source terms of the latter two special cases in order to match his/her problem.

1.6.1 Rocket Performance

This is the case considered by the NASA CEC⁽¹⁾ code. With the assumption of isentropic flow and in the absence of momentum and energy source terms, the conservation equations reduce to:

$$\left. \begin{aligned} \rho u A &= \text{const} \\ h + \frac{1}{2} u^2 &= \text{const} \\ s &= \text{const} \end{aligned} \right\} \quad (96)$$

In Eq. (96), the momentum equation is replaced by the entropy equation. With the further assumption of zero velocity and complete combustion in the combustion chamber, the flow velocity can be evaluated from:

$$u = \sqrt{2(h_c - h)} \quad , \quad (97)$$

where h_c is the mixture enthalpy per kilogram of mixture in the combustor. If there is no combustor heat loss, h_c is equal to h_r , the reactant enthalpy per kilogram of reactants. In the present code, we have considered combustor heat loss denoted by h_ℓ with the units of energy per kilogram of reactants. With heat loss, h_c becomes

$$h_c = h_r - h_\ell \quad . \quad (98)$$

h_f must be specified by the user (see Subsection 2.1.4.2). Like the NASA CEC code, combustion and throat parameters are always calculated while the rocket exit conditions are evaluated for specified pressure ratios or area ratios.

Rocket performance is obtained by first determining combustion properties in the rocket chamber and then determining exhaust properties at various stations in the nozzle exit including the throat.

1.6.1.1 Combustion conditions

Combustion temperature and equilibrium compositions are obtained by the program for an assigned chamber pressure and enthalpy (in the program $HP = \text{TRUE}$). From the combustion compositions and temperature, the combustion entropy s_c and other combustion properties are determined.

1.6.1.2 Exit conditions

Exit conditions may be desired for assigned pressure ratios or area ratios. Throat conditions, however, are always determined by the program after combustion conditions are completed and before any assigned pressure ratios or other assigned area ratios are considered. Isentropic expansion is assumed.

For an assigned pressure ratio, equilibrium compositions and exit temperature are determined for the pressure p corresponding to the assigned pressure ratio and for the combustion entropy s_c (in the program, $SP = \text{TRUE}$). For throat and other assigned area ratios, iteration procedures are used to determine the correct pressure ratios. These procedures are described below.

After equilibrium compositions and temperatures are obtained for an assigned pressure ratio or area ratio, other rocket parameters like the Mach number may be determined.

1.6.1.3 Throat conditions

Throat conditions may be determined by locating the pressure ratio for which area ratio is a minimum or, equivalently, for which the flow velocity is equal to the

velocity of sound. The second procedure is used for rocket nozzle problems. This pressure ratio is determined by iteration.

The initial estimate for the pressure ratio at the throat is obtained from

$$\frac{p_c}{p_t} = \left(\frac{\gamma_S + 1}{2} \right)^{\gamma_S / (\gamma_S - 1)} \quad (99)$$

The program uses the value of γ_S from the combustor point.

Equilibrium properties for p_t , from Eq. (99), and for s_c are obtained as for any exit point. From these properties, u^2 and a^2 are calculated and the following test for convergence is made:

$$\left| \frac{u^2 - a^2}{u^2} \right| < 0.4 \times 10^{-4} \quad (100)$$

This criterion is equivalent to ensuring that, at the throat, the Mach number which is equal to u/a is within the value of $1 \pm 0.2 \times 10^{-4}$.

If the convergence test is not met, an improved estimate of the throat pressure ratio is obtained from the following iteration formula:

$$\left(\frac{p_c}{p_t} \right)_{k+1} = \left\{ \frac{p_c/p_t}{1 + (u^2 - a^2) / [(\lambda_S + 1)n_g RT]} \right\}_k \quad (101)$$

A maximum of four iterations on throat pressure ratio is permitted. Usually, no more than two are required.

1.6.1.4 Discontinuities

A special procedure for obtaining throat conditions when the velocity of sound is discontinuous is given in Ref. (5). The three steps in this procedure are

summarized here for completeness. Steps 1 and 2 are used for all throat calculations while step 3 is used only for the special case of discontinuities at the throat. Case 5612 in Appendix E of the NASA CEC⁽¹⁾ manual illustrates this particular kind of problem.

- Step 1. Obtain an initial estimate of throat pressure ratio by means of Eq. (99). For the first chamber pressure in case 5612, this gives $p_c/p_t = 1.7469$. The temperature for this estimate is 2820 K (the melting point of BeO) with liquid and solid BeO both present.
- Step 2. Obtain a second estimate of throat pressure ratio by means of Eq. (101). For case 5612, this gives $p_c/p_t = 1.6161$. The temperature for this estimate is 2846 K which is above the melting point with no BeO(s) present. The sequence of steps 1 and 2 (namely, liquid and solid at one estimate of throat pressure ratio and liquid only at the next estimate) indicates that discontinuities exist at the throat. In this event, proceed with Step 3. Otherwise, continue with the usual procedure of using Eq. (101) until convergence.
- Step 3. Estimate the pressure ratio at the melting point where the solid phase just begins to appear by means of

$$\ln p_t = \ln p + \left(\frac{\partial \ln p}{\partial \ln T} \right)_S (\ln T_m - \ln T) \quad , \quad (102)$$

where the derivative is given by Eq. (72). The values for the right side of Eq. (102) are for the point in Step 2.

In case 5612, Eq. (102) gave $P_c/P_t = 1.7282$ for which the mole fraction of BeO(s) equaled 0.00005. The correct value for which the mole fraction of BeO(s) is zero is $P_c/P_t = 1.7277$ so that the error in P_c/P_t using Eq. (102) is 0.0005 (0.03 percent). In the NASA CEC⁽¹⁾ code, an iteration scheme is used to obtain the pressure ratios corresponding to the assigned area ratios.

1.6.1.5 Empirical formulas for initial estimates of p_c/p_e for specified area ratios

Initial estimates of pressure ratios corresponding to subsonic area ratios are obtained from the following empirical formulas

$$\ln \frac{p_c}{p_e} = \frac{\ln (p_c/p_t)}{A_e/A_t + 10.587 [\ln (A_e/A_t)]^3 + 9.454 \ln (A_e/A_t)} \quad \frac{A_e}{A_t} \geq 1.09 \quad (103)$$

and

$$\ln \frac{p_c}{p_e} = \frac{0.9 \ln (p_c/p_t)}{A_e/A_t + 10.587 [\ln (A_e/A_t)]^3 + 9.454 \ln (A_e/A_t)} \quad 1.0001 < \frac{A_e}{A_t} < 1.09 \quad (104)$$

When an assigned supersonic area ratio requires an initial estimate of pressure ratio to be obtained from an empirical formula, the following formulas are used:

$$\ln \frac{p_c}{p_e} = \ln \frac{p_c}{p_t} + \sqrt{3.294 \left(\ln \frac{A_e}{A_t} \right)^2 + 1.535 \ln \frac{A_e}{A_t}} \quad 1.0001 < \frac{A_e}{A_t} < 2 \quad (105)$$

and

$$\ln \frac{p_c}{p_e} = \gamma_S + 1.4 \ln \frac{A_e}{A_t} \quad \frac{A_e}{A_t} \geq 2 \quad (106)$$

In Eq. (106), the value of γ_S is that determined for throat conditions. The equilibrium properties which are obtained for the initial and each subsequently improved estimate of p_c/p_e are used in Eqs. (107) and (108) below to obtain the improved estimates of p_c/p_e .

1.6.1.6 Analytic expression for improved estimates of p_c/p_e

From Table 1 of Ref. (6), the following derivative may be obtained:

$$\left[\frac{\partial \ln(p_c/p_e)}{\partial \ln(A_e/A_t)} \right]_S = \frac{1}{[1/\gamma_S - n_g RT/2(h_c - h)]} = \frac{\gamma_S u^2}{u^2 - a^2} \quad (107)$$

This derivative is used in the following correction formula to obtain an improved estimate for p_c/p_e :

$$\left(\ln \frac{p_c}{p_e} \right)_{k+1} = \left(\ln \frac{p_c}{p_e} \right)_k + \left\{ \left[\frac{\partial \ln(p_c/p_e)}{\partial \ln(A_e/A_t)} \right]_S \right\}_k \left[\ln \frac{A_e}{A_t} - \left(\ln \frac{A_e}{A_t} \right)_k \right] \quad (108)$$

where the subscript k refers to the k^{th} estimate.

The iteration procedure is continued until

$$\left| \left(\ln \frac{p_c}{p_e} \right)_{k+1} - \left(\ln \frac{p_c}{p_e} \right)_k \right| < 0.00004 \quad (109)$$

with a maximum of 10 iterations permitted. Generally, convergence is reached within two to four iterations.

1.6.2 Magnetohydrodynamics (MHD) Channel Performance

The flow models describing the motion of an ionized fluid are well developed (see for example, Sutton and Sherman⁽⁷⁾). In the absence of friction, these models lead to the following momentum and energy source terms for MHD channel flows:

$$F = J_y B \quad (110a)$$

$$q = J_x E_x + J_y E_y \quad (110b)$$

where J_y and J_x are the x (axial direction) and y components of current density (amp/m²), B is the magnetic field applied in the positive z direction (Tesla), E_x and E_y are the x and y components of the electric field (volts/m).

In ionized flows, the conservation equations are complemented with Maxwell's equations which, in the limit of MHD flows, reduce to the Ohm's law given below:

$$J_y = \frac{\sigma}{1 + \beta^2} (E_y - uB + \beta E_x) \quad (111)$$

$$J_x = \frac{\sigma}{1 + \beta^2} [E_x - \beta(E_y - uB)] \quad (112)$$

Here, σ is the electrical conductivity (mho/m) and β is the Hall parameter (dimensionless). Both σ and β depend on pressure, temperature, and species concentration. In this code, we use a subroutine developed by H. Cohen⁽⁸⁾ to evaluate σ and β . A description of this subroutine, denoted by CONDUC, is given in Subsection 2.4.2.2.

1.6.2.1 MHD conservation equations

The conservation equations, Eqs. (1) - (4), state equations, Eqs. (5) and (6), and Eqs. (111) and (112) can be solved uniquely if four parameters are specified along the MHD channel axis. In this analysis, we specify the axial profile of the following parameters.

- Pressure, velocity, or area;
- Applied magnetic field;
- The load factor $K \equiv E_y/uB$, and
- Axial current density, which is assumed equal to zero.

With $J_x = 0$ and with the definition of the load factor, the conservation equations for an MHD channel flow reduce to:

Mass.

$$\rho u A = \text{const.} \quad (113)$$

Species

$$\rho u \frac{dn_i}{dx} = \dot{w}_i \quad (i = ME+1, \dots, NT) \quad (114)$$

Momentum

$$\rho u \frac{du}{dx} + \frac{dp}{dx} = \sigma u B^2 (K - 1) \quad (115)$$

Energy

$$\rho u \frac{dh}{dx} + \rho u^2 \frac{du}{dx} = \sigma u^2 B^2 K (K - 1) \quad (116)$$

The condition $J_x = 0$ leads to:

$$E_x = \beta u B (K - 1) \quad (117)$$

Since a large axial electric field, E_x , can lead to destructive arcing between the electrodes, Eq. (117) can be used to limit the magnitude of E_x below a specified value, denoted by EXIN in the program (see Subsection 2.1.4.1). Under this requirement, either u , B , or K must be described by Eq.(117). In the current code, we change the magnetic field to control the magnitude of E_x . A default value of 2.4 kV/m is selected for EXIN.

Equations (113) - (117) are not complete until $\dot{w}_i$ ($i > ME$) are specified. These can be determined once the elementary chemical reactions controlling the concentration of species i ($i > ME$) are known. Here, we assume that the elementary chemical reactions have the following form:

where ν_{ri} (ν'_{ri}) is the stoichiometric coefficient of i -th reactant (product) species in the r -th reaction, A_i a representation of i -th species, k_{rf} the forward rate constant of r -th reaction and L the total number of reactions. Since, in general, the elementary reactions are two or three body reactions, then at most, all but three ν_{ri} or ν'_{ri} are zero. Note that each reaction must contain at least one species with index i greater than ME . Let $\dot{w}_{ri}$ be the rate of production per unit volume of i -th species due to r -th reaction, then:

$$\dot{w}_{ri} = (\nu'_{ri} - \nu_{ri}) \rho k_{rf} \left(10^{-6} N_0 \rho \right)^{\left(\sum_{i=1}^{NT} \nu_{ri} - 1 \right)} \times \left[\prod_{i=1}^{NT} n_i^{\nu_{ri}} - \frac{1}{K_r(p)} \prod_{i=1}^{NT} n_i^{\nu'_{ri}} \right] \quad (119)$$

with k_{rf} in molecule-cm³-sec units. $N_0 = 6.02 \times 10^{26}$ is the number of molecules per kilogram-mole of a species, ρ is the mixture density, and $K_r(p)$ is the equilibrium constant given by:

$$K_r(p) = \left(\frac{p_{atm}}{n_g} \right)^{\sum_{i=1}^{NT} (\nu_{ri} - \nu'_{ri})} \exp \left(- \frac{\Delta G_{r0}}{RT} \right) \quad (r=1, \dots, L) \quad (120)$$

where

$$\Delta G_{r0} = \sum_{i=1}^{NT} (\nu'_{ri} - \nu_{ri}) \mu_i^0 \quad (121)$$

μ_i^0 is the i-th species standard state Gibbs free energy. The forward rate constant k_{rf} has the following functional form:

$$k_{rf} = a_r T^{b_r} \exp \left(- \frac{c_r}{T} \right) \quad (r=1, \dots, L) \quad (122)$$

with a_r , b_r and c_r constants. (See the sample problem number (3.3.1.1) of Section 3). $\dot{w}_i$, used in Eq. (114), is given by:

$$\dot{w}_i = \sum_{r=1}^L \dot{w}_{ri} \quad (123)$$

1.6.2.2 Solution of conservation equations

In order to determine the mixture properties along the channel, the conservation equations must be solved together with the partial Gibbs free energy minimization of the system. In the PACKAGE code, these equations are solved using a forward marching technique described by Gear⁽⁹⁾.

The derivatives in the conservation equations [cf. Eqs. (113) - (116)] are readily uncoupled when pressure or velocity is specified along the channel. The uncoupling yields first order differential equations for dh/dx , and du/dx or dp/dx . When area is

specified, however, the derivative uncoupling is somewhat complicated. In Appendix A, It is shown that when area is given dp/dx satisfies the following equation:

$$(\mathcal{M}^2 - 1) \frac{dp}{dx} = - \frac{\rho u^2}{A} \frac{dA}{dx} + \frac{u}{TC_{p, NE}} \left(\frac{\partial \ln V}{\partial \ln T} \right)_{p, NE} (q - Fu) - u^2 \phi - F, \quad (124)$$

where

$$\begin{aligned} \phi = & \frac{1}{\rho u} \left(- \frac{RT}{PV^2} \right) \left\{ \sum_{i=1}^{ME} \dot{w}_i \sum_{j=1}^{\ell} a_{ij} \left(\frac{\partial \pi_j}{\partial \ln p} \right)_{T, NE} + \left[1 - \frac{N}{N+M} \left(\frac{\partial \ln N}{\partial \ln p} \right)_{T, NE} \right] \sum_{i=ME+1}^{NG} \dot{w}_i \right\} \\ & + \frac{R}{uC_{p, NE}} \left\{ - \sum_{i=1}^{ME} \dot{w}_i \sum_{j=1}^{\ell} a_{ij} \left(\frac{\partial \pi_j}{\partial \ln T} \right)_{p, NE} + \sum_{i=ME+1}^{NG} \dot{w}_i \left[\frac{h_i}{RT} + \frac{N}{N+M} \left(\frac{\partial \ln N}{\partial \ln T} \right)_{p, NE} \right] \right. \\ & \left. + \sum_{i=NG+1}^{NT} \dot{w}_i \frac{h_i}{RT} \right\} \left(\frac{\partial \ln V}{\partial \ln T} \right)_{p, NE}, \quad (125) \end{aligned}$$

and $\mathcal{M}$ is the flow Mach number. The derivatives on the right-hand side of Eqs. (124) and (125) together with $\mathcal{M}$, $\gamma_{S, NE}$ and $C_{p, NE}$ are evaluated after the minimization of Gibbs free energy (see Subsection 1.3.1.3). Equation (124) can now be used to solve for du/dx and dh/dx from Eqs. (115) and (116). Note, that in Eq. (125), $\dot{w}_i$ for $i \leq ME$ refers to the net production rate of equilibrium pool species as a result of their participation in the rate controlled reactions. In the model used here, these reactions play no direct role in evaluating the concentration, n_i ($i \leq ME$), of these species which are determined from the minimization of partial Gibbs free energy of the system. The minimization, however, requires the concentration of the chemical elements in the equilibrium pool which depend on the amount of chemical elements that are lost to or gained from the

nonequilibrium pool species. Since the amount of chemical elements lost or gained from the equilibrium pool, as a result of rate controlled chemical reactions, is equal to the amount gained or lost by the nonequilibrium pool, then knowing the production rate of nonequilibrium pool species is sufficient to evaluate the properties of the equilibrium pool species. Therefore, a knowledge of $\dot{w}_i$ ($1 \leq ME$) is only required when using Eq. (125).

For supersonic channels, we have included the option of starting rate controlled chemistry either from the throat or from the channel entrance. When the solution of conservation equations begin at the throat, the variation of pressure, area, or velocity must be specified between the throat and the channel entrance. The present model only considers cases when there is a linear pressure drop between the throat and the channel entrance with the channel entrance pressure specified. The solution begins by first setting the magnetic field equal to zero. It is then turned on when the calculated pressure equals the assigned channel entrance pressure

1.6.2.3 Initial conditions

All the flow variables must be specified at some point $x = x_0$ along the channel in order to get a unique solution from the conservation equations. For all channel problems, we define $x_0 = 0$ as the channel entrance. The mixture parameters at the entrance point are determined when the flow upstream of the channel is known. At their entrance, MHD channels are attached to a device with properties identical to that of a rocket. That is, it is composed of a combustor, where the reactants are burned, a converging-diverging nozzle, where the combustion products are accelerated to supersonic velocities, and an exit plane which is connected to the MHD channel and defines the channel entrance. For supersonic channels, the entrance is located downstream of the throat, while for subsonic channels, it is located upstream of the throat. In either case, we assume total chemical equilibrium

from the combustor to the throat and zero magnetic field upstream of the channel entrance. Therefore, the methods described in the rocket performance section can be used to evaluate the combustor, throat and rocket exit (i. e. channel entrance) properties. When rate controlled chemistry begins at the throat the position of the throat must be specified as a negative x (see sample problem 3.3.1.4 and Subsection 2.1.7.2)

1.6.2.4 Procedure for obtaining the flow variables

The following is a list of procedures used to obtain the flow variables along the channel.

- Solve the conservation Eqs., (113) - (116), to determine p , h , and n_i ($i > ME$) at $x = x_0 + \Delta x$ in terms of initial conditions given at x_0 .
- Determine the concentration of chemical elements contained in the nonequilibrium pool, which is:

$$\sum_{j=ME+1}^{NT} a_{ij} n_j \quad (i=1, \dots, \ell),$$

then subtract this value from b_i^0 , the total amount of i -th chemical element concentration (see Eq. (9)) to get the concentration of i -th chemical elements in the equilibrium pool at $x = x_0 + \Delta x$.

- Determine the enthalpy contained in the nonequilibrium pool, which is:

$$\sum_{i=ME+1}^{NT} n_i (H_T^0)_i$$

then subtract it from h to get the enthalpy of the equilibrium pool at $x = x_0 + \Delta x$.

- Use p , n_i ($i > ME$), the reduced enthalpy, and the reduced chemical element concentrations to minimize partial Gibbs free energy and get concentrations n_i ($i \leq ME$) of the equilibrium pool species, temperature, density, and the remaining flow variables such as $C_{p,NE}$ and $\gamma_{S,NE}$, at $x = x_0 + \Delta x$.

1.6.3 Fully Chemical Rate Controlled Channel Flows

A fully chemical rate controlled flow model is developed for the analysis of uniformly mixed reacting mixtures when all the elementary reactions and their rate constants, which control the history of the mixture composition, are known. This type of channel flow is described by Eqs. (1) through (4) with the concentration of all species $i=1, \dots, NT$ given by Eq. (2). The minimization of the Gibbs free energy is no longer required. The mixture temperature is calculated using the iteration equation given by Eq. (32).

In the absence of equilibrium species, certain equations derived in the previous subsection are greatly simplified. With $N=0$, i.e., no equilibrium species Eqs. (41) and (42) become:

$$\left. \begin{aligned} \left(\frac{\partial \ln V}{\partial \ln T} \right)_{p, NE} &= 1 \\ \left(\frac{\partial \ln V}{\partial \ln p} \right)_{T, NE} &= -1 \end{aligned} \right\}, \quad (126)$$

hence, Eqs. (67) and (70) reduce to:

$$\left. \begin{aligned} C_{p, NE} &= n_g^R + C_{V, NE} \\ \gamma_{S, NE} &= \gamma \end{aligned} \right\} \quad (127)$$

For the area specified channel flows, the terms containing summations over $i=1$ to ME in Eq. (125) are eliminated. With ME , the number of gaseous species in the equilibrium pool, equal to zero and using the equation of state, Eq. (125) becomes:

$$\varphi = -\frac{1}{un_g} \sum_{i=1}^{NG} \dot{w}_i + \frac{R}{uC_{p, NE}} \sum_{i=1}^{NT} \dot{w}_i \frac{h_i}{RT} \quad (128)$$

The first summation on the right-hand side of Eq. (128) is proportional to the rate of change of the gaseous species molar concentration and can be written as:

$$\sum_{i=1}^{NG} \dot{w}_i = \rho u \frac{dn_g}{dx} \quad (129)$$

The second summation in Eq. (128) is proportional to the rate of energy released as a result of chemical reactions. Let Q_c , the chemically released heat per kilogram of mixture, be defined as:

$$\rho u \frac{dQ_c}{dx} = - \sum_{i=1}^{NT} \dot{w}_i h_i \quad (130)$$

Equation (124) now reduces to:

$$(\mathcal{M}^2 - 1) \frac{dp}{dx} = \rho u^2 \left\{ -\frac{1}{A} \frac{dA}{dx} + \frac{1}{n_g} \frac{dn_g}{dx} + \frac{1}{C_{p, NE}} \left[\frac{(q - Fu)}{\rho u} + \frac{dQ_c}{dx} \right] \right\} \quad (131)$$

With $\rho = p/(n_g RT)$, $C_{p, NE} = (\gamma - 1/\gamma) n_g R$, and $u^2 = \mathcal{M}^2 \gamma n_g RT$, Eq. (131) reduces to its more familiar form which is:

$$(\mathcal{M}^2 - 1) \frac{dp}{p} = \gamma \mathcal{M}^2 \left[-\frac{dA}{A} + \frac{dn_g}{n_g} + \frac{\gamma - 1}{\gamma} \frac{d(Q_c + Q_{nc})}{n_g RT} \right] \quad (132)$$

where Q_{nc} is defined as a nonchemical energy source per kilogram of mixture defined by:

$$\rho u \frac{dQ_{nc}}{dx} = q - Fu \quad . \quad (133)$$

For this type of flow, the initial conditions are determined once the reactant concentrations, temperature, pressure, and velocity are specified at the channel entrance. For more details, see Subsection 3.3.4.

1.6.4 Special Options

This subsection contains special options for modifying the channel flow. The first is concerned with the modeling of heat loss through the channel walls, and the second with the modeling of a two-stage combustor.

1.6.4.1 Channel Heat Loss Model

A simple heat loss term is included in the code for estimating the effects of heat loss through the channel walls. The program, however, is written in such a way that the user can readily replace the simple model with other more realistic ones. Here, it is assumed that the heat loss term, denoted by q_L , can be represented by:

$$q_L = \rho u \frac{h(T_w, p_{av}) - H(T, p)}{Z} \quad , \quad (134)$$

where $h(T_w, p_{av})$ is the static enthalpy of the mixture evaluated at an average wall temperature T_w , and pressure p_{av} . $H(T, p)$ is the stagnation enthalpy of the mixture at a given point in the channel and Z is a characteristic length selected by the user. For MHD flows with such a heat loss model, q_L must be added to the right-hand side of Eq. (116). For nonMHD flows with this heat loss model, Eq. (116) reduces to:

$$\frac{dH(T, p)}{dx} = \frac{h(T_w, p_{av}) - H(T, p)}{Z} \quad . \quad (135)$$

The solution of Eq. (135) is:

$$\frac{H(T, p) - h(T_w, p_{av})}{H(T_0, p_0) - h(T_w, p_{av})} = \exp\left(-\frac{x}{Z}\right) \quad , \quad (136)$$

where T_0 , p_0 refer to the initial conditions. From Eq. (136), we note that the characteristic length Z is an effective e-folding length.

1.6.4.2 Two-Stage Combustor Option

Two-stage combustors are devices which are intended to reduce the concentration of condensed species in coal fired MHD channels. This is accomplished by first burning the coal with part of the oxidizer in the first stage, leading to colder temperatures and, hence, higher concentration of condensed species; second, rejecting part or all of the condensed species from the first stage; and third, burning the remaining first stage combustion products with the remaining oxidizer and accelerating the products of the second stage towards the channel entrance.

Since chemical equilibrium is assumed in both stages of the combustor, only two thermodynamic parameters are required to evaluate all the parameters of the mixture in either stage. The two parameters chosen to minimize Gibbs free energy are enthalpy and pressure. Since minimization is subject to the conservation of chemical elements, the parameters to be specified in each stage are: pressure, enthalpy per kilogram of reactants, and number of moles of each chemical element per kilogram of reactants. In each stage "per kilogram" is with respect to the total mass of species in the respective stage. The derivation of these variables for each stage is straightforward and will not be repeated here. Only the basic elements are described below.

Let Y_i^F ($i = 1, \dots, s$) be the mass fraction of i -th fuel species in total fuel (i. e., $\sum_{i=1}^s Y_i^F = 1$), Y_i^O ($i = 1, \dots, m$) the mass fraction of i -th oxidizer species in total oxidizer (i. e., $\sum_{i=1}^m Y_i^O = 1$), θ_i the fraction of i -th fuel species injected into the second stage, β_i the fraction of i -th oxidizer species injected into the second stage and $(O/F)_T$ the total oxygen to fuel ratio, then in the first stage of the combustor we have:

$$H_1 = \frac{\sum_{i=1}^s (1 - \theta_i) Y_i^F H_i^F + (O/F)_T \sum_{i=1}^m (1 - \beta_i) Y_i^O H_i^O}{\sum_{i=1}^s (1 - \theta_i) Y_i^F + (O/F)_T \sum_{i=1}^m (1 - \beta_i) Y_i^O}, \quad (137)$$

and

$$b_{1j} = \frac{\sum_{i=1}^s a_{ji}^F (1 - \theta_i) Y_i^F / M_i^F + (O/F)_T \sum_{i=1}^m a_{ji}^O (1 - \beta_i) Y_i^O / M_i^O}{\sum_{i=1}^s (1 - \theta_i) Y_i^F + (O/F)_T \sum_{i=1}^m (1 - \beta_i) Y_i^O} \quad (138)$$

In the above equation, H_1 is the reactant enthalpy per kilogram of reactants, H_i enthalpy of i -th species per kilogram of i -th species, M_i molecular weight of i -th species, b_{1j} kilogram-moles of j -th chemical element per kilogram of mixture, and a_{ji} stoichiometric coefficient of j -th chemical element in i -th species. Subscripts F and O refer to fuel and oxidizer, respectively. Given Y_i^F , Y_i^O , $(O/F)_T$, and the reactant temperatures, we can determine H_1 and b_{1j} . With combustion pressure also specified, the PACKAGE Code can evaluate the temperature and composition of the combustion products using equilibrium chemistry.

Let n_{1j} ($j = 1, \dots, NT$) be the kilogram-moles of j -th species per kilogram of combustion products in the first stage. If α is the fraction of condensed species rejected from the first stage, we can show that H_1^α , and b_{1j}^α , the enthalpy and kilogram-moles of j -th chemical element per kilogram of the remaining species in the first stage, are given by:

$$H_1^\alpha = \frac{H_1 - \alpha \sum_{i=MG+1}^{NT} n_{1i} H_i}{1 - \alpha \sum_{i=MG+1}^{NT} n_{1i} M_i} , \quad (139)$$

and

$$b_{1j}^\alpha = \frac{b_{1j} - \alpha \sum_{i=MG+1}^{NT} a_{ji} n_{1i}}{1 - \alpha \sum_{i=MG+1}^{NT} n_{1i} M_i} . \quad (140)$$

Note that H_i , the enthalpy of i -th species, is calculated at the temperature of combustion products.

Adding the remaining fractions of the fuel and oxidizer to the first stage mixture, we can determine H_2 and b_{2j} , the enthalpy and kilogram-moles of j -th chemical element per kilogram of the mixture in the second stage. These are given by:

$$H_2 = \frac{AH_1^\alpha + \sum_{i=1}^s \theta_i Y_i^F H_i^F + (O/F)_T \sum_{i=1}^m \beta_i Y_i^O H_i^O}{A + \sum_{i=1}^s \theta_i Y_i^F + (O/F)_T \sum_{i=1}^m \beta_i Y_i^O} , \quad (141)$$

and

$$b_{2j} = \frac{A b_{1j}^\alpha + \sum_{i=1}^s a_{ji}^F \theta_i Y_i^F / M_i^F + (O/F)_T \sum_{i=1}^m a_{ji}^O \beta_i Y_i^O / M_i^O}{A + \sum_{i=1}^s \theta_i Y_i^F + (O/F)_T \sum_{i=1}^m \beta_i Y_i^O} , \quad (142)$$

where

$$A \equiv \left(1 - \alpha \sum_{M \in G+1}^{NT} n_{1i} M_i \right) \left[\sum_{i=1}^s (1 - \theta_i) Y_i^F + (O/F)_T \sum_{i=1}^m (1 - \beta_i) Y_i^O \right]. \quad (143)$$

Note that H_i^F and H_i^O are calculated at temperatures T_i^F and T_i^O which can be arbitrarily specified by the user. With H_2 , b_{2j} , and second stage pressure known, equilibrium chemistry is used to evaluate the temperature and species concentration of the combustion products within the second stage. Downstream of the second stage, the PACKAGE code treats the problem as if the first stage did not exist.

In the above derivation, we have assumed seed is part of the fuel. Let index $i = s$ represent the seed, then, for the special case where the seed is injected into the second stage and the remaining fuel in the first stage, Eqs. (141) to (143) become somewhat simplified, since for such a case $\theta_i = 0$ ($i = 1, \dots, s-1$) and $\theta_s = 1$.

1.7 Input Calculations

A number of options are provided in the program for specifying input and these options are discussed in detail in the sections describing the computer program. Part of the input concerns reactants. The total reactant may be composed of a number of reactants and each of these reactants may be specified as an oxidant or a fuel. If the total reactant contains more than one oxidant, these oxidants may be combined into a total oxidant by specifying the relative proportion of each oxidant. Similarly, if the total reactant contains more than one fuel, they may be combined into a total fuel by specifying the relative proportion of each fuel. The overall properties of the total reactant (such as elemental compositions b_i^0 , enthalpy g_0 , molecular weight M_0 , and positive and negative oxidation states V^+ and V^-) can then be calculated by specifying the relative amounts of total oxidant and total fuel.

In order to obtain assigned properties for the total reactant, each reactant j must be specified as either a fuel or an oxidant even though a reactant may ordinarily be thought of as inert (as, for example, N_2). Letting the superscript k equal 1 for

oxidant and 2 for fuel, the kilogram-atoms of the i^{th} element per kilogram of total oxidant or total fuel is

$$b_i^{(k)} = \sum_{j=1}^{\text{NREAC}} a_{ij}^{(k)} n_j^{(k)} \quad \begin{matrix} i = 1, \dots, l \\ k = 1, 2 \end{matrix} \quad (144)$$

where NREAC is the total number of reactants and where $n_j^{(k)}$ is the number of kilogram-moles of the j^{th} reactant per kilogram of total oxidant ($k = 1$) or total fuel ($k = 2$). If the amounts of oxidants and fuels are specified in terms of weights, then $n_j^{(k)}$ is obtained by

$$n_j^{(k)} = \frac{W_j^{(k)}}{M_j^{(k)} \sum_{j=1}^{\text{NREAC}} W_j^{(k)}} \quad \begin{matrix} j = 1, \dots, \text{NREAC} \\ k = 1, 2 \end{matrix} \quad (145)$$

where $W_j^{(k)}$ is the weight of the j^{th} reactant and $M_j^{(k)}$ is the molecular weight of the j^{th} reactant. If, however, amounts of oxidants and fuels are specified in terms of kilogram-moles $N_j^{(k)}$, then

$$n_j^{(k)} = \frac{N_j^{(k)}}{\sum_{j=1}^{\text{NREAC}} N_j^{(k)} M_j^{(k)}} \quad \begin{matrix} j = 1, \dots, \text{NREAC} \\ k = 1, 2 \end{matrix} \quad (146)$$

The $M_j^{(k)}$ may be calculated from the atomic weights of the chemical elements M_i as follows:

$$M_j^{(k)} = \sum_{i=1}^l a_{ij}^{(k)} M_i \quad \begin{matrix} j = 1, \dots, \text{NREAC} \\ k = 1, 2 \end{matrix} \quad (147)$$

The $b_i^{(k)}$ may be combined by means of the following equation to give the kilogram-atoms per kilogram of total reactant:

$$b_i^0 = \frac{b_i^{(2)} + (O/F)b_i^{(1)}}{1 + (O/F)} \quad i = 1, \dots, l \quad (148)$$

where O/F is the oxidant to fuel weight ratio.

Formulas analogous to Eqs. (144) and (148) may be used to obtain other properties of the total oxidant, total fuel, and total reactant (such as enthalpies and molecular weights). Scaled enthalpy of total oxidant ($k=1$) or total fuel ($k=2$) $\mathcal{H}^{(k)}$, (kg-mole/kg)^(k), is given by:

$$\mathcal{H}^{(k)} = \sum_{j=1}^{NREAC} \frac{(H_T^0)^{(k)} n_j^{(k)}}{RT} \quad k = 1, 2 \quad (149)$$

where $(H_T^0)^{(k)}$ is the enthalpy of the j^{th} reactant, (J/kg-mole) _{j} ^(k). Scaled enthalpy of total reactant $\mathcal{H}_0$, kg-mole/kg, is given by:

$$\mathcal{H}_0 = \frac{h_0}{RT} = \frac{\mathcal{H}^{(2)} + (O/F)\mathcal{H}^{(1)}}{1 + (O/F)} \quad (150)$$

Molecular weight of total oxidant ($k=1$) or total fuel ($k=2$):

$$M^{(k)} = \frac{1}{\sum_{j=1}^{NREAC} n_j^{(k)}} \quad k = 1, 2 \quad (151)$$

Molecular weight of total reactant, kg/kg-mole:

$$M_0 = \frac{[(O/F) + 1] M^{(1)} M^{(2)}}{M^{(1)} + (O/F) M^{(2)}} \quad (152)$$

(If $M^{(1)} = 0$, $M_0 = M^{(2)}$ and if $M^{(2)} = 0$, $M_0 = M^{(1)}$.)

In the event that an equivalence ratio is specified, it is calculated using elemental oxidation states. Let V_i^+ and V_i^- be positive and negative oxidation states of the i^{th} element in its commonly occurring compounds. At least one of these will be zero. Thus, for example, the negative oxidation state for chlorine is -1 and its positive oxidation state is zero. The oxidation states per kilogram of total oxidant or total fuel are:

$$V^{+(k)} = \sum_{i=1}^l V_i^+ b_i^{(k)} \quad k = 1, 2 \quad (153)$$

$$V^{-(k)} = \sum_{i=1}^l V_i^- b_i^{(k)} \quad k = 1, 2 \quad (154)$$

The positive and negative oxidation states for the total reactant are then

$$V^+ = \frac{V^{+(2)} + (O/F)V^{+(1)}}{1 + (O/F)} \quad (155)$$

$$V^- = \frac{V^{-(2)} + (O/F)V^{-(1)}}{1 + (O/F)} \quad (156)$$

Equivalence ratio is now defined as

$$r = - \frac{V^+}{V^-} \quad (157)$$

2. COMPUTER PROGRAM - PACKAGE

The PACKAGE computer program is written in standard FORTRAN IV. It is designed to run on any operating system that will accommodate the program's relatively large size. At Aerodyne Research, Inc., PACKAGE is run on a PRIME 400. Current storage is just under 450 K bytes.

Due to the accuracy required in some calculations, DOUBLE PRECISION statements are necessary for some variables on 32 bit machines (such as the PRIME 400 or the IBM 360/370 computer). These statements can be commented out on machines with larger word size like the CDC 6600. Data and Equivalence statements as well as functions pertaining to double precision variables must also be changed to reflect the the proper variable type.

PACKAGE requires thermodynamic data (associated with FORTRAN LOGICAL UNIT 7) for many of its calculations. This data is expressed in the form of seven coefficient polynomial fits over two temperature ranges as generated by the PAC⁽⁴⁾ (Properties and Coefficients) program (see Subsection 1.5.2). Since thermodynamic data are updated periodically, the answers for the sample problems, given in Section 3, may change somewhat from time to time.

Execution of the PACKAGE code requires allocation of five file units of which two are inputs, two are outputs, and one is designated for input/output. These files are described and defined in Table I.

This section is divided into five parts. Part one (Subsection 2.1) contains a comprehensive description of required input data. Part two (Subsection 2.2) contains a complete description of all possible outputs. Part three (Subsection 2.3) describes the program in modular form, while part four (Subsection 2.4) gives a complete specification of all routines. Part five (Subsection 2.5) deals with program modification with respect to storage, application modules, and input/output modules.

2.1 Description of Program Input

Required data is input from two files. Channel input data is read from FORTRAN LOGICAL UNIT 11 and will be discussed later. Program input data is read from FORTRAN LOGICAL UNIT 5 (card images). An input flow diagram is shown on the next page.

Program input data (LOGICAL UNIT 5) will be discussed under five categories. Two of the categories are required and three are optional. The two required categories and the code names by which they will be referred to are as follows:

- (a) Data pertaining to reactants (REACTANTS cards), and
- (b) Namelist data which include the type of problem, required schedules, and options (NAMELISTS input).

The first optional category of input data is the library of thermodynamic data for reaction products (THERMO data).

The second optional category of input data include chemical formulas of species which are singled out for special purposes. OMIT, SOLUTION, and INSERT are control codes used by the program to identify this type of input.

The third set of optional cards pertain to finite rate chemistry and are identified in subroutines ROCKET or MHD by the control codes SPEC, DLIT, REACTANT, PRODUCT, and KFRR.

The THERMO, REACTANTS, NAMELISTS, and SPEC codes are punched on separate cards, each preceding their appropriate data cards. The OMIT, SOLUTION, INSERT, DLIT, REACTANT, PRODUCT, and KFRR codes are on the same card as the data. The required order of the data cards is as follows:

- (1) THERMO code card,
- (2) THERMO data (these cards and the preceding THERMO code card may be omitted if the thermodynamic data are to be read from file),
- (3) REACTANTS code card along with two-stage indicator,
- (4) REACTANTS cards,
- (5) OMIT, SOLUTION, and INSERT cards (if any),

INPUT DATA

PROGRAM INPUT

CHANNEL INPUT

- (6) NAMELISTS code card,
- (7) NAMELIST data,
- (8) SPEC code card (if any),
- (9) SPEC DATA (if any), and
- (10) REACTION RATE cards (if any); these include DLIT, REACTANT, PRODUCT, and KFRR (forward reaction rate constant) cards.

In a particular run, there must be a set of REACTANTS cards (items 3 and 4), each followed by any number of sets in any order of OMIT, SOLUTION, and INSERT cards (item 5) and NAMELIST input (items 6 and 7). There may also be one SPEC card followed by the appropriate SPEC input (items 8 and 9). These are required if NEQPT=1 from namelist RKTINP (see description of SPEC data). Furthermore, the REACTION RATE cards (item 10) are used if the global point counter (denoted by IPP) reaches the value of NEQPT set in namelist RKTINP. NEQPT is used to flag finite rate chemistry.

Program input data contains two namelists for input: INPT2, required for all runs, and RKTINP, required for solutions along a given channel.

Figure 1 shows a flow chart of the main program which controls the reading, processing, and storing of input data. Examples of input cards for several typical problems are given in Section 3. Each category of input data is discussed in detail in the following sections.

2.1.1 THERMO DATA

The library of thermodynamic data for reaction products are in functional form. The order and format of the THERMO data, as well as a listing of a sample thermo data table, are detailed in Appendix D.

THERMO data may be read either from cards or from file. If the data are read from cards, the program will write the data on logical unit 7. During a computer run,

the appropriate reaction products data consistent with each set of REACTANTS cards will be automatically selected from logical unit 7 and stored in the program.

THERMO data may be read from cards for each run. However, a permanent tape or disk file containing the data may be made during any run by using the appropriate control cards preceding the operating deck.

When adding, removing, or changing data for various species in the file, the entire set of THERMO data must be included in the input for making a new file.

Data for one or more species may be omitted from consideration during any particular run (without removing the data from the file) by using OMIT cards (see Subsection 2.1.3 on OMIT and INSERT).

2.1.2 REACTANTS Cards

This set of cards is "required" input. The first card in the set contains the word REACTANTS punched in card columns 1 to 9 and a twostage indicator, which is "TWOSTG" if set, punched in card columns 16 to 21 (see discussion of two-stage combustor in Subsection 2.1.2.3). The last card in the set is blank. Between the first and last cards may be any number of cards up to a maximum of 30, one for each reactant species being considered. The cards for each reactant must give the chemical formula and the relative amount of the reactant. The format and contents of the cards are summarized in Table II.

2.1.2.1 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). For examples, see sample problems in Section 3. Weight fraction must be specified when the two-stage combustor option is used.

There are optional variables which may be set in namelist INPT2 that indicate relative amounts of total fuel to total oxidants. For this situation, each reactant must be specified a fuel or an oxidized by keypunching an F or O, respectively, in

column 72 of the REACTANTS card. The amounts given on the REACTANTS cards are relative to total fuel or total oxidant rather than total reactant. As an alternative, all reactants may be designated as fuel, or oxidizer or left undesignated. In these cases, the relative amounts of the reactants are completely specified by the values on the REACTANTS cards.

Note, for an NEQPT = 1 problem (see Subsection 2.1.4.2), all reactants must be specified as F or O (a combination is not permitted).

There are four options for indicating relative amounts of total fuel to total oxidant. They include:

- 1) Equivalence ratio (equivalents of fuel/equivalents of oxidant)
(ERATIO = TRUE in namelist INPT2)
- 2) Weight of oxidant/weight of fuel (O/F)(ERATIO = FALSE in namelist INPT2)
- 3) Fuel percent by weight (FPCT = TRUE in namelist INPT2)
- 4) Fuel to air ratio (FA = TRUE in namelist INPT2)

The FPCT and FA options have not been used at Aerodyne Research, Inc.

For each option, the values are given in the MIX array of INPT2 (described in Subsection 2.1.4.1).

The purpose of using the variable MIX to permit the use of one set of reactant cards with any number of values (up to 15) of the variables such as equivalence ratio (ERATIO = T). For channel calculations, and when the liquid solution model is used, only one set of these variables is allowed.

2.1.2.2 Reactant Enthalpy

Assigned enthalpy values for reactants are required for HP and channel problems. The values for the individual reactants are either keypunched on the REACTANTS cards or calculated from the THERMO data.

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 THERMO data for the temperature given in card columns 64 to 71.

When the program is calculating the individual reactant enthalpy values from the THERMO data, the following two conditions are required:

- 1) The reactant must also be one of the species in the set of THERMO data. For example, $\text{NH}_3(\text{g})$ is in the set of THERMO data but $\text{NH}_3(\text{l})$ is not. Therefore, if $\text{NH}_3(\text{g})$ is used as a reactant, its enthalpy could be calculated automatically, but that of $\text{NH}_3(\text{l})$ could not be;
- 2) The temperature T must be in the range $T_{\text{low}}/1.2 \leq T \leq T_{\text{high}} \times 1.2$ where T_{low} to T_{high} is the temperature range of the THERMO data.

2.1.2.3 Two-stage combustor option

- 1) Punch TWOSTG in columns 16 - 21 of Reactants card (also set TWOSTG = T in INPT2);
- 2) Specify the fraction (0.0 to 1.0) of each reactant added in the second stage. This value appears in columns 73 - 80 in format F8.5.
- 3) When this option is used, the relative amounts of fuel and oxidizer must be in terms of weight fractions. Anything else will not run.

2.1.3 OMIT, SOLUTION and/or INSERT Cards

OMIT, SOLUTION and/or INSERT cards may follow the REACTANTS cards. Their inclusion is optional. They contain the names of particular species in the library of thermodynamic data for the specific purposes to be discussed. Each card contains the word OMIT (in card columns 1 to 4), SOLUTION (in card columns 1 to 8), or INSERT (in card columns 1 to 6) and the names of one to four species starting in columns 16, 31, 46, and 61. The names must be exactly the same as they appear in the THERMO data.

2.1.3.1 OMIT cards

These cards list species in the THERMO data to be omitted from the chemical system under consideration. If OMIT cards are not used, the program will use all those species in the THERMO data which are consistent with the chemical system being considered. The program is limited to 200 OMIT species per run.

2.1.3.2 INSERT cards

These cards contain the names of condensed species only. They have been included as options for three reasons.

The first and most important reason for including the INSERT card option is that, in rare instances, it is impossible to obtain convergence without the use of an INSERT card. This occurs when, by considering gases only, the temperature becomes extremely low (say several degrees Kelvin). In these rare cases, the use of an INSERT card containing the name of the required condensed species will 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 reason is that if one knows that one or several particular condensed species will be present among the final equilibrium compositions for the 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 was 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. For all other assigned points, the inclusion of condensed species is handled automatically by the program.

The third reason is for cases where $NEQPT = 1$ in namelist RKTINP and chemically rate controlled pure condensed species appear on DLIT cards. For proper execution, they must also appear on the INSERT card.

The program is limited to 30 INSERT species per run.

2.1.3.3 SOLUTION cards

These cards contain the names of condensed species to be included in the ideal liquid solution model. The program is limited to 16 species for the solution model.

2.1.4 NAMELIST Input

The NAMELISTS code card precedes the NAMELIST input. There are two namelists to be input. These are: INPT2, required for all problems and RKTINP, which is optional. The variables in each namelist are listed in Tables III and IV. Note, variables not used are left over from the NASA CEC code.⁽¹⁾ Some additional information about some of these variables follows.

2.1.4.1 INPT2 namelist

A complete list of all variables input by this namelist is listed in Table III. A description of the more important variables and their function is given below.

Pressure Units - The program assumes the pressure in the P schedule to be in units of atmospheres unless either PSIA = T, NSQM = T, or MMHG = T.

Relative Amounts of Fuel(s) and Oxidizer(s) - These quantities may be specified by assigning 1 to 15 values for either ERATIO, FPCT, or FA (see Subsection 2.1.2.1) for TP, SP, or HP problems. 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.)

TP, HP, or SP Problems - In these problems, from 1 to 26 values of T or P may be assigned. However, only one value of entropy (~~S~~) may be assigned in INPT2 for the SP problem. Moreover, only one value of enthalpy is permitted for the HP problem. This value of enthalpy is not assigned in INPT2 but calculated by the program using data from REACTANTS cards (Eqs. (192) to (195) of Section 1). In a TP problem, if 26 values of T and 26 values of P are assigned in INPT2, properties will be calculated for the 676 possible P and T combinations. If the solution model is being used, only one P and MIX value may be used with more than one T.

Printing Mole Fractions of Trace Species - The program automatically prints compositions of species with mole fractions greater than 5×10^{-6} in F-format. The TRACE option permits printing of smaller mole fractions. If the variable TRACE is set to some positive value, mole fractions greater than or equal to this value will be printed. When this option is used, a special E-format for mole fraction output is used automatically. A TRACE value of 1. E-38 is the lowest recommended value to be used by the program.

Intermediate Output - Intermediate output will be listed for whatever point IDEBUG is set equal to and for all the following points. As an example, setting IDEBUG = 3 will result in intermediate output for all points, except the first two, appearing on Logical Unit 6. Debug output can also be obtained by setting IPRRKT to a nonzero value (Subsection 2.1.4.2) or IMPRNT to a nonzero value (Subsection 2.1.7.1). IPRRKT and IMPRNT outputs appear on Logical Unit 1.

Two-Stage Combustor Problems - The required INPT2 NAMELIST parameters for two-stage combustor problems are:

- (1) TWOSTG = TRUE and
- (2) ALPH, the fraction (0.0 to 1.0) of condensed species rejected from the first stage.

Channel Problems - The required INPT2 NAMELIST parameters for channel problems are:

- (1) One and only one chamber pressure P;
- (2) RKT = TRUE;
- (3) DXI, print point increment in the channel (Meters);
- (4) ACCURC, relative accuracy obtained in each integration step (Recommended value is 10^{-3});
- (5) HMIN, smallest step size used to obtain the desired accuracy before aborting the program (recommended value is 10^{-30}).

Additional INPT2 parameters required for MHD channel calculations (see equations in Subsection 1.6.2.1) are:

- (6) XK, load factor (dimensionless);
- (7) BZ, magnetic field (Tesla);
- (8) EXIN, maximum allowable magnitude of axial electric field (Volts/Meters) Recommended value is 2400. This variable causes BZ to be changed if the calculated values exceed EXIN. Note, EXIN = 0.0 will set BZ = constant throughout the channel.

Consider Ions - Set IONS = TRUE.

2.1.4.2 RKTNP namelist

This namelist follows the INPT2 namelist. A list of variables and their definition is given in Table IV. For channel problems, one pressure ratio PCP or one area ratio (either SUBAR or SUPAR) must be assigned. Pressure ratio and area ratio must not include values for the chamber and throat inasmuch as these values are assigned or calculated automatically by the program.

The remaining optional input parameters are described below:

NEQPT flags the initiation of rate controlled chemistry. This occurs at the point where the global counter (IPP) equals the value assigned to NEQPT. Note that the program assigns IPP = 1 and IPP = 2 to the combustor and the throat respectively, where chemical equilibrium is assumed. IPP = 3 refers to the point where the pressure ratio (PCP) or area ratio (SUBAR or SUPAR) is assigned. IPP = 3 defines the channel entrance with X (axial position in the channel) set to 0.0 meters. IPP is incremented immediately after storing a channel output print point.

There are four modes of calculation pertaining to NEQPT:

- (1) NEQPT = 100000 (default value) implies total chemical equilibrium for all IPP. Note, if you expect IPP to exceed 100000, this value must be increased to prevent finite rate chemistry;
- (2) NEQPT = 4 implies partial-equilibrium/partial-rate-controlled chemical calculations begin from the channel entrance. The conditions at the channel entrance are calculated assuming equilibrium chemistry and are used as the initial conditions for subsequent rate controlled calculations;
- (3) NEQPT = 3 implies that partial-equilibrium/partial-rate-controlled chemical calculations begin from the throat. This option is used when channel entrance velocity is supersonic. Furthermore, the user must specify a pressure profile from the throat to the channel entrance

(the program can not execute using an area or velocity profile).
See Subsection 2.1.7.2 for additional information
regarding this special channel profile option.

- (4) NEQPT = 1 implies rate control chemistry is initiated immediately. In this program, the concept of combustor (IPP = 1) and throat (IPP = 2) implies chemical equilibrium. For NEQPT=1, the starting position is defined to be out of equilibrium and occur at $X = 0.0$ meters. Since $X = 0.0$ position refers to the channel entrance (IPP = 3), it was necessary for output purposes to set all variables associated with IPP = 1 and IPP = 2 equal to the corresponding values at IPP = 3. Note, that NEQPT = 1 is the only option available to simulate fully finite rate controlled chemistry.
- (5) It is possible for NEQPT to have values such as 5, 6, . . . , 11, etc. (NEQPT = 2 is not allowed). This implies that finite rate chemistry begins at the previous point (IPP = 4 if NEQPT = 5). It is recommended, however, that NEQPT be either 10000 (left blank) or 4, 3, or 1.

HPATH and SPATH options indicate whether enthalpy (H) or entropy (S) are used to minimize Gibbs free energy (using Eqs. (38) or (39), respectively) in the channel. Since enthalpy is directly calculated from the channel equations, use of HPATH option is recommended, except for isentropic flows when entropy remains constant. Notice HPATH and SPATH can never be equal to each other. If HPATH = TRUE (SPATH = FALSE), then upon entrance into the channel, HP is set to HPATH and SP is set to SPATH.

HTLOSS is an assigned combustor heat loss (cal/gm) to be subtracted from the computer enthalpy of the reactants. The default value is zero.

IPRRKT is used for additional debug output appearing on Logical Unit 1 (see Table V and Subsection 2.2.3.3).

CHNHLS is an assigned mixture enthalpy at an average channel wall temperature. It is required when channel heat loss option, described in Subsection 1.6.4.1, is used. Additionally, variables NUMHLS and TCHFNL must be input.

NUMHLS must be set to 1 when CHNHLS is used.

TCHFNL is the wall temperature for which CHNHLS is assigned. The program will stop and output the results when the calculated temperature falls within ten degrees of TCHFNL. This variable can also be used to stop calculations, even when the heat loss option is not being used.

CHNLEN and TCNINP are used with CHNHLS. CHNLEN is an assigned characteristic length (see Subsection 1.6.4.1). TCHINP should be equal to TCHFNL.

TCEST is the initial temperature estimate to be used by Subroutine EQLBRM for RKT problems. (Default value is 3000.0 K)

2.1.5 SPEC and SPEC Data Cards

The SPEC card flags rate controlled chemical problems for the case when NEQPT = 1. This card contains a required assigned value for the channel entrance velocity. The SPEC card, read immediately after the NAMELIST data, contains the word SPEC in columns 1 - 4 as well as an initial flow velocity (UEINP in m/sec) in columns 13 - 23 in E 11.4 format. The SPEC card cannot be used unless NEQPT = 1.

Immediately following this card is a set of SPEC data cards containing the names of the species to be placed in the nonequilibrium chemistry group. These species, which initiate the chemical reaction, must have appeared in the reactants cards, and must appear in the DLIT cards (see discussion of DLIT cards). Each card contains up to three sets of species names along with the appropriate position of this species in the REACTANTS cards (i.e., 1 for first, 2 for second, etc.). There are at most 30 such inputs (10 cards) allowed. The input format is 3(3A4, I3, 8X), which implies that species names begin in columns 1, 24, and 47, while their position in the reactants cards is indicated by an integer ending in columns 15, 38, and 61. The last input card must be a blank card. See example in Subsection 3.4.1.1.

2.1.6 Reaction Rate Cards

For partial equilibrium/partial finite rate chemical problems (IPP = NEQPT), one must specify all the species which participate in the reactions. These species belong either to the equilibrium or rate controlled pool. Furthermore, one also needs to specify the chemical reaction equations as well as their rate constants. There are four types of RATE cards: DLIT, REACTANT, PRODUCT, and KFRR cards.

2.1.6.1 DLIT cards

These cards (or card) list those species in the THERMO data that are rate controlled. Each card contains the word DLIT (in columns 1 to 4) and the names of from one to four species starting in columns 16, 31, 46, and 61.

The DLIT cards must be the first in the series of REACTION rate cards. The DLIT series of cards is terminated by a blank card. The number of species on DLIT cards must not exceed 30. All SPEC data species must appear on a DLIT card. If a condensed species is part of the liquid solution, it cannot also appear on the DLIT card. Furthermore, if a pure condensed species is on the DLIT card and NEQPT = 1, that species must also appear on an INSERT card.

2.1.6.2 REACTANT and PRODUCT cards

These cards contain the species names and their stoichiometric coefficients in a chemical reaction. Each card contains the word REACTANT (column 1 to 8) for the reactants side of the equation, or PRODUCT (column 1 to 7) for the product side of the chemical equation. From one to four names of species may be on each card, starting in columns 16, 31, 46, and 61. The stoichiometric coefficients for each species (in F3.0 format) start in columns 13, 28, 43, and 58, respectively. Therefore, at most, there can be four species on each side of the chemical equation.

Third body reactions are allowed by using the species name, THIRD BODY, in the appropriate place.

NOTE: There should be at least one rate controlled species in each reaction.

2.1.6.3 KFRR cards

This card describes the forward rate constant of the reactions described by the REACTANT/PRODUCT cards. The card contains the word KFRR (in columns 1 to 4) and three numbers stating in columns 13, 23, and 33 (format (12X, 3E10.4)).

$$k = aT^b \exp(-c/T)$$

where

T is absolute temperature (in $^{\circ}\text{K}$)

a is the first number on the KFRR card (in molecule - cm^3 - sec units)

b is the second number on the KFRR card (unitless)

c is the third number on the KFRR card (in $^{\circ}\text{K}$).

NOTE: If a species is listed in a DLIT card and not in the REACTANT/PRODUCT cards, it is considered frozen. If a species is listed in the REACTANT/PRODUCT card but not in the DLIT card, it is considered to be in the equilibrium pool.

2.1.7 CHANNEL INPUTS

The main function of this input is to specify either velocity, pressure, or area profiles along the channel. Channel input parameters are read from FORTRAN file unit 11. There are two distinct data card types. The program requires the first data card. In certain cases, the second set of data cards may be omitted.

2.1.7.1 DATA CARD TYPE(1) - NAMELIST CHNLIN

This card contains five pieces of data (NMPATH, IMPRNT, XXSTOP, UEINP, ITYPE) to be inputted in namelist format by calling for NAMELIST CHNLIN. The variables for this namelist are listed in Table VI.

- (1) NMPATH describes the specified profile option to use for a given run.

NMPATH = 0 (default value) implies a constant velocity, equal to the channel entrance velocity, along the channel. This will select Model 4 in Table VII.

NMPATH = 1 refers to Model 1 in Table VII. It implies a specified velocity profile will be input along the channel.

NMPATH = 2 refers to Model 2 in Table VII. It implies a specified pressure profile will be input along the channel.

NMPATH = 3 refers to Model 3 in Table VII. It implies a specified area ratio profile will be input along the channel.

NMPATH = -1 or -2 or -3 corresponds to a constant velocity, pressure, or area profile along the channel. The calculated value at the channel entrance will be used.

- (2) IMPRNT is for CHANNEL debug output originating from subroutines EQLBRM, MHD, and DIFFUN.

IMPRNT = 0 for no debug output

IMPRNT = 1 or 2 or 3, etc., for increasing output (see Table VIII and Subsection 2.2.3.3).

- (3) XXSTOP is the value of the independent variable (axial coordinate in the channel in meters) for which the program will stop executing (STOP 5). All outputs prior to this point will be written in the output file. The default value of 0.0 defaults to 10 times the print step size. That is, a possible 10 output points may be generated. Note, if no channel calculations are desired, then XXSTOP must be set to a small value, such as 0.0001. XXSTOP is the most practical way of stopping program execution in the channel.
- (4) UEINP is the initial channel velocity in Meters/sec. If this value is left at 0.0, the program will calculate the initial velocity based on the equation:

$$UEINP = \sqrt{2 * 8314.3 * (H_{SUM}(1) - H_{SUM}(NPTM1))} ,$$

where

$H_{SUM}(1)$ = enthalpy at point 1 divided by the gas constant

$NPTM1 = NPT - 1 = 3$ when UEINP is calculated.

Also, if NEQPT = 1, then UEINP has already been input by the SPEC card (leave this field blank). However, a nonzero value input here will override the value input on the SPEC card.

- (5) ITYPE refers to the set of equations to be solved.

ITYPE = 1 for MHD problems with a simple wall heat loss

ITYPE = 999 or negative number sets the force (FFF) and heat (QQQ) terms equal to 0.0.

ITYPE = 0 defaults to ITYPE = 1

Note, Subroutine SETEQU has been written so that the user can add realistic force (FFF) and heat (QQQ) terms by adding appropriate equations corresponding to new ITYPE values (2, 3, 4, ...).

The force (FFF) and heat (QQQ) terms are set up in subroutine SETEQU. Currently, the program only considers ITYPE = 1 or ITYPE = 999 problems. If the user wishes to consider other FFF and QQQ terms, he must formulate them in SETEQU.

2.1.7.2 DATA CARD TYPE (2) - CHANNEL PROFILE

These cards contain the profiles of the specified variable, dictated by the NMPATH value, as a function of the axial distance in the channel. If NMPATH is zero or negative, these cards should be omitted (unless a special channel profile is desired). The user is allowed to input up to ninety pairs of data points (if more is required, see appropriate comments in the main program). Enter the independent (XINDP = axial distance in meters) and dependent variable (DUMMIN = velocity, pressure, or area ratio) anywhere in columns 1 through 10 and 11 through 20, respectively. The input format is 2F10.0. Since these are discrete values in the channel, the intermediate points are determined by a third order interpolation.

SPECIAL CHANNEL PROFILE (STARTING AT THE THROAT)

When rate controlled chemistry starts from the throat, NEQPT = 3, one wishes to integrate from the throat to the channel entrance. In this case, the following changes must be made to the appropriate independent (XINDP) and dependent (DUMMIN) variable pairs input by data card type 2. XINDP (1) must specify the axial position of the throat relative to the channel entrance (meters). Note, this value will be negative since the channel entrance is defined to be at 0.0 meters. DUMMIN(1) must specify the pressure at the channel entrance (atm). A linear pressure profile is assumed from the throat to the channel entrance. The subsequent data cards (if any) must specify a velocity (NMPATH = 1) or pressure (NMPATH = 2) or area ratio (NMPATH = 3) profile in the channel. Note, XINDP(2) must be set equal to 0.0 meters for these profiles. A constant velocity, pressure, or area profile, equal to their channel entrance value, will be generated whenever a channel profile is not specified. Note, NMPATH cannot be less than zero when NEQPT = 3.

2.2 Description of Program Output

The program yields five major categories of output. The first, denoted by INPUT DATA, prints the input data as well as all information related to the users choice of inputs. The second, defined as TABLES OF RESULTS, contains the computed output data at each print point. The third, denoted as OPTIONAL DATA, describes results concerning the computational procedures. Categories four and five are STOP CODES and ERROR MESSAGES, respectively. An output flow diagram is shown on the next page.

2.2.1 INPUT DATA

INPUT DATA have been previously described. The general procedure used in this program is to list the input as they are read in and before they are processed in the program. The purpose is to show, in as clear a way as possible, what is actually on the input cards. All problems list the following input data:

- (1) The word REACTANTS
- (2) Reactant Data
- (3) INSERT and/or OMIT and/or SOLUTION Card Data
- (4) The word NAMELISTS
- (5) All data in namelist INPT2 given in Table III
- (6) A list of the chemical elements in the system being considered
- (7) Following the INPT2 data is the statement "SPECIES BEING CONSIDERED IN THIS SYSTEM." Each species in the list is preceded by some identification such as J12/65. The J refers to JANAF data, and 12/65 indicates the date of the JANAF table. Entries beginning with L were generated at NASA-Lewis Research Center, while those with no identifying letter originated at Aerodyne Research on the indicated date.
- (8) A list of species in the liquid solution (when applicable)
- (9) The namelist RKTINP data given in Table IV are listed

BASIC PROGRAM OUTPUT

- (10) The current value of O/F, following by a listing of the enthalpies and the kilogram-atm per kilogram of each element of the total fuel and oxidant, and of the total reactant
- (11) All data associated with SPEC card (if applicable) including initial concentration of rate controlled species appearing on the SPEC DATA CARD
- (12) DLIT CARD data
- (13) Chemical elements which only appear in the nonequilibrium pool
- (14) Species composed of elements in (13), and not appearing on DLIT cards. These species are eliminated from consideration
- (15) Channel input data described in Table VI and Subsection 2.1.7
- (16) Chemical equations and rates.

2.2.2 TABLES OF RESULTS

The final output of the program is in the form of tables that are designed to be self-explanatory. If IONS = TRUE, and intermediate output from CONDUCT is printed. This includes the number density of the positive and negative ions and the conductivity. This output occurs at each print point. The features of the tables are:

- (1) Heading
- (2) Case Number
- (3) Reactant Data
- (4) Proportion of Oxidant to Fuel
- (5) Mixture Properties (P , T , ρ , h , S , M , $(\partial \ln V / \partial \ln T)_p$, C_p , γ_s , U , TOTAL H , B , β , a , ELEC DENS, IONIC DENS, σ , σ (without ions), ELECTRON COLLISION FREQ. These variables are defined in Subsection 2.4.11.
- (6) Channel problems list additionally p_c/p_e , $\mathcal{M}$ (Mach number), A_e/A_t , and molecular weight of mixture
- (7) Equilibrium Composition in Mole Fractions

- (8) Species in solution at the last report station (if applicable)
- (9) Nonequilibrium composition in mole fractions (if applicable)
- (10) List of species with mole fractions less than TRACE (Subsection 2.1.4.1).

2.2.3 OPTIONAL DATA

This includes information concerning iteration convergence, intermediate output, and programmer controlled debug output.

2.2.3.1 Information concerning the iteration convergence

All problems, except for NEQPT = 1 when NS =1, print information regarding iteration for each point on FORTRAN LOGICAL UNIT 6. Following the data on kilogram-atoms per kilogram of the reactants is a line containing the letters PT and the chemical symbols of the chemical elements of the problem. The numbers under PT refer to the points corresponding to the columns in the final table. The numbers under the chemical symbols are the values of $\pi_i = -\lambda_i/RT$ (λ_i are Lagrange Multipliers). The last column (without a heading) is the number of iterations required to converge to equilibrium composition.

In general, there is only one line for each point unless there has been an addition or deletion of a condensed species.

2.2.3.2 Intermediate output concerning iteration procedure

The option of printing intermediate output concerning the iteration procedure is provided primarily as a means of obtaining additional information for debugging purposes. There is usually no point in using the option when the program is working well. This output is written to FORTRAN LOGICAL UNIT 6. We have used this option in the past for the following reasons:

- (1) To find programming errors,
- (2) To study the iteration process and rate of convergence,
- (3) To verify that thermodynamic data have been properly prepared, and
- (4) To study the test for inclusion of condensed species.

As discussed in Subsection 2.1.4.1, intermediate output for point N and the following points is obtained by setting IDEBUG = N.

Table IX is a sample of the intermediate output for a first iteration. It was obtained by setting IDEBUG = 1. Following the first line, which gives the iteration number, is the iteration matrix. The line underneath the chemical symbols contains the solution to this matrix. The next line contains some additional information in regard to the matrix, that is, T, N (ENN), ln N (ENNL), P, ln(P/n_j), and λ. The next group of lines contain information on the individual species used in setting up the preceding matrix and the values of Δln n_j obtained from the matrix solution and Eq. (23). The information on the individual species includes the chemical symbol, n_j, ln n_j, Δ(ln n_j), dimensionless enthalpy, dimensionless entropy ($S_j^0/R \equiv S_j^0/R$), negative dimensionless standard state Gibbs free energy ($-G_j^0/RT \equiv -\mu_j^0/RT$), and negative dimensionless Gibbs free energy ($-G_j/RT \equiv -\mu_j/RT$).

The two derivative matrices and their solutions are also given for this point. These derivative matrices are set up after convergence. This is followed by two lines of output which summarize the results for the point NPT. The printed variables are labeled POINT, P, T, H/R, S/R, MW, CP/R, DLVPT, DLVTP, GAMMA(S), and V. The corresponding FORTRAN symbols (defined in Appendix B) are NPT, PPP, TTT, HSUM, SSUM, WM, CPR, DLVPT, DLVTP, GAMMAS, VLM, respectively.

Table X is part of the intermediate output showing the test for condensed phases after convergence. For a sample problem, it shows the results of testing the condensed species after convergence with Al₂O₃(s) being the only condensed species present. The notation G0-SUM(AIJ*PI) refers to the quantity given in Eq. (79). This quantity, as previously mentioned, must be negative for a condensed species not included in the previous convergence to be now considered for inclusion. Further, only that species with the most negative value will be included. In Table X, it may be seen that only one species, Al₂O₃(s), has a positive value for IUSE which means it was the only condensed species in the previous convergence. Assume the temperature for the previous convergence (not shown in Table X) is

670 K. The free energy test is not made for the following species because their temperature range does not include this temperature: $\text{Al}(\ell)$, $\text{AlCl}_3(\text{s})$, $\text{Al}_2\text{O}_3(\ell)$, $\text{H}_2\text{O}(\text{s})$, $\text{H}_2\text{O}(\ell)$, $\text{Mg}(\ell)$, $\text{MgCl}_2(\ell)$, $\text{MgO}(\ell)$, and $\text{S}(\text{s})$. The following species have positive values of $G^\circ\text{-SUM}(\text{AIJ*PI})$: $\text{C}(\text{s})$, $\text{MgCl}_2(\text{s})$, and $\text{MgO}(\text{s})$. The largest negative value for all preceding species tested is shown by MAX NEG DELTA G. After all condensed species have been tested, only that species with the largest negative value, in this case $\text{MgO}(\text{s})$, is included as a possible species and the iteration procedure is restarted. After convergence, the next test for condensed species (not shown in Table X), gave no negative values for $G^\circ\text{-SUM}(\text{AIJ*PI})$ which completes the test for condensed species for this point.

If a singular matrix occurs in subroutine GAUSS, the coefficients are output by a call to DBGOUT (see description of DBGOUT in Subsection 2.4.23). This will be printed to FORTRAN Logical Unit 1.

2.2.3.3 Debug output (all printed on FORTRAN Logical Unit 1)

There are two input variables (IPRRKT and IMPRNT) which control programmer debug output. There will be no extra debug output if each is set = 0. As the size of each variable increases, the quantity of output is correspondingly increased. IPRRKT is input in namelist RKTINP and yields potential output from Subroutines ROCKET, EQLBRM, MHD, SETEQU, and DIFFUN. IMPRNT is a channel input variable and yields potential output from Subroutines SETEQU, EQLBRM, MHD, and DIFFUN. In many cases, these variables yield output due to calls to Subroutine DBGOUT. If this is the case, the output will take the following form:

***** N DEBUG PTS. FOR HP = (0 or 1) AND SP = (1 or 0) DBG OUTPUT NO.(I3)

NUMBER	VALUE
1	FORMAT (G13.5)
2	:
:	:
:	:
N	FORMAT (G13.5)

The quantity of output is additive. For example, if IMPRNT = 1, we will get a set of outputs. If IMPRNT = 2, we will get the same set of output plus some additions. This same procedure is true for IPRRKT.

As with the intermediate output, there is no point in turning on the debug options if the program is working well.

The use of these debug options is not recommended unless one has a good understanding of the flow charts of the above mentioned subroutines. For more details, see Table V for IPRRKT output and Table VIII for IMPRNT output.

2.2.4 STOP Codes

The following STOP code conditions have been added to aid the user in discovering error conditions:

- (1) STOP is a normal stop occurring in MAIN at line 358, unless an error message is specified. Abnormal stops can result from Subroutines MHD and SRCHCC with appropriate error messages (lines 213 and 1112 in MHD and line 218 in SRCHCC).
- (2) STOP 2 can result from Subroutine ROCKET under the path where NEQPT = 1 for fully finite rate controlled chemistry. This error can occur if the SPEC card is incorrect or if all species were eliminated from the equilibrium pool (lines 233 or 489).
- (3) STOP 4 is an error message from Subroutine EQLBRM (lines 209 or 222) under finite rate conditions. See Subsection 2.2.5.4, error message (5).
- (4) STOP 5 is a user requested stop occurring when either the position in the channel exceeds the input XXSTOP value or the calculated temperature is less than the input TMPSTP value. XXSTOP is set by namelist CHNLIN (Subsection 2.1.7.1) and TMPSTP is set by namelist RKTINP (Subsection 2.1.4.2). This is not an error stop and all output, up to that point, will be printed. For all runs, this is the most likely normal termination. It occurs at line 869 of Subroutine ROCKET, but is flagged in MHD.

- (5) STOP 6 occurs for channel calculations when area is specified and the local Mach number approaches 1.0. This stop is flagged in DIFFUN whenever the Mach number squared is within 0.0001 of 1.0. Prior to this stop, all output through the previous point will be printed, as well as an appropriate message. This stop occurs at line number 187 of Subroutine DIFFUN.
- (6) The computer code allows for a maximum of 32 differential equations to be solved. STOP 7 indicates that the maximum number of allowed equations has been exceeded. It occurs in Subroutine MHD at lines 389, 410, 511, 552 and 596.
- (7) STOP 10 occurs when there is not enough storage for an NEQPT = 1 problem. The stop occurs at line number 193 of Subroutine MHD.
- (8) STOP 20 occurs when there is an error in Subroutine EQLBRM resulting in the temperature being set to zero. The stop occurs at lines 174 and 188 of Subroutine DIFFUN. Another cause of this stop in DIFFUN is when the calculated temperature is less than TCHFNL + 10.0 (see Subsection 2.1.4.2). Prior to this stop, all output through the previous point will be printed.
- (9) STOP 30 occurs when NEQPT = 1 and the number of species in the equilibrium pool, NS, is equal to zero. To correct the problem, add a new species to the reactants data in such a way that it will not affect the calculations. This can be done by including a small quantity of an inert species, such as Ar, as a new reactant. Be sure not to include this species in the SPEC data cards. This occurs at line 467 of Subroutine ROCKET.

2.2.5 Error Messages

2.2.5.1 Error messages in the MAIN program

- (1) ERROR - VOLUME MAY NOT BE ASSIGNED
Main program, line number 356. This occurs if either TV, HV, or SV is true. The program will stop since this type of calculation has been removed (though it exists in the NASA CEC code).

(2) ERROR IN ABOVE CARD. CONTENTS IGNORED

Main program, line number 165. This message indicates a keypunching error in a control card, a missing control card, or an extraneous card. The entire contents of this card are ignored by the program.

(3) ERROR IN ORDER OF CARDS FOR (Name of species)

Main program, line number 204. The cards containing THERMO data for the species named are out of order.

(4) ERROR IN REACTANT CARDS

Main program, line number 174. This is due to an error in a chemical symbol such as the symbol not being left-adjusted or not included in BLOCK DATA. Program stops.

2.2.5.2 Error messages in Subroutine SRCHCC

(1) ***. . . * FATAL ERROR NOT ENOUGH SPECIES STORAGE CHANGE
VALUE OF NSPCMX AND APPROPRIATE VECTORS IN COMMON IN
THE MAIN PGM

INSUFFICIENT STORAGE FOR FOLLOWING (Number of) SPECIES
Subroutine SRCHCC, line numbers 206, 207, and 212. This statement shows that for the chemical system under consideration, the program found more possible species in THERMO data than can be accommodated by storage reserved for the thermodynamic data in labeled commons (see discussion of increased storage, Subsection 2.4.1). This excess number of species is given in the error message. When this situation occurs, the names of the possible species are printed and control is returned to the main program and the program stops.

This situation can be resolved in two ways. First, the program can be recompiled with dimensions increased to accommodate the excess species (see Subsection 2.5.1 on Changing Number of Possible Reaction Species). Secondly, OMIT cards can be used to eliminate the required number of excess species.

The program is currently dimensioned for 300 species.

- (2) NEW SIZE GREATER 600 CHANGE SIZE OF SUB (600,3) ARRAY IN ALL ROUTINES

Subroutine SRCHCC, line number 214. The maximum number of species allowable for expansion in the commons is 600. If you require more than 600, you must increase the size of the SUB array in labeled COMMON/SPECE1/in all subroutines as well as follow all the instructions given in the discussion of the previous SRCHCC error message.

- (3) TOO MANY CONDENSED SPECIES PROGRAM ALLOWS (number) LAST (number) IGNORED UPDAT TEMP (NC,2) VECTOR IN COMMON/SPECE1/ EVERYWHERE

Subroutine SRCHCC, line number 199. One exceeded the maximum number of condensed species allowed. The overflow numbers were ignored and the program continued to execute. To fix this problem, update NCMAX in the MAIN program, and increase the size of the TEMP array appearing in labeled COMMON/SPECE1/in all subroutines. Currently, 175 condensed species are allowed.

- (4) JANAF TABLE ERROR AT BLOCK (number)

Subroutine SRCHCC, line number 216. An error occurred in reading the THERMO data from the JANAF table. The program lists the error line and stops.

2.2.5.3 Error messages in Subroutine HCALC

- (1) REACTANT (number) IS NOT IN THERMO DATA

Subroutine HCALC, line number 194. As discussed in the Subroutine HCALC section, enthalpies can be calculated by the program only for those reactants that are also included as reaction species in the thermodynamic data. The error message is printed when this condition is not met and the program stops.

- (2) **REACTANT TEMPERATURE OUT OF RANGE OF THERMO DATA**
Subroutine HCALC, line number 190. Subroutine HCALC permits calculation of thermodynamic data for reactants for temperatures that extend up to 20 percent beyond the temperature range over which the data were fit. However, if the assigned temperature is more than 20 percent beyond this range, the error message is printed and the program stops.

2.2.5.4 Error messages in Subroutine EQLBRM

- (1) **DERIVATIVE MATRIX SINGULAR**
Subroutine EQLBRM, line number 351. This situation occurs very rarely inasmuch as, if singularities in the matrix solutions occur, they generally occur first in the iteration matrices and the program does not get as far as the derivative matrices. However, it is possible for the iteration matrix to just barely avoid being singular and for the derivative matrix to be singular. When this occurs, the above message is printed, DLVPT is set equal to -1, and the program continues.
- (2) **SINGULAR MATRIX ITERATION (number) VARIABLE (number)**
Subroutine EQLBRM, line 358. Singularities may occur in the course of obtaining a matrix solution in GAUSS. When they occur, the program restarts with new estimates as discussed in the Singularities section (Subsection 1.4.6). However, if the singularity occurs again, even with new estimates, the above message is printed and control is returned to the main program and the program stops. One possible way to get through this difficulty, discussed in the Singularities section, is to assign a slightly modified equivalence ratio of O/F.
- (3) **LOW TEMPERATURE IMPLIES SPECIES SHOULD HAVE BEEN INCLUDED ON AN INSERT CARD, RESTART**
Subroutine EQLBRM, line numbers 355 and 757. This message can occur only for an HP problem. It occurs only when the omission of an important condensed product of reaction causes the program to seek a combustion

temperature that is unrealistically low ($T < 100\text{K}$). When this occurs, the program stops.

(4) PHASES OF A CONDENSED SPECIES ARE OUT OF ORDER

Subroutine EQLBRM, line number 1056. This statement is written when the thermodynamic data for three or more condensed phases of a species are not in a permitted order as discussed in Appendix D. After the statement is written, a table of output for all completed points is written and program stops.

(5) ERROR STOP 4 I $B\theta(I)$ $B\theta N(I)$ DIFFERENCE

Subroutine EQLBRM, line numbers 208 and 219. This occurs when $B\theta N(I)$, number of moles of I-th chemical element per kilogram of mixture in the nonequilibrium pool, exceeds $B\theta(I)$, its maximum value. This should never occur as $B\theta N(I)$ should approach, but never exceed $B\theta(I)$. If this does happen, your problem is most likely formulated incorrectly.

(6) DID NOT CONVERGE ON ELECTRON BALANCE

Subroutine EQLBRM, line number 653. When this occurs, the program stops after outputting the current results. Either set IONS = FLASE or omit some ions.

(7) THE TEMPERATURE = (degrees K) IS OUT OF RANGE FOR POINT
(Number)

Subroutine EQLBRM, line number 1472. This message is printed whenever the converged temperature for the indicated point is outside the temperature range read in on the card following the THERMO control card. This temperature range, which at present is 300 to 5000 K, is the one over which the gas phase thermodynamic data were fit. Generally, the thermodynamic data can be extrapolated a short distance without much loss in accuracy. However, to prevent large errors due to extrapolation if $TLOW/1.5 > T > 1.25*THIGH$, then after the message has been printed, the program writes the output for all completed points and then stops.

(8) N ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREMENTS
FOR THE POINT (Number)

Subroutine EQLBRM, line number 704. As indicated in Subsection 1.4.2, compositions are typically obtained in 3 to 12 iterations. The number (N=35) was arbitrarily selected for RKT=TRUE problems to indicate that if convergence has not been reached by that number, the problem probably will not converge at all. This situation occurs rarely. All completed points up to this point are printed and the program stops. If the cause of nonconvergence is not obvious from the output, it is recommended that the problem be rerun with intermediate output.

The number of iterations (N) is increased for the following special cases:

- (1) 50 if TRACE is nonzero (see INPT2 namelist)
- (2) 100 if TP=TRUE Problem (see INPT2 namelist)
- (3) 70 if SP=TRUE or HP=TRUE Problem (see INPT2 namelist)

2.2.5.5 Error messages in Subroutine ROCKET

(1) DID NOT CONVERGE FOR AREA RATIO = (Value of area ratio)

Subroutine ROCKET, line number 842. The program permits a maximum of 10 iterations to converge to the pressure ratio corresponding to the assigned area ratio. The usual number of iterations required is 1 to 5. The only situation in which the number of iterations has exceeded 10, in our experience, has been for an assigned area ratio very close to 1 such as $1. < A_e/A_t < 1.001$. This is due to the fact that the converged throat conditions do not correspond exactly to an area ratio of 1.

(2) ERROR INCORRECT SPEC CARD FOR NEQPT = 1 PROB

Subroutine ROCKET, line number 231. Under the path NEQPT = 1, fully finite rate controlled chemistry, this error will occur if a faulty SPEC card is input. The resulting error yields a STOP 2.

(3) PROGRAM STOPS WHEN IPP = (Value) IS .GE. NPP = (Value)

NPP IS SET TWICE IN ROCKET

Subroutine ROCKET, line number 871. The variable NPP was arbitrarily set to 500 in Subroutine ROCKET lines 142 and 895. If the global point

counter (IPP) exceeds this value, the program will stop executing. To correct this problem, reset NPP at the appropriate two lines.

- (4) **SUPERSONIC PRESSURE RATIOS MUST BE IN ASCENDING ORDER POINTS OUT OF ORDER WERE OMITTED FROM FROZEN CALCULATIONS**
Subroutine ROCKET line numbers 778 and 922. Program continues on to the next point after the above message.
- (5) **ERROR . . . FOR PROBLEM WHERE NEQPT = 1 . . . NS = 0**
NEED AT LEAST 1 REACTANT SPECIES IN EQUIL POOL . . . STOP 30
Subroutine ROCKET, line numbers 463 and 464. There were no species in the equilibrium pool for an NEQPT = 1 problem. A solution is to add a small quantity of an inert species (such as Ar) to the reactant cards, and rerun.

2.2.5.6 Error messages in Subroutine MHD

- (1) **ERROR - SOLUTION SPECIES ON DLIT CARD**
Subroutine MHD, line number 211. A species appearing in the liquid solution, also appeared on the DLIT card as a rate controlled species. This is a fatal error resulting in a STOP.
- (2) ******* KFLAG = (negative number)**
Subroutine MHD, line number 1101. When solving the set of channel equations, Gear's method returned an insoluble condition. It will repeat the calculations with a smaller step size and new starting conditions. This is not a fatal error.
- (3) **ERROR - KFLAG = (negative number)**
Subroutine MHD, line number 1106. This appears after the previous message if on the subsequent try KFLAG was still negative. This error will cause the program to stop after it outputs the results through the previous point. A possible fix is to decrease both the accuracy requirements (ACCURC) and the step size (DXI) inputted on namelist INPT2.
- (4) **NOT ENOUGH STORAGE FOR FINITE RATE EQUATIONS**
Subroutine MHD, line number 184. This message occurs when the addition of finite rate equations exceeds the appropriate storage allocation. See error messages (1), (2), and (3) in Subsection 2.2.5.2 for more details. A stop 10 will result if this is an NEQPT = 1 problem.

2.3 Modular Form of the Program

In order to facilitate adding or deleting applications of the chemical equilibrium part of the program, the program was set up in seven modules. These modules are concerned with general input, additional input processing, two applications, equilibrium calculations, channel calculations, and output. The general flow of these modules and associated routines are given in the following diagram:

A subroutine tree diagram is given in Figure 2. From these diagrams, it is clear, for example, that the MHD application which is a special channel application could be eliminated by omitting Subroutines MHD, DIFSUB, and DIFFUN and by omitting the statements which call MHD in Subroutine ROCKET.

Some detail of the individual routines are given in Subsection 2.4.

The present subsection gives: (1) the general purpose of each module, and (2) some common variables set by the module.

2.3.1 General Input Module

This module is controlled by the main program. A flow diagram of the main program is given in Figure 1. The module sets up the input required by all application modules. Some of these input data include the following:

- (1) THERMO data. The main program reads the thermodynamic data cards for all species and writes the data on FORTRAN LOGICAL UNIT 7. Subroutine SRCHCC reads in the data for the appropriate species for a particular chemical system from unit 7 and stores the data in the program.
- (2) REACTANTS cards. These cards are read and processed by subroutine REACT.
- (3) INPT2 namelist data. The main program initializes the variables, reads and writes the INPT2 data, and converts some of the data to the form required by the remainder of the program.
- (4) BLOCK DATA. These data are set for the entire computer run.
- (5) Composition estimates. These estimates and associated variables are set for the first iterations for the first point only.

The variables having to do with composition which are used directly by the equilibrium module include ENN, ENNL, IQ1, IUSE, JSOL, JLIQ, EN(1,J), ENLN(), and EMM. (All common variables are defined in Appendix B.) The remaining variables set in the general input module, which are used by the equilibrium module, include A, COEF, IONS, LLMT, RR, NS, NLM, NC, IDEBUG, TEMP, TRACE, and TMID. These latter variables usually remain unchanged for an entire problem set.

2.3.2 Application Modules

Each application module is called from the main program according to the type of problem designated in namelist INPT2. The module controls the flow of the program until the problem is completed. Control is then returned to the main program. Subroutine THERMP, Figure 3, shows an example of an application module. An application module is responsible for the following items:

- (1) Reading any additional input for the particular problem (namelist RKTINP and CHNLIN for channel applications).
- (2) Doing any calculation peculiar to the problem.
- (3) Calling routines which are contained in the additional input processing module, as required.
- (4) Calling Subroutine MHD (from Subroutine ROCKET) to set channel inputs and control channel calculations.
- (5) Setting a point number NPT and setting certain variables required for the assigned thermodynamic states for that point if they have not already been set in the main program. These variables are set as follows for various assigned states:

Variable	Temperature and pressure	Enthalpy and pressure	Entropy and pressure
TP	True	False	False
HP	False	True	False
SP	False	False	True
TT	T_0	Estimated T	Estimated T
PP	P_0	P_0	P_0
SØ	---	---	S_0
HSUBØ	---	h_0/R	---

Estimated T is set equal to 3000 K for the first point only. For succeeding points, the temperature estimate is set equal to the value of some previous converged point.

- (6) Calling the equilibrium module (Subroutine EQLBRM).
- (7) Printing special output for the problem, calling the output module to print general output, printing debug output through subroutine DBGOUT.

2.3.3 Equilibrium Module

The equilibrium module calculates compositions and thermodynamic properties for a particular point NPT. The module is controlled by subroutine EQLBRM which is diagrammed in Figure 4.

Subroutine EQLBRM calls for subroutines: (1) CPHS to calculate thermodynamic functions of the individual species, (2) MATRIX to set up the solution matrix, (3) GAUSS to solve the set of equations, and (4) DBGOUT to output special debug variables.

Common variables either calculated or set by the EQLBRM module include CPR, CPSUM, DLVPT, DLVTP, EN, ENLN, ENN, GAMMAS, H θ , HSUM, JLIQ, JSOL, PPP, S, SSUM, TOTN, TTT, VLM, and WM. These variables are described in Appendix B.

2.3.4 Additional Input Processing Module

The additional input processing module consists of a set of routines which are called for various purposes:

- (1) NEWOF is called by an application module to adjust values of b_i^0 , r , and h_0/R for each O/F. See Appendix E.
- (2) SAVE is called to save or move composition data from one point to another. The purpose is to use the calculated results from some previous point as initial estimates for the current point.
- (3) HCALC is called from NEWOF - to calculate enthalpies for reactants where one or more REACTANTS cards had zeros in columns 37 and 38.
- (4) CPHS is called by HCALC, EQLBRM, and DIFFUN to calculate thermodynamic functions for an individual reactant using the THERMO data.

Variables set by this module which are required by the equilibrium module include B θ , HSUB θ , and EQRAT. See Appendix B.

2.3.5 Output Module

The output module consists of the five subroutines VARFMT, EFMT, OUT1, OUT2, and OUT3. OUT1 lists data given on the REACTANTS cards as well as O/F, %F, and r. OUT2 lists the properties P_{atm} , T, ρ (g/cc), H(cal/g), s (cal/(g) (K)), M (molecular weight of the gas), $(\partial \ln V / \partial \ln P)_T$, $(\partial \ln V / \partial \ln T)_P$, c_p (cal/(g) (K)), γ_s , U(M/sec), TOTAL H (cal/g), B (Tesla), β (Hall parameter), a(speed of sound), ELEC DENS, IONIC DENS, σ (MHO/M), σ (without NEG IONS), and electron collision FREQUENCY (1/sec). OUT3 lists equilibrium composition (mole fractions), species in solution at last report station, composition of nonequilibrium species, and trace species. The above variables are defined in Subsection 2.4.11.

Subroutines VARFMT and EFMT are called from OUT2 and OUT3. VARFMT adjusts the number of decimal places in a variable format according to the size of the numbers. EFMT sets up a special E-type format for printing density ρ and mole fractions.

2.3.6 Channel Calculations

In channel problems, the channel calculation module defines the system of differential equations using DIFFUN and SETEQU, and solves them using DIFSUB, EQLBRM, CPHS, and CONDUCT.

2.4 Routines

The program consists of a main program, 23 subroutines, 1 function, and block data. A description of the function of each of these is given in the following subsections.

Most program variables used in these sections are in labeled common and are defined in Appendix B.

2.4.1 Main Program

A flow chart of the main program is given in Figure 1. Generally, the routine performs the following functions:

- (1) Reads code cards THERMO, REACTANTS, OMIT, INSERT, SOLUTION and NAMELISTS and directs flow of the program accordingly.
- (2) Stores THERMO data on file unit 7.
- (3) Calls subroutine REACT to read and process REACTANTS cards.
- (4) Reads OMIT, INSERT, and SOLUTION cards and stores the species names.
- (5) Initializes variables in namelist INPT2.
- (6) Reads and writes namelist INPT2.
- (7) Stores the number of pressures in NP.
- (8) Stores values of O/F in OXF array. If O/F values have not been input directly, they are calculated as follows:

Values in MIX (Table III)	Code (Table III)	O/F calculation in main program
Oxidant to fuel weight ratio, O/F	ERATIO = .FALSE.	OXF(i) = O/F
Fuel to air weight ratio, f/a	FA = .TRUE.	OXF(i) = 1/(f/a)
Percent fuel, %F	FPCT = .TRUE.	OXF(i) = (100-%F) (%F)
Equivalence ratio, r	ERATIO = .TRUE.	$\text{OXF}(i) = \frac{-rV^{-(2)} - V^{+(2)}}{rV^{-(1)} + V^{+(1)}}$
Not specified		$\text{OXF}(i) = \frac{\text{WP}(1)}{\text{WP}(2)}$

The parameters $V^{\pm}$ are defined in Subsection 1.7. The parameters WP(1) and WP(2) are defined in Appendix B.

- (9) Makes necessary adjustments to consider charge balance if IONS = TRUE. This is done by adding 1 to NLM and E to LLMT array.
- (10) Calls SRCHCC to pull required THERMO data from file unit 7 and to store the data in the program.
- (11) Sets up indices for the processing of ideal condensed solutions.
- (12) Sets initial estimates for compositions. These estimates are set with each INPT2 read. They are used only for the first point in the lists of variables in namelist (e. g., the first O/F and the first T and P in a TP problem). All succeeding points use the results from a previous point for estimates.

For the first point, the program assigns an estimate of 0.1 for N, the total number of kilogram-moles per kilogram in the equilibrium pool. The initial estimate of number of moles of each equilibrium gaseous species per kilogram of mixture n_j is set equal to $0.1/\text{MG}$ where MG is the total number of gaseous species in the equilibrium pool. Condensed species are assigned zero moles. (See Subsection 1.4.1).

- (12) Sets IUSE(j) positive for condensed species listed on INSERT cards (see IUSE array described in Subsection 2.4.3).
- (13) Calls THERMP if TP, HP, or SP is true.

2.4.2 Subroutine REACT

The purpose of subroutine REACT is to read and process the data on the REACTANTS cards. The subroutine is called from the main program after a REACTANTS code card has been read. The data on these cards are described in Subsection 2.1.2 and Table II.

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

The FORTRAN symbols for the properties read from the REACTANTS cards and their associated properties discussed in INPUT CALCULATIONS are as follows:

Property	FORTRAN symbol
$a_{ij}^{(k)}$	ANUM(j,m) ^a
$W_j^{(k)}$	PECWT(j) (if no M in cc 53)
$N_j^{(k)}$	PECWT(j) (if M in cc 53)
$(H_T^O)_j^{(k)}$	ENTH(j) (if 00 not in cc 37 and 38)
$\rho_j^{(k)}$	DENS(j) ^b used for TWOSTG = TRUE problem only

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

^bFor two-stage combustor, it refers to the fraction of that j species added to the second stage.

If there are several oxidants, their properties are combined by Subroutine REACT into properties of a total oxidant using the relative proportion of each oxidant given on the REACTANTS cards. Similarly, if there are several fuels, their properties are combined into properties of a total fuel. The total oxidant and total fuel properties discussed in Subsection 2.1.2.1 and their associated FORTRAN symbols are as follows:

Property	FORTTRAN symbol	Equation
$b_i^{(k)}$	BØP(i, k)	(187)
$M_j^{(k)}$	RMW(j)	(190)
$\mathcal{H}(k)_T$	HPP(k) (If ØØ not in cc 37 and 38)	(192)
$\mathcal{H}(k)_T$	HPP(k) (If ØØ not in cc 37 and 38)	(194)
$M^{(k)}$	AM(k)	(196)
$V^+(k)$	VPLS(k)	(200)
$V^-(k)$	VMIN(k)	(201)
$W_j^{(k)} / \sum_{j=1}^{NREAC} W_j^{(k)}$	PECWT(j)	

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

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

A provision is made for eliminating a second file search when two consecutive sets of REACTANTS cards contain the same elements. This is done by saving the element symbols (LLMT(ℓ)) in LLMTS(ℓ), the kilogram-atoms per kilogram BØP(ℓ , k) in SBØP(ℓ , K), and the number of elements (NLM) in NLS. Note: for channel problems, only one set of REACTANTS cards are allowed.

Atomic weights M_i used in Eq. (190) are stored in ATOM(2, i). The corresponding chemical symbols are stored in ATOM(1, i). The oxidation states of the chemical elements V_i^+ or V_i^- used in Eqs. (200) and (201) are stored in ATOM(3, i). The ATOM array is stored by BLOCK DATA.

2.4.3 Subroutine SRCHCC

Subroutine SRCHCC reads the THERMO data from file on FORTRAN LOGICAL UNIT 7 and stores the appropriate data in the program.

A check is made in this routine to prevent THERMO data from exceeding their storage allotments. These variables are all in labeled common SPECE1 thru SPECE6 and are currently dimensioned for 300 species (Appendix B). However, this dimension may be reduced to save storage (see Subsection 2.5.1).

SRCHCC is called from the main program when the logical variable NEWR is true (see Figure 1). NEWR is set true in REACT to indicate a new chemical system. REACT also stores chemical element symbols for the current chemical system in LLMT array. SRCHCC stores THERMO data in the program for each species whose elements are included in the LLMT array (unless the species name was listed on an OMIT card).

The THERMO data are stored in common variables TLOW, TMID, THIGH, SUB, A, COEF, and TEMP. SRCHCC writes out the names and dates of species whose data are stored in the program.

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

The various condensed phases of a species are expected to be adjacent in the THERMO data as they are read from file unit 7. These phases must be either in increasing or decreasing order according to their temperature intervals.

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

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

- (1) They indicate which species are to be included in the current iteration ($IUSE(j) < 0$ for excluded species and $IUSE(j) \geq 0$ for included species).
- (2) They indicate multiple phases of the same species if absolute values of $IUSE(j)$ are equal.

The $IUSE(j)$ are initialized in Subroutine SRCHCC and the main program as follows:

- (1) $IUSE(j) = 0$ for all gaseous species.
- (2) $IUSE(j) = n$ for all condensed species whose names have been listed on INSERT cards. The number n indicates the species was the n^{th} condensed species whose THERMO data were read from file 7.
- (3) $IUSE(j) = -n$ for all condensed species not listed on INSERT cards where n is defined in (2).
- (4) $IUSE(j) = -n-1000$ for liquid species in solution and $IUSE(j) = -n-2000$ for the solid phases of the same species. n is defined as in (2).

These initial values of $IUSE(j)$ may be adjusted later in Subroutine EQLBRM. For condensed species (or liquid solution), the sign is adjusted as species (or liquid solution) are included or excluded in the current iteration. When a liquid freezes out of solution, $IUSE(j)$ is reset to $-n$, for both the liquid and solid phases.

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

2.4.4 Subroutine HCALC

The purpose of HCALC is to calculate thermodynamic properties for reactants under certain circumstances.

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

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

Property	FORTTRAN symbol	Equation	Conditions
$\mathcal{H}(k)T$	HPP(k)	(192)	HP, RKT problem if $\phi\phi$ in cc 37 and 38
h_o/R	HSUB ϕ	(193)	HP, RKT problem of $\phi\phi$ in cc 37 and 38

2.4.5 Subroutine SAVE

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

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

- (1) ISV positive. Transfer compositions for point just completed for use as initial estimates for next point (transfer EN (ISV,J) to EN(NPT,J)).
- (2) ISV negative. Save values of ENLN(J) for gases and EN(NPT,J) for condensed in SLN(J), ENN in ENSAVE, ENNL in ENLSAV, IQ1 in IQSAVE, JSOL in JSOLS, JLIQ in JLIQS, and NLM in LL1. (These values are saved because they are to be used as initial estimates for

some future point and they may be overwritten in the meantime.) Make ISV positive and transfer EN(ISV, J) to EN(NPT, J).

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

2.4.6 Subroutine NEWOF

This subroutine combines the properties of total oxidant and total fuel calculated in Subroutine REACT with an O/F value to give properties for the total reactant. NEWOF is called for each mixture assigned in the MIX array in INPT2 namelist. It is called from either THERMP or ROCKET. The calculated properties and corresponding FORTRAN symbols are as follows:

Property	FORTTRAN symbol	Equation
b_i^o	BØ(j)	(191)
h_o/R	HSUBØ	(193)
r	EQRAT	(204)

Subroutine HCALC is called by NEWOF to calculate the enthalpies for each reactant that has zeros keypunched in card columns 37 and 38 in its REACTANTS card (see Table II).

Values of HPP(2), HPP(1), HSUBØ, BØP(i, 2), BØP(i, 1) and BØ(i) are printed out.

2.4.7 Subroutine EQLBRM

Subroutine EQLBRM is the control routine for the equilibrium module which calculates equilibrium compositions and thermodynamic properties for a particular point. A brief overview of the tasks controlled by EQLBRM will be listed below. A more detailed explanation is shown in the flow diagram given in Figure 4.

General flow in EQLBRM is:

- (1) Initialize control variables.
- (2) If there is only one equilibrium species, skip to Task (11).
- (3) Initialize additional variables for iteration technique.
- (4) Call MATRIX and GAUSS to determine problem solution
- (5) If a singularity exists, skip to Task (14).
- (6) Obtain corrections to the estimates.
- (7) Remove solution and/or ions, if necessary.
- (8) Check on convergence requirements for AMBDA, SUM, AA (for condensed species), trace species, ions, and entropy for SP problems. If any test fails, reiterate by repeating Task (4). However, if the maximum number of iterations was exceeded, jump to Task (15). Otherwise, set CONVG = TRUE.
- (9) Is it necessary to consider condensed species in the model? Should a condensed species be added or its phase changed? Should the solution model be considered? If so, have any species been frozen out of solution? If any answer is yes, then reiterate by returning to Task (4).
- (10) Calculate equilibrium properties and return to the calling program (unless an unrealistic calculation dictates further iterations).
- (11) Initialize variables for special iteration method used for a one-variable equilibrium system.
- (12) Call CPHS to obtain thermodynamic data of all species, including nonequilibrium species.
- (13) Iterate until this system passes the convergence requirements, skip to Task (10), or exceeds the number of allowed iterations, skip to Task (15).
- (14) Print a message alerting one to a singularity. If it is a correctable singularity, remove an equation to be solved, and skip to Task (4). Otherwise, skip to Task (16).

- (15) Check on two special conditions involving condensed species and/or solution (assuming this was the cause of convergence failure). Thus, it is possible to set CONVG = TRUE and jump to Task (9), or reset an initial condition and jump to Task (3). However, the general flow will yield an appropriate convergence failure message as well as debug output (assuming IMPRNT is nonzero).
- (16) Set the calculated temperature (TT) to 0.0 and return to the calling routine. Zero temperature will force the program to stop executing, and output results through the previous point.

Several common variables must be set before EQLBRM is called. These variables and the modules setting them are summarized as follows:

Module	Variables
Input	ENN, ENNL, IQ1, IUSE(j), JSOL, } for first iteration, JLIQ, EN(NPT, j), ENLN(j), EMM } first point only COEF(k, i, j), TEMP(n, k), IONS, LLMT(l), RR, NS, NSK, NLM, NC, IDEBUG, TRACE, TMID, NSOL For TP, HP, and SP problems, TP, HP, SP, and SØ (if SP is true) are all set.
Application	TT, PP, NPT. In addition, if not previously set in Input: TP, HP, SP, and SØ (if SP is true).
Additional input processing	BØ, EQRAT, and HSUBØ

Common variables set by EQLBRM include TTT(NPT), PPP(NPT), SSUM(NPT), HSUM(NPT), CPR(NPT), GAMMAS(NPT), VLM(NPT), WM(NPT), DLVPT(NPT), DLVTP(NPT), TOTN(NPT), ENN, EN(NPT, j), ENLN(j), IUSE(j), JLIQ, JSOL, and ENNS. See Appendix B.

2.4.8 Subroutine CPHS

Subroutine CPHS calculates thermodynamic properties using Eqs. (90), (91), and (92) for species numbering from 1 to NSK for an assigned temperature TT. It uses either one of two sets of coefficients: COEF(2, i, j) for the temperature interval TLOW to TMID and COEF(1, i, j) for the interval TMID to THIGH. The index j is the jth species and the index i (i = 1 to 7) refers to the ith coefficient.

The properties calculated and their corresponding FORTRAN symbols are as follows:

Property	FORTTRAN symbol
$\left(\frac{S_T^0}{R}\right)_j$	S(j) j = JS1, . . . , NSK
$\left(\frac{H_T^0}{RT}\right)_j$	H(j) j = JS1, . . . , NSK
$\sum_{j=JS1}^{NSK} n_j \left(\frac{C_p^0}{R}\right)_j$	CPSUM (one of the terms in Eq. (59))
$n_j \left(\frac{C_p^0}{R}\right)_j$	CPSUM (when CPHS is called by HCALC)

The index JS1 is always set equal to 1 in all routines calling CPHS except HCALC. In the latter event, JS1 and NSK are both set equal to the index j of a particular species. Note, NSK is the total number of species in the system. NSK equals NS in the absence of rate controlled chemistry (for more details, see MHD subroutine described in Subsection 2.4.18).

2.4.9 Subroutine MATRIX

This subroutine sets up the matrices pertaining to the iteration equations. The assigned thermodynamic state being set up is specified by the following codes:

Assigned Thermodynamic State	Codes
TP	TP = .TRUE. CONVG = .FALSE.
HP	HP = .TRUE. CONVG = .FALSE.
SP	SP = .TRUE. CONVG = .FALSE.

After convergence of any of the previous 3 problems, setup of the derivative matrices is specified by the following codes:

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

2.4.10 Subroutine GAUSS

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

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

2.4.11 Subroutines OUT1, OUT2, and OUT3

These subroutines write statements common to all problems. OUT1 writes statements giving the data on REACTANTS and on O/F, percent fuel, equivalence ratio.

OUT2 writes the statements for printing values of pressure, temperature, density, enthalpy, entropy, molecular weight, $(\partial \ln V / \partial \ln P)_T$, $(\partial \ln V / \partial \ln T)_P$, heat capacity, γ_S , velocity, stagnation enthalpy, magnetic field, Hall parameter, sonic velocity, electron density, ionic density, conductivity, conductivity without ions, and electron collision frequency. These variables and corresponding labels are printed with a variable format described in BLOCK DATA.

OUT3 writes statements giving the mole fractions of equilibrium species, nonequilibrium species, solution species, and trace species.

2.4.12 Subroutine VARFMT

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

2.4.13 Subroutine EFMT

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

2.4.14 Subroutine THERMP

This subroutine is the application module for TP, HP, and SP problems. Common variables, which must be set according to the assigned thermodynamic states, are given as follows. For these problems, the variables TP, HP, SP, and $S\emptyset$ are set or read in the main program. HSUB $\emptyset$ is set either in NEWOF or HCALC. The general flow of the routine is given in Figure 3.

Indices run from 1 to NP ($NP \leq 26$) for assigned pressure P and from 1 to NT ($NT \leq 26$) for assigned temperature T . NP and NT are set in the main program.

2.4.15 Subroutine ROCKET

This subroutine is the control program for the CHANNEL problems. A flow diagram for this subroutine is given in Figure 5. Subroutine ROCKET obtains the required thermodynamic properties for equilibrium performance by calling Subroutine EQLBRM. Rocket performance parameters are then obtained by calling Subroutine RKTOUT. In addition to calling RKTOUT, and in addition to using controls common to all problems (discussed in Subsection 2.3), Subroutine ROCKET also does the following:

- (1) It reads and processes the input data in RKTINP namelist.
- (2) It calculates estimates for throat pressure ratios.
- (3) It calculates estimates for pressure ratios corresponding to assigned area ratios (if any).
- (4) Since models describing the flow in the upstream region of an MHD channel are identical to that of a rocket with converging - diverging nozzle, ROCKET can also be used to evaluate the combustion product properties of the MHD combustor and the channel entrance under both subsonic and supersonic conditions.
- (5) It controls the flow and initialization for fully nonequilibrium chemistry problem in a one-dimensional flow channel for a multi-phase mixture. This includes reading SPEC and SPEC DATA cards.
- (6) Inputs the necessary variable to allow for a simple heat loss from the combustor.
- (7) Controls and outputs calculations pertaining to a two-stage combustor.
- (8) Contains the normal termination message and stop condition (STOP 5).

2.4.16 Subroutine RKTOUT

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

It is also the control program for writing channel performance output. It contains the write statements that apply specifically to channel parameters and it calls Subroutines OUT1, OUT2, and OUT3 for the write statements common to all problems. The channel parameters are printed with the variable format, FMT, described in BLOCK DATA.

Subroutine RKTOUT is called from Subroutines ROCKET, MHD, and DIFFUN.

2.4.17 BLOCK DATA

BLOCK DATA contains atomic data stored in ATOM(i, j) and many of the variables used with the variable format, FMT. The ATOM variables are defined in Appendix B. The format variables are stored in the common labeled OUPT and are described here.

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

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

where the spaces are stored as blanks.

Some variables set in BLOCK DATA to modify FMT are as follows:

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

For example, setting FMT(5) equal to F3, would result in a format statement appearing as (, 3A4, A2, F9.3, etc.)

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

Variable	Stored Label
FP	P, ATM
FT	T, DEG K
FH	H, CAL G
FS	S, CAL (G)(K)
FM	M, MOL WT
FV	(DLV DLP)T
FD	(DLV DLT)P
FC	CP, CAL (G)(K)
FG	GAMMA (S)
FL	SON VEL, M SEC
FR1	PC P
FC1	CF
FN	MACH NUMBER
FR	CSTAR, FT/SEC
FI	ISP, LB-SEC LB
FA	IVAC, LB-SEC LB
FA1, FA2	AE/AT

2.4.18 Subroutine MHD

MHD has four basic functions. These include reading channel input data from FORTRAN LOGICAL UNIT 11, reading reaction rate cards from FORTRAN LOGICAL UNIT 5, isolating nonequilibrium from equilibrium species, and controlling the solution of the channel differential equations. A flow diagram for this subroutine is given in Figure 6.

The channel inputs were discussed in detail in program input Subsection 2.1. One function of this subroutine is to choose which flow parameter is specified along the channel and, therefore, which equations should be solved.

The reaction rate cards were also discussed in the program input section. When IPP = NEQPT, this subroutine does the following (see discussion of NEQPT in Subsection 2.1.4.2):

- (1) Defines NOMIT as the total number of species in the nonequilibrium pool (i. e. , counts the number of species on the DLIT cards).
- (2) Sets NS = NSK - NOMIT where NSK is the total number of species in the mixture (defined in MAIN).
- (3) Isolates the nonequilibrium species from the equilibrium species. Locates the equilibrium species in the first NS positions and the nonequilibrium species in the (NS + 1) through NSK positions. It also reorders all parameters (such as SUB, IUSE, EN, ENLN, COEF, A, etc.) associated with each species.
- (4) Reduces the number of equations (IQ1) solved by MATRIX, whenever a condensed species, with IUSE(j) greater than zero, appears on the DLIT card.
- (5) Outputs the chemical reactions

Subroutine MHD sets the number of differential equations to be solved. This becomes NOMIT + 2, when velocity or pressure is assigned, and NOMIT + 3, when area is assigned. It also sets all initial values necessary for channel calculations.

The solution of the differential equations, which is the last function of MHD, is performed by repetitive calls to Subroutine DIFSUB. DIFSUB is called until the independent variable (distance) is beyond the report interval as defined by DXI of namelist INPT2. MHD then recalculates the conditions and compositions at the report stations. This is performed by additional calls to INTERP, EQLBRM, and CONDOC. Note, intermediate conditions and compositions are calculated from DIFSUB by calls to DIFFUN (see Subsection 2.4.20). Control is then returned to ROCKET, where these values are stored for output by RKTOUT.

MHD also contains a mechanism for controlling the integration steps, which maximizes the efficiency of the integration technique. When the axial position in the channel exceeds the stop position XXSTOP, read from CHANNEL inputs, control immediately returns to ROCKET, where RKTOUT is called to output all results prior to this point. The program will then terminate with a STOP 5 message.

If the calculated temperature falls below a minimum value TMPSTP (set by TCHFNL of RKTNP), control immediately returns to ROCKET where RKTOUT is called to output all results prior to this point. Execution is terminated by a STOP 5.

2.4.19 Subroutine DIFSUB

DIFSUB is a routine that solves a system of ordinary differential equations. This multistep, multiorder technique was written by Gear.⁽⁵⁾ DIFSUB has one major advantage over other numerical methods, which solve initial value - ordinary differential equations. It can handle a set of "stiff" differential equations, which are typical of most chemically reacting systems.

DIFSUB has been modified from Gear's original code by the addition of a Gaussian elimination section, instead of a strict matrix inversion. This speeds up execution of larger systems.

DIFSUB calls the subroutine DIFFUN which evaluates the derivatives of the equations. DIFSUB uses two INPT2 namelist variables, ACCURC and HMIN. If for a given step, the truncation error for each equation is greater than ACCURC, then the integration step size is reduced. If the truncation error is much less, then the step size is increased. HMIN is the minimum step size allowed by the integration technique before the method aborts.

2.4.20 Subroutine DIFFUN

DIFFUN (flow diagram shown in Figure 7) is called from Subroutine DIFSUB. It does the following tasks:

- (1) Retrieves previous differential equation solutions.
- (2) Generates new set of $B\phi N(I)$, where $B\phi N(I)$ is number of moles of I^{th} chemical element per kilogram of mixture in the nonequilibrium pool.

- (3) Determines remaining flow variables (e.g. temperature, and the concentration of species of the equilibrium pool) by calling Subroutine EQLBRM.
- (4) Determines fluid conductivity, when required, by calling Subroutine CONDUCT.
- (5) For each rate equation, it calculates the backward chemical rates using the thermodynamic data. It also calculates the net production rate of species in the nonequilibrium pool (i.e. sets up the NOMIT differential equations).
- (6) Determines the force term (FFF) and heat term (QQQ) by calling Subroutine SETEQU.
- (7) Sets up channel differential equations which describe the conservation equations of mass, rate controlled species, momentum, and enthalpy. Depending on which assigned profile is being used (see Table VII), real function INTERP is called to interpolate one of the following assigned channel inputs:
 - (i) velocity and its derivative
 - (ii) pressure and its derivative
 - (iii) area ratio and its derivative
- (8) If the returned temperature from EQLBRM is set to 0.0 or falls below a minimum value TDIFUN (set by TCHFNL of RKTINP), DIFFUN will call RKTOUT to output all results prior to this point. Execution is terminated by a STOP 20. Additionally, much of the debug output requested by channel input (IMPRNT) and RKTINP input (IPRRKT) is printed from this subroutine.

2.4.21 Subroutine SETEQU

This subroutine is called from DIFFUN. Its function is to calculate the force term (FFF) and the energy term (QQQ) which are used in the conservation equations. The user can specify the functional form of FFF and QQQ. The current code contains the models described in Subsection 1.6. Other models can be added to this subroutine and controlled by the ITYPE variable described in namelist CHNLIN.

2. 4. 22 Subroutine CONDUCT

CONDUCT was written by Dr. Howard Cohen of the M. I. T. Energy Laboratory. It calculates the conductivity of open cycle MHD generators without slag, using the Demetriades and Argyropoulos algorithm.⁽⁶⁾ It also calculates the electron collision frequency. Cross sections, based on the compilations of Spencer,^(7, 8) are tabulated for temperatures from 1700 to 3000°K; outside this range, an extrapolation is used. Ion number density and conductivity are output from this subroutine.

2. 4. 23 Subroutine DBGOUT

DBGOUT will output a vector for debug purposes. This routine is called from subroutines EQLBRM, GAUSS, ROCKET, MHD, SETEQU, and DIFFUN. The call statement will contain five variables NUMOUT, HP, SP, DXOUTP, NUMDBG where: NUMOUT is the number of outputs to print; HP and SP symbolize any two logical variable passed in the call statement, DXOUTP is the output vector, and NUMDBG is the debug output reference number. The output format will read HP = 1 or 0 and SP = 0 or 1, where 1 implies true and 0 implies false. The use of calls to this routine is controlled by the CHNLIN input IMPRNT as well as RKTINP input IPRRKT. To understand these outputs, consult Tables V and VIII and Subsections 2.1.7.1 and 2.1.4.2.

2. 4. 24 Real Function INTERP

This function will perform up to a tenth order interpolation on a vector as well as return its first derivative. It is used in connection with channel inputs in Subroutines MHD and DIFFUN.

2.5 Modification of the Program

2.5.1 Modification of the Required Storage

The storage requirements can be changed by changing the dimensions of the total number of species, condensed species, chemical elements, and channel input profile. The current configuration consists of 300 total species (of which 175 can be condensed species), 30 chemical elements, and 90 channel inputs. It is a simple matter to change the dimension of the total species and channel inputs by making one set of changes in the MAIN program. However, changes in the dimension of chemical elements and condensed species, require additional changes in most of the remaining subroutines.

The dimension of the total species can be increased or decreased by changing the value of NSPCMX (line number 122 in MAIN), as well as the dimension of the variables S, ENLN, H₀, DELN, IUSE, SLN, SCONMX, OMIT, DATE, EN, COEF, A, and XMWC residing in commons SPECE1, SPECE2, SPECE3, SPECE4, SPECE5, SPECE6, SPECE7, SPECE8, SPECE9, KGM, THMF, STOIC, and TSTG. These changes are required only in the MAIN program. A maximum of 600 species are allowed by the above changes. To increase the size beyond this number, requires increasing the size of the SUB array residing in common SPECE1. Unfortunately, this change must occur in all subroutines where common SPECE1 resides.

The dimension of condensed species can be increased or decreased by changing the value of NCMAX (line number 123) in the MAIN program. In addition, one must also change the dimension of the TEMP array in all subroutines containing common SPECE1.

The most cumbersome change occurs in changing the dimension of chemical elements. This requires changing the value of NELMX (line number 124 in MAIN) which indicates how many elements are allowed. In addition, one must change the dimension of variables LLMT, B₀, B₀N, A, and XELMC residing in commons MISC, NEQ, STOIC, and TSTG in all subroutines.

The dimension of channel input profile vectors can be increased or decreased by changing the value of NUMV (line number 125 in MAIN), as well as the dimension

of the variables XINDP, DUMMIN, VELIN, PRESIN, and AREAIN residing in commons MIKE0, MIKE5, MIKE1, MIKE2, and MIKE3. These changes are required only in the MAIN program.

The amount of storage required per variable and the current storage requirement, is listed in Table XI. The equations used to determine the storage, also appear in this table.

2.5.2 Eliminating an Application

Any application module may be removed simply by removing the statement calling the controlled subroutine (THERMP, ROCKET, and/or MHD) and removing the subroutines in the application module (see Figure 2). The calling statements to THERMP and ROCKET are near the end of the main program. Subroutine ROCKET calls subroutine MHD at lines 288 and 860.

2.5.3 Adding an Application

An application may be added by doing the following:

- (1) Giving the type of problem a name and including the name in the main program in the following places:
 - (a) Namelist INPT2,
 - (b) Logical statement, and
 - (c) Statement setting it to false before the INPT2 read;
- (2) Programming an application module is described in Subsection 2.3.2.
- (3) Calling the module when the name variable is true after the INPT2 namelist data have been processed in the main program.

2.5.4 Modifying Input and Output Modules

The input modules may be modified as long as the common variables used by EQLBRM are properly set. These variables are indicated in the description of the modules.

The listed output may be modified. Labeled common variables which are calculated by the equilibrium module and which are used on subroutine OUT2 and OUT3 include HSUM, SSUM, CPR, DLVTP, DLVPT, GAMMAS, PPP, TTT, VLM, TOTN, and EN. (Variables are defined in Appendix B.)

The units in the output may be changed in OUT2 and RKTOUT. Either a variable format (FMT) or a special E-format (subroutine EFMT) is used for all output. The variable format (FMT) is described in the section "BLOCK DATA" and the adjustments in number of decimal places may be reset in the output routines. The parameter labels may be adjusted in the DATA statements in BLOCK DATA, the output routines, or in the application module itself.

2.5.5 Changing Temperature Dependences in Subroutine EQLBRM

As the temperature varies, the phase of condensed species may change or freeze out of the liquid solution in the equilibrium composition. These conditions occur in Subroutine EQLBRM and are controlled by the following temperature variables (appearing in Data statements).

<u>Variable</u>	<u>Value</u>	<u>Comment</u>
TTCRIT	150.0	A condensed species is flagged for possible phase change whenever the current temperature is within TTCRIT of its melting temperature
TMELTM	150.0	Phase change if current temperature within (melting temperature - TMELTM)
TMELTP	150.0	Phase change if current temperature within (melting temperature + TMELTP)
TMELTS	150.0	Species frozen out of solution whenever the current temperature is lower than is (melting temperature - TMELTS)
TPMLTS	50.0	TMELTS is set to TPMLTS for TP Prob.

3. SAMPLE PROBLEMS

This section contains sample problems which are intended to show the basic input/output formats for different types of problems. This is done in four subsections. The simplest problems are considered in the first subsection (3.1). These are TP (temperature and pressure assigned), HP (enthalpy and pressure assigned), and SP (entropy and pressure assigned) problems. Channel problems, without rate controlled chemistry and with/without the two stage combustor option, are considered in the second Subsection (3.2). The third Subsection (3.3) contains partial equilibrium/partial rate controlled channel problems with different input options, such as, velocity, area, or pressure assigned along the channel. Fully chemical rate controlled channel flow is considered in the last subsection.

In all the following sample problems, thermodynamic data is read from file unit 7. Therefore, no THERMO DATA cards are used.

Tables XII and XIII list section cross references of descriptions and examples of input types and problem types, respectively.

3.1 TP, HP, and SP Problems

This problem set will demonstrate how to execute a TP, HP, and SP problem.

3.1.1 Input Data

The same program input file, with slight modifications, is used for all three problems. The first 17 input lines, common to these problems, are the following:

```

REACTANTS      XXXSTG
C 5.46166H 4.56349N 0.07139S 0.03431O 0.900000 0.74800 -21782.0S 298.00F 0.0
SI0.80718FE0.09769AL0.43349MG0.11413O 2.525260.09524 -288546.4S 298.00F 0.0
P 2.020000 5.00000 0.00046 -351350.0S 298.00F 0.0
CA0.26213NA0.01290K 0.01496TI0.010010 0.296040.01905 -48221.1S 298.00F 0.0
K 2.000000C 1.000000 3.00000 0.09185 -274900.0S 298.00F 0.0
H 2.000000 1.00000 0.04540 -68288.0L 298.00F 0.0
N 2.00000 00 0.75426 4100.6G 166.000 0.0
O 2.00000 00 0.23195 4326.2G 166.000 0.0
AR1.00000 00 0.01379 2823.4G 166.000 0.0

SOLUTION      AL2O3(L)      SIO2(L)      TI2O3(L)      KALO2(L)
SOLUTION      KALSI2O6(L)    KALSI3O8(L)  FE3O4(L)      KALSI04(L)
SOLUTION      K2SI2O5(L)    K2CO3(L)     K2SO4(L)
OMIT          MGSIO3(S)     MGSIO3(L)
INSERT        FEO(L)        CAO(S)
NAMELISTS

```


A description of these lines is given below.

DATA CARD 1 - This is the REACTANTS code card containing the letters REACTANTS in columns 1 - 9 and the letters XXXSTG in columns 16 - 21 indicating this is not a two stage combustor problem.

DATA CARDS 2 through 10 - This is the set of REACTANTS data described in Table II. Note, the $\beta\beta$ in columns 37 and 38 of oxidizing species N_2 , O_2 , and Ar tells the program to calculate the enthalpy of these species at the input temperature, which is 1660 K in this case. When this happens the input enthalpies given in columns 54 - 62 are overridden for these species.

DATA CARD 11 - A blank card to terminate the REACTANTS data input

DATA CARDS 12 through 16 - These contain the list of species to be either placed in the liquid solution, omitted from calculation, or inserted in the calculation (see Subsection 2.1.3 for more detail).

These cards can appear in mixed random order.

DATA CARD 17 - This is the NAMELISTS code card, columns 1 - 9.

For TP, HP, and SP problems, this flags additional input data that is contained in INPT2.

INPT2 DATA CARDS

These cards contain input information peculiar to each problem. For a description of the contents of these cards, see Table III.

3.1.1.1 TP problem

DATA CARD (18)	\$/ INPT2	KASE = 101, P(1) = 4.5, ERATIO = T, MIX = 1.087 TP = T, TRACE = 1.0E - 7, IONS = T, T = 1600., 2000., 1800., 2400., 2800. \$/ END
----------------	----------------------	---

CARD (19)	BLANK	CARD
-----------	-------	------

CARD	STOP	CARD
------	------	------

INPT2 DATA CARD - The variables contained in this namelist are described in Table III. For this problem TP = TRUE indicating temperature T, and pressure P, are assigned. If solution is used, only one pressure value is permitted. Notice, the assigned temperatures are listed in an arbitrary order. These are sorted by the program in descending order so that the solution model will be used properly. Note also, that for TP problems the reactant enthalpies and temperatures listed on the data cards 2-9 are overridden.

3.1.1.2 HP problem

DATA CARD (18)	\$/ INPT2	KASE = 102, P(1) = 4.5, ERATIO = T, MIX = 1.087, HP = T, TRACE = 1.0E - 7, IONS = T \$/ END
----------------	----------------------	--

CARD (19)	BLANK	CARD
-----------	-------	------

CARD (20)	STOP	CARD
-----------	------	------

INPT2 DATA CARD - The variables contained in this namelist are described in Table III. For this problem HP = TRUE, indicating enthalpy, H, and pressure, P, are assigned. If solution option is used only one pressure value is permitted. For this problem, enthalpy is evaluated internally by the code using the data supplied on Cards 2-9. Therefore, no enthalpy value is given in INPT2.

3.1.1.3 SP problem

DATA CARD (18)	%INPT2	KASE = 103, P(1) = 4.5, ERATIO = T, MX = 1.087
		SP = T, TRACE = 1.0E-7, IONS = T, S0 = 2.0374
		%END
CARD (19)	BLANK	CARD
CARD (20)	STOP	CARD

INPT2 DATA CARD - The variables contained in this namelist are described in Table III. For this problem, SP = TRUE indicating pressure, P, and entropy, S (denoted by S0 in the input data) are assigned. If solution option is used, only one pressure value is permitted. Only one value of entropy can be assigned. The units of entropy used are (cal/gm - K).

3.1.2 Output Data

As in the case of input data, sections of the output data are common to all problems. The code first outputs part of the input data exactly as they appear on the input data cards. For the problems being considered, this is information contained on Cards 1 through 17. Following this output is a list of all possible variables, some with multiple values, that are contained in the INPT2 namelist. For a given problem, however, only a fraction of these variables are generally specified in the INPT2 Data cards (Data card (18) in this problem set). Since a total of 26 assigned temperatures

are permitted by the program, then 26 values of temperature, T, will be printed in the output. The nonzero values correspond to those which are assigned by the user in the INPT2 Data cards. The same discussion applies to variables P (pressure) and MIX (either O/F ratio or equivalence ratio). Note that, variable V is not used in this code so it should be ignored. The variable RHO contains the same values as the variable P. Most of the remaining variables appearing in the INPT2 output data are logical with a default value of false. Those which have been used in this program are: ERATIO, TP, HP, SP, RKT, IONS, and TWOSTG. The nonlogical variables appearing in the INPT2 output, but not listed in the INPT2 input data, have their default values printed in the output. Following INPT2 output is a list of chemical elements which are contained in the chemical species listed on the reactant cards (Cards 2-9 for this case). For TP problems this list is also repeated for each value of assigned INPT2 temperature. A table of all chemical species which are listed in file unit 7 and are composed of any combination of chemical elements within the system is printed out next. A second list of chemical elements follows. For IONS = T problems this list also includes the electron as one of the chemical elements. Species in the liquid solution, the oxygen to fuel ratio, enthalpy and number of moles of chemical elements per kilogram of fuel, per kilogram of oxidizer and per kilogram of total mixture appear next.

Information concerning the iteration procedure (i. e., solution of Eqs. (34) - (39) of Section 1) are given next. For each calculation point this contains a list of chemical elements, the point number, the calculated values of $\pi_i = -\lambda_i/RT$, where λ_i is the i^{th} Lagrange multiplier (see Eq. (12) of Section 1), and the number of iteration needed for convergence. The number of π_i is equal to the number of chemical elements. For each point, the iteration is continued until the lowest Gibbs free energy is achieved. This may require addition or removal of condensed species from the mixture. Each time a condensed species is added or removed from the mixture it is indicated in the output and the calculated value of π_i are listed for the new mixture. If IONS = T, the program prints out number density of all the ions in the system together with the mixture conductivity. This output procedure is repeated for all points.

If the current temperature is much less than the freezing point of one or more condensed species in the liquid solution, these species are removed from the solution and a new equilibrium composition is obtained. For TP problems, species are removed from the liquid solution when the mixture temperature is 50 K below the freezing temperature of each species. For other problems, this temperature difference is set at 150 K. These values can be changed by the user (see Subsection 2.5.5). Following this output is the list of reactants and their properties as they appear in the reactant input cards. However, for species on reactant cards which contained $\emptyset\emptyset$ on columns 37 and 38, the output enthalpy may differ from their corresponding values appearing on the reactant input cards. This is because, for these species, the enthalpy is evaluated by the code using the temperature that is on the reactant input cards. This value of enthalpy overrides the value listed on the reactant cards. The last group of output data corresponds to the thermodynamic and other properties of the mixture and is self-explanatory.

While major parts of the output data are the same for all types of problems, there are certain output data which are peculiar to each problem type. For the three cases considered in this subsection, these peculiarities are given below.

3.1.2.1 Output data for TP problems

The output for this problem is given in Sample Output 1. All of this output is described in Subsection 3.1.2. Note, that the five values of temperature, the values of pressure, mix, and trace, which are specified in the INPT2 namelist (see Subsection 3.1.1.1) are printed out. The logical variables ERATIO, TP, and IONS, which are set equal to true in the INPT2 namelist, are also listed as true in the output. For TP problems, the temperatures can be listed randomly in the INPT2 namelist. The program, however, sorts them in the descending order. Hence, the maximum temperature corresponds to point one of the output data. Also, after the thermodynamic properties of each point are calculated, the solution is removed from the mixture and reconsidered at the next point. Referring to Sample Output 1, pages 6-8, note that at all points, the solution is added to the mixture. However, as the temperature gets lower, certain species are removed from the solution. This is done at points 3 and 4 where $\text{Al}_2\text{O}_3(l)$, $\text{Ti}_2\text{O}_3(l)$, etc., are removed. A species that is removed from the solution will not be considered part of the solution unless the problem is restarted. The number of species in liquid solution at the last calculation point are printed out below the species mole fraction output.

Sample Output 1, TP Problem
(12 Output Pages)

```

1
REACTANTS      XXXSTG
C 5.4617 H 4.5635 N 8.8714 S 8.8343 O 8.9888 8.74888 -21782.88 S 298.888 8 F 8.88888
SI 8.8872 FE 8.8977 AL 8.4335 MG 8.1141 O 2.5253 8.95248E-81 -288546.44 S 298.888 8 F 8.88888
P 2.8888 O 5.8388 8.8888 8.8888 8.8888 8.46888E-83 -351358.88 S 298.888 8 F 8.88888
CA 8.2621 NA 8.8129 K 8.8149 TI 8.8188 O 8.2968 8.19858E-81 -48221.18 S 298.888 8 F 8.88888
K 2.8888 C 1.8188 O 3.8888 8.8888 8.8888 8.91858E-81 -274988.88 S 298.888 8 F 8.88888
H 2.8888 O 1.8388 8.8888 8.8888 8.8888 8.45488E-81 -58288.88 L 298.888 8 F 8.88888
N 2.8888 8.8888 8.8888 8.8888 8.8888 8.75426 4188.68 G 1668.888 8 O 8.88888
O 2.8888 8.8888 8.8888 8.8888 8.8888 8.23195 4326.28 G 1668.888 8 O 8.88888
AR 1.8888 8.8888 8.8888 8.8888 8.8888 8.13798E-81 2823.48 G 1668.888 8 O 8.88888
SOLUTION      AL2O3(L)      SiO2(L)      Ti2O3(L)      KAlO2(L)
SOLUTION      KAlSi2O6(L)      KAlSi3O8(L)      Fe3O4(L)      KAlSiO4(L)
SOLUTION      K2Si2O5(L)      K2CO3(L)      K2SO4(L)
OMIT          MgSiO3(S)      MgSiO3(L)
INSERT        FeO(L)      CaO(S)
NAME LIST8
1
@INPT2
KASE = 181,
T = 1688.88 , 2288.88 , 1838.88 , 2488.88 ,
2888.88 , 8.88888 , 8.88888 , 8.88888 , 8.88888 , 8.88888 ,
8.88888 , 8.88888 , 8.88888 , 8.88888 , 8.88888 ,
8.88888 , 8.88888 , 8.88888 , 8.88888 , 8.88888 ,
8.88888 , 8.88888 ,
P = 4.58888 , 8.88888 , 8.88888 , 8.88888 ,
8.88888 , 8.88888 , 8.88888 , 8.88888 , 8.88888 ,
8.88888 , 8.88888 , 8.88888 , 8.88888 , 8.88888 ,
8.88888 , 8.88888 , 8.88888 , 8.88888 , 8.88888 ,
8.88888 , 8.88888 ,
PSIA = F,
MATHG = F,
NSOM = F,
V = 8.88888 , 8.88888 , 8.88888 , 8.88888 ,
8.88888 , 8.88888 , 8.88888 , 8.88888 , 8.88888 ,
8.88888 , 8.88888 , 8.88888 , 8.88888 ,
RHO = 4.58888 , 8.88888 , 8.88888 , 8.88888 ,
8.88888 , 8.88888 , 8.88888 , 8.88888 , 8.88888 ,
8.88888 , 8.88888 , 8.88888 , 8.88888 , 8.88888 ,
8.88888 , 8.88888 , 8.88888 , 8.88888 , 8.88888 ,
8.88888 , 8.88888 ,
ERAT-O= T,
OXFL = F,
FPCT = F,
FA = F,
MIX = 1.88788 , 8.88888 , 8.88888 , 8.88888 ,
8.88888 , 8.88888 , 8.88888 , 8.88888 , 8.88888 ,
8.88888 , 8.88888 , 8.88888 , 8.88888 , 8.88888 ,
8.88888 ,
TP = T,
HP = F,
SP = F,
IV = F,

```

UV = F,
 SV = F,
 RKT = F,
 SHOCK = F,
 DECN = F,
 OTTO = F,
 CR = 0.000000,
 SS = 0.000000/000000,
 IONS = T,
 IDEBUG = 0,
 TRACE = 0.100000E-06,
 SIUNIT = F,
 DXI = 0.000000,
 NITER = 0,
 NSTOP = 0,
 NFOL = F,
 BZ = 0.000000,
 XK = 0.000000,
 ACCURC = 0.100000E-02,
 HMIN = 0.100000E-14,
 ALPH = 0.000000,
 EXIN = 2400.00,
 TWOSTG = F,
 *END
 LLMT =

S-10

C
 H
 N
 S
 O
 SI
 FE
 AL
 MG
 P
 CA
 NA
 K
 TI
 AR

LLMT =

C
 H
 N
 S
 O
 SI
 FE
 AL
 MG
 P
 CA
 NA
 K
 TI
 AR

LLMT -

C H N S O S I F E A L M G P C A N A K T I A R

LLMT -

C H N S O S I F E A L M G P C A N A K T I A R

2
11

LLMT -

C H N S O S I F E A L M G P C A N A K T I A R

LLMT -

C H N S O S I F E

AL
MG
P
CA
NA
K
LI
AR

SSPECIES BEING CONSIDERED IN THIS SYSTEM

S-16

J12/65 AL(S)
J12/62 ALN(S)
J12/67 ALOH
J12/68 ALJ2H
J 6/68 AL2O2+
L 5/66 AR
J 9/65 C-
J12/71 CH+
J 6/63 CN
J 9/65 CO
3/3/7 CO3-
J 6/61 CS2
J 9/65 C2H4
J12/69 C3
J12/68 CA(S)
BAR 73 CACO3(S)
J 6/78 CAOH+
102/67 E
J 3/65 FE
4/13/7 FEO-
10/78 FEO2H2
J 6/66 FES04(S)
10/78 FES04(L)
J 3/64 FALO
J12/69 HCP
J 6/63 HNO3
11/65 H2O(L)
J12/65 H2SO4(L)
3/3/7 HSI-
3/3/7 K-
534/76 KALSI308(S)
J12/61 KO
J12/70 KOH(L)
10/78 K2O(L)
12/79 K2SIO3(L)
J12/70 MG+
10/78 MGJ(L)
J12/71 MG(S)
J12/67 MG2SIO4(L)
J 9/65 NH3
J 6/72 NO2-
J12/64 N2O
J 6/62 NA(S)
3/3/7 NA-
J12/70 NAH(L)
J 3/66 NA2CO3(S)
12/70 NA2O2H2

J12/65 AL(L)
J 3/67 ALN
J12/67 ALOH+
10/78 ALO2H2
J 6/72 AL2O3(S)
L12/66 AR+
3/3/7 CAL
J12/72 CH2
J12/70 CN+
J 3/61 COS
3/7/7 CO3-
J12/69 C2
L 5/72 C2H6
J 6/68 C3O2
J12/68 CA(L)
J 6/71 CAO(S)
J12/71 CAO2H2(S)
J 3/65 FE(S)
3/1/78 FE+
10/78 FEOH
J 6/66 FE2H3(S)
BAR 73 FE32(S)
J 6/66 FE2S3O12(S)
L12/69 HCN
3/8/7 HK
J 3/64 HO2
J 3/61 H2O
J12/66 H2SO4
J12/61 K(S)
10/78 KALO2(S)
H10/77 KALSI308(L)
7/29/8 KO+
J12/70 KOH
J12/70 K2O2H2
PB1/77 K2SIO5(L)
J12/66 MGO3(S)
10/78 MGO
J 6/71 MGS
J 3/61 N
J 6/63 NO
J12/64 NO3
J12/70 N2O+
J 6/62 NA(L)
J 3/63 NAH
J12/70 NAOH
J 3/66 NA2CO3(L)
J12/66 NA2SO4(S)

J12/65 AL
J 6/70 ALO
J12/67 ALOH-
J 6/72 AL2O
J 6/75 AL2O3(L)
J 3/61 C(S)
3/3/7 C3-
J 3/61 CH2O
J12/70 CN-
3/3/7 COS-
J 6/62 CP
J12/69 C2-
J 3/67 C2N
J12/69 C4
J12/68 CA
J 6/71 CAO(L)
J 12/7 CAO2H2
J 3/65 FE(S)
J 6/65 FEO(S)
4/20/7 FEO2
BAR 73 FES(S)
J 6/65 FE2O3(S)
J 9/65 H
J12/70 HCO
J12/70 HNCO
12/21/ HPO2
L 2/69 H2O2
3/25/7 H3O+
J12/61 K(L)
H10/77 KALO2(L)
3/8/7 KCN
J12/67 KO-
J12/71 KOH+
J12/71 K2SO4(S)
J 9/62 MG(S)
J12/66 MGH
10/78 MGOH
L 7/76 MGS04(S)
J12/70 NCO
3/3/7 NO-
3/3/7 NO3-
J 9/64 N2O4
J 6/62 NA
J12/67 NAO
J12/71 NAOH+
J 6/68 NA2O(S)
J12/66 NA2SO4(S)

J 6/65 AL+
J 6/70 ALO+
J12/68 ALO2
J 6/72 AL2O+
10/78 AL6O13SI2(S)
J 3/61 C
3/3/7 C2H-
J 6/69 CH3
J 6/66 CNN
J 9/65 CO2
J12/62 CS
J 3/67 C2H
J 3/61 C2N2
J12/69 C5
J12/70 CA+
J12/74 CAO
J12/71 CAS(S)
J 3/65 FE(S)
J 6/65 FEO(L)
4/13/7 FEO2-
BAR 73 FES(S)
10/78 FE2O3(L)
J 6/66 H+
J12/70 HCO+
J 3/63 HNO
J 3/61 H2
3/8/7 H2P
3/3/7 HP-
J 6/62 K
H10/77 KALSIO4(L)
J 3/66 K2CO3(S)
J12/70 KOH(S)
J12/61 K2
J12/71 K2SO4(S)
J 9/62 MG(L)
J 3/64 MGN
J 6/68 MGOH+
L 7/76 MGS04(L)
J12/71 NH
J 6/66 NO+
J 9/65 N2
J12/64 N2O5
J 3/65 NA+
J12/67 NAO-
J 6/62 NA2
J 6/68 NA2O(S)
J12/66 NA2SO4(S)

J 6/63 ALH
J 12/7 ALO-
3/8/7 ALO2-
J 9/65 AL2O2
3/8/7 ALS
L12/66 C+
J12/67 CH
J 3/61 CH4
J12/70 CN2
4/12/7 CO2-
3/3/7 CS-
J 3/61 C2H2
J 9/66 C2O
J12/68 CA(S)
BAR 73 CACO3(S)
J 6/70 CAOH
BAR 73 CASO4(S)
J 3/65 FE(L)
J 9/66 FEO
J 6/66 FEO2H2(S)
BAR 73 FES(S)
J 6/65 FE3O4(S)
J 9/65 H-
3/8/7 HCO3-
J 6/63 HNO2
L11/65 H2O(S)
J12/65 H2S
3/3/7 HS-
J 3/65 K+
H10/77 KALSI2O6(L)
J 3/66 K2CO3(L)
J12/70 KOH(S)
J 6/63 K2O(S)
J12/71 K2SO4(L)
J 9/62 MG
J12/65 MGO(S)
10/78 MGO2H2
10/78 MG2SIO4(S)
J12/65 NH2
J 9/64 NO2
J12/65 N2H4
J12/70 N3
534/76 NAALSI308(S)
J12/70 NAOH(S)
J 3/66 NA2CO3(S)
J 6/68 NA2O(L)
J12/66 NA2SO4(L)

K11/74	NA2SO4	C 4/76	NA2SIO3(S)	J 4/76	NA2SIO3(L)	J 4/76	NA2SIO5(S)	J 4/76	NA2SIO5(L)
J 6/62	O	J 12/66	O+	J 6/65	O-	J 12/70	OH	J 12/70	OH+
J 12/70	OH-	J 9/65	O2	J 12/66	O2-	J 6/61	O3	J 6/62	P
J 6/61	P(S)	J 12/66	P+	3/3/7	P-	J 6/67	PH	J 6/62	PH3
J 9/62	PN	J 6/71	PO	3/3/7	PO-	1/1/0	PO2	7/11/7	PO2-
10/5/7	PO3	2/14/9	PO3-	J 6/67	PS	J 6/61	P2	J 6/61	P4
J 12/65	S(S)	J 12/65	S(L)	J 6/71	S	J 12/66	S+	3/3/7	S-
J 6/67	SH	J 6/61	SN	J 6/71	SO	3/3/7	SO-	J 6/61	SO2
3/3/7	SO2-	J 9/65	SO3	3/3/7	SO3-	J 12/65	S2	3/3/7	S2-
J 6/64	S8	J 3/67	SI(S)	J 3/67	SI(L)	J 3/67	SI	J 12/71	SI+
3/3/7	SI-	10/78	SIC(S)	J 3/67	SIC	J 3/67	SIC2	J 12/69	SIH
J 12/71	SIH+	J 12/60	SIH4	J 3/67	SIN	J 9/67	SIO	J 6/67	SIO2(S)
J 6/67	SIO2(S)	J 6/67	SIO2(S)	J 6/67	SIO2(L)	J 9/67	SIO2	10/78	SIO2H2
J 12/71	SIS	J 3/67	SI2	J 3/67	SI2C	J 3/67	SI2N	J 3/67	SI3
8/79	TI(S)A	8/79	TI(S)B	8/79	TI(L)	8/79	TI	8/79	TI+
3/79	TIO(S)A	8/79	TIO(S)B	8/79	TIO(L)	8/79	TIO	8/79	TIO2(S)A
8/79	TIO2(S)B	8/79	TIO2(L)	8/79	TIO2	8/79	TI2O3(S)	8/79	TI2O3(L)
8/79	TI3O5(S)A	8/79	TI3O5(S)B	8/79	TI3O5(L)	8/79	TI5O7(S)	8/79	TI5O7(L)
8/79	TIC(S)	8/79	TIC(L)	8/79	TIN(S)	8/79	TIN(L)		
329	16	117	61	0	9	755			

C
H
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SI
FE
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G
P
CA
NA
K
TI
AR
E

3-18

SPECIES IN SOLUTION

AL2O3(L)
SIO2(L)
TI2O3(L)
KALO2(L)
KALSIO6(L)
KALSIO8(L)
FE2O3(L)
KALSIO4(L)
K2SIO5(L)
K2CO3(L)
K2SO4(L)

NOF = 6.688484

ENTHALPY
(KCAL) (DEG K) / KG
NOF-AVMS/AG
C
H
N

EFFECTIVE FUEL

HEP(2)
-0.46314276E 03
BEP(1,2)
0.47734685E-01
0.44111375E-01
0.61591272E-03

EFFECTIVE OXIDANT

HEP(1)
0.18411401E 03
BEP(1,1)
0.00000000E 00
0.00000000E 00
0.53319950E-01

MIXTURE

HSUB0
0.99278503E 02
B0(1)
0.62150983E-02
0.57763495E-02
0.46926081E-01

[illegible][illegible]

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 2							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 CAOH+	2.018E 15	2 K+	1.763E 20	3 NA+	1.321E 17		
1 AL02-	3.216E 15	2 CO2-	4.390E 16	3 FEO-	1.202E 16	4 FEO2-	4.263E 18
5 H-	3.421E 15	6 HCO3-	1.781E 16	7 HS-	1.425E 16	8 K-	2.137E 15
9 KO-	2.493E 16	10 NO2-	7.673E 15	11 O-	4.756E 16	12 OH-	1.260E 18
13 O2-	8.317E 15	14 PO2-	9.806E 19	15 PO3-	5.636E 19	16 S-	2.269E 15
17 SO-	1.593E 16	18 SO2-	2.071E 17				
CONDUCTIVITY = 0.4648 (MHO/M)							
AL2O3(L) REMOVED FROM SOLUTION AS IT IS 50.03 DEG K BELOW MELTING PT							
Ti2O3(L) REMOVED FROM SOLUTION AS IT IS 50.00 DEG K BELOW MELTING PT							
3	-16.989 -11.843 -12.885 -20.413	-19.353 -20.527 -8.743 -23.566	-22.032 -23.408 -24.865 -23.665	-21.848 -25.968			
	-24.441 -21.654 17.000						
ADD SOLUTION							
3	-16.699 -11.743 -12.882 -20.100	-19.508 -29.856 -11.965 -38.377	-21.957 -23.146 -24.754 -23.630	-23.131 -25.651			
	-24.435 -22.232 8.000						
ADD Ti3O5(S)B							
3	-16.700 -11.743 -12.882 -20.101	-19.507 -29.857 -11.965 -38.377	-21.957 -23.147 -24.755 -23.630	-23.131 -31.005			
	-24.435 -22.232 3.000						
ADD MG2Si4(S)							
3	-16.690 -11.739 -12.882 -20.091	-19.513 -29.904 -11.945 -38.380	-26.992 -23.144 -24.753 -23.629	-23.072 -30.997			
	-24.435 -22.197 4.000						
ADD CAO(S)							
3	-16.689 -11.732 -12.882 -20.090	-19.513 -29.902 -11.945 -38.377	-26.992 -23.144 -29.595 -23.632	-23.075 -30.996			
	-24.435 -22.199 4.000						
ADD TiO2(S)B							
3	-10.544 -10.307 -12.892 -16.100	-24.004 -20.640 -6.342 -31.176	-22.641 -20.756 -25.104 -22.925	-21.334 -23.511			
	-24.435 -19.172 10.000						
REMOVE TiO5(S)B							
3	-16.689 -11.732 -12.882 -20.089	-19.513 -29.901 -11.944 -38.376	-26.992 -23.143 -29.595 -23.632	-23.074 -32.492			
	-24.435 -22.198 10.000						

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 3															
ION		DENS (M-3)		ION		DENS (M-3)		ION		DENS (M-3)		ION		DENS (M-3)	
1	K+	9.255E	19	2	NA+	7.591E	16								
1	FE02-	5.483E	15	2	HS-	4.489E	15	3	OH-	5.588E	15	4	PO2-	5.782E	19
5	PO3-	3.473E	19	6	SO2-	8.564E	15								
CONDUCTIVITY =		0.0036 (MHO/M)													
FE104(L) REMOVED FROM SOLUTION AS TT IS 50.00 DEG K BELOW MELTING PT KALO2(L) REMOVED FROM SOLUTION AS TT IS 50.00 DEG K BELOW MELTING PT KALS104(L) REMOVED FROM SOLUTION AS TT IS 50.00 DEG K BELOW MELTING PT KALS1206(L) REMOVED FROM SOLUTION AS TT IS 50.00 DEG K BELOW MELTING PT SIO2(L) REMOVED FROM SOLUTION AS TT IS 50.00 DEG K BELOW MELTING PT															
4	-15.737	-11.603	-12.710	-18.519	-21.007	-19.135	-7.102	-24.152	-21.765	-21.255	-25.083	-22.871	-21.333	-24.113	
	-24.218	-24.382	17.090												
ADD SOLUTION															
4	-15.485	-11.526	-12.707	-18.250	-21.142	-36.540	-6.984	-24.998	-21.677	-21.196	-24.965	-22.835	-21.542	-23.838	
	-24.214	-24.354	7.090												
ADD AL601(S)I2(S)															

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  4   -15.465  -11.516  -12.707  -18.229  -21.153  -33.988  -6.982  -32.757  -21.676  -21.172  -24.964  -22.835  -21.600  -23.817
    -24.214  -24.383   5.000
ADD TI3O5(S)B
  4   -15.466  -11.516  -12.707  -18.230  -21.152  -33.989  -6.983  -32.757  -21.676  -21.172  -24.964  -22.835  -21.600  -32.950
    -24.214  -24.383   3.000
ADD H32SI04(S)
  4   -15.459  -11.513  -12.707  -18.222  -21.156  -33.995  -6.983  -32.747  -28.010  -21.170  -24.964  -22.835  -21.570  -32.944
    -24.214  -24.365   4.000
ADD FE3O4(S)
  4   -15.452  -11.508  -12.707  -18.215  -21.160  -33.986  -10.178  -32.742  -28.007  -21.164  -24.965  -22.835  -21.570  -32.937
    -24.214  -24.364   3.000
ADD CAO(S)
  4   -15.454  -11.502  -12.707  -18.217  -21.159  -33.985  -10.179  -32.744  -28.009  -21.165  -31.622  -22.839  -21.576  -32.939
    -24.214  -24.367   4.000
ADD AL2O3(S)
  4   -15.439  -11.408  -12.706  -18.201  -21.166  -31.443  -10.170  -33.576  -29.266  -20.912  -31.615  -22.842  -28.058  -32.927
    -24.212  -27.661   8.000
REMOVE AL6O13SI2(S)
  4   -15.452  -11.501  -12.707  -18.215  -21.160  -33.717  -10.178  -33.586  -28.142  -21.153  -31.622  -22.839  -21.665  -32.938
    -24.214  -24.417  10.000
ADD TIO2(S)A
  4   -9.540  -10.153  -12.707  -15.853  -25.409  -24.997  -4.513  -27.212  -24.004  -19.954  -27.372  -22.010  -20.028  -25.856
    -24.214  -20.662   9.000
REMOVE TI3O5(S)B
  4   -15.452  -11.501  -12.707  -18.214  -21.160  -33.716  -10.178  -33.585  -28.142  -21.152  -31.621  -22.839  -21.665  -34.353
    -24.214  -24.417  10.000
ADD FALO2(S)
  4   -15.445  -11.494  -12.707  -18.207  -21.163  -33.414  -10.174  -33.580  -28.286  -21.079  -31.618  -22.840  -22.330  -34.347
    -24.213  -24.782   3.000
REMOVE AL6O13SI2(S)
  4   -15.448  -11.497  -12.707  -18.210  -21.162  -33.470  -10.176  -33.933  -28.261  -21.114  -31.619  -22.840  -21.980  -34.350
    -24.213  -24.591   4.000
ADD FEO(L)
  4   -19.279  -12.473  -12.707  -22.182  -19.163  -37.480  -12.841  -36.907  -30.254  -24.824  -33.618  -23.565  -22.923  -38.348
    -24.213  -25.806   5.000
REMOVE FE3O4(S)
  4   -15.456  -11.499  -12.707  -18.219  -21.157  -33.479  -10.846  -33.939  -28.266  -21.120  -31.624  -22.841  -21.982  -34.358
    -24.213  -24.594   6.000

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ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 4													
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)						
1 K+	8.678E 19	2 NA+	2.781E 16										
1 HS-	4.606E 15	2 PO2-	5.525E 19	3 PO3-	3.152E 19	4 SO2-	1.829E 15						
CONDUCTIVITY = 0.0003 (MHO/M)													
5	-14.208 -11.330 -12.520 -16.240 -23.106 -17.444 -5.189 -24.966 -21.666 -19.315 -25.443 -21.946 -20.754 -21.828												
	-23.975 -27.460 18.000												
ADD SOLUTION													
5	-13.956 -11.253 -12.518 -16.022 -23.241 -40.495 -5.068 -25.812 -21.564 -19.271 -25.322 -21.903 -20.984 -21.553												
	-23.971 -27.437 8.000												
ADD AL6O13SI2(S)													
5	-13.937 -11.442 -12.518 -15.996 -23.251 -37.378 -5.070 -35.612 -21.566 -19.265 -25.324 -21.903 -21.185 -21.533												
	-23.971 -27.529 6.000												

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ADD TI3O5(S)B
5 -13.938 -11.242 -12.518 -15.997 -23.251 -37.379 -5.071 -35.613 -21.566 -19.265 -25.325 -21.904 -21.186 -35.448
-23.971 -27.530 3.000
ADD Ti3SiO4(S)
5 -13.935 -11.239 -12.518 -15.994 -23.253 -37.404 -5.073 -35.601 -30.216 -19.266 -25.328 -21.904 -21.143 -35.446
-23.971 -27.506 5.000
ADD Fe3O4(S)
5 -13.928 -11.235 -12.518 -15.983 -23.256 -37.395 -9.704 -35.596 -30.213 -19.266 -25.329 -21.905 -21.143 -35.440
-23.971 -27.502 4.000
ADD CAO(S)
5 -13.932 -11.229 -12.513 -15.992 -23.254 -37.396 -9.706 -35.600 -30.217 -19.266 -34.214 -21.910 -21.149 -35.443
-23.971 -27.508 4.000
ADD KALO2(S)
5 -13.928 -11.220 -12.517 -15.972 -23.255 -36.244 -9.705 -35.982 -30.791 -19.212 -34.213 -21.914 -23.465 -35.441
-23.969 -28.691 5.000
REMOVE AL6O13Si2(S)
5 -13.930 -11.224 -12.517 -15.977 -23.255 -36.547 -9.706 -37.528 -30.640 -19.243 -34.214 -21.913 -21.921 -35.442
-23.973 -27.904 5.000
ADD TiO2(S)A
5 -7.077 -9.902 -12.517 -15.905 -28.375 -26.200 -2.878 -29.614 -25.573 -18.751 -29.093 -20.833 -19.593 -26.908
-23.973 -22.865 9.000
REMOVE TI3O5(S)B
5 -13.929 -11.224 -12.517 -15.976 -23.255 -36.546 -9.705 -37.527 -30.640 -19.243 -34.213 -21.912 -21.920 -37.148
-23.973 -27.903 12.000
ADD Fe2SiO3(L)
5 -13.928 -11.222 -12.517 -15.973 -23.255 -36.382 -9.705 -37.116 -30.721 -19.233 -34.213 -21.913 -22.331 -37.148
-23.969 -28.113 3.000
ADD FeO(S)
5 -16.683 -11.920 -12.517 -18.765 -21.807 -39.281 -11.636 -39.290 -32.168 -20.980 -35.661 -22.476 -23.054 -40.044
-23.969 -29.428 5.000
REMOVE Fe3O4(S)
5 -13.936 -11.224 -12.517 -15.980 -23.251 -36.391 -10.192 -37.123 -30.726 -19.233 -34.218 -21.915 -22.333 -37.157
-23.969 -28.120 6.000

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ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 5		ION		DENS (M-3)
					DENS (M-3)				
1	K+	2.498E 19	2	NA+	1.292E 16				
1	HS-	2.611E 15	2	PO2-	1.626E 19		3	PO3-	8.717E 18
CONDUCTIVITY =		6.0000 (MHO/M)							

1
THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED TEMPERATURE AND PRESSURE

CASE NO. 101

CHEMICAL FORMULA		WT FRACTION (SEE NOTE)			ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	C 5.46166 H 4.56349	N 0.07139	S 0.03431	O 0.90000	0.74800	-21782.000	S	298.00 0.0000
FUEL	SI 0.87718 FE 0.09759	AL 0.43349	MG 0.11413	O 2.52526	0.09524	-293546.438	S	298.00 0.0000
FUEL	P 2.00000 O 0.00000				0.00046	-351350.000	S	298.00 0.0000
FUEL	CA 0.20213 NA 0.01200	K 0.01486	TI 0.01001	O 0.29604	0.01905	-48221.102	S	298.00 0.0000
FUEL	K 2.00000 C 1.00000	O 3.00000			0.09185	-274900.000	S	298.00 0.0000
FUEL	H 2.00000 O 1.00000				0.04540	-68283.000	L	298.00 0.0000
OXIDANT	N 2.00000				0.75426	10512.871	G	1660.00 0.0000
OXIDANT	O 2.00000				0.23195	11101.393	G	1660.00 0.0000

OXIDANT AR 1.00000
 O/F= 6.6885 PERCENT FUEL= 13.0065 EQUIVALENCE RATIO= 0.01379 6765.552 G 1660.00 0.0000
 REACTANT DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	4.5000	4.5000	4.5000	4.5000	4.5000
T, DEG K	2808	2130	2030	1800	1600
RHO, G/CC	5.7306-4	6.9051-4	8.3241-4	9.2441-4	1.0411-3
H, CAL/G	197.1	-72.1	-224.0	-288.6	-355.5
S, CAL/(G)(K)	2.2091	2.1063	2.0374	2.0025	1.9630
M, MOL WT	29.342	30.219	30.357	30.341	30.374
(DLV/DLP)T	-1.01222	-1.00287	-1.00050	-1.00031	-1.00056
(DLV/DLT)P	1.2972	1.0124	1.0067	1.0055	1.0090
CP, CAL/(G)(K)	0.8119	0.4604	0.3389	0.3309	0.3335
GAMMA (S)	1.1470	1.1885	1.2427	1.2497	1.2487
VELOCITY, M/SEC			0.30	0.00	0.00
TOTAL H(CAL/G)			-224.00	-288.57	-355.51
MAG FLD(TESLA)			0.30	0.00	0.00
BETA			0.00	0.00	0.00
SON VEL, M/SEC	955.3	885.9	825.0	785.1	739.5
ELEC DENS	2.744 20	1.615 19	1.434 17	1.163 16	3.071 14
IONIC DENS	6.094 20	3.368 20	1.852 20	1.736 20	4.998 19
SIGMA (RHO/M)	8.8654	0.4648	0.0036	0.0003	0.0000
W/O IONS	9.5130	0.4359	0.0037	0.0003	0.0000
CFRQ (1/SEC)	8.724 11	9.788 11	1.128 12	1.271 12	1.331 12

MOLE FRACTIONS

ALO2	1.288 -7	1.292-10	2.813-14	1.618-13	2.384-16
ALO2-	1.690 -7	2.323-10	3.250-14	2.567-13	3.308-16
ALO2H	1.159 -6	6.916 -9	2.689-11	1.093 -9	1.879-11
ALO2H2	1.196 -6	2.190 -8	6.193-10	9.832 -8	9.425 -9
AL2O3(L)	6.3850-7	1.3485-8	0.0000 0	0.0000 0	0.0000 0
AR	8.7889-3	9.0200-3	9.0629-3	9.0732-3	9.0755-3
CO	6.9688-2	3.0921-2	3.4142-2	3.3300-2	3.2193-2
COS	3.1334-8	2.4823-8	2.5293-7	1.5110-6	1.3296-5
CO2	1.1221-1	1.4777-1	1.5343-1	1.5448-1	1.5562-1
CA	1.459 -5	2.083 -7	1.088 -9	3.453-11	4.537-13
CAQ(S)	0.0000 0	1.0233-3	1.1714-3	1.1306-3	1.1323-3
CAO	1.234 -5	1.403 -7	2.025-10	2.548-12	1.049-14
CAOH	6.5923-4	4.2010-5	9.4341-7	7.5273-8	3.1352-9
CAO2H2	4.5893-4	1.0967-4	8.4801-6	1.4747-6	1.6511-7
E	2.327 -5	1.166 -6	8.634 -9	6.311-10	1.456-11
FE	1.9471-4	3.3704-5	1.0828-6	1.5728-7	7.1264-9
FEQ(S)	0.0000 0	0.0000 0	0.0000 0	0.0000 0	4.3791-4
FEQ(L)	0.0000 0	0.0000 0	0.0000 0	4.3105-4	0.0000 0
FEQ	1.755 -4	3.465 -5	4.653 -7	3.422 -8	6.538-10
FLOH	8.6017-6	3.4311-6	1.8478-7	3.5400-8	2.2590-9
FEQ?	2.681 -5	6.538 -6	4.173 -8	1.709 -9	1.561-11
FEQ2-	2.473 -6	3.079 -7	3.252-10	7.409-12	1.913-14
FLO2H2	1.7715-5	4.1421-5	1.4426-5	9.2315-6	2.7143-6
FE3O4(L)	2.83 -2	1.0597-4	1.4127-4	0.0000 0	0.0000 0
H	3.1456-3	4.5047-4	4.3423-5	1.1126-5	1.9097-6
HK	2.3221-6	7.3012-7	1.8395-7	2.0587-7	4.4602-8

HNO	7.126	-7	8.642	-8	2.545	-9	2.295	-10	1.139	-11
HO2	2.668	-6	1.831	-7	8.927	-10	2.214	-11	2.166	-13
HPO2	9.156	-9	1.7186	-8	7.6884	-8	1.5987	-7	2.1999	-7
H2	6.3745	-3	3.6679	-3	4.8543	-3	4.6485	-3	5.6356	-3
H2O	6.9981	-2	8.8829	-2	8.2415	-2	8.1457	-2	8.1808	-2
H2O2	2.376	-7	3.789	-8	9.162	-10	6.892	-11	2.744	-12
H2S	6.8842	-8	5.9374	-8	8.2194	-7	5.9763	-6	6.8267	-5
K	1.7727	-3	9.4559	-4	3.2110	-4	4.2311	-4	1.1085	-4
K+	3.7416	-5	1.2735	-5	5.5715	-6	4.7093	-6	1.2041	-6
KALO2(S)	8.8838	8	8.8888	8	8.8888	8	1.8568	-3	1.3315	-3
KALO2(L)	1.8860	-3	1.7718	-3	1.8969	-3	8.8708	8	8.8888	8
KALSI04(L)	1.2598	-5	1.4798	-5	4.8173	-6	8.8888	8	8.8888	8
KALSI206(L)	6.3148	-5	6.9521	-5	5.8585	-6	8.8888	8	8.8888	8
KALSI308(L)	7.4217	-6	8.7207	-5	4.5733	-5	8.9784	-4	6.2372	-4
K2CO3(L)	4.641	-11	1.844	-9	1.348	-8	2.127	-7	1.042	-6
KO	5.1190	-5	9.9686	-6	2.9946	-7	7.1444	-8	2.1930	-9
KOH	1.3650	-3	1.7953	-3	1.1575	-3	2.2171	-3	9.3473	-4
K2SO4(L)	2.927	-11	1.677	-10	3.884	-8	1.522	-7	1.715	-6
K2SI03(L)	8.8888	8	8.8888	8	8.8888	8	8.8888	8	7.7148	-4
K2SI205(L)	3.8631	-6	2.7591	-4	9.2338	-4	3.4464	-4	3.7836	-4
MG	7.676	-5	4.474	-6	4.661	-8	3.981	-9	7.613	-11
MGH	2.975	-7	1.137	-8	1.819	-10	7.986	-12	1.455	-13
MCO	2.677	-5	8.362	-7	1.328	-9	2.925	-11	1.832	-13
MGOH	3.8213	-4	7.6557	-5	2.3961	-6	3.9580	-7	1.8218	-8
MGO2H2	1.2529	-5	9.8683	-6	9.2311	-7	3.1933	-7	3.7472	-8
MG2SI04(S)	8.8888	8	8.8888	8	2.5535	-4	2.5696	-4	2.5736	-4
MG2SI04(L)	8.8888	8	2.1833	-4	8.8888	8	8.8888	8	8.8888	8
3-1-1 NO	1.435	-6	4.371	-8	3.552	-10	1.443	-11	2.639	-13
6-1-1 NO2	9.2539	-3	1.5513	-3	4.6375	-5	4.8749	-6	1.9312	-7
N2	3.818	-6	2.444	-7	9.565	-10	1.983	-11	1.536	-13
N2O	6.8206	-1	7.8483	-1	7.8887	-1	7.8890	-1	7.8988	-1
NA	9.225	-7	1.561	-7	4.724	-9	4.221	-10	2.863	-11
NAO	4.1629	-5	3.3611	-5	2.7871	-5	2.3325	-5	1.8772	-5
NAOH	1.119	-6	3.455	-7	2.627	-8	4.279	-9	4.258	-10
O	1.3580	-5	2.3844	-5	3.8985	-5	3.4828	-5	3.9481	-5
O-	3.876	-3	1.513	-4	8.687	-7	2.518	-8	3.827	-10
OH	3.350	-7	3.435	-9	9.421	-13	6.734	-15	8.177	-18
OH-	9.7779	-3	1.3893	-3	9.6702	-5	1.2952	-5	1.8492	-6
O2	1.813	-6	9.899	-8	3.364	-10	1.400	-11	1.548	-13
PN	1.3889	-2	1.3991	-3	7.6137	-6	1.9677	-7	2.8841	-9
PO	1.2963	-7	9.8313	-8	6.2581	-7	1.9280	-6	4.2750	-6
PO2	5.8845	-6	2.8511	-6	4.3378	-6	4.7831	-6	2.8888	-6
PO2-	1.8188	-5	1.8992	-5	1.4683	-5	1.3358	-5	6.3574	-6
PO3	7.1821	-6	7.8835	-6	3.4889	-6	2.9986	-6	7.8397	-7
PO3-	1.7565	-7	2.8973	-7	1.1688	-7	5.4794	-8	1.1418	-8
PS	1.9126	-6	4.3789	-6	2.8987	-6	1.7187	-6	4.2316	-7
S	4.879	-10	4.294	-10	3.859	-8	5.867	-7	1.861	-5
SH	2.6284	-6	4.1575	-7	2.3374	-7	1.3385	-7	1.3531	-7
SO	6.6551	-7	2.2255	-7	5.3093	-7	1.1598	-6	2.9813	-6
SO2	1.8860	-4	4.2541	-5	2.8641	-5	2.3764	-5	1.7426	-5
SO3	1.8124	-3	1.1133	-3	1.1313	-3	1.1293	-3	1.8377	-3
S2	2.9851	-7	1.9784	-7	3.7545	-3	1.1269	-8	2.3858	-9
SIO	1.529	-9	9.517	-10	2.426	-8	2.924	-7	5.715	-6
SIO2(L)	2.435	-3	6.887	-5	2.186	-7	1.747	-9	1.799	-11
SIO2	6.6763	-4	2.3717	-3	1.3811	-3	8.8888	8	8.8888	8
	2.555	-4	8.383	-6	1.748	-8	7.641	-11	4.173	-13

TIO 3.563 -7 1.648 -8 3.387-11 4.729-13 1.458-15
 TIO2(S)A 0.0000 0 0.0000 0 0.0000 0 4.5143-5 4.5155-5
 TIO2(S)B 0.0000 0 0.0000 0 4.5044-5 0.0000 0 0.0000 0
 TIO2 4.229 -5 8.514 -6 4.761 -8 1.180 -9 7.401-12
 TI2O3(L) 5.3877-7 1.8176-5 0.0000 0 0.0000 0 0.0000 0

0 SPECIES IN SOLUTION AT LAST STATION

KFIS1308(L) K2CO3(L) K2SO4(L) K2SI2O5(L)

0 ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-06 FOR ALL ASSIGNED CONDITIONS

AL(S)	AL(L)	AL	AL+	ALH	ALN(S)	ALN	ALO	ALO+	ALO-
ALOH	ALOH+	ALOH-	AL2O	AL2O+	AL2O2	AL2O2+	AL2O3(S)	AL6O13SI2(S)	ALS
AR+	C(S)	C	C+	C-	CAL	C3-	C2H-	CH	CH+
CH2	CH2O	CH3	CH4	CN	CN+	CN-	CNN	CN2	COS-
CO2-	CO3-	CO4-	CP	CS	CS-	CS2	C2	C2-	C2H
C2H2	C2H4	C2H6	C2N	C2N2	C2O	C3	C3O2	C4	C5
CA(S)	CA(S)	CA(L)	CA+	CACO3(S)	CACO3(S)	CAO(L)	CAOH+	CAO2H2(S)	CAS(S)
CASO4(S)	FE(S)	FE(S)	FE(S)	FE(L)	FE+	FEO-	FEO2H2(S)	FEO3H3(S)	FES(S)
FES(S)	FES(S)	FESO4(S)	FES2(S)	FE2O3(S)	FE2O3(L)	FE3O4(S)	FE2S3O12(S)	H+	H-
H2LO	H2N	HCO	HCO+	HCO3-	HCP	HNCO	HNO2	HNO3	H2O(S)
H2O(L)	H2P	H2SO4(L)	H2SO4	H3O+	HP-	HS-	HSI-	K(S)	K(L)
K-	KALS1308(S)	KCN	K2CO3(S)	KO+	KO-	KOH(S)	KOH(S)	KOH(L)	KOH+
K2	K2O(S)	K2O(L)	K2O2H2	K2SO4(S)	K2SO4(S)	MG(S)	MG(L)	MG+	MGCO3(S)
MGN	MGO(S)	MGO(L)	MGOH+	MGS(S)	MGS	MGSO4(S)	MGSO4(L)	NCO	NH
NH2	NH3	NO-	NO+	NO2-	NO3	NO3-	N2H4	N2O+	N2O4
N2O5	N3	NA(S)	NA(L)	NA+	NAALS1308(S)	NA-	NAH	NAO-	NAOH(S)
NAOH(L)	NAOH+	NA2	NA2CO3(S)	NA2CO3(S)	NA2CO3(L)	NA2O(S)	NA2O(S)	NA2O(L)	NA2O2H2
NA2SO4(S)	NA2SO4(S)	NA2SO4(S)	NA2SO4(L)	NA2SO4	NA2SIO3(S)	NA2SIO3(L)	NA2SI2O5(S)	NA2SI2O5(L)	O+
CH+	O2-	O3	P	P(S)	P+	P-	PH	PH3	PO-
P2	P4	S(S)	S(L)	S+	S-	SN	SO-	SO2-	SO3-
S2-	S8	SI(S)	SI(L)	SI	SI+	SI-	SIC(S)	SIC	SIC2
SIH	SIH+	SIH4	SIN	SIO2(S)	SIO2(S)	SIO2(S)	SIO2H2	SIS	SI2
SI2C	SI2N	SI3	TI(S)A	TI(S)B	TI(L)	TI	TI+	TIO(S)A	TIO(S)B
TIO(L)	TIO2(L)	TI2O3(S)	TI3O5(S)A	TI3O5(S)B	TI3O5(L)	TI5O7(S)	TI5O7(L)	TIC(S)	TIC(L)
TIN(S)	TIN(L)								

0 NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

STOP

3.1.2.2 Output data for HP problems

The output data for the HP problems considered here is given in Sample Output 2. Comparison of Sample Outputs 1 and 2 show that these outputs are almost the same. For HP problems, no input value is given for temperature T, and HP is set equal to TRUE instead of TP. Note that the thermodynamic properties of this case are practically identical to that of the TP case at 2808 K temperature and 4.5 atm pressure. This just shows that, for a given mixture at chemical equilibrium, any two thermodynamic variables can be used to determine the remaining mixture properties.

3.1.2.3 Output data for SP problems

The output data for the SP problem considered here is given in Sample Output 3. It differs from the HP problem output in the fact that the assigned value (in cal/gam-K) of the entropy (S^θ) is given in the INPT2 output data. Note, that the entropy and pressure for this case are identical to entropy and pressure for the TP case when $T = 2000$ K. Therefore, we expect identical thermodynamic properties. The only difference between the two cases is the mixture composition. This occurs because, when SP is TRUE, a liquid species is removed from the solution when the mixture temperature is 150 K below the melting point of that species, while in a TP case, a species is removed when the temperature is 50 K below its melting point.

Sample Output 2, HP Problem
(7 Output Pages)

```

1
REACTANTS      XXXSTG
C 5.4617 H 4.5635 N 0.0714 S 0.0343 O 0.9000 0.74800 -21782.00 S 298.000 0 F 0.00000
SI 0.8072 FE 0.0977 AL 0.4335 MG 0.1141 O 2.5253 0.95240E-01 -288546.44 S 298.000 0 F 0.00000
P 2.0000 O 5.0000 0.0000 0.0000 0.0000 0.46000E-03 -351350.00 S 298.000 0 F 0.00000
CA 0.2621 NA 0.0129 K 0.0149 TI 0.0100 O 0.2960 0.19050E-01 -48221.10 S 298.000 0 F 0.00000
K 2.0000 C 1.0000 O 3.0000 0.0000 0.0000 0.91850E-01 -274900.00 S 298.000 0 F 0.00000
H 2.0000 O 1.0000 0.0000 0.0000 0.0000 0.45400E-01 -68288.00 L 298.000 0 F 0.00000
N 2.0000 0.0000 0.0000 0.0000 0.0000 0.75426 4100.60 G 1660.000 0 O 0.00000
O 2.0000 0.0000 0.0000 0.0000 0.0000 0.23195 4326.20 G 1660.000 0 O 0.00000
AR 1.0000 0.0000 0.0000 0.0000 0.0000 0.13790E-01 2823.40 G 1660.000 0 O 0.00000
SOLUTION      AL2O3(L)      SiO2(L)      Ti2O3(L)      KAlO2(L)
SOLUTION      KAlSi2O6(L)      KAlSi3O8(L)      Fe3O4(L)      KAlSiO4(L)
SOLUTION      K2Si2O5(L)      K2CO3(L)      K2SO4(L)
OMIT          MgSiO3(S)      MgSiO3(L)
INSERT        FeO(L)      CaO(S)
NAMELISTS

```

```

1
$INPT2
KASE = 102,
T = 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000,
P = 4.50000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000,
PSIA = F,
MMHG = F,
NSQM = F,
V = 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000,
RHO = 4.50000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000,
ERATIO= T,
OXFL = F,
FPCT = F,
FA = F,
MIX = 1.008700, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000,
TP = F,
HP = T,
SP = F,
TV = F,

```

UV = F,
 SV = F,
 RKT = F,
 SHOCK = F,
 DETN = F,
 OTTO = F,
 CR = 0.000000 ,
 S0 = 0.0000000000
 IONS = T,
 IDEBUG= 0,
 TRACE = 0.100000E-06,
 SIUNIT= F,
 DXI = 0.000000 ,
 NITER = 0,
 NSTOP = 0,
 NEOL = F,
 BZ = 0.000000 ,
 XK = 0.000000 ,
 ACCURC= 0.100000E-02,
 RMIN = 0.100000E-14,
 ALPH = 0.000000 ,
 EXIN = 2400.00 ,
 TWOSTG= F,
 SEND
 LLMT =

C
 H
 N
 S
 O
 SI
 FE
 AL
 MG
 P
 CA
 NA
 K
 TI
 AR

3-26

#SPECIES BEING CONSIDERED IN THIS SYSTEM

J12/65 AL(S)	J12/65 AL(L)
J12/62 ALN(S)	J 3/67 ALN
J12/67 ALOH	J12/67 ALOH+
J12/68 ALO2H	10/78 ALO2H2
J 6/68 AL2O2+	J 6/72 AL2O3(S)
L 5/66 AR	L12/66 AR+
J 9/65 C-	3/8/7 CAL
J12/71 CH+	J12/72 CH2
J 6/69 CN	J12/70 CN+
J 9/65 CO	J 3/61 COS
3/3/7 CO3-	3/7/7 CO4-
J 6/61 CS2	J12/69 C2
J 9/65 C2H4	L 5/72 C2H6
J12/69 C3	J 6/68 C3O2
J12/68 CA(S)	J12/68 CA(L)

J12/65 AL
J 6/70 ALO
J12/67 ALOH-
J 6/72 AL2O
J 6/75 AL2O3(L)
J 3/61 C(S)
3/3/7 C3-
J 3/61 CH2O
J12/70 CN-
3/3/7 COS-
J 6/62 CP
J12/69 C2-
J 3/67 C2N
J12/69 C4
J12/68 CA

J 6/65 AL+
J 6/70 ALO+
J12/68 ALO2
J 6/72 AL2O+
10/78 AL6O13SI2(S)
J 3/61 C
3/3/7 C2H-
J 6/69 CH3
J 6/66 CNH
J 9/65 CO2
J12/62 CS
J 3/67 C2H
J 3/61 C2N2
J12/69 C5
J12/70 CA+

J 6/63 ALH
J 12/7 ALO-
3/8/7 ALO2-
J 9/65 AL2O2
3/8/7 ALS
L12/66 C+
J12/67 CH
J 3/61 CH4
J12/70 CN2
4/12/7 CO2-
3/3/7 CS-
J 3/61 C2H2
J 9/66 C2O
J12/68 CA(S)
BAR 73 CAC03(S)

BAR 73 CACO3(S)
 J 6/78 CAOH+
 L02/67 E
 J 3/65 FE
 4/13/7 FEO-
 10/78 FEO2H2
 J 6/66 FESO4(S)
 10/78 FESO4(L)
 J 3/64 HALO
 J12/69 HCP
 J 6/63 HNO3
 L11/65 H2O(L)
 J12/66 H2SO4(L)
 3/3/7 HSI-
 3/3/7 K-
 GS4/76 KALSI308(S)
 J12/67 KO
 J12/78 KOH(L)
 10/78 K2O(L)
 12/79 K2SIO3(L)
 J12/78 MG+
 10/78 MGO(L)
 J12/71 MGS(S)
 J12/67 MG2SIO4(L)
 J 9/65 NH3
 J 6/72 NO2-
 J12/64 N2O
 J 6/62 NA(S)
 3/3/7 NA-
 J12/78 NAOH(L)
 J 3/66 NA2CO3(S)
 J12/78 NA2O2H2
 K11/74 NA2SO4
 J 6/62 O
 J12/78 OH-
 J 6/61 P(S)
 J 9/62 PN
 10/5/7 PO3
 J12/65 S(S)
 J 6/67 SH
 3/3/7 SO2-
 J6/64 S8
 3/3/7 SI-
 J12/71 SIH+
 J 6/67 SIO2(S)
 J12/71 SIS
 8/79 TI(S)A
 8/79 TIO(S)A
 8/79 TIO2(S)B
 8/79 TI3O5(S)A
 8/79 TIC(S)
 329 16

CHNS

117

J 6/71 CAO(S)
 J12/71 CAO2H2(S)
 J 3/65 FE(S)
 3/1/78 FE+
 10/78 FEOH
 J 6/66 FEO3H3(S)
 BAR 73 FES2(S)
 J 6/66 FE2S3O12(S)
 L12/69 HCN
 3/8/7 HK
 J 3/64 HO2
 J 3/61 H2O
 J12/66 H2SO4
 J12/61 K(S)
 10/78 KALO2(S)
 H10/77 KALSI308(L)
 7/29/8 KO+
 J12/78 KOH
 J12/78 K2O2H2
 PB7/77 K2SIO5(L)
 J12/66 MGCO3(S)
 10/78 MGO
 J 6/71 MGS
 J 3/61 N
 J 6/63 NO
 J12/64 NO3
 J12/78 N2O+
 J 6/62 NA(L)
 J 3/63 NAH
 J12/78 NAOH
 J 3/66 NA2CO3(L)
 J12/66 NA2SO4(S)
 J 4/76 NA2SIO3(S)
 L12/66 O+
 J 9/65 O2
 L12/66 P+
 J 6/71 PO
 2/14/9 PO3-
 J12/65 S(L)
 J 6/61 SN
 J 9/65 SO3
 J 3/67 SI(S)
 10/78 SIC(S)
 J12/68 SIH4
 J 6/67 SIO2(S)
 J 3/67 SI2
 8/79 TI(S)B
 8/79 TIO(S)B
 8/79 TIO2(L)
 8/79 TI3O5(S)B
 8/79 TIC(L)
 61

8

J 6/71 CAO(L)
 J 12/7 CAO2H2
 J 3/65 FE(S)
 J 6/65 FEO(S)
 4/20/7 FEO2
 BAR 73 FES(S)
 J 6/65 FE2O3(S)
 J 9/65 H
 J12/78 HCO
 J12/78 HMCO
 12/21/ HPO2
 L 2/69 H2O2
 3/25/7 H3O+
 J12/61 K(L)
 H10/77 KALO2(L)
 3/8/7 KCN
 J12/67 KO-
 J12/71 KOH+
 J12/71 K2SO4(S)
 J 9/62 MG(S)
 J12/66 MGH
 10/78 MGOH
 L 7/76 MGSO4(S)
 J12/78 NCO
 3/3/7 NO-
 3/3/7 NO3-
 J 9/64 N2O4
 J 6/62 NA
 J12/67 NAO
 J12/71 NAOH+
 J 6/68 NA2O(S)
 J12/66 NA2SO4(S)
 J 4/76 NA2SIO3(L)
 J 6/65 O-
 J12/66 O2-
 3/3/7 P-
 3/3/7 PO-
 J 6/67 PS
 J 6/71 S
 J 6/71 SO
 3/3/7 SO3-
 J 3/67 SI(L)
 J 3/67 SIC
 J 3/67 SIN
 J 6/67 SIO2(L)
 J 3/67 SI2C
 8/79 TI(L)
 8/79 TIO(L)
 8/79 TIO2
 8/79 TI3O5(L)
 8/79 TIN(S)
 9 755

J12/74 CAO
 J12/71 CAS(S)
 J 3/65 FE(S)
 J 6/65 FEO(L)
 4/13/7 FEO2-
 BAR 73 FES(S)
 10/78 FE2O3(L)
 J 6/66 H+
 J12/78 HCO+
 J 3/63 HNO
 J 3/61 H2
 3/8/7 H2P
 3/3/7 HP-
 J 6/62 K
 H10/77 KALSI04(L)
 J 3/66 K2CO3(S)
 J12/78 KOH(S)
 J12/61 K2
 J12/71 K2SO4(S)
 J 9/62 MG(L)
 J 3/64 MGN
 J 6/68 MGOH+
 L 7/76 MGSO4(L)
 J12/71 NH
 J 6/66 NO+
 J 9/65 N2
 J12/64 N2O5
 J 3/65 NA+
 J12/67 NAO-
 J 6/62 NA2
 J 6/68 NA2O(S)
 J12/66 NA2SO4(S)
 J 4/76 NA2SIO5(S)
 J12/78 OH
 J 6/61 O3
 J 6/67 PH
 1/1/8 PO2
 J 6/61 P2
 L12/66 S+
 3/3/7 SO-
 J12/65 S2
 J 3/67 SI
 J 3/67 SIC2
 J 9/67 SIO
 J 9/67 SIO2
 J 3/67 SI2N
 8/79 TI
 8/79 TIO
 8/79 TI2O3(S)
 8/79 TI5O7(S)
 8/79 TIN(L)

J 6/78 CAOH
 BAR 73 CASO4(S)
 J 3/65 FE(L)
 J 9/66 FEO
 J 6/66 FEO2H2(S)
 BAR 73 FES(S)
 J 6/65 FE3O4(S)
 J 9/65 H-
 3/8/7 HCO3-
 J 6/63 HNO2
 L11/65 H2O(S)
 J12/65 H2S
 3/3/7 HS-
 J 3/65 K+
 H10/77 KALSI206(L)
 J 3/66 K2CO3(L)
 J12/78 KOH(S)
 J 6/63 K2O(S)
 J12/71 K2SO4(L)
 J 9/62 MG
 J12/65 MGO(S)
 10/78 MGO2H2
 10/78 MG2SIO4(S)
 J12/65 NH2
 J 9/64 NO2
 J12/65 N2H4
 J12/78 N3
 GS4/76 NAALSI308(S)
 J12/78 NAOH(S)
 J 3/66 NA2CO3(S)
 J 6/68 NA2O(L)
 J12/66 NA2SO4(L)
 J 4/76 NA2SIO5(L)
 J12/78 OH+
 J 6/62 P
 J 6/62 PH3
 7/11/7 PO2-
 J 6/61 P4
 3/3/7 S-
 J 6/61 SO2
 3/3/7 S2-
 J12/71 SI+
 J12/69 SIH
 J 6/67 SIO2(S)
 10/78 SIO2H2
 J 3/67 SI3
 8/79 TI+
 8/79 TIO2(S)A
 8/79 TI2O3(L)
 8/79 TI5O7(L)

O
S
I
F
E
A
L
M
G
P
C
A
N
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K
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A
R
E

SPECIES IN SOLUTION

AL2O3 (L)
 SiO2 (L)
 Ti2O3 (L)
 KAlO2 (L)
 KAlSi2O6 (L)
 KAlSi3O8 (L)
 Fe3O4 (L)
 KAlSiO4 (L)
 K2Si2O5 (L)
 K2CO3 (L)
 K2SO4 (L)

DOF = 6.688484

ENTHALPY
(KG-MOL) (DEG K) /KG
ØKG-ATOMS/KG

3-28

CHNSO
SIFEAL
MG
P
CANAK
TIAR
E

EFFECTIVE FUEL

```
HPP(2)
-0.46814276E+03
BOP(I,2)
0.47784686E-01
0.44411376E-01
0.61591272E-03
0.29600743E-03
0.15532037E-01
0.92621811E-03
0.11209674E-03
0.49741857E-03
0.13096121E-03
0.64814049E-05
0.30382284E-03
0.14304126E-04
0.13461588E-02
0.11487569E-04
0.00000000E+00
0.00000000E+00
```

EFFECTIVE OXIDANT

[illegible]

MIXTURE

HSUB#
 0.99278503E-02
 B0(I)
 0.62150983E-02
 0.57763495E-02
 0.46926081E-01
 0.38500097E-04
 0.14631987E-01
 0.12046822E-03
 0.14579822E-04
 0.64696564E-04
 0.17033421E-04
 0.84300154E-06
 0.39126411E-04
 0.19254976E-05
 0.17508765E-03
 0.14941265E-05
 0.30030060E-03
 0.00000000E-00

#PT	C	H	N	S	O	SI	FE	AL	MG	P	CA	NA	K	TI
1	-18.474	-12.110	-13.481	-23.309	-16.399	-23.077	-12.547	-21.756	-22.870	-26.969	-23.920	-25.752	-23.168	-28.689
REMOVE CAO(S)														
1	-18.473	-12.109	-13.481	-23.308	-16.399	-23.077	-12.547	-21.756	-22.870	-27.046	-23.987	-25.752	-23.168	-28.688
REMOVE FE0(L)														
1	-18.439	-12.098	-13.489	-23.282	-16.396	-23.073	-14.678	-21.707	-22.873	-27.043	-23.962	-25.777	-23.181	-28.656
ADD SOLUTION														

1 -18.393 -12.874 -13.500 -23.247 -16.394 -23.336 -14.789 -28.223 -22.884 -27.181 -23.941 -25.812 -23.657 -28.637
 -25.218 -15.843 7.888

ION		DENS (M-3)	ION		DENS (M-3)	ION		DENS (M-3)	ION		DENS (M-3)
1	CA+	9.618E 15	2	CAOH+	1.489E 17	3	K+	4.415E 28	4	KOH+	7.996E 15
5	NA+	3.839E 17									
1	ALO-	1.186E 17	2	ALO2-	1.999E 18	3	CN-	2.282E 15	4	CO2-	5.782E 17
5	CO3-	6.473E 15	6	FEO-	2.657E 17	7	FEO2-	2.915E 19	8	H-	1.611E 17
9	HCO3-	5.128E 16	10	HS-	9.571E 16	11	K-	3.219E 16	12	KO-	3.339E 17
13	NO-	5.982E 16	14	NO2-	2.868E 17	15	NAO-	6.197E 15	16	O-	3.956E 18
17	OH-	2.148E 19	18	O2-	7.812E 17	19	PO-	3.376E 15	20	PO2-	8.467E 19
21	PO3-	2.254E 19	22	S-	3.843E 16	23	SO-	2.235E 17	24	SO2-	9.899E 17
25	SO3-	4.954E 15									

CONDUCTIVITY = 8.8746 (MHO/M)

1
 THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED PRESSURES

CASE NO. 182

CHEMICAL FORMULA		WT FRACTION (SEE NOTE)			ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL C	5.46166 H 4.56349	N 8.87139	S 8.83431	O 8.98888	8.74888	-21782.888	S	298.88
FUEL SI	8.88718 FE 8.89769	AL 8.43349	MG 8.11413	O 2.52526	8.89524	-288546.438	S	298.88
FUEL P	2.88888 O 5.88888				8.88846	-351358.888	S	298.88
FUEL CA	8.26213 NA 8.81298	K 8.81486	TI 8.81881	O 8.29684	8.81985	-48221.182	S	298.88
FUEL H	2.88888 C 1.88888	O 3.88888			8.89185	-274988.888	S	298.88
FUEL K	2.88888 O 1.88888				8.84548	-68288.888	L	298.88
OXIDANT N	2.88888				8.75426	18512.871	G	1668.88
OXIDANT O	2.88888				8.23195	11181.393	G	1668.88
OXIDANT AR	1.88888				8.81379	6765.552	G	1668.88

O/F= 6.6885 PERCENT FUEL= 13.8865 EQUIVALENC RATIO= 1.8878 REACTANT DENSITY= 8.8888

OTHERMODYNAMIC PROPERTIES

P, ATM 4.5888
 T, DEG K 2888
 RHO, G/CC 5.7388-4
 H, CAL/G 197.3
 S, CAL/(G)(K) 2.2892
 M, MOL WT 29.341
 (DLV/DLP)T -1.81222
 (DLV/DLT)P 1.2972
 CP, CAL/(G)(K) 8.8128
 GAMMA (S) 1.1478
 SON VEL, M/SEC 955.3
 ELEC DENS 2.747 28
 IONIC DENS 6.896 28
 SIGMA (MHO/M) 8.8746
 W/O IONS 9.5238
 FREQ (1/SEC) 8.723 11

MOLE FRACTIONS

ALO2	1.2918-7
ALO2-	1.6951-7
ALO2H	1.1619-6
ALO2H2	1.1983-6
AL2O3(L)	6.4889-7
AR	8.7887-3
CO	6.9718-2
CO2	1.1218-1
CA	1.4654-5
CAO	1.2353-5
CAOH	6.5939-4
CAO2H2	4.5873-4
E	2.3298-5
FE	1.9474-4
FeO	1.7552-4
FeOH	8.6811-6
FeO2	2.6884-5
FeO2-	2.4719-6
FeO2H2	1.7694-5
Fe3O4(L)	2.8175-7
H	3.1495-3
HK	2.3233-6
HNO	7.1314-7
HO2	2.6626-6
H2	6.3769-3
H2O	6.9973-2
H2O2	2.3773-7
K	1.7731-3
K+	3.7448-5
KALO2(L)	1.8865-3
KALSIO4(L)	1.2583-5
KALSI2O6(L)	6.3883-5
KALSI3O8(L)	7.3886-6
KO	5.1213-5
KOH	1.3645-3
K2SI2O5(L)	3.8487-6
MG	7.6883-5
MGH	2.9771-7
MGO	2.6787-5
MGOH	3.8287-4
MGO2H2	1.2519-5
N	1.4376-6
NO	9.2563-3
NO2	3.8198-6
N2	6.8285-1
N2O	9.2384-7
NA	4.1633-5
NAO	1.1175-6
NAOH	1.3495-5
O	3.8797-3
O-	3.3549-7
OH	9.7839-3
OH-	1.8147-6
O2	1.3817-2

3-30

PM 1.2978-7
 PO 5.8869-6
 PO2 1.8138-5
 PO2- 7.1885-6
 PO3 1.7561-7
 PO3- 1.9112-6
 S 2.6233-6
 SH 6.6689-7
 SO 1.1866-4
 SO2 1.8123-3
 SO3 2.9849-7
 SIO 2.4369-3
 SIO2(L) 6.6635-4
 SIO2 2.5568-4
 TIO 3.5661-7
 TIO2 4.2297-5
 TI2O3(L) 5.3724-7

#SPECIES IN SOLUTION AT LAST STATION

AL2O3(L)	FE3O4(L)	KALO2(L)	KALSIO4(L)	KALSI2O6(L)	KALSI3O8(L)	K2CO3(L)	K2SO4(L)	K2SIO2O5(L)	SIO2(L)
SIO2(L)	TI2O3(L)								

#ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN $8.18888E-86$ FOR ALL ASSIGNED CONDITIONS

AL(S)	AL(L)	AL	AL+	ALH	ALN(S)	ALN	ALO	ALO+	ALO-
ALOH	ALOH+	ALOH-	AL2O	AL2O+	AL2O2	AL2O2+	AL2O3(S)	AL6O13SIO2(S)	ALS
AR+	C(S)	C	C+	C-	CAL	C3-	C2H-	CH	CH+
CH2	CH2O	CH3	CH4	CN	CN+	CN-	CNN	CN2	CO5
COS-	CO2-	CO3-	CO4-	CP	CS	CS-	CS2	C2	C2-
C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2O	C3	C3O2	C4
C5	CA(S)	CA(S)	CA(L)	CA+	CACO3(S)	CACO3(S)	CAO(S)	CAO(L)	CAOH+
CAO2H2(S)	CAS(S)	CASO4(S)	FE(S)	FE(S)	FE(S)	FE(L)	FE+	FE(S)	FE(L)
FE0-	FE02H2(S)	FE03H3(S)	FES(S)	FES(S)	FES(S)	FES04(S)	FES2(S)	FE2O3(S)	FE2O3(L)
FE3O4(S)	FE2S3O12(S)	H+	H-	HALO	HCN	HCO	HCO+	HCO3-	HCP
HNCO	HNO2	HNO3	HPO2	H2O(S)	H2O(L)	H2P	H2S	H2SO4(L)	H2SO4
H3O+	HP-	HS-	HSI-	K(S)	K(L)	K-	KALO2(S)	KALSI3O8(S)	KCN
K2CO3(S)	K2CO3(L)	KO+	KO-	KOH(S)	KOH(S)	KOH(L)	KOH+	K2	K2O(S)
K2O(L)	K2O2H2	K2SO4(S)	K2SO4(S)	K2SO4(L)	K2SIO3(L)	MG(S)	MG(L)	MG+	MGC03(S)
MGN	MGO(S)	MGO(L)	MGOH+	MGS(S)	MGS	MGS04(S)	MGS04(L)	MG2SIO4(S)	MG2SIO4(L)
NCO	NH	NH2	NH3	NO-	NO+	NO2-	NO3	NO3-	N2H4
N2O+	N2O4	N2O5	N3	NA(S)	NA(L)	NA+	NAALSI3O8(S)	NA-	NAH
NAO-	NAOH(S)	NAOH(L)	NAOH+	NA2	NA2CO3(S)	NA2CO3(S)	NA2CO3(L)	NA2O(S)	NA2O(S)
NA2O(L)	NA2O2H2	NA2SO4(S)	NA2SO4(S)	NA2SO4(S)	NA2SO4(L)	NA2SO4	NA2SIO3(S)	NA2SIO3(L)	NA2SIO2O5(S)
NA2SIO2O5(L)	O+	OH+	O2-	O3	P	P(S)	P+	P-	PH
PH3	PO-	PS	P2	P4	S(S)	S(L)	S+	S-	SN
SO-	SO2-	SO3-	S2	S2-	S8	SI(S)	SI(L)	SI	SI+
SI-	SIC(S)	SIC	SIC2	SIH	SIH+	SIH4	SIN	SIO2(S)	SIO2(S)
SIO2(S)	SIO2H2	SIS	SI2	SI2C	SI2N	SI3	TI(S)A	TI(S)B	TI(L)
TI	TI+	TIO(S)A	TIO(S)B	TIO(L)	TIO2(S)A	TIO2(S)B	TIO2(L)	TI2O3(S)	TI3O5(S)A
TI3O5(S)B	TI3O5(L)	TI5O7(S)	TI5O7(L)	TIC(S)	TIC(L)	TIN(S)	TIN(L)		

#NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

1

STOP

Sample Output 3, SP Problem
(7 Output Pages)

1

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REACTANTS      XXXSTG
C 5.4617 H 4.5635 N 0.0714 S 0.0343 O 0.9000 0.74800 -21782.00 S 298.000 0 F 0.00000
SI 0.0072 FE 0.0977 AL 0.4335 MG 0.1141 O 2.5253 0.95240E-01 -288546.44 S 298.000 0 F 0.00000
P 2.0000 O 5.0000 0.0000 0.0000 0.0000 0.0000 0.46000E-03 -351350.00 S 298.000 0 F 0.00000
CA 0.2621 NA 0.0129 K 0.0149 TI 0.0100 O 0.2960 0.19050E-01 -48221.10 S 298.000 0 F 0.00000
K 2.0000 C 1.0000 O 3.0000 0.0000 0.0000 0.0000 0.91850E-01 -274900.00 S 298.000 0 F 0.00000
H 2.0000 O 1.0000 0.0000 0.0000 0.0000 0.0000 0.45400E-01 -68288.00 L 298.000 0 F 0.00000
N 2.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.75426 4100.60 G 1660.000 0 O 0.00000
O 2.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.23195 4326.20 G 1660.000 0 O 0.00000
AR 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.13790E-01 2823.40 G 1660.000 0 O 0.00000
SOLUTION      AL2O3(L)      SiO2(L)      Ti2O3(L)      KAlO2(L)
SOLUTION      KAlSi2O6(L)      KAlSi3O8(L)      Fe3O4(L)      KAlSiO4(L)
SOLUTION      K2Si2O5(L)      K2CO3(L)      K2SO4(L)
OMIT          MGSiO3(S)      MGSiO3'(L)
INSERT        FeO(L)      CaO(S)
NAMELISTS
1
$INPT2
KASE = 103,
T = 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 ,
P = 4.50000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 ,
PSIA = F,
MMHG = F,
NSQM = F,
V = 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 ,
RHO = 4.50000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 ,
ERATIO= T,
OXFL = F,
FPCY = F,
Fh = F,
MIX = 1.08700 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 ,
TP = F,
HP = F,
SP = T,
TV = F,

```

UV = F,
 SV = F,
 RKT = F,
 SHOCK = F,
 DETN = F,
 OTTO = F,
 CR = 0.000000 ,
 S0 = 2.0374000000
 IONS = T,
 IDEBUG= 0,
 TRACE = 0.100000E-06,
 SIUNIT= F,
 DXI = 0.000000 ,
 NITER = 0,
 NSTOP = 0,
 NEQL = F,
 BZ = 0.000000 ,
 XK = 0.000000 ,
 ACCURC= 0.100000E-02,
 HMIN = 0.100000E-14,
 ALPH = 0.000000 ,
 EXIN = 2400.00 ,
 TWOSTG= F,
 \$END
 LLMT =

3-36

C
 H
 N
 S
 O
 SI
 FE
 AL
 MG
 P
 CA
 NA
 K
 TI
 AR

0SPECIES BEING CONSIDERED IN THIS SYSTEM

J12/65 AL(S)	J12/65 AL(L)
J12/62 ALN(S)	J 3/67 ALN
J12/67 ALOH	J12/67 ALOH+
J12/68 ALO2H	10/78 ALO2H2
J 6/68 AL202+	J 6/72 AL203(S)
L 5/66 AR	L12/66 AR+
J 9/65 C-	3/8/7 CAL
J12/71 CH+	J12/72 CH2
J 6/69 CN	J12/70 CN+
J 9/65 CO	J 3/61 COS
3/3/7 CO3-	3/7/7 CO4-
J 6/61 CS2	J12/69 C2
J 9/65 C2H4	L 5/72 C2H6
J12/69 C3	J 6/63 C3O2
J12/68 CA(S)	J12/68 CA(L)

J12/65 AL
J 6/70 ALO
J12/67 ALOH-
J 6/72 AL20
J 6/75 AL203(L)
J 3/61 C(S)
3/3/7 C3-
J 3/61 CH2O
J12/70 CN-
3/3/7 COS-
J 6/62 CP
J12/69 C2-
J 3/67 C2N
J12/69 C4
J12/68 CA

J 6/65 AL+
J 6/70 ALO+
J12/68 ALO2
J 6/72 AL20+
10/78 AL6013SI2(S)
J 3/61 C
3/3/7 C2H-
J 6/69 CH3
J 6/66 CNN
J 9/65 CO2
J12/62 CS
J 3/67 C2H
J 3/61 C2N2
J12/69 C5
J12/70 CA+

J 6/63 ALH
J 12/7 ALO-
3/8/7 ALO2-
J 9/65 AL202
3/8/7 ALS
L12/66 C+
J12/67 CH
J 3/61 CH4
J12/70 CN2
4/12/7 CO2-
3/3/7 CS-
J 3/61 C2H2
J 9/66 C2O
J12/68 CA(S)
BAR 73 CACO3(S)

BAR 73 CACO3(S) J 6/71 CAO(S) J 6/71 CAO(L) J12/74 CAO J 6/78 CAOH
 J 6/78 CAOH+ J12/71 CAO2H2(S) J 12/7 CAO2H2 J12/71 CAS(S) BAR 73 CASO4(S)
 L82/67 E J 3/65 FE(S) J 3/65 FE(S) J 3/65 FE(S) J 3/65 FE(L) J 3/65 FE(L)
 J 3/65 FE J 8/1/78 FE+ J 6/65 FEO(S) J 6/65 FEO(L) J 9/66 FEO
 4/13/7 FEO- 18/78 FEOH 4/28/7 FEO2 J 13/7 FEO2- J 6/66 FEO2H2(S)
 18/78 FEO2H2 J 6/66 FEO3H3(S) BAR 73 FES(S) BAR 73 FES(S)
 J 6/66 FESO4(S) BAR 73 FES2(S) J 6/65 FE2O3(S) 18/78 FE2O3(L) J 6/65 FE3O4(S)
 18/78 FE3O4(L) J 6/66 FE2S3O12(S) J 9/65 H J 6/66 H+ J 9/65 H-
 J 3/64 HALO L12/69 HCN J12/78 HCO J12/78 HCO+ J 3/8/7 HCO3-
 J12/69 HCP 3/8/7 HK J12/78 HNCO J 3/63 HNO J 6/63 HNO2
 J 6/63 HNO3 J 3/64 HO2 12/21/ HPO2 J 3/61 H2 L11/65 H2O(S)
 L11/65 H2O(L) J 3/61 H2O L 2/69 H2O2 3/8/7 H2P J12/65 H2S
 J12/66 H2SO4(L) J12/66 H2SO4 3/25/7 H3O+ 3/3/7 HP- 3/3/7 HS-
 3/3/7 HSI- J12/61 K(S) J12/61 K(L) J 6/62 K J 3/65 K+ J 3/65 K+
 3/3/7 K- 18/78 KALO2(S) H18/77 KALO2(L) H18/77 KALSIO4(L) H18/77 KALSIO4(L)
 GS4/76 KALSIO3(S) H18/77 KALSIO3(L) 3/8/7 KCN J 3/66 K2CO3(S) J 3/66 K2CO3(L)
 J12/67 KO 7/29/8 KO+ J12/67 KO- J12/78 KOH(S) J12/78 KOH(S)
 J12/78 KOH(L) J12/78 KOH J12/71 KOH+ J12/61 K2 J 6/63 K2O(S)
 18/78 K2O(L) J12/78 K2O2H2 J12/71 K2SO4(S) J12/71 K2SO4(L)
 12/79 K2SIO3(L) 28/7/7 K2SIO2O5(L) J 9/62 MG(S) J 9/62 MG(L) J 9/62 MG
 J12/78 MG+ J12/66 MGCO3(S) J12/66 MGH J 3/64 MGN J12/65 MGO(S)
 18/78 MGO(L) 18/78 MGO 18/78 MGOH J 6/68 MGOH+ 18/78 MGO2H2
 J12/71 MGS(S) J 6/71 MGS L 7/76 MGSO4(S) L 7/76 MGSO4(L) 18/78 MG2SIO4(S)
 J12/67 MG2SIO4(L) J 3/61 N J12/78 NCO J12/71 NH J12/65 NH2
 J 9/65 NH3 J 6/63 NO 3/3/7 NO- J 6/66 NO+ J 9/64 NO2
 J 6/72 NO2- J12/64 NO3 3/3/7 NO3- J 9/65 N2 J12/65 N2H4
 J12/64 N2O J12/78 N2O+ J 9/64 N2O4 J12/64 N2O5 J12/78 N3
 J 6/62 NA(S) J 6/62 NA(L) J 6/62 NA J 3/65 NA+ GS4/76 NAALSIO3(S)
 3/3/7 NA- J 3/63 NAH J12/67 NAO J12/67 NAO- J12/78 NAOH(S)
 J12/78 NAOH(L) J12/78 NAOH J12/71 NAOH+ J 6/62 NA2 J 3/66 NA2CO3(S)
 J 3/66 NA2CO3(S) J 3/66 NA2CO3(L) J 6/68 NA2O(S) J 6/68 NA2O(L)
 J12/78 NA2O2H2 J12/66 NA2SO4(S) J12/66 NA2SO4(S) J12/66 NA2SO4(L)
 K11/7 NA2SO4 J 4/76 NA2SIO3(S) J 4/76 NA2SIO3(L) J 4/76 NA2SIO3(L)
 J 6/62 O L12/66 O+ J 6/65 O- J12/78 OH J12/78 OH+
 J12/78 OH- J 9/65 O2 J12/66 O2- J 6/61 O3 J 6/62 P
 J 6/61 P(S) L12/66 P+ 3/3/7 P- J 6/67 PH J 6/62 PH3
 J 9/62 PN J 6/71 PO 3/3/7 PO- J 6/67 PS 7/11/7 PO2-
 18/5/7 PO3 J 6/67 PO3- J 6/67 PS J 6/61 P2 J 6/61 P4
 J12/65 S(S) J12/65 S(L) J 6/71 S L12/66 S+ 3/3/7 S-
 J 6/67 SH J 6/61 SN J 6/71 SO 3/3/7 SO- J 6/61 SO2
 3/3/7 SO2- J 9/65 SO3 3/3/7 SO3- J12/65 S2 3/3/7 S2-
 J6/64 S8 J 3/67 SI(S) J 3/67 SI(L) J 3/67 SI J12/71 SI+
 3/3/7 SI- 18/78 SIC(S) J 3/67 SIC J 3/67 SIC2 J12/69 SIH
 J12/71 SIH+ J12/68 SIH4 J 3/67 SIN J 9/67 SIO J 6/67 SIO2(S)
 J 6/67 SIO2(S) J 6/67 SIO2(S) J 6/67 SIO2(L) J 9/67 SIO2 18/78 SIO2H2
 J12/71 SIS J 3/67 SI2 J 3/67 SI2C J 3/67 SI2N J 3/67 SI3
 8/79 TI(S)A 8/79 TI(S)B 8/79 TI(S)B 8/79 TI(L) 8/79 TI+
 8/79 TIO(S)A 8/79 TIO(S)B 8/79 TIO(L) 8/79 TIO2 8/79 TIO2(S)A
 8/79 TIO2(S)B 8/79 TIO2(L) 8/79 TIO2 8/79 TI2O3(S)
 8/79 TI3O5(S)A 8/79 TI3O5(S)B 8/79 TI3O5(L) 8/79 TI5O7(S)
 8/79 TIC(S) 8/79 TIC(L) 8/79 TIN(S) 8/79 TIN(L)
 329 16 117 61 9 755

C
 H
 N
 S

O
SI
FE
AL
MG
P
CA
NA
K
TI
AR
E

Species in Solution

AL2O3(L)
SiO2(L)
Ti2O3(L)
KALO2(L)
KALSI2O6(L)
KALSI3O8(L)
FE3O4(L)
KALSIO4(L)
K2Si2O5(L)
K2CO3(L)
K2SO4(L)

PDF = 6.688484

ENTHALPY (KG-MOL)(DEG K)/KG		EFFECTIVE FUEL HPP(2)		EFFECTIVE OXIDANT HPP(1)		MIXTURE HSUB#								
#KG-ATOMS/KG		BOP(I,2)		BOP(I,1)		B#(I)								
3-30	C	0.47784686E-01	0.00000000E 00	0.62150983E-02										
	H	0.44411376E-01	0.00000000E 00	0.57763495E-02										
	N	0.61591272E-03	0.53849950E-01	0.46926081E-01										
	S	0.29600743E-03	0.00000000E 00	0.38500097E-04										
	O	0.15532037E-01	0.14497420E-01	0.14631987E-01										
	SI	0.92621811E-03	0.00000000E 00	0.12046822E-03										
	FE	0.11209674E-03	0.00000000E 00	0.14579822E-04										
	AL	0.49741857E-03	0.00000000E 00	0.64696564E-04										
	MG	0.13096121E-03	0.00000000E 00	0.17033421E-04										
	P	0.64814049E-05	0.00000000E 00	0.84300154E-06										
	CA	0.30082284E-03	0.00000000E 00	0.39126411E-04										
	NA	0.14804160E-04	0.00000000E 00	0.19254976E-05										
	K	0.13461588E-02	0.00000000E 00	0.17508765E-03										
	TI	0.11487569E-04	0.00000000E 00	0.14941265E-05										
	AR	0.00100000E 00	0.34519879E-03	0.30030060E-03										
E	0.00000000E 00	0.00000000E 00	0.00000000E 00											
SPT	C	H	N	S	O	SI	FE	AL	MG	P	CA	NA	K	TI
1	-16.699	-11.777	-12.842	-19.974	-19.731	-20.203	-11.483	-23.712	-21.969	-22.978	-30.218	-23.484	-21.733	-25.539
	-24.387	-22.251	18.000											
AL2O3(L) REMOVED FROM SOLUTION AS TT IS 150.00 DEG K BELOW MELTING PT														
TI2O3(L) REMOVED FROM SOLUTION AS TT IS 150.00 DEG K BELOW MELTING PT														
ADD SOLUTION														
1	-16.644	-11.724	-12.878	-20.030	-19.557	-29.947	-11.450	-38.532	-21.947	-23.075	-29.623	-23.612	-23.111	-25.581
	-24.430	-22.276	8.000											
REMOVE FEO(L)														
1	-16.678	-11.732	-12.879	-20.069	-19.534	-29.891	-11.952	-38.420	-21.959	-23.109	-29.632	-23.620	-23.134	-25.620


```

-24.431 -22.282 4.0000
ADD TI3O5(S)B
1 -16.682 -11.733 -12.879 -20.074 -19.530 -29.886 -11.954 -38.414 -21.960 -23.115 -29.628 -23.622 -23.134 -31.031
-24.431 -22.275 3.0000
ADD MG2SIO4(S)
1 -16.690 -11.732 -12.882 -20.091 -19.513 -29.902 -11.945 -38.377 -26.992 -23.144 -29.595 -23.633 -23.075 -30.996
-24.435 -22.198 4.0000
ADD TIO2(S)B
1 -14.177 -10.926 -13.209 -17.824 -20.041 -20.542 -10.797 -28.618 -21.143 -22.383 -23.590 -24.512 -22.405 -23.167
-24.845 -16.446 9.0000
REMOVE TI3O5(S)B
1 -16.689 -11.732 -12.882 -20.090 -19.513 -29.900 -11.944 -38.376 -26.991 -23.144 -29.594 -23.633 -23.074 -32.492
-24.435 -22.197 9.0000

```

ION		DENS (M-3)	ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 1		ION		DENS (M-3)
1	K+	9.257E 19	2	NA+	7.592E 16		
1	FE02-	5.411E 15	2	HS-	4.490E 15	3	OH-
5	PO3-	3.474E 19	6	SO2-	8.571E 15	4	PO2-
CONDUCTIVITY =		0.0036 (MHO/M)					

1
THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED
ENTROPY AND PRESSURE

CASE NO. 103

CHEMICAL FORMULA		WT FRACTION (SEE NOTE)			ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	C 5.46166 H 4.56349 N 0.07139 S 0.03431 O 0.90000	0.74800	-21782.0000	S	298.00	0.0000		
FUEL	SI 0.80718 FE 0.09769 AL 0.43349 MG 0.11413 O 2.52526	0.09524	-288546.438	S	298.00	0.0000		
FUEL	P 2.00000 O 5.00000	0.00046	-351350.0000	S	298.00	0.0000		
FUEL	CA 0.26213 NA 0.01200 K 0.01486 TI 0.01001 O 0.29604	0.01905	-48221.102	S	298.00	0.0000		
FUEL	K 2.00000 C 1.00000 O 3.00000	0.09185	-274900.0000	S	298.00	0.0000		
FUEL	H 2.00000 O 1.00000	0.04540	-68288.0000	L	298.00	0.0000		
OXIDANT	N 2.00000	0.75426	10512.871	G	1660.00	0.0000		
OXIDANT	O 2.00000	0.23195	11101.393	G	1660.00	0.0000		
OXIDANT	AR 1.00000	0.01379	6765.552	G	1660.00	0.0000		
O/F= 6.6885 PERCENT FUEL= 13.0065 EQUIVALENCE RATIO= 1.0870 REACTANT DENSITY= 0.0000								

#THERMODYNAMIC PROPERTIES

P, ATM 4.5000
 T, DEG K 2000
 RHO, G/CC 8.3238-4
 H, CAL/G -224.0
 S, CAL/(G)(K) 2.0374
 M, MOL WT 30.357
 (DLV/DLP)T -1.00050
 (DLV/DLT)P 1.0067
 CP, CAL/(G)(K) 0.3389
 GAMMA (S) 1.2426
 SON VEL, M/SEC 825.0
 ELEC DENS 1.436 17
 IONIC DENS 1.852 20

1
3
0

SIGMA (MHO/M) 8.8836
W/O IONS 8.8837
FREQ (1/SEC) 1.128 12

MOLE FRACTIONS

AR	9.8629-3
CO	3.4142-2
COS	2.5277-7
CO2	1.5342-1
CAO(S)	1.1714-3
CAOH	9.4423-7
CAO2H2	8.4852-6
FE	1.8836-6
FEO	4.6572-7
FEOH	1.8498-7
FEO2H2	1.4438-5
FE3O4(L)	1.4127-4
H	4.8447-5
HK	1.8481-7
H2	4.8541-3
H2O	8.2415-2
H2S	8.2136-7
K	3.2119-4
K+	5.5727-6
KALO2(L)	1.8969-3
KALSiO4(L)	4.8185-6
KALSi2O6(L)	5.8635-6
KALSi3O8(L)	4.5748-5
KO	2.9972-7
KOH	1.1577-3
K2Si2O5(L)	9.2325-4
MGOH	2.3981-6
MGO2H2	9.2365-7
MG2SiO4(S)	2.5534-4
NO	4.6414-5
N2	7.8847-1
NA	2.7872-5
NAOH	3.8983-5
O	8.6175-7
OH	9.6778-5
O2	7.6233-6
PN	6.2553-7
PO	4.3374-6
PO2	1.4682-5
PO2-	3.4815-6
PO3	1.1698-7
PO3-	2.8911-6
S	2.3375-7
SH	5.3883-7
SO	2.8643-5
SO2	1.1313-3
SiO	2.4893-7
SiO2(L)	1.3814-3
TiO2(S)B	4.5844-5

#SPECIES IN SOLUTION AT LAST STATION

FE3O4(L)	KALO2(L)	KALSIO4(L)	KALSI2O6(L)	KALSI3O8(L)	K2CO3(L)	K2SO4(L)	K2SI2O5(L)	SIO2(L)	
AL(S)	AL(L)	AL	AL+	ALH	ALN(S)	ALN	ALO	ALO+	ALO-
ALOH	ALOH+	ALOH-	ALO2	ALO2-	ALO2H	ALO2H2	AL2O	AL2O+	AL2O2
AL2O2+	AL2O3(S)	AL2O3(L)	AL6O13SI2(S)	ALS	AR+	C(S)	C	C+	C-
CAL	C3-	C2H-	CH	CH+	CH2	CH2O	CH3	CH4	CN
CN+	CN-	CNN	CN2	COS-	CO2-	CO3-	CO4-	CP	CS
CS-	CS2	C2	C2-	C2H	C2H2	C2H4	C2H6	C2N	C2N2
C2O	C3	C3O2	C4	C5	CA(S)	CA(S)	CA(L)	CA	CA+
CACO3(S)	CACO3(S)	CAO(L)	CAO	CAOH+	CAO2H2(S)	CAS(S)	CASO4(S)	E	FE(S)
FE(S)	FE(S)	FE(L)	FE+	FEO(S)	FEO(L)	FEO-	FEO2	FEO2-	FEO2H2(S)
FEO3H3(S)	FES(S)	FES(S)	FES(S)	FESO4(S)	FES2(S)	FE2O3(S)	FE2O3(L)	FE3O4(S)	FE2S3O12(S)
H+	H-	HALO	HCN	HCO	HCO+	HCO3-	HCP	HNCO	HNO
HNO2	HNO3	HO2	HPO2	H2O(S)	H2O(L)	H2O2	H2P	H2SO4(L)	H2SO4
H3O+	HP-	HS-	HSI-	K(S)	K(L)	K-	KALO2(S)	KALSI3O8(S)	KCN
K2CO3(S)	K2CO3(L)	KO+	KO-	KOH(S)	KOH(S)	KOH(L)	KOH+	K2	K2O(S)
K2O(L)	K2O2H2	K2SO4(S)	K2SO4(S)	K2SO4(L)	K2SIO3(L)	MG(S)	MG(L)	MG	MG+
MGC03(S)	MGH	MGN	MGO(S)	MGO(L)	MGO	MGOH+	MGS(S)	MGS	MGSO4(S)
MGS04(L)	MG2SIO4(L)	N	NCO	NH	NH2	NH3	NO-	NO+	NO2
NO2-	NO3	NO3-	N2H4	N2O	N2O+	N2O4	N2O5	N3	NA(S)
NA(L)	NA+	NAALSI3O8(S)	NA-	NAH	NAO	NAO-	NAOH(S)	NAOH(L)	NAOH+
NA2	NA2CO3(S)	NA2CO3(S)	NA2CO3(L)	NA2O(S)	NA2O(S)	NA2O(L)	NA2O2H2	NA2SO4(S)	NA2SO4(S)
NA2SO4(S)	NA2SO4(L)	NA2SO4	NA2SIO3(S)	NA2SIO3(L)	NA2SI2O5(S)	NA2SI2O5(L)	O+	O-	OH+
OH-	O2-	O3	P	P(S)	P+	P-	PH	PH3	PO-
PS	P2	P4	S(S)	S(L)	S+	S-	SN	SO-	SO2-
SO3	SO3-	S2	S2-	S8	SI(S)	SI(L)	SI	SI+	SI-
SIC(S)	SIC	SIC2	SIH	SIH+	SIH4	SIN	SIO2(S)	SIO2(S)	SIO2(S)
SIO2	SIO2H2	SIS	SI2	SI2C	SI2N	SI3	TI(S)A	TI(S)B	TI(L)
TI	TI+	TIO(S)A	TIO(S)B	TIO(L)	TIO	TIO2(S)A	TIO2(L)	TIO2	TI2O3(S)
TI2O3(L)	TI3O5(S)A	TI3O5(S)B	TI3O5(L)	TI5O7(S)	TI5O7(L)	TIC(S)	TIC(L)	TIN(S)	TIN(L)

#NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

1

STOP

14-3

3.2 Channel Problems With Equilibrium Chemistry

In this subsection, INPUT/OUTPUT formats and their description are considered for channel flows with equilibrium chemistry. Three problems are considered. All are for MHD channel flows with conservation equations given by Eqs. (113),(115)-(116) of Section 1. In the first problem, channel entrance pressure ratio is specified, while in the second the channel entrance subsonic area ratio is given. In the third problem, we have used the two stage option of the code.

3.2.1 Input Data

For this type of problem, the REACTANTS, OMIT, SOLUTION, and INSERT cards are similar to those described in Subsection 3.1.1. The INPT2 data is also similar except, as described below, other variables peculiar to channel problems must be specified. Two additional input data are required for the channel problems, these are: RKTNP namelist, described in Table IV and CHANNEL input data (Unit 11), described in Table VI. The function of these input data will become clear as we discuss the three special problems considered here.

3.2.1.1 Input data when channel entrance pressure is specified

For this problem, the first 17 input cards are identical to that of the TP problem considered in Subsection 3.1.1.1. The description of the remaining input cards follow:

Data Card (18)	\$INPT2	KASE = 104, PC(1) = 4.5, DXI = 0.25, BZ = 6., XK = 0.8, ERATIO = T, MIX = 1.037, RKT = T, TRACE = 1.0E - 7, IONS = T, ACCURC = 1.0E-3, EXIN = 2100., HMIN = 1.0E - 30 \$END
Data Card (19)	\$RKTNP	PCP(1) = 1.428, HPATH = T, SPATH = F, IPRRKT = 1, TCHFNL = 1200. \$END

Data Card (20) BLANK CARD

Data Card (21) STOP CARD

INPT2 DATA CARD - The variables contained in this namelist are described in Table III. For channel Problems, the logical variable RKT is always set equal to TRUE. Note that only one value of P(1) is allowed.

RKTINP DATA CARD - This namelist is described in Table IV. Only one value of PCP(1), channel entrance pressure ratio, is allowed. For all channel problems HPATH and SPATH must be set equal to TRUE and FALSE respectively.

CHANNEL INPUT DATA (From FORTRAN logical Unit 11)

```
$CHNLIN            NMPATH = 0, IMPRNT = 2,  
                    XXSTOP = 2.51  
                    $END
```

CHNLIN DATA - The variables listed in this namelist are described in Table VI

3.2.1.2 Input data when channel entrance area ratio is specified.

For this problem, the first 17 input cards are identical to that of the TP problem considered in Subsection 3.1.1.1. The description of the remaining input cards follow:

```
DATA CARD (18)       $INPT2       KASE = 106, P(1) = 4.5, DXI = 0.25, BZ = 6.,  
                                    XK = 0.8, ERATIO = F, MIX = 6.6885, RKT = T,  
                                    TRACE = 1.0E-7, IONS = T, ACCURC = 1.0E-3,  
                                    EXIN = 2100.0, HMIN = 1.0E-30  
                                    $END
```

DATA CARD (19) \$RKTINP HPATH = T, SPATH = F,
 IPRRKT = 1, TCHENL = 1200.,
 SUBAR(1) = 1.0425 \$END

DATA CARD (20) BLANK CARD

DATA CARD (21) STOP

INPT2 DATA CARD - The variables contained in this namelist are described in Table III. Note that for this case, ERATIO = FALSE, therefore, the value of MIX variable equals the O/F ratio. Only one P(1) value is allowed.

RKTINP DATA CARD - This namelist is described in Table IV. For this problem a subsonic area ratio, SUBAR is specified. Only one value of SUBAR(1) is allowed.

CHANNEL INPUT DATA (From FORTRAN logical Unit 11)

\$CHNLIN NMPATH = 0, IMPRNT = 2, XXSTOP = 2.51
 \$END

CHNLIN DATA - The variables listed in this namelist are described in Table VI.

3.2.1.3 Input data for a two stage combustor model with channel entrance pressure specified

The first 17 input data cards for this problem are shown below.

REACTANTS		TWO STG						
C	5.46166H	4.56349N	0.07139S	0.03431O	0.900000	7.4800	-21782.0S	298.00F
E	10.80718FE	0.0769AL	0.43349MG	0.11413O	2.525260	0.29524	-288545.4S	298.00F
P	2.000000	5.000000					-351350.0S	298.00F
C	0.26213N	0.0129FK	0.01486TI	0.01001O	0.296040	0.01905	-40221.1S	298.00F
K	2.000000	1.000000	0.000000				-274900.0S	298.00F
H	2.000000	1.000000					-68288.0L	298.00F
N	2.000000						0.75426	4100.6G
O	2.000000						0.23195	4326.2G
AR	1.000000						0.01379	2823.4G

SOLUTION	AL2O3(L)	SiO2(L)	TI2O3(L)	KALO2(L)
SOLUTION	KALSI2O6(L)	KALSI3O8(L)	FE3O4(L)	KALSI4O4(L)
SOLUTION	K2SI2O5(L)	K2CO3(L)	K2SO4(L)	
OMIT	K2SI3O3(S)	K2SI3O3(L)		
INSERT	FeO(L)	CrO(S)		
NAMELISTS				

These 17 cards are basically the same as those of the TP problem shown in Subsection 3.1.1.1. The differences are the appearance of the letters TWO STG on the first card and the presence of the nonzero values on the last two columns of each card. The letters TWO STG flag a two-stage combustor. In this case the numbers on the last two columns of each card become the fraction of the REACTANT, shown on the same card, that is injected into the second stage. For the problem considered here, all fuel, except K_2CO_3 , and half of the oxidizer is injected into the first stage, while all of the K_2CO_3 and the remaining half of the oxidizer is injected into the second stage. The description of the remaining input cards follow.

DATA CARD (18) \$INPT2 KASSE = 1.05, P(1) = 4.5, DXI = 0.25,
 BZ = 6., XK = 0.8, ERATIO = T, MDX = 1.057,
 RKT = T, TRACE = 1.0E-7, IONS = T,
 ACCURC = 1.0E-3, EXIN = 2100.0,
 TWO STG = T, ALPH = 0.999, HMIN = 1.0E-30
 \$END

DATA CARD (19) \$RKTNP PCP(1) = 1.428, HPATH = T, SPATH = F.
 IPRRKT = 1, TCHFNL = 1200.
 \$END

DATA CARD (20) BLANK CARD

DATA CARD (21) STOP

INPT2 DATA CARD - The variables contained in this namelist are described in Table III. Note that for this case, TWOSTG = TRUE must appear in this input card. The fraction of condensed species rejected from the the first stage, denoted by ALPH, also appears here. Only one value of P(1) is allowed.

RKTNP DATA CARD - This namelist is described in Table IV. Only one value of PCP(1) is allowed.

CHANNEL INPUT DATA (From FORTRAN logical Unit 11)

```
$CHNLIN                NMPATH = 0, IMPRNT = 2, XXSTOP = 0.51,  
                         $END
```

CHNLIN DATA - The variables listed in this namelist are described in Table VI.

3.2.2 Output Data

The output data for channel problems is basically the same as that for other types of problems, see Subsection 3.1.2. In addition to the type of output described in Subsection 3.1.2, channel problems contain output related to the RKTNP and CHANNEL input data. All variables, some with multiple values, contained in the RKTNP namelist are printed out. This output appears just after the list of output that contains species in the solution. For the channel problems considered in this code a single value of SUBAR, a single value of SUPAR, or a single value of PCP is allowed.

Therefore, a single nonzero variable is printed out for the combined arrays SUBAR, SUPAR, and PCP. The remaining variables appearing in the RKTINP output, and not appearing in RKTINP input, have their default value. Output data corresponding to CHANNEL input data appear just after the printout of ion number density and conductivity for point two or three. This list contains the input data that is specified on the \$CHNLIN input data.

In more general channel problems, CHANNEL INPUTS also contain data which specifies the profiles of either the velocity, pressure, or area ratio along the channel axis. In such a case, the values of the independent variable (i.e., channel axis) and the corresponding values of the dependent variable are listed. If the dependent variable is a constant but not specified in CHANNEL INPUTS input data its value will be assigned by the program. The assigned value will be equal to the channel entrance value of the corresponding dependent variable. This value will then be printed out.

In the following, the output data corresponding to the three channel problems considered in this subsection are discussed.

3.2.2.1 Output data when channel entrance velocity is specified

The output for this problem is given in Sample Output (4). The sections containing the contents of the reactant cards and INPT2 data are the same as those of other problems such as the one described in Subsection 3.1.2.1. In the INPT2 data, however, RKT is set equal to TRUE flagging a channel problem. The output corresponding to the RKTINP contains zero values for all the SUBAR and SUPAR arrays and a single value for the PCP array. The remaining variables appearing in this output but not appearing in the RKTINP input card have their default values listed. The output data corresponding to channel input is shown on Output page 6 under CHANNEL INPUTS. All variables contained in this namelist are printed out. If the variable is not assigned in CHNLIN input data, its default value will appear. The values of dependent and independent variables are also shown under this output. If the dependent variable is a constant, a pair of constant values appear. The remaining output data has already been discussed in Subsection 3.1.2.

**Sample Output 4, Channel Problem With
Entrance Velocity Specified
(12 Output Pages)**

1

```

REACTANTS      XXXSTG
C 5.4617 H 4.5635 N 0.0714 S 0.0343 O 0.9000 0.74800 -21782.00 S 298.000 0 F 0.00000
SI 0.8072 FE 0.0977 AL 0.4335 MG 0.1141 O 2.5253 0.95240E-01 -288546.44 S 298.000 0 F 0.00000
P 2.0000 O 5.0000 0.0000 0.0000 0.0000 0.46000E-03 -351350.00 S 298.000 0 F 0.00000
CA 0.2621 NA 0.0129 K 0.0149 TI 0.0100 O 0.2960 0.19050E-01 -48221.10 S 298.000 0 F 0.00000
K 2.0000 C 1.0000 O 3.0000 0.0000 0.0000 0.91850E-01 -274900.00 S 298.000 0 F 0.00000
H 2.0000 O 1.0000 0.0000 0.0000 0.0000 0.45400E-01 -68288.00 L 298.000 0 F 0.00000
N 2.0000 0.0600 0.0000 0.0000 00 0.0000 0.75426 4100.60 G 1660.000 0 O 0.00000
O 2.0000 0.0000 0.0000 0.0000 00 0.0000 0.23195 4326.20 G 1660.000 0 O 0.00000
AR 1.0000 0.0000 0.0000 0.0000 00 0.0000 0.13790E-01 2823.40 G 1660.000 0 O 0.00000
SOLUTION      AL2O3(L)      SiO2(L)      Ti2O3(L)      KAlO2(L)
SOLUTION      KAlSi2O6(L)      KAlSi3O8(L)      Fe3O4(L)      KAlSiO4(L)
SOLUTION      K2Si2O5(L)      K2CO3(L)      K2SO4(L)
OMIT          MGSiO3(S)      MGSiO3(L)
INSERT        FEO(L)      CAO(S)
NAMELISTS
1
$INPT2
KASE = 104,
T = 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
P = 4.50000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 ,
PSIA = F,
MMHG = F,
NSQM = F,
V = 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
RHO = 4.50000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 ,
ERATIO= T,
OXFL = F,
FPCT = F,
FA = F,
MIX = 1.00000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 ,
TP = F,
HP = F,
SP = F,
TV = F,

```

UV = F,
 SV = F,
 RKT = T,
 SHOCK = F,
 DETN = F,
 OTTO = F,
 CR = 0.000000 ,
 SS = 0.000000000000 ,
 IONS = T,
 IDEBUG= 0,
 TRACE = 0.100000E-06,
 SIUNIT= F,
 DXI = 0.250000 ,
 NITER = 0,
 NSTOP = 0,
 NEOL = F,
 BZ = 6.00000 ,
 XK = 0.000000 ,
 ACCURC= 0.100000E-02,
 HMIN = 0.100000E-29,
 ALPH = 0.000000 ,
 EXIN = 2100.00 ,
 TWOSTG= F,
 \$END
 LLMT =

3-52

C
 H
 N
 S
 O
 SI
 FE
 AL
 MG
 P
 CA
 NA
 K
 TI
 AR

#SPECIES BEING CONSIDERED IN THIS SYSTEM

J12/65 AL(S)	J12/65 AL(L)
J12/62 ALN(S)	J 3/67 ALN
J12/67 ALOH	J12/67 ALOH+
J12/68 ALO2H	10/78 ALO2H2
J 6/68 AL2O2+	J 6/72 AL2O3(S)
L 5/66 AR	L12/66 AR+
J 9/65 C-	3/8/7 CAL
J12/71 CH+	J12/72 CH2
J 6/69 CN	J12/70 CN+
J 9/65 CO	J 3/61 COS
3/3/7 CO3-	3/7/7 CO4-
J 6/61 CS2	J12/69 C2
J 9/65 C2H4	L 5/72 C2H6
J12/69 C3	J 6/68 C3O2
J12/63 CA(S)	J12/63 CA(L)

J12/65 AL
J 6/70 ALO
J12/67 ALOH-
J 6/72 AL2O
J 6/75 AL2O3(L)
J 3/61 C(S)
3/3/7 C3-
J 3/61 CH2O
J12/70 CN-
3/3/7 COS-
J 6/62 CP
J12/69 C2-
J 3/67 C2N
J12/69 C4
J12/63 CA

J 6/65 AL+
J 6/70 ALO+
J12/68 ALO2
J 6/72 AL2O+
10/78 AL6O13SI2(S)
J 3/61 C
3/3/7 C2H-
J 6/69 CH3
J 6/66 CNH
J 9/65 CO2
J12/62 CS
J 3/67 C2H
J 3/61 C2N2
J12/69 C5
J12/70 CA+

J 6/63 ALH
J 12/7 ALO-
3/8/7 ALO2-
J 9/65 AL2O2
3/8/7 ALS
L12/66 C+
J12/67 CH
J 3/61 CH4
J12/70 CN2
4/12/7 CO2-
3/3/7 CS-
J 3/61 C2H2
J 9/66 C2O
J12/68 CA(S)
BAR 73 CACO3(S)

BAR 73	CACO3(S)	J 6/71	CAO(S)	J 6/71	CAO(L)	J12/74	CAO	J 6/78	CAOH
J 6/78	CAOH+	J12/71	CAO2H2(S)	J 12/7	CAO2H2	J12/71	CAS(S)	BAR 73	CASO4(S)
L82/67	E	J 3/65	FE(S)	J 3/65	FE(S)	J 3/65	FE(S)	J 3/65	FE(L)
J 3/65	FE	J1/78	FE+	J 6/65	FEO(S)	J 6/65	FEO(L)	J 9/66	FEO
4/13/7	FEO-	18/78	FEOH	4/28/7	FEO2	4/13/7	FEO2-	J 6/66	FEO2H2(S)
18/78	FEO2H2	J 6/66	FEO3H3(S)	BAR 73	FES(S)	BAR 73	FES(S)	BAR 73	FES(S)
J 6/66	FES04(S)	BAR 73	FES2(S)	J 6/65	FE2O3(S)	18/78	FE2O3(L)	J 6/65	FE3O4(S)
18/78	FE3O4(L)	J 6/66	FE2S3O12(S)	J 9/65	H	J 6/66	H+	J 9/65	H-
J 3/64	HALO	L12/69	HCN	J12/78	HCO	J12/78	HCO+	3/8/7	HCO3-
J12/69	HCP	J12/78	HK	J12/78	HNCO	J 3/63	HNO	J 6/63	HNO2
J 6/63	HNO3	J 3/64	HO2	12/21/	HPO2	J 3/61	H2	L11/65	H2O(S)
L11/65	H2O(L)	J 3/61	H2O	L 2/69	H2O2	3/8/7	H2P	J12/65	H2S
J12/66	H2SO4(L)	J12/66	H2SO4	3/25/7	H3O+	3/3/7	HP-	3/3/7	HS-
3/3/7	HSI-	J12/61	K(S)	J12/61	K(L)	J 6/62	K	J 3/65	K+
3/3/7	K-	18/78	KALO2(S)	H18/77	KALO2(L)	H18/77	KALSIO4(L)	H18/77	KALSIO2O6(L)
GS4/76	KALSIO3O8(S)	H18/77	KALSIO3O8(L)	3/8/7	KCN	J 3/66	K2CO3(S)	J 3/66	K2CO3(L)
J12/67	KO	7/29/8	KO+	J12/67	KO-	J12/78	KOH(S)	J12/78	KOH(S)
J12/78	KOH(L)	J12/78	KOH	J12/71	KOH+	J12/61	K2	J 6/63	K2O(S)
18/78	K2O(L)	J12/78	K2O2H2	J12/71	K2SO4(S)	J12/71	K2SO4(S)	J12/71	K2SO4(L)
12/79	K2SIO3(L)	H87/77	K2SIO2O5(L)	J 9/62	MG(S)	J 9/62	MG(L)	J 9/62	MG
J12/78	MG+	J12/66	MGCO3(S)	J12/66	MGH	J 3/64	MGN	J12/65	MGO(S)
18/78	MGO(L)	18/78	MGO	18/78	MGOH	J 6/68	MGOH+	18/78	MGO2H2
J12/71	MGS(S)	J 6/71	MGS	L 7/76	MGSO4(S)	L 7/76	MGSO4(L)	18/78	MG2SIO4(S)
J12/67	MG2SIO4(L)	J 3/61	N	J12/78	NCO	J12/71	NH	J12/65	NH2
J 9/65	NH3	J 6/63	NO	3/3/7	NO-	J 6/66	NO+	J 9/64	NO2
J 6/72	NO2-	J12/64	NO3	3/3/7	NO3-	J 9/65	N2	J12/65	N2H4
J12/64	N2O	J12/78	N2O+	J 9/64	N2O4	J12/64	N2O5	J12/78	N3
J 6/62	NA(S)	J 6/62	NA(L)	J 6/62	NA	J 3/65	NA+	GS4/76	NAALSIO3O8(S)
3/3/7	NA-	J 3/63	NAH	J12/67	NAO	J12/67	NAO-	J12/78	NAOH(S)
J12/78	NAOH(L)	J12/78	NAOH	J12/71	NAOH+	J 6/62	NA2	J 3/66	NA2CO3(S)
J 3/66	NA2CO3(S)	J 3/66	NA2CO3(L)	J 6/68	NA2O(S)	J 6/68	NA2O(S)	J 6/68	NA2O(L)
J12/78	NA2O2H2	J12/66	NA2SO4(S)	J12/66	NA2SO4(S)	J12/66	NA2SO4(S)	J12/66	NA2SO4(L)
K11/74	NA2SO4	J 4/76	NA2SIO3(S)	J 4/76	NA2SIO3(L)	J 4/76	NA2SIO2O5(S)	J 4/76	NA2SIO2O5(L)
J 6/62	O	L12/66	O+	J 6/65	O-	J12/78	OH	J12/78	OH+
J12/78	OH-	J 9/65	O2	J12/66	O2-	J 6/61	O3	J 6/62	P
J 6/61	P(S)	L12/66	P+	3/3/7	P-	J 6/67	PH	J 6/62	PH3
J 9/62	PN	J 6/71	PO	3/3/7	PO-	1/1/8	PO2	7/11/7	PO2-
18/5/7	PO3	2/14/9	PO3-	J 6/67	PS	J 6/61	P2	J 6/61	P4
J12/65	S(S)	J12/65	S(L)	J 6/71	S	L12/66	S+	3/3/7	S-
J 6/67	SH	J 6/61	SN	J 6/71	SO	3/3/7	SO-	J 6/61	SO2
3/3/7	SO2-	J 9/65	SO3	3/3/7	SO3-	J12/65	S2	3/3/7	S2-
J6/64	S8	J 3/67	SI(S)	J 3/67	SI(L)	J 3/67	SI	J12/71	SI+
3/3/7	SI-	18/78	SIC(S)	J 3/67	SIC	J 3/67	SIC2	J12/69	SIH
J12/71	SIH+	J12/68	SIH4	J 3/67	SIN	J 9/67	SIO	J 6/67	SIO2(S)
J 6/67	SIO2(S)	J 6/67	SIO2(S)	J 6/67	SIO2(L)	J 9/67	SIO2	18/78	SIO2H2
J12/71	SIS	J 3/67	SI2	J 3/67	SI2C	J 3/67	SI2N	J 3/67	SI3
8/79	TI(S)A	8/79	TI(S)B	8/79	TI(L)	8/79	TI	8/79	TI+
8/79	TIO(S)A	3/79	TIO(S)B	8/79	TIO(L)	8/79	TIO	8/79	TIO2(S)A
8/79	TIO2(S)B	8/79	TIO2(L)	8/79	TIO2	8/79	TI2O3(S)	8/79	TI2O3(L)
8/79	TI3O5(S)A	8/79	TI3O5(S)B	8/79	TI3O5(L)	8/79	TI5O7(S)	8/79	TI5O7(L)
8/79	TIC(S)	8/79	TIC(L)	8/79	TIN(S)	8/79	TIN(L)		
329	16	117	61	8	9	755			

O
SI
TE
AL
MG
P
CA
NA
K
TI
AR
E

SSPECIES IN SOLUTION

AL2O3(L)
SiO2(L)
Ti2O3(L)
KALO2(L)
KALSI2O6(L)
KALSI3O8(L)
FE3O4(L)
KALCIO4(L)
K2SI2O5(L)
K2CO3(L)
K2SO4(L)

*RKTINP

EQL = T,

FROZ = F,

4-5-3 SUBAR = 0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,

SUPAR = 0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,

PCP = 1.42800, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,

0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,

0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,

TCEST = 3000.00,
NFZ = 1,

NEOPT = 100000,
HTLOSS = 0.000000,

HPATH = T,
SPATH = F,

NUMHLS = 0,
CHNLIN = 1.000000,

CHNHLS = 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000,

0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
TCHINP = 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,

0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000,

TCHENL = 1200.00,
IPRRT = 1,

\$END
\$OF = 6.688484

[illegible]

ION		DENS (M-3)		ION		DENS (M-3)		ION		DENS (M-3)		ION		DENS (M-3)	
1	CA+	9.618E 15		2	CAOH+	1.489E 17		3	K+	4.415E 28		4	KOH+	7.996E 15	
5	NA+	3.839E 17													
1	ALO-	1.186E 17		2	ALO2-	1.999E 18		3	CN-	2.282E 15		4	CO2-	5.782E 17	
5	CO3-	6.473E 15		6	FEO-	2.657E 17		7	FEO2-	2.915E 19		8	H-	1.611E 17	
9	HCO3-	5.128E 16		10	HS-	9.571E 16		11	K-	3.219E 16		12	KO-	3.339E 17	
13	NO-	5.982E 16		14	NO2-	2.868E 17		15	NAO-	6.197E 15		16	O-	3.956E 18	
17	OH-	2.148E 19		18	O2-	7.812E 17		19	PO-	3.376E 15		20	PO2-	8.467E 19	
21	PO3-	2.254E 19		22	S-	3.843E 16		23	SO-	2.235E 17		24	SO2-	9.899E 17	
25	SO3-	4.954E 15													
CONDUCTIVITY =		8.8746 (MHO/M)													
2	-18.858	-12.332	-13.662	-23.523	-16.726	-24.864	-14.125	-29.919	-23.821	-27.487	-24.198	-25.927	-23.844	-29.833	
	-25.619	-15.983	4.888												
ADD CAO(S)															
2	-18.854	-12.329	-13.663	-23.526	-16.725	-24.853	-14.135	-29.892	-23.824	-27.486	-24.655	-25.931	-23.846	-29.829	
	-25.621	-15.895	3.888												
PC/PT= 1.739138		T= 2646.26													

2 -18.854 -12.329 -13.663 -23.526 -16.725 -24.053 -14.135 -29.890 -23.023 -27.406 -24.654 -25.931 -23.846 -29.028
 -25.620 -15.895 1.000
 PC/PT= 1.738415 T= 2646.38

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 2			
ION	DENS (M-3)	ION	DENS (M-3)
1 CA+	1.347E 15	2 CAOH+	2.566E 16
5 NA+	1.505E 17	3 K+	2.072E 20
4 KOH+	1.738E 15		
1 ALO-	1.161E 16	2 ALO2-	2.825E 17
5 FEO-	9.784E 16	6 FEO2-	1.583E 19
9 HS-	2.548E 16	10 K-	9.644E 15
13 NO2-	4.969E 16	14 NAO-	1.928E 15
17 O2-	1.475E 17	18 PO2-	5.529E 19
21 SO-	5.722E 16	22 SO2-	3.612E 17
23 SO3-	1.666E 15		
3 CO2-	1.468E 17	4 CO3-	1.444E 15
7 H-	3.441E 16	8 HCO3-	1.672E 16
11 KO-	1.010E 17	12 NO-	1.051E 16
15 O-	8.636E 17	16 OH-	6.389E 18
19 PO3-	1.875E 19	20 S-	9.500E 15

CONDUCTIVITY = 5.8165 (MHO/M)

3 -18.694 -12.239 -13.605 -23.434 -16.600 -23.758 -14.372 -29.287 -22.975 -27.334 -24.301 -25.890 -23.779 -28.887
 -25.474 -15.582 3.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 3			
ION	DENS (M-3)	ION	DENS (M-3)
1 CA+	3.004E 15	2 CAOH+	5.208E 16
5 NA+	2.098E 17	3 K+	2.708E 20
4 KOH+	3.004E 15		
1 ALO-	2.712E 16	2 ALO2-	5.799E 17
5 FEO-	1.415E 17	6 FEO2-	1.997E 19
9 HS-	4.080E 16	10 K-	1.495E 16
13 NO2-	8.419E 16	14 NAO-	2.957E 15
17 O2-	2.627E 17	18 PO-	1.511E 15
21 S-	1.567E 16	22 SO-	9.359E 16
23 SO2-	5.217E 17		
3 CO2-	2.423E 17	4 CO3-	2.506E 15
7 H-	6.025E 16	8 HCO3-	2.520E 16
11 KO-	1.567E 17	12 NO-	1.977E 16
15 O-	1.511E 18	16 OH-	9.951E 18
19 PO2-	6.465E 19	20 PO3-	2.016E 19
24 SO3-	2.486E 15		

CONDUCTIVITY = 6.8299 (MHO/M)

*****CHANNEL INPUTS*****

NMPATH= 1
 IMPRNT= 2
 XXSTOP= 2.5100
 VEINP= 0.00000
 ITYPE= 1

INDEPENDENT VARIABLE

0.00000

1.00000

DEPENDENT VARIABLE

744.58826

744.58826

4 -18.717 -12.252 -13.614 -23.448 -16.616 -23.792 -14.347 -29.353 -22.983 -27.345 -24.343 -25.899 -23.791 -28.906
 -25.497 -15.621 1.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 4			
ION	DENS (M-3)	ION	DENS (M-3)
1 CA+	2.728E 15	2 CAOH+	4.769E 16
5 NA+	2.007E 17	3 K+	2.613E 20
4 KOH+	2.793E 15		

1	ALO-	2.460E 16	2	ALO2-	5.338E 17	3	CO2-	2.267E 17	4	CO3-	2.328E 15
5	FEO-	1.347E 17	6	FEO2-	1.930E 19	7	H-	5.614E 16	8	HCO3-	2.377E 16
9	HS-	3.832E 16	10	K-	1.412E 16	11	KO-	1.478E 17	12	NO-	1.823E 16
13	NO2-	7.857E 16	14	NAO-	2.792E 15	15	O-	1.410E 18	16	OH-	9.396E 18
17	O2-	2.442E 17	18	PO-	1.424E 15	19	PO2-	6.311E 19	20	PO3-	1.986E 19
21	S-	1.470E 16	22	SO-	8.776E 16	23	SO2-	4.962E 17	24	SO3-	2.352E 15

CONDUCTIVITY = 6.7268 (MHO/M)

5 -18.739 -12.265 -13.624 -23.462 -16.633 -23.827 -14.321 -29.421 -22.991 -27.357 -24.386 -25.908 -23.802 -28.925
 -25.520 -15.660 1.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 5

ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 CA+	2.473E 15	2 CAOH+	4.361E 16	3 K+	2.520E 20	4 KOH+	2.594E 15
5 NA+	1.919E 17						
1 ALO-	2.227E 16	2 ALO2-	4.905E 17	3 CO2-	2.118E 17	4 CO3-	2.160E 15
5 FEO-	1.280E 17	6 FEO2-	1.864E 19	7 H-	5.225E 16	8 HCO3-	2.239E 16
9 HS-	3.596E 16	10 K-	1.332E 16	11 KO-	1.393E 17	12 NO-	1.679E 16
13 NO2-	7.322E 16	14 NAO-	2.632E 15	15 O-	1.313E 18	16 OH-	8.863E 18
17 O2-	2.267E 17	18 PO-	1.341E 15	19 PO2-	6.159E 19	20 PO3-	1.956E 19
21 S-	1.377E 16	22 SO-	8.222E 16	23 SO2-	4.716E 17	24 SO3-	2.224E 15

CONDUCTIVITY = 6.6227 (MHO/M)

6 -18.763 -12.278 -13.633 -23.476 -16.650 -23.863 -14.294 -29.490 -22.999 -27.368 -24.429 -25.917 -23.814 -28.944
 -25.543 -15.700 1.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 6

ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 CA+	2.238E 15	2 CAOH+	3.981E 16	3 K+	2.429E 20	4 KOH+	2.405E 15
5 NA+	1.833E 17						
1 ALO-	2.013E 16	2 ALO2-	4.502E 17	3 CO2-	1.977E 17	4 CO3-	2.001E 15
5 FEO-	1.216E 17	6 FEO2-	1.800E 19	7 H-	4.857E 16	8 HCO3-	2.108E 16
9 HS-	3.373E 16	10 K-	1.256E 16	11 KO-	1.311E 17	12 NO-	1.545E 16
13 NO2-	6.817E 16	14 NAO-	2.480E 15	15 O-	1.222E 18	16 OH-	8.353E 18
17 O2-	2.103E 17	18 PO-	1.261E 15	19 PO2-	6.009E 19	20 PO3-	1.926E 19
21 S-	1.289E 16	22 SO-	7.695E 16	23 SO2-	4.479E 17	24 SO3-	2.101E 15

CONDUCTIVITY = 6.5187 (MHO/M)

7 -18.786 -12.292 -13.643 -23.490 -16.667 -23.900 -14.267 -29.559 -23.008 -27.380 -24.473 -25.927 -23.826 -28.964
 -25.567 -15.740 1.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 7

ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 CA+	2.022E 15	2 CAOH+	3.630E 16	3 K+	2.340E 20	4 KOH+	2.228E 15
5 NA+	1.750E 17						
1 ALO-	1.816E 16	2 ALO2-	4.124E 17	3 CO2-	1.844E 17	4 CO3-	1.851E 15
5 FEO-	1.154E 17	6 FEO2-	1.736E 19	7 H-	4.509E 16	8 HCO3-	1.983E 16

9 HS-	3.159E 16	18 K-	1.182E 16	11 KO-	1.233E 17	12 NO-	1.418E 16
13 NO2-	6.337E 16	14 NAO-	2.334E 15	15 O-	1.135E 18	16 OH-	7.863E 18
17 O2-	1.947E 17	18 PO-	1.185E 15	19 PO2-	5.859E 19	20 PO3-	1.897E 19
21 S-	1.205E 16	22 SO-	7.194E 16	23 SO2-	4.249E 17	24 SO3-	1.983E 15
CONDUCTIVITY = 6.4127 (MHO/M)							

8 -18.818 -12.305 -13.653 -23.505 -16.684 -23.938 -14.240 -29.631 -23.016 -27.391 -24.518 -25.936 -23.838 -28.984
-25.591 -15.782 1.0000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 8							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 CA+	1.824E 15	2 CAOH+	3.305E 16	3 K+	2.253E 20	4 KOH+	2.062E 15
5 NA+	1.670E 17						
1 ALO-	1.635E 16	2 ALO2-	3.772E 17	3 CO2-	1.717E 17	4 CO3-	1.710E 15
5 FEO-	1.094E 17	6 FEO2-	1.673E 19	7 H-	4.181E 16	8 HCO3-	1.862E 16
9 HS-	2.956E 16	10 K-	1.112E 16	11 KO-	1.158E 17	12 NO-	1.300E 16
13 NO2-	5.882E 16	14 NAO-	2.194E 15	15 O-	1.053E 18	16 OH-	7.393E 18
17 O2-	1.800E 17	18 PO-	1.112E 15	19 PO2-	5.711E 19	20 PO3-	1.867E 19
21 S-	1.125E 16	22 SO-	6.717E 16	23 SO2-	4.028E 17	24 SO3-	1.869E 15
CONDUCTIVITY = 6.3057 (MHO/M)							

9 -18.834 -12.319 -13.663 -23.519 -16.702 -23.978 -14.212 -29.703 -23.025 -27.403 -24.564 -25.945 -23.851 -29.004
-25.615 -15.824 1.0000

3-50

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 9							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 CA+	1.643E 15	2 CAOH+	3.004E 16	3 K+	2.168E 20	4 KOH+	1.906E 15
5 NA+	1.592E 17						
1 ALO-	1.470E 16	2 ALO2-	3.444E 17	3 CO2-	1.597E 17	4 CO3-	1.578E 15
5 FEO-	1.035E 17	6 FEO2-	1.611E 19	7 H-	3.871E 16	8 HCO3-	1.748E 16
9 HS-	2.764E 16	10 K-	1.045E 16	11 KO-	1.087E 17	12 NO-	1.190E 16
13 NO2-	5.453E 16	14 NAO-	2.060E 15	15 O-	9.757E 17	16 OH-	6.944E 18
17 O2-	1.662E 17	18 PO-	1.043E 15	19 PO2-	5.564E 19	20 PO3-	1.837E 19
21 S-	1.050E 16	22 SO-	6.266E 16	23 SO2-	3.814E 17	24 SO3-	1.760E 15
CONDUCTIVITY = 6.1979 (MHO/M)							

10 -18.858 -12.333 -13.674 -23.534 -16.720 -24.018 -14.183 -29.776 -23.033 -27.414 -24.610 -25.955 -23.863 -29.025
-25.640 -15.867 1.0000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 10							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 CA+	1.476E 15	2 CAOH+	2.726E 16	3 K+	2.085E 20	4 KOH+	1.759E 15
5 NA+	1.517E 17						
1 ALO-	1.318E 16	2 ALO2-	3.140E 17	3 CO2-	1.483E 17	4 CO3-	1.454E 15
5 FEO-	9.795E 16	6 FEO2-	1.550E 19	7 H-	3.580E 16	8 HCO3-	1.638E 16
9 HS-	2.581E 16	10 K-	9.810E 15	11 KO-	1.019E 17	12 NO-	1.088E 16
13 NO2-	5.048E 16	14 NAO-	1.933E 15	15 O-	9.027E 17	16 OH-	6.514E 18

17 O2-	1.531E 17	18 PO2-	5.419E 19	19 PO3-	1.807E 19	20 S-	9.782E 15
21 SO-	5.838E 16	22 SO2-	3.609E 17	23 SO3-	1.656E 15		
CONDUCTIVITY = 6.0892 (MHO/M)							

11 -18.882 -12.347 -13.684 -23.549 -16.739 -24.060 -14.154 -29.851 -23.042 -27.426 -24.658 -25.965 -23.876 -29.047
 -25.665 -15.910 1.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 11

ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 CA+	1.325E 15	2 CAOH+	2.470E 16	3 K+	2.004E 20	4 KOH+	1.622E 15
5 NA+	1.444E 17						
1 ALO-	1.180E 16	2 ALO2-	2.857E 17	3 CO2-	1.376E 17	4 CO3-	1.337E 15
5 FEO-	9.256E 16	6 FEO2-	1.491E 19	7 H-	3.306E 16	8 HCO3-	1.534E 16
9 HS-	2.409E 16	10 K-	9.199E 15	11 KO-	9.539E 16	12 NO-	9.928E 15
13 NO2-	4.666E 16	14 NAO-	1.811E 15	15 O-	8.339E 17	16 OH-	6.104E 18
17 O2-	1.409E 17	18 PO2-	5.275E 19	19 PO3-	1.777E 19	20 S-	9.106E 15
21 SO-	5.432E 16	22 SO2-	3.411E 17	23 SO3-	1.556E 15		
CONDUCTIVITY = 5.9797 (MHO/M)							

12 -18.907 -12.362 -13.695 -23.563 -16.758 -24.104 -14.125 -29.927 -23.051 -27.438 -24.706 -25.974 -23.888 -29.068
 -25.690 -15.955 1.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 12

ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 CA+	1.186E 15	2 CAOH+	2.234E 16	3 K+	1.926E 20	4 KOH+	1.494E 15
5 NA+	1.374E 17						
1 ALO-	1.055E 16	2 ALO2-	2.596E 17	3 CO2-	1.275E 17	4 CO3-	1.228E 15
5 FEO-	8.737E 16	6 FEO2-	1.432E 19	7 H-	3.048E 16	8 HCO3-	1.435E 16
9 HS-	2.245E 16	10 K-	8.616E 15	11 KO-	8.920E 16	12 NO-	9.044E 15
13 NO2-	4.306E 16	14 NAO-	1.695E 15	15 O-	7.692E 17	16 OH-	5.713E 18
17 O2-	1.294E 17	18 PO2-	5.133E 19	19 PO3-	1.746E 19	20 S-	8.467E 15
21 SO-	5.049E 16	22 SO2-	3.222E 17	23 SO3-	1.461E 15		
CONDUCTIVITY = 5.8692 (MHO/M)							

13 -18.932 -12.376 -13.705 -23.578 -16.778 -24.148 -14.095 -30.004 -23.060 -27.449 -24.755 -25.984 -23.901 -29.091
 -25.716 -16.001 1.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 13

ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 CA+	1.060E 15	2 CAOH+	2.017E 16	3 K+	1.849E 20	4 KOH+	1.374E 15
5 NA+	1.306E 17						
1 ALO-	9.406E 15	2 ALO2-	2.354E 17	3 CO2-	1.179E 17	4 CO3-	1.126E 15
5 FEO-	8.237E 16	6 FEO2-	1.374E 19	7 H-	2.807E 16	8 HCO3-	1.340E 16
9 HS-	2.091E 16	10 K-	8.061E 15	11 KO-	8.331E 16	12 NO-	8.224E 15
13 NO2-	3.960E 16	14 NAO-	1.584E 15	15 O-	7.083E 17	16 OH-	5.341E 18
17 O2-	1.187E 17	18 PO2-	4.993E 19	19 PO3-	1.716E 19	20 S-	7.864E 15
21 SO-	4.688E 16	22 SO2-	3.039E 17	23 SO3-	1.370E 15		

CONDUCTIVITY = 5.7579 (MHO/M)

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THEORETICAL MHD CORE PERFORMANCE

SPC = 66.1 PSIA
CASE NO. 104

CASE NO. 104						WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC		
CHEMICAL FORMULA												
FUEL	C	5.46166	H	4.56349	N 0.07139	S 0.03431	O 0.90000	0.74800	-21782.000	S	298.00	0.0000
FUEL	SI	0.80718	FE	0.09769	AL 0.43349	MG 0.11413	O 2.52526	0.09524	-288546.438	S	298.00	0.0000
FUEL	P	2.00000	O	5.00000				0.00046	-351350.000	S	298.00	0.0000
FUEL	CA	0.26213	NA	0.01290	K 0.01486	TI 0.01001	O 0.29604	0.01905	-48221.102	S	298.00	0.0000
FUEL	K	2.00000	C	1.00000	O 3.00000			0.09185	-274900.000	S	298.00	0.0000
FUEL	H	2.00000	O	1.00000				0.04540	-68288.000	L	298.00	0.0000
OXIDANT	N	2.00000						0.75426	10512.871	G	1660.00	0.0000
OXIDANT	O	2.00000						0.23195	11101.393	G	1660.00	0.0000
OXIDANT	AR	1.00000						0.01379	6765.552	G	1660.00	0.0000
O/F=		6.6885	PERCENT FUEL=		13.0065	EQUIVALENCE RATIO=		1.0870	REACTANT DENSITY=		0.0000	

O/F= 6.6885 PERCENT FUEL= 13.0065 EQUIVALENCE RATIO= 1.0870 REACTANT DENSITY= 0.0000

AXIAL STATION (M)														
	CHAMBER	THROAT	0.0000	0.2500	0.5000	0.7500	1.0000	1.2500	1.5000	1.7500	2.0000	2.2500	2.5000	
PC/P	1.0000	1.7384	1.4280	1.4698	1.5135	1.5590	1.6066	1.6564	1.7084	1.7628	1.8197	1.8792	1.9416	
P, ATM	4.5000	2.5886	3.1513	3.0616	2.9733	2.8864	2.8009	2.7168	2.6341	2.5528	2.4730	2.3946	2.3177	
T, DEG K	2808	2646	2703	2696	2689	2681	2674	2667	2659	2652	2644	2637	2629	
RHO, G/CC	5.7300-4	3.5336-4	4.1970-4	4.0899-4	3.9840-4	3.8794-4	3.7763-4	3.6745-4	3.5741-4	3.4751-4	3.3775-4	3.2815-4	3.1869-4	
H, CAL/G	197.3	95.7	131.0	126.8	122.6	118.3	114.0	109.6	105.2	100.7	96.2	91.6	87.0	
S, CAL/(G)(K)	2.2092	2.2092	2.2092	2.2096	2.2100	2.2104	2.2108	2.2112	2.2116	2.2120	2.2124	2.2129	2.2133	
M, MOL WT	29.341	29.643	29.538	29.550	29.561	29.573	29.585	29.597	29.610	29.622	29.634	29.647	29.660	
(DLV/DLP)T	-1.01222	-1.00981	-1.01080	-1.01070	-1.01059	-1.01048	-1.01037	-1.01025	-1.01013	-1.01001	-1.00989	-1.00977	-1.00964	
(DLV/DLP)P	1.2972	1.2053	1.2834	1.2818	1.2800	1.2782	1.2763	1.2743	1.2722	1.2700	1.2676	1.2652	1.2626	
CP, CAL/(G)(K)	0.8120	0.7357	0.8094	0.8075	0.8054	0.8032	0.8009	0.7984	0.7957	0.7929	0.7899	0.7867	0.7833	
GAMMA (S)	1.1470	1.1452	1.1443	1.1443	1.1444	1.1444	1.1445	1.1446	1.1446	1.1447	1.1448	1.1450	1.1451	
VELOCITY, M/SEC			744.59	744.59	744.59	744.59	744.59	744.59	744.59	744.59	744.59	744.59	744.59	
TOTAL H(CAL/G)			197.28	193.09	188.85	184.56	180.23	175.86	171.44	166.97	162.46	157.90	153.29	
MAG FLD(TESLA)			6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	
BETA			1.67	1.72	1.76	1.81	1.86	1.92	1.97	2.03	2.09	2.15	2.22	
SON VEL, M/SEC	955.3	922.0	933.0	931.7	930.3	928.8	927.4	926.0	924.5	923.1	921.6	920.1	918.6	
ELEC DENS	2.747 20	1.089 20	1.528 20	1.466 20	1.405 20	1.346 20	1.288 20	1.231 20	1.177 20	1.123 20	1.071 20	1.021 20	9.722 19	
IONIC DENS	6.096 20	3.059 20	3.097 20	3.768 20	3.642 20	3.519 20	3.398 20	3.281 20	3.165 20	3.053 20	2.943 20	2.836 20	2.731 20	
SIGMA (MHO/M)	8.8746	5.8165	6.8299	6.7268	6.6227	6.5187	6.4127	6.3057	6.1979	6.0892	5.9797	5.8692	5.7579	
W/O IONS	9.5230	6.2364	7.3245	7.2146	7.1034	6.9925	6.8793	6.7652	6.6502	6.5342	6.4172	6.2992	6.1804	
FREQ (1/SEC)	8.723 11	5.278 11	6.305 11	6.140 11	5.973 11	5.817 11	5.659 11	5.503 11	5.350 11	5.198 11	5.049 11	4.902 11	4.758 11	
MACH NUMBER	0.0000	1.0000	0.7930	0.7992	0.8004	0.8016	0.8029	0.8041	0.8054	0.8066	0.8079	0.8092	0.8106	
AE/AT		1.0000	1.0425	1.0698	1.0983	1.1279	1.1587	1.1908	1.2242	1.2591	1.2955	1.3334	1.3730	
TOTAL MOL WT	29.266	29.530	29.442	29.451	29.461	29.471	29.481	29.491	29.502	29.512	29.522	29.533	29.544	

MOLE FRACTIONS

ALO2	1.2918-7	2.4179-8	4.4802-8	4.1972-8	3.9270-8	3.6693-8	3.4239-8	3.1906-8	2.9692-8	2.7593-8	2.5606-8	2.3727-8	2.1954-8	
ALO2-	1.6951-7	3.9196-8	6.7545-8	6.3822-8	6.0232-8	5.6784-8	5.3457-8	5.0265-8	4.7203-8	4.4272-8	4.1468-8	3.8790-8	3.6236-8	
ALO2H	1.1619-6	3.1861-7	5.1251-7	4.8755-7	4.6335-7	4.3991-7	4.1722-7	3.9533-7	3.7419-7	3.5383-7	3.3423-7	3.1537-7	2.9727-7	
ALO2H2	1.1983-6	3.7935-7	5.7721-7	5.5173-7	5.2692-7	5.0279-7	4.7935-7	4.5663-7	4.3460-7	4.1330-7	3.9270-7	3.7279-7	3.5359-7	

AL2O3(L)	6.4009-7	2.8374-7	3.8186-7	3.7188-7	3.6196-7	3.5212-7	3.4236-7	3.3271-7	3.2317-7	3.1377-7	3.0448-7	2.9533-7	2.8632-7
AR	8.7887-3	8.8679-3	8.8414-3	8.9443-3	8.8472-3	8.8502-3	8.8532-3	8.8563-3	8.8594-3	8.8625-3	8.8656-3	8.8688-3	8.8720-3
CO	6.9710-2	5.8906-2	6.2597-2	6.2181-2	6.1761-2	6.1336-2	6.0906-2	6.0472-2	6.0033-2	5.9590-2	5.9142-2	5.8689-2	5.8232-2
CO2	1.1218-1	1.2463-1	1.2039-1	1.2086-1	1.2134-1	1.2183-1	1.2232-1	1.2282-1	1.2332-1	1.2383-1	1.2434-1	1.2486-1	1.2538-1
CA	1.4604-5	6.8005-6	9.8866-6	9.5009-6	9.1237-6	8.7548-6	8.3941-6	8.0418-6	7.6978-6	7.3623-6	7.0351-6	6.7164-6	6.4060-6
CAO(S)	0.0000-0	4.2325-4	2.0332-4	2.3178-4	2.5989-4	2.8766-4	3.1509-4	3.4215-4	3.6885-4	3.9518-4	4.2113-4	4.4669-4	4.7187-4
CAO	1.2353-5	5.0967-6	7.7655-6	7.4119-6	7.0685-6	6.7347-6	6.4107-6	6.0964-6	5.7918-6	5.4968-6	5.2113-6	4.9352-6	4.6685-6
CAOH	6.5939-4	3.9271-4	5.2261-4	5.0616-4	4.8994-4	4.7394-4	4.5818-4	4.4265-4	4.2737-4	4.1233-4	3.9753-4	3.8299-4	3.6870-4
CAO2H2	4.5873-4	3.2755-4	4.0337-4	3.9749-4	3.8670-4	3.7601-4	3.6543-4	3.5495-4	3.4458-4	3.3433-4	3.2420-4	3.1418-4	3.0429-4
E	2.3298-5	1.5116-5	1.7799-5	1.7526-5	1.7250-5	1.6975-5	1.6694-5	1.6412-5	1.6127-5	1.5839-5	1.5550-5	1.5258-5	1.4965-5
FE	1.9474-4	1.3823-4	1.9104-4	1.9097-4	1.9090-4	1.9081-4	1.9071-4	1.9060-4	1.9047-4	1.9033-4	1.9016-4	1.8997-4	1.8975-4
FEO	1.7552-4	1.7242-4	1.7468-4	1.7448-4	1.7426-4	1.7401-4	1.7375-4	1.7346-4	1.7315-4	1.7281-4	1.7244-4	1.7203-4	1.7159-4
FEOH	8.6011-6	8.4052-6	8.5049-6	8.4795-6	8.4535-6	8.4267-6	8.3993-6	8.3709-6	8.3417-6	8.3115-6	8.2802-6	8.2477-6	8.2139-6
FE02	2.6804-5	2.7492-5	2.7531-5	2.7510-5	2.7485-5	2.7456-5	2.7422-5	2.7384-5	2.7340-5	2.7291-5	2.7235-5	2.7173-5	2.7103-5
FE02-	2.4719-6	2.1965-6	2.3263-6	2.3080-6	2.2891-6	2.2700-6	2.2500-6	2.2293-6	2.2080-6	2.1860-6	2.1633-6	2.1399-6	2.1157-6
FE02H2	1.7694-5	2.4316-5	2.1752-5	2.1950-5	2.2152-5	2.2359-5	2.2571-5	2.2789-5	2.3011-5	2.3239-5	2.3472-5	2.3710-5	2.3954-5
FE3O4(L)	2.8175-7	2.4723-6	1.1339-6	1.2275-6	1.3305-6	1.4442-6	1.5699-6	1.7089-6	1.8628-6	2.0334-6	2.2227-6	2.4331-6	2.6670-6
H	3.1495-3	2.0985-3	2.4318-3	2.3952-3	2.3585-3	2.3217-3	2.2847-3	2.2476-3	2.2104-3	2.1731-3	2.1356-3	2.0980-3	2.0603-3
HK	2.3233-6	1.4766-6	1.7362-6	1.7013-6	1.6665-6	1.6319-6	1.5975-6	1.5633-6	1.5294-6	1.4956-6	1.4621-6	1.4288-6	1.3958-6
HNO	7.1314-7	3.2874-7	4.3639-7	4.2130-7	4.0648-7	3.9192-7	3.7763-7	3.6362-7	3.4988-7	3.3642-7	3.2324-7	3.1033-7	2.9771-7
HO2	2.6626-6	1.2778-6	1.6812-6	1.6272-6	1.5738-6	1.5211-6	1.4691-6	1.4179-6	1.3674-6	1.3176-6	1.2687-6	1.2205-6	1.1731-6
H2	6.3769-3	5.4144-3	5.7291-3	5.6947-3	5.6601-3	5.6252-3	5.5900-3	5.5545-3	5.5187-3	5.4826-3	5.4462-3	5.4096-3	5.3726-3
H2O	6.9973-2	7.3882-2	7.2532-2	7.2686-2	7.2842-2	7.2998-2	7.3155-2	7.3313-2	7.3472-2	7.3632-2	7.3793-2	7.3954-2	7.4117-2
H2O2	2.3773-7	1.1897-7	1.5364-7	1.4875-7	1.4392-7	1.3916-7	1.3447-7	1.2985-7	1.2530-7	1.2083-7	1.1643-7	1.1211-7	1.0787-7
K	1.7731-3	1.7655-3	1.7700-3	1.7719-3	1.7739-3	1.7758-3	1.7778-3	1.7797-3	1.7817-3	1.7836-3	1.7855-3	1.7874-3	1.7893-3
K+	3.7440-5	2.8757-5	3.1547-5	3.1247-5	3.0944-5	3.0635-5	3.0330-5	3.0023-5	2.9714-5	2.9404-5	2.9092-5	2.8779-5	2.8464-5
KALO2(L)	1.8065-3	1.7430-3	1.7652-3	1.7629-3	1.7605-3	1.7581-3	1.7558-3	1.7534-3	1.7511-3	1.7487-3	1.7463-3	1.7442-3	1.7420-3
KALSiO4(L)	1.2583-5	1.7086-5	1.5933-5	1.6074-5	1.6209-5	1.6338-5	1.6463-5	1.6581-5	1.6693-5	1.6798-5	1.6896-5	1.6986-5	1.7068-5
KALSi2O6(L)	6.3003-5	1.0984-4	9.7449-5	9.8906-5	1.0030-4	1.0163-4	1.0288-4	1.0406-4	1.0515-4	1.0616-4	1.0706-4	1.0785-4	1.0853-4
KALSi3O8(L)	7.3886-6	3.9269-5	2.4197-5	2.5675-5	2.7225-5	2.8851-5	3.0557-5	3.2343-5	3.4208-5	3.6155-5	3.8183-5	4.0290-5	4.2477-5
KO	5.1213-5	3.4352-5	3.9900-5	3.9192-5	3.8484-5	3.7774-5	3.7063-5	3.6350-5	3.5637-5	3.4923-5	3.4208-5	3.3492-5	3.2777-5
KOH	1.3645-3	1.4034-3	1.3916-3	1.3908-3	1.3900-3	1.3892-3	1.3884-3	1.3875-3	1.3867-3	1.3858-3	1.3848-3	1.3839-3	1.3829-3
K2Si2O5(L)	3.0487-6	1.3851-5	8.6358-6	9.0614-6	9.5074-6	9.9743-6	1.0463-5	1.0973-5	1.1506-5	1.2061-5	1.2640-5	1.3242-5	1.3868-5
MG	7.6803-5	6.9039-5	7.1809-5	7.1652-5	7.1490-5	7.1325-5	7.1154-5	7.0979-5	7.0800-5	7.0615-5	7.0425-5	7.0229-5	7.0027-5
MGH	2.9771-7	1.7743-7	2.1352-7	2.0888-7	2.0428-7	1.9970-7	1.9516-7	1.9065-7	1.8618-7	1.8174-7	1.7734-7	1.7298-7	1.6865-7
MGO	2.6787-5	1.8605-5	2.1330-5	2.1010-5	2.0688-5	2.0365-5	2.0040-5	1.9713-5	1.9384-5	1.9054-5	1.8721-5	1.8388-5	1.8052-5
MGOH	3.8207-4	3.9967-4	3.9376-4	3.9432-4	3.9489-4	3.9546-4	3.9605-4	3.9663-4	3.9723-4	3.9783-4	3.9843-4	3.9905-4	3.9966-4
MG02H2	1.2519-5	1.5493-5	1.4369-5	1.4453-5	1.4538-5	1.4626-5	1.4715-5	1.4807-5	1.4902-5	1.4998-5	1.5098-5	1.5200-5	1.5304-5
N	1.4376-6	5.3936-7	7.7076-7	7.3964-7	7.0926-7	6.7961-7	6.5068-7	6.2248-7	5.9501-7	5.6826-7	5.4225-7	5.1695-7	4.9237-7
NO	9.2563-3	6.2126-3	7.2212-3	7.0996-3	6.9774-3	6.8547-3	6.7313-3	6.6075-3	6.4832-3	6.3583-3	6.2330-3	6.1073-3	5.9811-3
NO2	3.0198-6	1.5089-6	1.9594-6	1.8986-6	1.8384-6	1.7790-6	1.7202-6	1.6622-6	1.6049-6	1.5484-6	1.4926-6	1.4377-6	1.3837-6
N2	6.8205-1	6.8976-1	6.8713-1	6.8747-1	6.8776-1	6.8805-1	6.8835-1	6.8865-1	6.8895-1	6.8926-1	6.8957-1	6.8988-1	6.9019-1
N2O	9.2304-7	4.7045-7	6.0299-7	5.8436-7	5.6598-7	5.4786-7	5.3000-7	5.1241-7	4.9508-7	4.7802-7	4.6125-7	4.4475-7	4.2854-7
NA	4.1633-5	4.2411-5	4.2141-5	4.2204-5	4.2268-5	4.2332-5	4.2397-5	4.2463-5	4.2529-5	4.2596-5	4.2664-5	4.2732-5	4.2800-5
NAO	1.1195-6	7.8103-7	8.9369-7	8.7884-7	8.6395-7	8.4902-7	8.3404-7	8.1902-7	8.0397-7	7.8889-7	7.7378-7	7.5864-7	7.4347-7
NAOH	1.3495-5	1.3593-5	1.3574-5	1.3546-5	1.3518-5	1.3489-5	1.3460-5	1.3430-5	1.3400-5	1.3369-5	1.3338-5	1.3307-5	1.3276-5
O	3.0797-3	1.7523-3	2.1655-3	2.1183-3	2.0710-3	2.0238-3	1.9765-3	1.9293-3	1.8821-3	1.8349-3	1.7879-3	1.7408-3	1.6939-3
O-	3.3549-7	1.1983-7	1.7602-7	1.6853-7	1.6122-7	1.5411-7	1.4714-7	1.4035-7	1.3373-7	1.2729-7	1.2103-7	1.1494-7	1.0903-7
OH	9.7839-3	6.9265-3	7.8350-3	7.7756-3	7.6653-3	7.5540-3	7.4418-3	7.3288-3	7.2148-3	7.0999-3	6.9842-3	6.8675-3	6.7500-3
CH-	1.8147-6	8.8605-7	1.1591-6	1.1235-6	1.0833-6	1.0537-6	1.0192-6	9.8526-7	9.5171-7	9.1860-7	8.8596-7	8.5379-7	8.2210-7
O2	1.3817-2	9.866-3	1.1277-2	1.1125-2	1.0972-2	1.0816-2	1.0657-2	1.0496-2	1.0333-2	1.0167-2	9.9989-3	9.8281-3	9.6549-3
PN	1.2910-7	9.2553-8	1.0373-7	1.0227-7	1.0082-7	9.9371-8	9.7938-8	9.6513-8	9.5098-8	9.3692-8	9.2295-8	9.0909-8	8.9534-8
PO	5.0869-6	4.1553-6	4.4599-6	4.4269-6	4.3937-6	4.3600-6	4.3264-6	4.2926-6	4.2586-6	4.2244-6	4.1901-6	4.1556-6	4.1209-6
PO2	1.0188-5	1.0187-5	1.0201-5	1.0201-5	1.0200-5	1.0200-5	1.0200-5	1.0199-5	1.0198-5	1.0197-5	1.0196-5	1.0195-5	1.0194-5
PO2-	7.1875-6	7.6715-6	7.5305-6	7.5466-6	7.5625-6	7.5791-6	7.5948-6	7.6103-6	7.6257-6	7.6409-6	7.6559-6	7.6707-6	7.6854-6
PO3	1.7561-7	1.7593-7	1.7671-7	1.7647-7	1.7621-7	1.7592-7	1.7564-7	1.7534-7	1.7502-7	1.7469-7	1.7434-7	1.7398-7	1.7360-7

PO3-	1.9112-6	2.6011-6	2.3477-6	2.3745-6	2.4019-6	2.4300-6	2.4585-6	2.4875-6	2.5172-6	2.5475-6	2.5784-6	2.6099-6	2.6421-6
S	2.6233-6	1.4527-6	1.7883-6	1.7469-6	1.7059-6	1.6653-6	1.6251-6	1.5854-6	1.5460-6	1.5070-6	1.4685-6	1.4304-6	1.3928-6
SH	6.6609-7	3.7261-7	4.5558-7	4.4452-7	4.3361-7	4.2284-7	4.1221-7	4.0171-7	3.9136-7	3.8116-7	3.7110-7	3.6119-7	3.5143-7
SO	1.1066-4	8.1559-5	9.0887-5	8.9779-5	8.8668-5	8.7554-5	8.6437-5	8.5317-5	8.4194-5	8.3069-5	8.1942-5	8.0812-5	7.9681-5
SO2	1.0123-3	1.0531-3	1.0400-3	1.0415-3	1.0430-3	1.0446-3	1.0462-3	1.0477-3	1.0493-3	1.0509-3	1.0525-3	1.0541-3	1.0557-3
SO3	2.9049-7	2.4582-7	2.6259-7	2.6020-7	2.5778-7	2.5532-7	2.5283-7	2.5030-7	2.4774-7	2.4514-7	2.4251-7	2.3984-7	2.3714-7
SIO	2.4369-3	1.5373-3	1.8933-3	1.8566-3	1.8190-3	1.7804-3	1.7409-3	1.7005-3	1.6593-3	1.6173-3	1.5745-3	1.5310-3	1.4869-3
SIO2(L)	6.6635-4	1.4661-3	1.1453-3	1.1786-3	1.2128-3	1.2479-3	1.2840-3	1.3210-3	1.3588-3	1.3974-3	1.4369-3	1.4770-3	1.5179-3
SIO2	2.5560-4	1.7176-4	2.0752-4	2.0377-4	1.9990-4	1.9591-4	1.9180-4	1.8759-4	1.8326-4	1.7883-4	1.7431-4	1.6969-4	1.6498-4
TIO	3.5661-7	2.0532-7	2.5247-7	2.4674-7	2.4102-7	2.3531-7	2.2961-7	2.2392-7	2.1824-7	2.1256-7	2.0690-7	2.0125-7	1.9561-7
TIO2	4.2297-5	4.0059-5	4.1296-5	4.1196-5	4.1088-5	4.0971-5	4.0846-5	4.0710-5	4.0564-5	4.0407-5	4.0238-5	4.0056-5	3.9860-5
TI2O3(L)	5.3724-7	1.9283-6	1.2206-6	1.2808-6	1.3450-6	1.4135-6	1.4867-6	1.5648-6	1.6482-6	1.7373-6	1.8325-6	1.9342-6	2.0429-6

0SPECIES IN SOLUTION AT LAST STATION

AL2O3(L)	FE3O4(L)	KALO2(L)	KALSIO4(L)	KALSI2O6(L)	KALSI3O8(L)	K2CO3(L)	K2SO4(L)	K28I2O5(L)	SIO2(L)
SIO2(L)	TI2O3(L)								

0ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-06 FOR ALL ASSIGNED CONDITIONS

AL(S)	AL(L)	AL	AL+	ALH	ALN(S)	ALN	ALO	ALO+	ALO-
ALOH	ALOH+	ALOH-	AL2O	AL2O+	AL2O2	AL2O2+	AL2O3(S)	AL6O13SI2(S)	AL5
AR+	C(S)	C	C+	C-	CAL	C3-	C2H-	CH	CH+
CH2	CH2O	CH3	CH4	CN	CN+	CN-	CNN	CN2	COS
COS-	CO2-	CO3-	CO4-	CP	CS	CS-	CS2	C2	C2-
C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2O	C3	C3O2	C4
C5	CA(S)	CA(S)	CA(L)	CA+	CACO3(S)	CACO3(S)	CAO(L)	CAOH+	CAO2H2(S)
CAS(S)	CASO4(S)	FE(S)	FE(S)	FE(S)	FE(L)	FE+	FEO(S)	FEO(L)	FEO-
FE02H2(S)	FE03H3(S)	FES(S)	FES(S)	FES(S)	FESO4(S)	FES2(S)	FE2O3(S)	FE2O3(L)	FE3O4(S)
FE2S3O12(S)	H+	H-	HALO	HCN	HCO	HCO+	HCO3-	HCP	HNCO
HNO2	HNO3	HPO2	H2O(S)	H2O(L)	H2P	H2S	H2SO4(L)	H2SO4	H3O+
HP-	HS-	HSI-	K(S)	K(L)	K-	KALO2(S)	KALSI3O8(S)	KCN	K2CO3(S)
K2CO3(L)	KO+	KO-	KOH(S)	KOH(S)	KOH(L)	KOH+	K2	K2O(S)	K2O(L)
K2O2H2	K2SO4(S)	K2SO4(S)	K2SO4(L)	K2SIO3(L)	MG(S)	MG(L)	MG+	MGCO3(S)	MGN
MGO(S)	MGO(L)	MGOH+	MGS(S)	MGS	MGSO4(S)	MGSO4(L)	MGSIO4(S)	MGSIO4(L)	NCO
NH	NH2	NH3	NC-	NO+	NO2-	NO3	NO3-	N2H4	N2O+
N2O4	N2O5	N3	NA(S)	NA(L)	NA+	NAALSI3O8(S)	NA-	NAH	NAO-
NAOH(S)	NAOH(L)	NAOH+	NA2	NA2CO3(S)	NA2CO3(S)	NA2CO3(L)	NA2O(S)	NA2O(S)	NA2O(L)
NA2O2H2	NA2SO4(S)	NA2SO4(S)	NA2SO4(S)	NA2SO4(L)	NA2SO4	NA2SIO3(S)	NA2SIO3(L)	NA2SIO5(S)	NA2SIO5(L)
O+	OH+	O2-	O3	P	P(S)	P+	P-	PH	PH3
PO-	PS	P2	P4	S(S)	S(L)	S+	S-	SN	SO-
SO2-	SO3-	S2	S2-	S8	SI(S)	SI(L)	SI	SI+	SI-
SIC(S)	SIC	SIC2	SIH	SIH+	SIH4	SIN	SIO2(S)	SIO2(S)	SIO2(S)
SIO2H2	SIS	SI2	SI2C	SI2N	SI3	TI(S)A	TI(S)B	TI(L)	TI
TI+	TIO(S)A	TIO(S)B	TIO(L)	TIO2(S)A	TIO2(S)B	TIO2(L)	TI2O3(S)	TI3O5(S)A	TI3O5(S)B
TI3O5(L)	TI5O7(S)	TI5O7(L)	TIC(S)	TIC(L)	TIN(S)	TIN(L)			

0NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

1

STOP 5 IS NORMAL CHANNEL STOP

IT OCCURS WHEN XPOSITION EXCEEDS INPUTTED XXSTOP VALUE

3.2.2.2 Output data when channel entrance area ratio is specified.

The output for this problem is given in Sample Output (5). The main difference between this output and the output for the previous problem is that in this case one value of SUBAR (i. e., subsonic area ratio) is specified in RKTINP output data instead of PCP. Since the format of the output data for this problem is the same as that of the previous problem, no further description will be given.

3.2.2.3 Output data for a two-stage combustor model with channel entrance velocity specified.

The output for this problem is given in Sample Output (6). The contents of the output associated with REACTANT, INPT2, and RKTINP for a two-stage combustor model have the same format as those of the previous two channel problems. The value of O/F and equivalence ratio appearing anywhere in the output refer to the total values of oxidizer and fuel available to the combustor. The output unique to this problem is a list of thermodynamic variables corresponding to the first stage prior to and after the rejection of a specified amount of condensed species. The first stage output data begins on output page 5 of Sample Output 6 with the list of enthalpy and number of moles of chemical elements per kilogram of fuel, oxidizer, and total mixture present in the first stage. These values correspond to the amount of oxidizer and fuel that is injected in the first stage. The fraction of each REACTANT injected in the second stage is the last number on the REACTANT cards. Since chemical equilibrium is assumed in the first stage, information concerning the minimization of Gibbs free energy appears next in the output. This is followed by the thermodynamic properties of the equilibrium mixture. Similar information concerning the properties of the first stage after the rejection of a specified percent of the condensed species is then printed out. The enthalpy and number of moles of chemical elements per kilogram of mixture in the second stage is printed out next. Beyond this point, the problem is treated like a single-stage combustor and hence, the output format is the same as that of the previous two problems.

**Sample Output 5, Channel Problem With
Entrance Area Ratio Specified
(13 Output Pages)**

```

1
REACTANTS      XXXSTG
C 5.4617 H 4.5635 N 0.0714 S 0.0343 O 0.9000 0.74800 -21782.00 S 298.000 0 F 0.00000
SI 0.8072 FE 0.0977 AL 0.4335 MG 0.1141 O 2.5253 0.95240E-01 -288546.44 S 298.000 0 F 0.00000
P 2.0000 O 5.0000 0.0000 0.0000 0.0000 0.46000E-03 -351350.00 S 298.000 0 F 0.00000
CA 0.2621 NA 0.0129 K 0.0149 TI 0.0100 O 0.2960 0.19050E-01 -48221.10 S 298.000 0 F 0.00000
K 2.0000 C 1.0000 O 3.0000 0.0000 0.0000 0.91850E-01 -274900.00 S 298.000 0 F 0.00000
H 2.0000 O 1.0000 0.0000 0.0000 0.0000 0.45400E-01 -68288.00 L 298.000 0 F 0.00000
N 2.0000 0.0000 0.0000 0.0000 0.0000 0.75426 4100.60 G 1660.000 0 O 0.00000
O 2.6000 0.0000 0.0000 0.0000 0.0000 0.23195 4326.20 G 1660.000 0 O 0.00000
AR 1.0000 0.0000 0.0000 0.0000 0.0000 0.13790E-01 2823.40 G 1660.000 0 O 0.00000
SOLUTION      AL2O3(L)      SiO2(L)      Ti2O3(L)      KAlO2(L)
SOLUTION      KAlSi2O6(L)      KAlSi3O8(L)      Fe3O4(L)      KAlSiO4(L)
SOLUTION      K2Si2O5(L)      K2CO3(L)      K2SO4(L)
OMIT          MGSiO3(S)      MGSiO3(L)
INSERT        FeO(L)      CAO(S)
NAMELISTS
1
$INPT2
KASE = 106,
T = 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 ,
P = 4.50000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 ,
PSIA = F,
MMHG = F,
NSQM = F,
V = 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 ,
RHO = 4.50000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 ,
ERATIO= F,
OXFL = F,
FPCT = F,
FA = F,
MIX = 6.68850 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 ,
TP = F,
HP = F,
SP = F,
TV = F,

```

UV = F,
 SV = F,
 RKT = T,
 SHOCK = F,
 DLTN = F,
 OTTO = F,
 CR = 0.000000 ,
 S0 = 0.000000000000 ,
 IONS = T,
 IDEBUG= 0 ,
 TRACE = 0.100000E-06 ,
 SIUNIT= F,
 DXI = 0.250000 ,
 NITER = 0 ,
 NSTOP = 0 ,
 NEL_ = F,
 BZ = 6.000000 ,
 XK = 0.800000 ,
 ACCURC= 0.100000E-02 ,
 HMIN = 0.100000E-29 ,
 ALPH = 0.000000 ,
 EXIN = 2100.00 ,
 TWOSTG= F,
 \$END
 LLMT =

3-68

C
 H
 N
 S
 O
 SI
 FE
 AL
 MG
 P
 CA
 NA
 K
 TI
 AR

00SPECIES BEING CONSIDERED IN THIS SYSTEM

J12/65 AL(S)	J12/65 AL(L)
J12/62 ALN(S)	J 3/67 ALN
J12/67 ALOH	J12/67 ALOH+
J12/68 ALO2H	10/78 ALO2H2
J 6/68 AL2O2+	J 6/72 AL2O3(S)
L 5/66 AR	L12/66 AR+
J 9/65 C-	3/8/7 CAL
J12/71 CH+	J12/72 CH2
J 6/69 CN	J12/70 CN+
J 9/65 CO	J 3/61 COS
3/3/7 CO3-	3/7/7 CO4-
J 6/61 CS2	J12/69 C2
J 9/65 C2H4	L 5/72 C2H6
J12/69 C3	J 6/68 C3O2
J12/68 CA(S)	J12/68 CA(L)

J12/65 AL
J 6/70 ALO
J12/67 ALOH-
J 6/72 AL2O
J 6/75 AL2O3(L)
J 3/61 C(S)
3/3/7 C3-
J 3/61 CH2O
J12/70 CN-
3/3/7 COS-
J 6/62 CP
J12/69 C2-
J 3/67 C2N
J12/69 C4
J12/68 CA

J 6/65 AL+
J 6/70 ALO+
J12/68 ALO2
J 6/72 AL2O+
10/78 AL6O13SI2(S)
J 3/61 C
3/3/7 C2H-
J 6/69 CH3
J 6/66 CNN
J 9/65 CO2
J12/62 CS
J 3/67 C2H
J 3/61 C2N2
J12/69 C5
J12/70 CA+

J 6/63 ALH
J 12/7 ALO-
3/8/7 ALO2-
J 9/65 AL2O2
3/8/7 ALS
L12/66 C+
J12/67 CH
J 3/61 CH4
J12/70 CN2
4/12/7 CO2-
3/3/7 CS-
J 3/61 C2H2
J 9/66 C2O
J12/68 CA(S)
BAR 73 CACO3(S)

BAR 73	CACO3(S)	J 6/71	CAO(S)	J 6/71	CAO(L)	J12/74	CAO	J 6/78	CAOH
J 6/78	CAOH+	J12/71	CAO2H2(S)	J 12/7	CAO2H2	J12/71	CAS(S)	BAR 73	CASO4(S)
L82/67	E	J 3/65	FE(S)	J 3/65	FE(S)	J 3/65	FE(S)	J 3/65	FE(L)
J 3/65	FE	8/1/78	FE+	J 6/65	FE0(S)	J 6/65	FE0(L)	J 9/66	FEO
4/13/7	FEO-	18/78	FEOH	4/28/7	FEO2	4/13/7	FEO2-	J 6/66	FEO2H2(S)
18/78	FEO2H2	J 6/66	FEO3H3(S)	BAR 73	FES(S)	BAR 73	FES(S)	BAR 73	FES(S)
J 6/66	FESO4(S)	BAR 73	FES2(S)	J 6/65	FE2O3(S)	18/78	FE2O3(L)	J 6/65	FE3O4(S)
18/78	FE3O4(L)	J 6/66	FE2S3O12(S)	J 9/65	H	J 6/66	H+	J 9/65	H-
J 3/64	HALO	L12/69	HCN	J12/78	HCO	J12/78	HCO+	3/8/7	HCO3-
J12/69	HCP	3/8/7	HK	J12/78	HNCO	J 3/63	HNO	J 6/63	HNO2
J 6/63	HNO3	J 3/64	HO2	12/21/	HPO2	J 3/61	H2	L11/65	H2O(S)
L11/65	H2O(L)	J 3/61	H2O	L 2/69	H2O2	3/8/7	H2P	J12/65	H2S
J12/66	H2SO4(L)	J12/66	H2SO4	3/25/7	H3O+	3/3/7	HP-	3/3/7	HS-
3/3/7	HSI-	J12/61	K(S)	J12/61	K(L)	J 6/62	K	J 3/65	K+
3/3/7	K-	18/78	KALO2(S)	H18/77	KALO2(L)	H18/77	KALSIO4(L)	H18/77	KALSIO2O6(L)
GS4/76	KALSIO3(S)	H18/77	KALSIO3(L)	3/8/7	KCN	J 3/66	K2CO3(S)	J 3/66	K2CO3(L)
J12/67	KO	7/29/8	KO+	J12/67	KO-	J12/78	KOH(S)	J12/78	KOH(S)
J12/78	KOH(L)	J12/78	KOH	J12/71	KOH+	J12/61	K2	J 6/63	K2O(S)
18/78	K2O(L)	J12/78	K2O2H2	J12/71	K2SO4(S)	J12/71	K2SO4(S)	J12/71	K2SO4(L)
12/79	K2SIO3(L)	PB7/77	K2SIO3(S)	J 9/62	MG(S)	J 9/62	MG(L)	J 9/62	MG
J12/78	MG+	J12/66	MGCO3(S)	J12/66	MGH	J 3/64	MGN	J12/65	MGO(S)
18/78	MGO(L)	18/78	MGO	18/78	MGOH	J 6/68	MGOH+	18/78	MGO2H2
J12/71	MGS(S)	J 6/71	MGS	L 7/76	MGSO4(S)	L 7/76	MGSO4(L)	18/78	MG2SIO4(S)
J12/67	MG2SIO4(L)	J 3/61	N	J12/78	NCO	J12/71	NH	J12/65	NH2
J 9/65	NH3	J 6/63	NO	3/3/7	NO-	J 6/66	NO+	J 9/64	NO2
J 6/72	NO2-	J12/64	NO3	3/3/7	NO3-	J 9/65	N2	J12/65	N2H4
J12/64	N2O	J12/78	N2O+	J 9/64	N2O4	J12/64	N2O5	J12/78	N3
J 6/62	NA(S)	J 6/62	NA(L)	J 6/62	NA	J 3/65	NA+	GS4/76	NAALSIO3(S)
3/3/7	NA-	J 3/63	NAH	J12/67	NAO	J12/67	NAO-	J12/78	NAOH(S)
J12/78	NAOH(L)	J12/78	NAOH	J12/71	NAOH+	J 6/62	NA2	J 3/66	NA2CO3(S)
J 3/66	NA2CO3(S)	J 3/66	NA2CO3(L)	J 6/68	NA2O(S)	J 6/68	NA2O(S)	J 6/68	NA2O(L)
J12/78	NA2O2H2	J12/66	NA2SO4(S)	J12/66	NA2SO4(S)	J12/66	NA2SO4(S)	J12/66	NA2SO4(L)
K11/74	NA2SO4	J 4/76	NA2SIO3(S)	J 4/76	NA2SIO3(L)	J 4/76	NA2SIO3(L)	J 4/76	NA2SIO3(L)
J 6/62	O	L12/66	O+	J 6/65	O-	J12/78	OH	J12/78	OH+
J12/78	OH-	J 9/65	O2	J12/66	O2-	J 6/61	O3	J 6/62	P
J 6/61	P(S)	L12/66	P+	3/3/7	P-	J 6/67	PH	J 6/62	PH3
J 9/62	PN	J 6/71	PO	3/3/7	PO-	1/1/8	PO2	7/11/7	PO2-
18/5/7	PO3	2/14/9	PO3-	J 6/67	PS	J 6/61	P2	J 6/61	P4
J12/65	S(S)	J12/65	S(L)	J 6/71	S	L12/66	S+	3/3/7	S-
J 6/67	SH	J 6/61	SN	J 6/71	SO	3/3/7	SO-	J 6/61	SO2
3/3/7	SO2-	J 9/65	SO3	3/3/7	SO3-	J12/65	S2	3/3/7	S2-
J6/64	S8	J 3/67	SI(S)	J 3/67	SI(L)	J 3/67	SI	J12/71	SI+
3/3/7	SI-	18/78	SIC(S)	J 3/67	SIC	J 3/67	SIC2	J12/69	SIH
J12/71	SIH+	J12/68	SIH4	J 3/67	SIN	J 9/67	SIO	J 6/67	SIO2(S)
J 6/67	SIO2(S)	J 6/67	SIO2(S)	J 6/67	SIO2(L)	J 9/67	SIO2	18/78	SIO2H2
J12/71	SIS	J 3/67	SI2	J 3/67	SI2C	J 3/67	SI2N	J 3/67	SI3
8/79	TI(S)A	8/79	TI(S)B	8/79	TI(L)	8/79	TI	8/79	TI+
8/79	TIO(S)A	8/79	TIO(S)B	8/79	TIO(L)	8/79	TIO	8/79	TIO2(S)A
8/79	TIO2(S)B	8/79	TIO2(L)	8/79	TIO2	8/79	TI2O3(S)	8/79	TI2O3(L)
8/79	TI3O5(S)A	8/79	TI3O5(S)B	8/79	TI3O5(L)	8/79	TI5O7(S)	8/79	TI5O7(L)
3/79	TIC(S)	8/79	TIC(L)	8/79	TIN(S)	8/79	TIN(L)		
329	16	117	61	8	9	755			

```

O
SI
FE
AL
MG
P
CA
NA
K
TI
AR
E
#SPECIES IN SOLUTION
AL2O3(L)
SIO2(L)
TI2O3(L)
KALO2(L)
KALSI2O6(L)
KALSI3O8(L)
FE3O4(L)
KALSIO4(L)
K2SI2O5(L)
K2CO3(L)
K2SO4(L)
$RKTINP
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FROZ = F,
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C 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 ,
SUPAR = 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
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PCP = 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
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TCEST = 3000.00 ,
NPFZ = 1,
NEOPT = 100000,
HTLOSS= 0.000000 ,
HPATH = T,
SPATH = F,
NUMHLS= 0,
CHNLEN= 1.00000 ,
CHNHLS= 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 ,
TCHINP= 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
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0.000000 ,
TCHFCAL= 1200.00
IPR:KLT= 1,
SEND
#OF = 6.688499

```

[illegible]

ION		DENS (M-3)	ION		DENS (M-3)		ION		DENS (M-3)		ION		DENS (M-3)	
1	CA+	9.618E 15	2	CAOH+	1.409E 17	3	K+	4.415E 20	4	KOH+	7.996E 15			
5	NA+	3.839E 17												
1	ALO-	1.186E 17	2	ALO2-	1.999E 18	3	CN-	2.281E 15	4	CO2-	5.782E 17			
5	CO3-	6.473E 15	6	PEO-	2.657E 17	7	PEO2-	2.915E 19	8	H-	1.611E 17			
9	HCO3-	5.120E 16	10	HS-	9.571E 16	11	K-	3.219E 16	12	KO-	3.339E 17			
13	NO-	5.902E 16	14	NO2-	2.069E 17	15	NAO-	6.197E 15	16	O-	3.956E 18			
17	OH-	2.140E 19	18	O2-	7.012E 17	19	PO-	3.376E 15	20	PO2-	8.467E 19			
21	PO3-	2.254E 19	22	S-	3.843E 16	23	SO-	2.235E 17	24	SO2-	9.899E 17			
25	SO3-	4.954E 15												
CONDUCTIVITY =		8.8746 (Mio/M)												
2	-18.858	-12.332	-13.662	-23.528	-16.726	-24.064	-14.125	-29.919	-23.021	-27.407	-24.198	-25.927	-23.844	-29.033
	-25.619	-15.903	4.000											
ADD CAO(S)														
2	-18.854	-12.329	-13.663	-23.526	-16.725	-24.053	-14.135	-29.892	-23.024	-27.406	-24.655	-25.931	-23.846	-29.029
	-25.621	-15.895	3.000											
PC/PT= 1.739130		T=	2546.20											

2 -18.854 -12.329 -13.663 -23.526 -16.724 -24.053 -14.135 -29.890 -23.023 -27.406 -24.654 -25.931 -23.846 -29.028
 -25.620 -15.895 1.000
 PC/PT= 1.738414 T= 2646.33

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 2							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 CA+	1.347E 15	2 CAOH+	2.566E 16	3 K+	2.072E 20	4 KOH+	1.738E 15
5 NA+	1.505E 17						
1 ALO-	1.161E 16	2 ALO2-	2.825E 17	3 CO2-	1.468E 17	4 CO3-	1.444E 15
5 FEO-	9.784E 16	6 FEO2-	1.583E 19	7 H-	3.441E 16	8 HCO3-	1.672E 16
9 HS-	2.548E 16	10 K-	9.644E 15	11 KO-	1.010E 17	12 NO-	1.051E 16
13 NO2-	4.969E 16	14 NAO-	1.928E 15	15 O-	8.636E 17	16 OH-	6.389E 18
17 O2-	1.475E 17	18 PO2-	5.529E 19	19 PO3-	1.875E 19	20 S-	9.500E 15
21 SO-	5.722E 16	22 SO2-	3.612E 17	23 SO3-	1.666E 15		
CONDUCTIVITY = 5.8165 (MHO/M)							

3 -18.686 -12.234 -13.602 -23.429 -16.594 -23.745 -14.384 -29.257 -22.972 -27.330 -24.284 -25.888 -23.776 -28.880
 -25.467 -15.567 3.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 3							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 CA+	3.127E 15	2 CAOH+	5.395E 16	3 K+	2.746E 20	4 KOH+	3.088E 15
5 NA+	2.134E 17						
1 ALO-	2.828E 16	2 ALO2-	6.007E 17	3 CO2-	2.483E 17	4 CO3-	2.575E 15
5 FEO-	1.441E 17	6 FEO2-	2.019E 19	7 H-	6.193E 16	8 HCO3-	2.571E 16
9 HS-	4.176E 16	10 K-	1.527E 16	11 KO-	1.600E 17	12 NO-	2.039E 16
13 NO2-	8.638E 16	14 NAO-	3.020E 15	15 O-	1.553E 18	16 OH-	1.017E 19
17 O2-	2.701E 17	18 PO-	1.545E 15	19 PO2-	6.515E 19	20 PO3-	2.022E 19
21 S-	1.607E 16	22 SO-	9.588E 16	23 SO2-	5.312E 17	24 SO3-	2.535E 15
CONDUCTIVITY = 6.8812 (MHO/M)							

3 -18.694 -12.239 -13.605 -23.433 -16.600 -23.758 -14.373 -29.286 -22.975 -27.334 -24.301 -25.890 -23.779 -28.887
 -25.474 -15.582 2.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 3							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 CA+	3.009E 15	2 CAOH+	5.214E 16	3 K+	2.710E 20	4 KOH+	3.007E 15
5 NA+	2.099E 17						
1 ALO-	2.716E 16	2 ALO2-	5.806E 17	3 CO2-	2.425E 17	4 CO3-	2.509E 15
5 FEO-	1.416E 17	6 FEO2-	1.998E 19	7 H-	6.031E 16	8 HCO3-	2.522E 16
9 HS-	4.003E 16	10 K-	1.496E 16	11 KO-	1.568E 17	12 NO-	1.979E 16
13 NO2-	8.427E 16	14 NAO-	2.960E 15	15 O-	1.513E 18	16 OH-	9.959E 18
17 O2-	2.629E 17	18 PO-	1.512E 15	19 PO2-	6.467E 19	20 PO3-	2.016E 19
21 S-	1.569E 16	22 SO-	3.367E 16	23 SO2-	5.221E 17	24 SO3-	2.487E 15
CONDUCTIVITY = 6.8318 (MHO/M)							

3 -18.694 -12.239 -13.605 -23.434 -16.600 -23.759 -14.372 -29.287 -22.975 -27.334 -24.301 -25.890 -23.779 -28.887

-25.474 -15.583 1.0000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 3		ION		DENS (M-3)		
					DENS (M-3)						
1	CA+	3.005E 15	2	CAOH+	5.209E 16	3	K+	2.709E 20	4	KOH+	3.005E 15
5	NA+	2.099E 17									
1	ALO-	2.711E 16	2	ALO2-	5.797E 17	3	CO2-	2.421E 17	4	CO3-	2.505E 15
5	FEO-	1.415E 17	6	FEO2-	1.996E 19	7	H-	6.022E 16	8	HCO3-	2.519E 16
9	HS-	4.078E 16	10	K-	1.494E 16	11	KO-	1.566E 17	12	NO-	1.976E 16
13	NO2-	8.415E 16	14	NAO-	2.956E 15	15	O-	1.510E 18	16	OH-	9.947E 18
17	O2-	2.625E 17	18	PO-	1.510E 15	19	PO2-	6.461E 19	20	PO3-	2.014E 19
21	S-	1.567E 16	22	SO-	9.354E 16	23	SO2-	5.215E 17	24	SO3-	2.485E 15
CONDUCTIVITY =		6.8270 (MHO/M)									

*****CHANNEL INPUTS*****

NMPATH= 1
 IMPRNT= 2
 XXSTOP= 2.5100
 UEINP= 0.00000
 ITYPE= 1

INDEPENDENT VARIABLE

0.00000

1.00000

DEPENDENT VARIABLE

744.61780

744.61780

4 -18.717 -12.252 -13.614 -23.448 -16.616 -23.792 -14.347 -29.353 -22.983 -27.345 -24.343 -25.899 -23.791 -28.906
 -25.497 -15.621 1.0000

3
1
73

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 4		ION		DENS (M-3)		
					DENS (M-3)						
1	CA+	2.728E 15	2	CAOH+	4.768E 16	3	K+	2.613E 20	4	KOH+	2.793E 15
5	NA+	2.007E 17									
1	ALO-	2.460E 16	2	ALO2-	5.337E 17	3	CO2-	2.266E 17	4	CO3-	2.328E 15
5	FEO-	1.347E 17	6	FEO2-	1.930E 19	7	H-	5.613E 16	8	HCO3-	2.377E 16
9	HS-	3.832E 16	10	K-	1.412E 16	11	KO-	1.478E 17	12	NO-	1.823E 16
13	NO2-	7.856E 16	14	NAO-	2.791E 15	15	O-	1.409E 18	16	OH-	9.396E 18
17	O2-	2.442E 17	18	PO-	1.424E 15	19	PO2-	6.311E 19	20	PO3-	1.986E 19
21	S-	1.470E 16	22	SO-	8.776E 16	23	SO2-	4.962E 17	24	SO3-	2.352E 15
CONDUCTIVITY =		6.7266 (MHO/M)									

5 -18.740 -12.265 -13.624 -23.462 -16.633 -23.827 -14.321 -29.421 -22.991 -27.357 -24.386 -25.908 -23.802 -28.925
 -25.520 -15.660 1.0000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 5		ION		DENS (M-3)		
					DENS (M-3)						
1	CA+	2.473E 15	2	CAOH+	4.360E 16	3	K+	2.520E 20	4	KOH+	2.593E 15
5	NA+	1.919E 17									
1	ALO-	2.227E 16	2	ALO2-	4.905E 17	3	CO2-	2.118E 17	4	CO3-	2.159E 15
5	FEO-	1.280E 17	6	FEO2-	1.864E 19	7	H-	5.224E 16	8	HCO3-	2.239E 16

9 HS-	3.596E 16	10 K-	1.332E 16	11 KO-	1.393E 17	12 NO-	1.679E 16
13 NO2-	7.322E 16	14 NAO-	2.632E 15	15 O-	1.313E 18	16 OH-	8.863E 18
17 O2-	2.267E 17	18 PO-	1.340E 15	19 PO2-	6.159E 19	20 PO3-	1.956E 19
21 S-	1.377E 16	22 SO-	9.221E 16	23 SO2-	4.716E 17	24 SO3-	2.224E 15

CONDUCTIVITY = 6.6225 (MHO/M)

6 -18.763 -12.278 -13.633 -23.476 -16.658 -23.863 -14.294 -29.498 -22.999 -27.368 -24.429 -25.917 -23.814 -28.944
-25.543 -15.788 1.0000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 6							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 CA+	2.238E 15	2 CAOH+	3.981E 16	3 K+	2.429E 20	4 KOH+	2.405E 15
5 NA+	1.833E 17						
1 ALO-	2.813E 16	2 ALO2-	4.581E 17	3 CO2-	1.977E 17	4 CO3-	2.881E 15
5 FEO-	1.216E 17	6 FEO2-	1.808E 19	7 H-	4.857E 16	8 HCO3-	2.108E 16
9 HS-	3.372E 16	10 K-	1.256E 16	11 KO-	1.311E 17	12 NO-	1.544E 16
13 NO2-	6.816E 16	14 NAO-	2.488E 15	15 O-	1.222E 18	16 OH-	8.353E 18
17 O2-	2.103E 17	18 PO-	1.261E 15	19 PO2-	6.888E 19	20 PO3-	1.926E 19
21 S-	1.289E 16	22 SO-	7.695E 16	23 SO2-	4.478E 17	24 SO3-	2.101E 15

CONDUCTIVITY = 6.5185 (MHO/M)

7 -18.786 -12.292 -13.613 -23.498 -16.667 -23.908 -14.267 -29.568 -23.888 -27.388 -24.473 -25.927 -23.826 -28.964
-25.567 -15.748 1.0000

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ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 7							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 CA+	2.822E 15	2 CAOH+	3.629E 16	3 K+	2.340E 20	4 KOH+	2.228E 15
5 NA+	1.758E 17						
1 ALO-	1.816E 16	2 ALO2-	4.123E 17	3 CO2-	1.843E 17	4 CO3-	1.851E 15
5 FEO-	1.154E 17	6 FEO2-	1.736E 19	7 H-	4.589E 16	8 HCO3-	1.983E 16
9 HS-	3.159E 16	10 K-	1.182E 16	11 KO-	1.233E 17	12 NO-	1.418E 16
13 NO2-	6.336E 16	14 NAO-	2.334E 15	15 O-	1.135E 18	16 OH-	7.862E 18
17 O2-	1.947E 17	18 PO-	1.185E 15	19 PO2-	5.859E 19	20 PO3-	1.897E 19
21 S-	1.205E 16	22 SO-	7.193E 16	23 SO2-	4.249E 17	24 SO3-	1.983E 15

CONDUCTIVITY = 6.4125 (MHO/M)

8 -18.818 -12.385 -13.653 -23.585 -16.684 -23.938 -14.248 -29.631 -23.816 -27.391 -24.518 -25.936 -23.838 -28.984
-25.591 -15.782 1.0000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 8							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 CA+	1.824E 15	2 CAOH+	3.384E 16	3 K+	2.253E 20	4 KOH+	2.862E 15
5 NA+	1.678E 17						
1 ALO-	1.635E 16	2 ALO2-	3.771E 17	3 CO2-	1.717E 17	4 CO3-	1.718E 15
5 FEO-	1.893E 17	6 FEO2-	1.673E 19	7 H-	4.188E 16	8 HCO3-	1.862E 16
9 HS-	2.956E 16	10 K-	1.112E 16	11 KO-	1.158E 17	12 NO-	1.388E 16
13 NO2-	5.882E 16	14 NAO-	2.194E 15	15 O-	1.053E 18	16 OH-	7.393E 18

17 O2-	1.888E 17	18 PO-	1.112E 15	19 PO2-	5.718E 19	20 PO3-	1.867E 19
21 S-	1.125E 16	22 SO-	6.717E 16	23 SO2-	4.827E 17	24 SO3-	1.869E 15
CONDUCTIVITY = 6.3856 (MHO/M)							

9 -18.834 -12.319 -13.663 -23.519 -16.782 -23.978 -14.212 -29.783 -23.825 -27.483 -24.564 -25.945 -23.851 -29.884
 -25.615 -15.824 1.888

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 9							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 CA+	1.642E 15	2 CAOH+	3.883E 16	3 K+	2.168E 28	4 KOH+	1.986E 15
5 NA+	1.592E 17						
1 ALO-	1.469E 16	2 ALO2-	3.444E 17	3 CO2-	1.597E 17	4 CO3-	1.578E 15
5 FEO-	1.835E 17	6 FEO2-	1.611E 19	7 H-	3.871E 16	8 HCO3-	1.748E 16
9 HS-	2.764E 16	10 K-	1.845E 16	11 KO-	1.887E 17	12 NO-	1.198E 16
13 NO2-	5.453E 16	14 NAO-	2.868E 15	15 O-	9.756E 17	16 OH-	6.943E 18
17 O2-	1.661E 17	18 PO-	1.843E 15	19 PO2-	5.564E 19	20 PO3-	1.837E 19
21 S-	1.858E 16	22 SO-	6.265E 16	23 SO2-	3.814E 17	24 SO3-	1.768E 15
CONDUCTIVITY = 6.1977 (MHO/M)							

18 -18.858 -12.333 -13.674 -23.534 -16.728 -24.819 -14.183 -29.776 -23.833 -27.414 -24.618 -25.955 -23.863 -29.825
 -25.648 -15.867 1.888

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 18							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 CA+	1.476E 15	2 CAOH+	2.725E 16	3 K+	2.885E 28	4 KOH+	1.759E 15
5 NA+	1.517E 17						
1 ALO-	1.318E 16	2 ALO2-	3.139E 17	3 CO2-	1.483E 17	4 CO3-	1.454E 15
5 FEO-	9.795E 16	6 FEO2-	1.558E 19	7 H-	3.579E 16	8 HCO3-	1.638E 16
9 HS-	2.581E 16	10 K-	9.818E 15	11 KO-	1.819E 17	12 NO-	1.888E 16
13 NO2-	5.847E 16	14 NAO-	1.932E 15	15 O-	9.826E 17	16 OH-	6.514E 18
17 O2-	1.531E 17	18 PO2-	5.418E 19	19 PO3-	1.887E 19	20 S-	9.781E 15
21 SO-	5.837E 16	22 SO2-	3.689E 17	23 SO3-	1.656E 15		
CONDUCTIVITY = 6.8898 (MHO/M)							

11 -18.882 -12.347 -13.684 -23.549 -16.739 -24.868 -14.154 -29.851 -23.842 -27.426 -24.658 -25.965 -23.876 -29.847
 -25.665 -15.911 1.888

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 11							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 CA+	1.325E 15	2 CAOH+	2.469E 16	3 K+	2.884E 28	4 KOH+	1.622E 15
5 NA+	1.444E 17						
1 ALO-	1.188E 16	2 ALO2-	2.857E 17	3 CO2-	1.376E 17	4 CO3-	1.337E 15
5 FEO-	9.255E 16	6 FEO2-	1.491E 19	7 H-	3.385E 16	8 HCO3-	1.534E 16
9 HS-	2.488E 16	10 K-	9.198E 15	11 KO-	9.538E 16	12 NO-	9.927E 15
13 NO2-	4.665E 16	14 NAO-	1.811E 15	15 O-	8.338E 17	16 OH-	6.184E 18
17 O2-	1.489E 17	18 PO2-	5.275E 19	19 PO3-	1.777E 19	20 S-	9.185E 15
21 SO-	5.432E 16	22 SO2-	3.411E 17	23 SO3-	1.556E 15		

CONDUCTIVITY = 5.9795 (MHO/M)

12 -18.987 -12.362 -13.655 -23.564 -16.758 -24.104 -14.125 -29.927 -23.051 -27.438 -24.786 -25.974 -23.888 -29.068
 -25.690 -15.955 1.0000

ION		DENS (M-3)	ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 12		ION		DENS (M-3)
1	CA+	1.186E 15	2	CAOH+	2.233E 16	3	K+
5	NA+	1.374E 17				4	KOH+
1	ALO-	1.055E 16	2	ALO2-	2.595E 17	3	CO2-
5	FEO-	8.736E 16	6	FEO2-	1.432E 19	7	H-
9	HS-	2.245E 16	10	K-	8.615E 15	11	KO-
13	NO2-	4.306E 16	14	NAO-	1.694E 15	15	O-
17	O2-	1.294E 17	18	PO2-	5.133E 19	19	PO3-
21	SO-	5.049E 16	22	SO2-	3.221E 17	23	SO3-

CONDUCTIVITY = 5.8690 (MHO/M)

13 -18.932 -12.376 -13.705 -23.578 -16.778 -24.148 -14.095 -30.004 -23.060 -27.449 -24.755 -25.984 -23.901 -29.091
 -25.716 -16.601 1.0000

ION		DENS (M-3)	ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 13		ION		DENS (M-3)
1	CA+	1.060E 15	2	CAOH+	2.017E 16	3	K+
5	NA+	1.306E 17				4	KOH+
1	ALO-	9.405E 15	2	ALO2-	2.354E 17	3	CO2-
5	FEO-	8.237E 16	6	FEO2-	1.374E 19	7	H-
9	HS-	2.090E 16	10	K-	8.061E 15	11	KO-
13	NO2-	3.968E 16	14	NAO-	1.584E 15	15	O-
17	O2-	1.187E 17	18	PO2-	4.993E 19	19	PO3-
21	SO-	4.687E 16	22	SO2-	3.039E 17	23	SO3-

CONDUCTIVITY = 5.7577 (MHO/M)

THEORETICAL MHD CORE PERFORMANCE

SPC = 66.1 PSIA
 CASE NO. 106

CHEMICAL FORMULA		WT FRACTION (SEE NOTE)		ENERGY CAL/MOL		STATE	TEMP DEG K	DENSITY G/CC
FUEL	C 5.46166 H 4.56349	N 0.07139	S 0.03431	O 0.900000	0.74800	-21782.000	S	298.00
FUEL	SI 0.80718 FE 0.09769	AL 0.43349	MG 0.11413	O 2.52526	0.09524	-288546.438	S	298.00
FUEL	P 2.00000 O 5.00000				0.00046	-351350.000	S	298.00
FUEL	CA 0.26213 NA 0.01290	K 0.01486	TI 0.01001	O 0.29604	0.01905	-48221.102	S	298.00
FUEL	K 2.00000 C 1.00000	O 3.00000			0.09185	-274903.000	S	298.00
FUEL	H 2.00000 O 1.00000				0.04540	-68288.000	L	298.00
OXIDANT	N 2.00000				0.75426	10512.871	G	1660.00
OXIDANT	O 2.00000				0.23195	11101.393	G	1660.00
OXIDANT	AR 1.00000				0.01379	6765.552	G	1660.00

O/F= 6.6385 PERCENT FUEL= 13.0064 EQUIVALENCE RATIO= 1.0870 REACTANT DENSITY= 0.0000

AXIAL STATION (M)

#	CHAMBER	THROAT	0.0000	0.250	0.500	0.750	1.000	1.250	1.500	1.750	2.000	2.250	2.500
PC/P	1.0000	1.7384	1.4280	1.4699	1.5135	1.5591	1.6067	1.6564	1.7084	1.7628	1.8197	1.8793	1.9417
P, ATM	4.5000	2.5886	3.1512	3.0615	2.9732	2.8863	2.8008	2.7167	2.6340	2.5527	2.4729	2.3945	2.3176
T, DEG K	2808	2546	2703	2696	2689	2681	2674	2667	2659	2652	2644	2637	2629
RHO, G/CC	5.7300-4	3.5336-4	4.1969-4	4.0898-4	3.9839-4	3.8793-4	3.7762-4	3.6744-4	3.5739-4	3.4750-4	3.3774-4	3.2813-4	3.1868-4
H, CAL/G	197.3	95.7	131.0	126.8	122.6	118.3	114.0	109.6	105.2	100.7	96.2	91.6	87.0
S, CAL/(G)(K)	2.2092	2.2092	2.2092	2.2096	2.2100	2.2104	2.2108	2.2112	2.2116	2.2120	2.2124	2.2129	2.2133
M, MOL WT	29.341	29.643	29.538	29.550	29.561	29.573	29.585	29.597	29.610	29.622	29.634	29.647	29.660
(DLV/DLP)T	-1.01222	-1.00981	-1.01080	-1.01070	-1.01059	-1.01048	-1.01037	-1.01025	-1.01013	-1.01001	-1.00989	-1.00977	-1.00964
(DLV/DLP)P	1.2972	1.2553	1.2834	1.2817	1.2800	1.2782	1.2763	1.2743	1.2722	1.2700	1.2676	1.2652	1.2626
CP, CAL/(G)(K)	0.8120	0.7857	0.8094	0.8075	0.8054	0.8032	0.8009	0.7984	0.7957	0.7929	0.7899	0.7867	0.7833
GAMMA (S)	1.1470	1.1452	1.1443	1.1443	1.1444	1.1444	1.1445	1.1446	1.1446	1.1447	1.1448	1.1450	1.1451
VELOCITY,M/SEC			744.62	744.62	744.62	744.62	744.62	744.62	744.62	744.62	744.62	744.62	744.62
TOTAL H(CAL/G)			197.28	193.09	188.85	184.56	180.24	175.86	171.44	166.97	162.46	157.90	153.29
MAG FLD(TESLA)			6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00
BETA			1.67	1.72	1.77	1.81	1.86	1.92	1.97	2.03	2.09	2.15	2.22
SON VEL,M/SEC	955.3	922.0	933.0	931.7	930.3	928.8	927.4	926.0	924.5	923.1	921.6	920.1	918.6
ELEC DENS	2.747 20	1.089 20	1.527 20	1.466 20	1.405 20	1.346 20	1.288 20	1.231 20	1.177 20	1.123 20	1.071 20	1.021 20	9.721 19
IONIC DENS)	6.096 20	3.059 20	3.897 20	3.768 20	3.642 20	3.519 20	3.398 20	3.281 20	3.165 20	3.053 20	2.943 20	2.835 20	2.731 20
SIGMA (MHO/M)	8.8746	5.8165	6.8270	6.7266	6.6225	6.5185	6.4125	6.3056	6.1977	6.0890	5.9795	5.8690	5.7577
W/O IONS	9.5229	6.2064	7.3215	7.2144	7.1033	6.9923	6.8791	6.7650	6.6500	6.5340	6.4170	6.2990	6.1802
FREQ (1/SEC)	8.723 11	5.278 11	6.305 11	6.140 11	5.978 11	5.817 11	5.659 11	5.503 11	5.350 11	5.198 11	5.049 11	4.902 11	4.758 11
MACH NUMBER	0.0000	1.0000	0.7931	0.7992	0.8004	0.8017	0.8029	0.8041	0.8054	0.8067	0.8080	0.8093	0.8106
AE/AT		1.0000	1.0425	1.0698	1.0983	1.1279	1.1587	1.1908	1.2242	1.2591	1.2955	1.3334	1.3730
3-77 TOTAL MOL WT	29.266	29.530	29.442	29.451	29.461	29.471	29.481	29.491	29.502	29.512	29.522	29.533	29.544

MOLE FRACTIONS

ALO2	1.2918-7	2.4179-8	4.4802-8	4.1968-8	3.9265-8	3.6689-8	3.4235-8	3.1903-8	2.9689-8	2.7590-8	2.5602-8	2.3724-8	2.1952-8
ALO2-	1.6951-7	3.9196-8	6.7518-8	6.3816-8	6.0225-8	5.6779-8	5.3452-8	5.0260-8	4.7199-8	4.4267-8	4.1463-8	3.8786-8	3.6232-8
ALO2H	1.1619-6	3.1869-7	5.1251-7	4.8751-7	4.6330-7	4.3987-7	4.1719-7	3.9529-7	3.7416-7	3.5380-7	3.3419-7	3.1534-7	2.9724-7
ALO2H2	1.1982-6	3.7935-7	5.7721-7	5.5169-7	5.2687-7	5.0276-7	4.7931-7	4.5659-7	4.3458-7	4.1327-7	3.9265-7	3.7276-7	3.5356-7
AL2O3(L)	6.4009-7	2.8374-7	3.8188-7	3.7186-7	3.6193-7	3.5210-7	3.4233-7	3.3269-7	3.2316-7	3.1375-7	3.0446-7	2.9531-7	2.8630-7
AR	8.7887-3	8.8679-3	8.8414-3	8.8443-3	8.8473-3	8.8502-3	8.8532-3	8.8563-3	8.8594-3	8.8625-3	8.8656-3	8.8688-3	8.8720-3
CO	6.9710-2	5.8905-2	6.2596-2	6.2180-2	6.1760-2	6.1335-2	6.0905-2	6.0471-2	6.0032-2	5.9589-2	5.9141-2	5.8688-2	5.8231-2
CO2	1.1218-1	1.2463-1	1.2039-1	1.2086-1	1.2134-1	1.2183-1	1.2232-1	1.2282-1	1.2332-1	1.2383-1	1.2434-1	1.2486-1	1.2539-1
CA	1.4604-5	6.8005-6	9.8862-6	9.5003-6	9.1231-6	8.7542-6	8.3935-6	8.0412-6	7.6973-6	7.3617-6	7.0346-6	6.7158-6	6.4054-6
CAO(S)	0.0000 0	4.2325-4	2.0334-4	2.3181-4	2.5993-4	2.8770-4	3.1512-4	3.4219-4	3.6889-4	3.9522-4	4.2117-4	4.4673-4	4.7191-4
CAO	1.2351-5	5.0967-6	7.7651-6	7.4115-6	7.0680-6	6.7343-6	6.4102-6	6.0960-6	5.7914-6	5.4963-6	5.2108-6	4.9348-6	4.6681-6
CAOH	6.5939-4	3.9260-4	5.2259-4	5.0613-4	4.8991-4	4.7392-4	4.5815-4	4.4263-4	4.2734-4	4.1230-4	3.9751-4	3.8297-4	3.6868-4
CAO2H2	4.5873-4	3.2755-4	4.0836-4	3.9747-4	3.8668-4	3.7600-4	3.6541-4	3.5494-4	3.4457-4	3.3432-4	3.2418-4	3.1417-4	3.0427-4
E	2.3298-5	1.5116-5	1.7792-5	1.7525-5	1.7250-5	1.6974-5	1.6694-5	1.6411-5	1.6126-5	1.5839-5	1.5549-5	1.5258-5	1.4964-5
FE	1.9474-4	1.8828-4	1.9104-4	1.9097-4	1.9090-4	1.9081-4	1.9071-4	1.9060-4	1.9047-4	1.9032-4	1.9016-4	1.8997-4	1.8975-4
FEO	1.7552-4	1.7242-4	1.7468-4	1.7448-4	1.7426-4	1.7401-4	1.7375-4	1.7346-4	1.7315-4	1.7281-4	1.7244-4	1.7203-4	1.7159-4
FEOH	8.6011-6	8.4052-6	8.5049-6	8.4795-6	8.4535-6	8.4267-6	8.3992-6	8.3709-6	8.3416-6	8.3114-6	8.2801-6	8.2476-6	8.2138-6
FEO2	2.6804-5	2.7493-5	2.7531-5	2.7510-5	2.7485-5	2.7456-5	2.7423-5	2.7384-5	2.7341-5	2.7291-5	2.7236-5	2.7173-5	2.7103-5
FEO2-	2.4719-6	2.1966-6	2.3254-6	2.3080-6	2.2891-6	2.2700-6	2.2500-6	2.2293-6	2.2080-6	2.1860-6	2.1633-6	2.1399-6	2.1157-6
FEO2H2	1.7694-5	2.4310-5	2.1752-5	2.1505-5	2.1252-5	2.1000-5	2.0748-5	2.0495-5	2.0242-5	2.0000-5	1.9757-5	1.9514-5	1.9271-5
FE3O4(L)	2.8175-7	2.4724-6	1.1340-6	1.2276-6	1.3307-6	1.4444-6	1.5702-6	1.7092-6	1.8631-6	2.0337-6	2.2231-6	2.4335-6	2.6675-6
H	3.1434-3	2.0985-3	2.4317-3	2.3951-3	2.3585-3	2.3216-3	2.2847-3	2.2476-3	2.2103-3	2.1730-3	2.1355-3	2.0979-3	2.0602-3
HK	2.3233-6	1.4761-6	1.7362-6	1.7012-6	1.6664-6	1.6318-6	1.5975-6	1.5633-6	1.5293-6	1.4955-6	1.4620-6	1.4288-6	1.3957-6
HNO	7.1314-7	3.2871-7	4.3637-7	4.2128-7	4.0646-7	3.9190-7	3.7762-7	3.6360-7	3.4986-7	3.3640-7	3.2322-7	3.1032-7	2.9770-7

HO2	2.6626-6	1.2778-6	1.6812-6	1.6271-6	1.5738-6	1.5211-6	1.4691-6	1.4178-6	1.3673-6	1.3176-6	1.2686-6	1.2205-6	1.1731-6
H2	6.3769-3	5.4143-3	5.7290-3	5.6946-3	5.6600-3	5.6251-3	5.5899-3	5.5544-3	5.5186-3	5.4825-3	5.4461-3	5.4094-3	5.3725-3
H2O	6.9973-2	7.3881-2	7.2532-2	7.2687-2	7.2842-2	7.2998-2	7.3155-2	7.3313-2	7.3472-2	7.3632-2	7.3793-2	7.3954-2	7.4117-2
H2O2	2.3773-7	1.1897-7	1.5364-7	1.4874-7	1.4391-7	1.3915-7	1.3446-7	1.2984-7	1.2530-7	1.2082-7	1.1643-7	1.1211-7	1.0786-7
K	1.7731-3	1.7654-3	1.7700-3	1.7719-3	1.7739-3	1.7758-3	1.7778-3	1.7797-3	1.7817-3	1.7836-3	1.7855-3	1.7874-3	1.7893-3
K+	3.7440-5	2.8757-5	3.1560-5	3.1246-5	3.0944-5	3.0635-5	3.0329-5	3.0022-5	2.9714-5	2.9404-5	2.9092-5	2.8778-5	2.8463-5
KALO2(L)	1.8065-3	1.7430-3	1.7652-3	1.7628-3	1.7605-3	1.7581-3	1.7558-3	1.7534-3	1.7511-3	1.7487-3	1.7465-3	1.7442-3	1.7420-3
KALSIO4(L)	1.2583-5	1.7086-5	1.5934-5	1.6074-5	1.6209-5	1.6339-5	1.6463-5	1.6581-5	1.6693-5	1.6798-5	1.6895-5	1.6986-5	1.7068-5
KALSI2O6(L)	6.3003-5	1.0984-4	9.7457-5	9.8908-5	1.0030-4	1.0163-4	1.0288-4	1.0406-4	1.0516-4	1.0616-4	1.0706-4	1.0785-4	1.0853-4
KALSI3O8(L)	7.3887-6	3.9269-5	2.4201-5	2.5677-5	2.7226-5	2.8854-5	3.0560-5	3.2345-5	3.4212-5	3.6158-5	3.8185-5	4.0293-5	4.2481-5
KO	5.1213-5	3.4353-5	3.9899-5	3.9192-5	3.8483-5	3.7773-5	3.7062-5	3.6349-5	3.5636-5	3.4922-5	3.4207-5	3.3491-5	3.2776-5
KOH	1.3645-3	1.4034-3	1.3916-3	1.3908-3	1.3900-3	1.3892-3	1.3884-3	1.3875-3	1.3867-3	1.3858-3	1.3848-3	1.3839-3	1.3829-3
K2SIO2O5(L)	3.0487-6	1.3851-5	8.6357-6	9.0622-6	9.5084-6	9.9751-6	1.0464-5	1.0974-5	1.1507-5	1.2062-5	1.2641-5	1.3243-5	1.3869-5
MG	7.6803-5	6.9038-5	7.1809-5	7.1651-5	7.1490-5	7.1324-5	7.1153-5	7.0979-5	7.0799-5	7.0614-5	7.0424-5	7.0228-5	7.0026-5
MGH	2.9771-7	1.7748-7	2.1351-7	2.0887-7	2.0427-7	1.9970-7	1.9515-7	1.9065-7	1.8617-7	1.8173-7	1.7733-7	1.7297-7	1.6864-7
MGO	2.6787-5	1.8605-5	2.1329-5	2.1009-5	2.0688-5	2.0365-5	2.0039-5	1.9712-5	1.9384-5	1.9053-5	1.8721-5	1.8387-5	1.8052-5
MGOH	3.8207-4	3.9967-4	3.9376-4	3.9432-4	3.9489-4	3.9546-4	3.9605-4	3.9663-4	3.9723-4	3.9783-4	3.9843-4	3.9905-4	3.9967-4
MGO2H2	1.2519-5	1.5493-5	1.4369-5	1.4553-5	1.4538-5	1.4626-5	1.4716-5	1.4807-5	1.4902-5	1.4998-5	1.5098-5	1.5200-5	1.5305-5
N	1.4376-6	5.3936-7	7.7072-7	7.3960-7	7.0922-7	6.7957-7	6.5064-7	6.2244-7	5.9497-7	5.6823-7	5.4221-7	5.1691-7	4.9234-7
NO	9.2564-3	6.2127-3	7.2211-3	7.0995-3	6.9773-3	6.8545-3	6.7312-3	6.6074-3	6.4830-3	6.3582-3	6.2329-3	6.1071-3	5.9810-3
NO2	3.0198-6	1.5089-6	1.9594-6	1.8986-6	1.8384-6	1.7789-6	1.7202-6	1.6621-6	1.6048-6	1.5483-6	1.4926-6	1.4377-6	1.3836-6
N2	6.8205-1	6.8976-1	6.8718-1	6.8747-1	6.8776-1	6.8806-1	6.8835-1	6.8865-1	6.8895-1	6.8926-1	6.8957-1	6.8988-1	6.9019-1
N2O	9.2305-7	4.7045-7	6.0297-7	5.8434-7	5.6597-7	5.4785-7	5.2998-7	5.1239-7	4.9506-7	4.7801-7	4.6123-7	4.4473-7	4.2852-7
NA	4.1633-5	4.2410-5	4.2141-5	4.2204-5	4.2268-5	4.2332-5	4.2397-5	4.2463-5	4.2529-5	4.2596-5	4.2664-5	4.2732-5	4.2800-5
NAO	1.1195-6	7.8101-7	8.9368-7	8.7883-7	8.6394-7	8.4900-7	8.3402-7	8.1901-7	8.0396-7	7.8887-7	7.7376-7	7.5862-7	7.4346-7
NAOH	1.3495-5	1.3593-5	1.3574-5	1.3546-5	1.3518-5	1.3489-5	1.3460-5	1.3430-5	1.3400-5	1.3369-5	1.3339-5	1.3307-5	1.3276-5
O	3.0797-3	1.7520-3	2.1655-3	2.1182-3	2.0710-3	2.0237-3	1.9764-3	1.9292-3	1.8820-3	1.8349-3	1.7878-3	1.7408-3	1.6939-3
O-	3.3549-7	1.1983-7	1.7594-7	1.6852-7	1.6121-7	1.5410-7	1.4713-7	1.4034-7	1.3372-7	1.2728-7	1.2102-7	1.1493-7	1.0903-7
OH	9.7839-3	6.9266-3	7.8849-3	7.7754-3	7.6651-3	7.5539-3	7.4417-3	7.3286-3	7.2147-3	7.0998-3	6.9840-3	6.8674-3	6.7499-3
OH-	1.8147-6	8.8660-7	1.1586-6	1.1234-6	1.0882-6	1.0536-6	1.0192-6	9.8521-7	9.5166-7	9.1856-7	8.8591-7	8.5374-7	8.2205-7
O2	1.3817-2	9.8665-3	1.1277-2	1.1125-2	1.0972-2	1.0816-2	1.0657-2	1.0496-2	1.0333-2	1.0167-2	9.9988-3	9.8280-3	9.6547-3
PN	1.2970-7	9.2555-8	1.0370-7	1.0227-7	1.0082-7	9.9368-8	9.7935-8	9.6510-8	9.5094-8	9.3688-8	9.2292-8	9.0906-8	8.9530-8
PO	5.0868-6	4.1557-6	4.4587-6	4.4268-6	4.3936-6	4.3599-6	4.3263-6	4.2925-6	4.2585-6	4.2244-6	4.1900-6	4.1555-6	4.1208-6
PO2	1.0188-5	1.5373-5	1.0198-5	1.0201-5	1.0201-5	1.0200-5	1.0200-5	1.0199-5	1.0198-5	1.0197-5	1.0196-5	1.0195-5	1.0194-5
PO2-	7.1805-6	7.6715-6	7.5255-6	7.5466-6	7.5625-6	7.5791-6	7.5948-6	7.6103-6	7.6257-6	7.6409-6	7.6559-6	7.6707-6	7.6854-6
PO3	1.7561-7	1.7593-7	1.7667-7	1.7647-7	1.7621-7	1.7592-7	1.7564-7	1.7534-7	1.7502-7	1.7469-7	1.7434-7	1.7398-7	1.7360-7
PO3-	1.9112-6	2.6011-6	2.3462-6	2.3746-6	2.4019-6	2.4301-6	2.4585-6	2.4876-6	2.5173-6	2.5475-6	2.5784-6	2.6100-6	2.6422-6
S	2.6233-6	1.4527-6	1.7882-6	1.7468-6	1.7058-6	1.6653-6	1.6251-6	1.5853-6	1.5459-6	1.5070-6	1.4684-6	1.4304-6	1.3927-6
SH	6.6600-7	3.7260-7	4.5555-7	4.4450-7	4.3359-7	4.2282-7	4.1218-7	4.0169-7	3.9134-7	3.8113-7	3.7108-7	3.6117-7	3.5141-7
SO	1.1066-4	8.1553-5	9.0884-5	8.9776-5	8.8665-5	8.7552-5	8.6434-5	8.5314-5	8.4192-5	8.3067-5	8.1939-5	8.0810-5	7.9678-5
SO2	1.0123-3	1.0531-3	1.0399-3	1.0415-3	1.0430-3	1.0446-3	1.0462-3	1.0477-3	1.0493-3	1.0509-3	1.0525-3	1.0541-3	1.0557-3
SO3	2.9049-7	2.4582-7	2.6259-7	2.6020-7	2.5778-7	2.5532-7	2.5283-7	2.5030-7	2.4774-7	2.4514-7	2.4251-7	2.3984-7	2.3714-7
SIO	2.4368-3	1.5373-3	1.8933-3	1.8565-3	1.8189-3	1.7803-3	1.7408-3	1.7005-3	1.6593-3	1.6172-3	1.5744-3	1.5309-3	1.4868-3
SIO2(L)	6.6635-4	1.4661-3	1.1453-3	1.1786-3	1.2128-3	1.2480-3	1.2841-3	1.3210-3	1.3588-3	1.3975-3	1.4369-3	1.4771-3	1.5180-3
SIO2	2.5560-4	1.7176-4	2.0752-4	2.0376-4	1.9989-4	1.9590-4	1.9180-4	1.8758-4	1.8326-4	1.7883-4	1.7430-4	1.6968-4	1.6497-4
TIO	3.5660-7	2.5532-7	2.5246-7	2.4673-7	2.4101-7	2.3530-7	2.2960-7	2.2391-7	2.1823-7	2.1255-7	2.0689-7	2.0124-7	1.9560-7
TIO2	4.2297-5	4.0059-5	4.1296-5	4.1196-5	4.1038-5	4.0971-5	4.0845-5	4.0710-5	4.0564-5	4.0407-5	4.0238-5	4.0056-5	3.9860-5
TI2O3(L)	5.3723-7	1.9286-6	1.2206-6	1.2809-6	1.3451-6	1.4136-6	1.4868-6	1.5649-6	1.6483-6	1.7374-6	1.8327-6	1.9344-6	2.0431-6

8 SPECIES IN SOLUTION AT LAST STATION

AL2O3(L) FE3O4(L) KALO2(L) KALSIO4(L) KALSI2O6(L) KALSI3O8(L) K2CO3(L) K2SO4(L) K2SIO2O5(L) SIO2(L)

SIO2(L) TI2O3(L)

8 ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-06 FOR ALL ASSIGNED CONDITIONS

AL(S)	AL(L)	AL	AL+	ALH	ALN(S)	ALN	ALO	ALO+	ALO-
ALOH	ALOH+	ALOH-	AL2O	ALH	AL2O2	AL2O2+	AL2O3(S)	AL6O13SI2(S)	ALS
AR+	C(S)	C	C+	C-	CAL	C3-	C2H-	CH	CH+

CH2	CH2O	CH3	CH4	CN	CN+	CN-	CNN	CN2	COS
COS-	CO2-	CO3-	CO4-	CP	CS	CS-	CS2	C2	C2-
C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2O	C3	C3O2	C4
C5	CA(S)	CA(S)	CA(L)	CA+	CACO3(S)	CACO3(S)	CAO(L)	CAOH+	CAO2H2(S)
CAS(S)	CASO4(S)	FE(S)	FE(S)	FE(S)	FE(L)	FE+	FE(S)	FE(L)	FEO-
FEO2H2(S)	FEO3H3(S)	FES(S)	FES(S)	FES(S)	FESO4(S)	FES2(S)	FE2O3(S)	FE2O3(L)	FE3O4(S)
FE2S3O12(S)	H+	H-	HALO	HCN	HCO	HCO+	HCO3-	HCP	HNCO
HNO2	HNO3	HPO2	H2O(S)	H2O(L)	H2P	H2S	H2SO4(L)	H2SO4	H3O+
HP-	HS-	HSI-	K(S)	K(L)	K-	KALO2(S)	KALSI3O8(S)	KCN	K2CO3(S)
K2CO3(L)	KO+	KO-	KOH(S)	KOH(S)	KOH(L)	KOH+	K2	K2O(S)	K2O(L)
K2O2H2	K2SO4(S)	K2SO4(S)	K2SO4(L)	K2SIO3(L)	MG(S)	MG(L)	MG+	MGCO3(S)	MGN
MGO(S)	MGO(L)	MGOH+	MGS(S)	MGS	MGSO4(S)	MGSO4(L)	MG2SIO4(S)	MG2SIO4(L)	NCO
NH	NH2	NH3	NO-	NO+	NO2-	NO3	NO3-	N2H4	N2O+
N2O4	N2O5	N3	NA(S)	NA(L)	NA+	NAALSI3O8(S)	NA-	NAH	NAO-
NAOH(S)	NAOH(L)	NAOH+	NA2	NA2CO3(S)	NA2CO3(S)	NA2CO3(L)	NA2O(S)	NA2O(S)	NA2O(L)
NA2O2H2	NA2SO4(S)	NA2SO4(S)	NA2SO4(S)	NA2SO4(L)	NA2SO4	NA2SIO3(S)	NA2SIO3(L)	NA2SIO3(S)	NA2SIO5(L)
O+	OH+	O2-	O3	P	P(S)	P+	P-	PH	PH3
PO-	PS	P2	P4	S(S)	S(L)	S+	S-	SN	SO-
SO2-	SO3-	S2	S2-	S8	SI(S)	SI(L)	SI	SI+	SI-
SIC(S)	SIC	SIC2	SIH	SIH+	SIH4	SIN	SIO2(S)	SIO2(S)	SIO2(S)
SIO2H2	SIS	SI2	SI2C	SI2N	SI3	TI(S)A	TI(S)B	TI(L)	TI
TI+	TIO(S)A	TIO(S)B	TIO(L)	TIO2(S)A	TIO2(S)B	TIO2(L)	TI2O3(S)	TI3O5(S)A	TI3O5(S)B
TI3O5(L)	TI5O7(S)	TI5O7(L)	TIC(S)	TIC(L)	TIN(S)	TIN(L)			

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

1

STOP 5 IS NORMAL CHANNEL STOP

IT OCCURS WHEN XPOSITION EXCEEDS INPUTTED XXSTOP VALUE

**Sample Output 6, Channel Problem With
Two Stage Combustor and Entrance Velocity
Specified
(15 Output Pages)**

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1
REACTANTS      TWOSTG
C 5.4617 H 4.5635 N 0.0714 S 0.0343 O 0.9000 0.74800 -21782.00 S 298.000 0 F 0.00000
SI 0.0072 FE 0.0977 AL 0.4335 MG 0.1141 O 2.5253 0.95240E-01 -288546.44 S 298.000 0 F 0.00000
P 2.0000 O 5.0000 0.0000 0.0000 0.0000 0.46000E-03 -351350.00 S 298.000 0 F 0.00000
CA 0.2621 NA 0.0129 K 0.0149 TI 0.0100 O 0.2960 0.19050E-01 -48221.10 S 298.000 0 F 0.00000
K 2.0000 C 1.0000 O 3.0000 0.0000 0.0000 0.91850E-01 -274900.00 S 298.000 0 F 1.00000
H 2.0000 O 1.0000 0.0000 0.0000 0.0000 0.45400E-01 -68288.00 L 298.000 0 F 0.00000
N 2.0000 0.0000 0.0000 0.0000 0.0000 0.75426 4100.60 G 1660.000 0 O 0.50000
O 2.0000 0.0000 0.0000 0.0000 0.0000 0.73195 4326.20 G 1660.000 0 O 0.50000
AR 1.0000 0.0000 0.0000 0.0000 0.0000 0.13790E-01 2823.40 G 1660.000 0 O 0.50000
SOLUTION      AL2O3(L)      SiO2(L)      Ti2O3(L)      KAlO2(L)
SOLUT ON      KAlSi2O6(L)      KAlSi3O8(L)      Fe3O4(L)      KAlSiO4(L)
SOLUTION      K2Si2O5(L)      K2CO3(L)      K2SO4(L)
OMIT          MgSiO3(S)      MgSiO3(L)
INSERT        FeO(L)      CAO(S)
NAMELISTS
1
$INPT2
KASE = 105,
T = 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000,
P = 4.50000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
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NSCM = F,
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FA = F,
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HP = F,
GP = F,
TV = F,

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 SV = F,
 RKT = T,
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 ACCURC= 0.100000E-02,
 HMIN = 0.100000E-29,
 ALPH = 0.999000,
 EXIN = 2100.00,
 TWGSG= T,
 \$END
 LLNT =

4
 00
 1
 3

C
 H
 N
 S
 O
 SI
 FE
 AL
 MG
 P
 CA
 NA
 K
 TI
 AR

0SPECIES BEING CONSIDERED IN THIS SYSTEM

J12/65 AL(S)	J12/65 AL(L)	J12/65 AL	J 6/65 AL+	J 6/63 ALH
J12/62 ALN(S)	J 3/67 ALN	J 6/70 ALO	J 6/70 ALO+	J 12/7 ALO-
J12/67 ALOH	J12/67 ALOH+	J12/67 ALOH-	J12/68 ALO2	3/8/7 ALO2-
J12/68 ALO2H	10/78 ALO2H2	J 6/72 AL2O	J 6/72 AL2O+	J 9/65 AL2O2
J 6/68 AL2O2+	J 6/72 AL2O3(S)	J 6/75 AL2O3(L)	10/78 AL6O13SI2(S)	3/8/7 ALS
L 5/66 AR	L12/66 AR+	J 3/61 C(S)	J 3/61 C	L12/66 C+
J 9/65 C-	3/8/7 CAL	3/3/7 C3-	3/3/7 C2H-	J12/67 CH
J12/71 CH+	J12/72 CH2	J 3/61 CH2O	J 6/69 CH3	J 3/61 CH4
J 6/69 CN	J12/70 CN+	J12/70 CN-	J 6/66 CNN	J12/70 CN2
J 9/65 CO	J 3/61 COS	3/3/7 COS-	J 9/65 CO2	4/12/7 CO2-
3/3/7 CO3-	3/7/7 CO4-	J 6/62 CP	J12/62 CS	3/3/7 CS-
J 6/61 CS2	J12/69 C2	J12/69 C2-	J 3/67 C2H	J 3/61 C2H2
J 9/65 C2H4	L 5/72 C2H6	J 3/67 C2N	J 3/61 C2N2	J 9/66 C2O
J12/69 C3	J 6/68 C3O2	J12/69 C4	J12/69 C5	J12/68 CA(S)
J12/68 CA(S)	J12/68 CA(L)	J12/68 CA	J12/70 CA+	BAR 73 CAC03(S)

CS-05

BAR 73	CACO3(S)	J 6/71	CAO(S)	J 6/71	CAO(L)	J 12/74	CAO	J 6/78	CAOH
J 6/78	CAOH+	J 12/71	CAO2H2(S)	J 12/7	CAO2H2	J 12/71	CAS(S)	BAR 73	CASO4(S)
L82/67	E	J 3/65	FE(S)	J 3/65	FE(S)	J 3/65	FE(S)	J 3/65	FE(L)
J 3/65	FE	8/1/78	FE+	J 6/65	FEO(S)	J 6/65	FEO(L)	J 9/66	FEO
4/13/7	FEO-	18/78	FEOH	4/28/7	FEO2	4/13/7	FEO2-	J 6/66	FEO2H2(S)
10/78	FEO2H2	J 6/66	FEO3H3(S)	BAR 73	FES(S)	BAR 73	FES(S)	BAR 73	FES(S)
J 6/66	FESO4(S)	BAR 73	FES2(S)	J 6/65	FE2O3(S)	18/78	FE2O3(L)	J 6/65	FE3O4(S)
18/78	FE.O4(L)	J 6/66	FE2S3O12(S)	J 9/65	H	J 6/66	H+	J 9/65	H-
J 3/64	HALO	L12/69	HCN	J 12/78	HCO	J 12/78	HCO+	3/8/7	HCO3-
J 12/69	HCP	3/8/7	HK	J 12/78	HNCO	J 3/63	HNO	J 6/63	HNO2
J 6/63	HNO3	J 3/64	HO2	12/21/	HPO2	J 3/61	H2	L11/65	H2O(S)
L11/65	H2O(L)	J 3/61	H2O	L 2/69	H2O2	3/8/7	H2P	J 12/65	H2S
J 12/66	H2SO4(L)	J 12/66	H2SO4	3/25/7	H3O+	3/3/7	HP-	3/3/7	HS-
3/3/7	HSI-	J 12/61	K(S)	J 12/61	K(L)	J 6/62	K	J 3/65	K+
3/3/7	K-	18/78	KALO2(S)	H18/77	KALO2(L)	H18/77	KALSIO4(L)	H18/77	KALSIO6(L)
GS4/76	KALSI3O8(S)	J 18/77	KALSI3O8(L)	3/8/7	KCN	J 3/66	K2CO3(S)	J 3/66	K2CO3(L)
J 12/67	KO	1/29/8	KO+	J 12/67	KO-	J 12/78	KOH(S)	J 12/78	KOH(S)
J 12/78	KOH(L)	J 12/78	KOH	J 12/71	KOH+	J 12/61	K2	J 6/63	K2O(S)
18/78	K2O(L)	J 12/78	K2O2H2	J 12/71	K2SO4(S)	J 12/71	K2SO4(S)	J 12/71	K2SO4(L)
12/79	K2SIO3(L)	837/77	K2SIO5(L)	J 9/62	MG(S)	J 9/62	MG(L)	J 9/62	MG
J 12/78	MG+	J 12/66	MGCO3(S)	J 12/66	MGH	J 3/64	MGN	J 12/65	MGO(S)
18/78	MGO(L)	18/78	MGO	18/78	MGOH	J 6/68	MGOH+	18/78	MGO2H2
J 12/71	MGS(S)	J 6/71	MGS	L 7/76	MGSO4(S)	L 7/76	MGSO4(L)	18/78	MGSIO4(S)
J 12/67	MG2SIO4(L)	J 3/61	N	J 12/78	NCO	J 12/71	NH	J 12/65	NH2
J 9/65	NH3	J 6/63	NO	3/3/7	NO-	J 6/66	NO+	J 9/64	NO2
J 6/72	NO2-	J 12/64	NO3	3/3/7	NO3-	J 9/65	N2	J 12/65	N2H4
J 12/64	N2O	J 12/78	N2O+	J 9/64	N2O4	J 12/64	N2O5	J 12/78	N3
J 6/62	NA(S)	J 6/62	NA(L)	J 6/62	NA	J 3/65	NA+	GS4/76	NAALSI3O8(S)
3/3/7	NA-	J 3/63	NAH	J 12/67	NAO	J 12/67	NAO-	J 12/78	NAOH(S)
J 12/78	NAOH(L)	J 12/78	NAOH	J 12/71	NAOH+	J 6/62	NA2	J 3/66	NA2CO3(S)
J 3/66	NA2CO3(S)	J 3/66	NA2CO3(L)	J 6/68	NA2O(S)	J 6/68	NA2O(S)	J 6/68	NA2O(L)
J 12/78	NA2O2H2	J 12/66	NA2SO4(S)	J 12/66	NA2SO4(S)	J 12/66	NA2SO4(S)	J 12/66	NA2SO4(L)
K11/74	NA2SO4	J 4/76	NA2SIO3(S)	J 4/76	NA2SIO3(L)	J 4/76	NA2SIO5(S)	J 4/76	NA2SIO5(L)
J 6/62	O	L12/66	O+	J 6/65	O-	J 12/78	OH	J 12/78	OH+
J 12/78	OH-	J 9/65	O2	J 12/66	O2-	J 6/61	O3	J 6/62	P
J 6/61	P(S)	L12/66	P+	3/3/7	P-	J 6/67	PH	J 6/62	PH3
J 9/62	PN	J 6/71	PO	3/3/7	PO-	1/1/8	PO2	7/11/7	PO2-
18/5/7	PO3	2/14/9	PO3-	J 6/67	PS	J 6/61	P2	J 6/61	P4
J 12/65	S(S)	J 12/65	S(L)	J 6/71	S	L12/66	S+	3/3/7	S-
J 6/67	SH	J 6/61	SN	J 6/71	SO	3/3/7	SO-	J 6/61	SO2
3/3/7	SO2-	J 9/65	SO3	3/3/7	SO3-	J 12/65	S2	3/3/7	S2-
J 6/64	S8	J 3/67	SI(S)	J 3/67	SI(L)	J 3/67	SI	J 12/71	SI+
3/3/7	SI-	18/78	SIC(S)	J 3/67	SIC	J 3/67	SIC2	J 12/69	SIH
J 12/71	SIH+	J 12/68	SIH4	J 3/67	SIN	J 9/67	SIO	J 6/67	SIO2(S)
J 6/67	SIO2(S)	J 6/67	SIO2(S)	J 6/67	SIO2(L)	J 9/67	SIO2	18/78	SIO2H2
J 12/71	SIS	J 3/67	SI2	J 3/67	SI2C	J 3/67	SI2N	J 3/67	SI3
8/79	TI(S)A	8/79	TI(S)B	8/79	TI(L)	8/79	TI	8/79	TI+
8/79	TIO(S)A	8/79	TIO(S)B	8/79	TIO(L)	8/79	TIO	8/79	TIO2(S)A
8/79	TIO2(S)B	8/79	TIO2(L)	8/79	TIO2	8/79	TI2O3(S)	8/79	TI2O3(L)
8/79	TI3O5(S)A	8/79	TI3O5(S)B	8/79	TI3O5(L)	8/79	TI5O7(S)	8/79	TI5O7(L)
8/79	TIC(S)	8/79	TIC(L)	8/79	TIN(S)	8/79	TIN(L)		

329

16

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61

8

9

755

C
H
N
S

```
O
SI
FE
AL
MG
P
CA
NA
K
TI
AR
E
#SPECIES IN SOLUTION
AL2O3(L)
SiO2(L)
Ti2O3(L)
KAlO2(L)
KAlSi2O6(L)
KAlSi3O8(L)
Fe3O4(L)
KAlSiO4(L)
K2Si2O5(L)
K2CO3(L)
K2SO4(L)
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O .000000 ,
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SEND
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FIRST STAGE PROPERTIES BEFORE SLAG REJECTION

HOF = 6.688483

ENTHALPY (KG-MOL)(DEG K)/KG #KG-ATOMS/KG		EFFECTIVE FUEL HPP(2) BPP(I,2)		EFFECTIVE OXIDANT HPP(1) BPP(I,1)		MIXTURE HPP(1) BPP(I,1)									
C	H	N	S	O	SI	FE	AL	MG	P	CA	NA	K	TI		
1	-12.215	-18.408	-13.202	-16.478	-21.631	-17.498	-8.459	-18.188	-19.898	-21.140	-23.962	-23.482	-25.386	-19.665	
1	-12.216	-18.408	-13.203	-16.480	-21.628	-17.500	-8.579	-18.184	-19.899	-21.146	-23.955	-23.484	-25.387	-19.667	
1	-12.435	-18.438	-13.255	-16.651	-21.325	-19.133	-9.330	-23.134	-20.043	-21.322	-23.392	-23.717	-30.622	-24.501	
1	-12.450	-18.440	-13.259	-16.665	-21.305	-19.118	-9.375	-23.068	-21.246	-21.333	-23.358	-23.731	-30.569	-24.445	
P, ATM	4.5000														
T, DEG K	2321														
RHO, G/CC	6.2216-4														
H, CAL/G	111.9														
S, CAL/(G)(K)	2.3112														
M, MOL WT	26.330														
(DLV/DLP)T	-1.00100														
(DLV/DLT)P	1.0538														
CP, CAL/(G)(K)	0.4547														
GAMMA (S)	1.2245														
SON VEL,M/SEC	947.3														
ELEC DENS	0.0000														
IONIC DENS	0.0000														
SIGMA (MHO/M)	0.0000														
W/O IONS	0.0000														
FREQ (1/SEC)	0.0000														

MOLE FRACTIONS

ALOH 3.5524-7
 ALO2H 7.9574-7
 ALO2H2 1.7074-5
 AL2O3(L) 1.4678-3
 AR 7.0946-3
 CO 2.6366-1
 COS 6.8048-5
 CO2 2.5843-2
 CS 3.7208-6
 CA 3.3996-6
 CAO(S) 1.6968-3
 CAO2H 1.0677-4
 CAO2H2 4.1726-5
 FE 6.4217-4
 FEO 1.4313-5
 FEOH 8.6877-6
 FEO2H2 1.7465-5
 FE3O4(L) 2.0674-6
 H 1.4856-3
 HCN 8.2052-7
 HCO 3.3143-7
 H2 8.7094-2
 H2O 4.7584-2
 H2S 5.8276-4
 HS- 1.2935-7
 K 5.1576-7
 KALO2(L) 8.4318-5
 KALSIO4(L) 8.7941-7
 KALSIO6(L) 4.8807-6
 KALSIO8(L) 1.3075-5
 KOH 1.3263-7
 K2SIO5(L) 5.0253-7
 MG 6.8415-5
 MGH 8.1938-7
 MGO 2.3288-7
 MGOH 1.7144-4
 MGO2H2 3.0099-6
 MG2SIO4(L) 2.8046-4
 NH2 1.9909-7
 NH3 1.1183-6
 NO 1.9003-5
 N2 5.5525-1
 NA 8.2615-5
 NA+ 1.7527-7
 NAH 4.5564-7
 NAOH 7.7203-6
 O 1.5717-6
 OH 1.3326-4
 O2 3.6261-7
 PN 1.0738-5
 PO 6.9354-6
 PO2 6.5678-7
 PS 2.1374-5
 S 1.0039-4
 SH 3.3262-4

SN 1.3345-6
 SO 2.6624-4
 SO2 1.8770-4
 S2 1.1761-4
 SIO 1.4480-3
 SIO2(L) 3.8889-3
 SIO2 4.4865-6
 SIS 1.9522-5
 TIO2 7.6404-7
 TI2O3(L) 3.4892-5

0SPECIES IN SOLUTION AT LAST STATION

AL2O3(L)	FE3O4(L)	KALO2(L)	KALSIO4(L)	KALSI2O6(L)	KALSI3O8(L)	K2CO3(L)	K2SO4(L)	K2SI2O5(L)	SIO2(L)
SIO2(L)	TI2O3(L)								

0ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-06 FOR ALL ASSIGNED CONDITIONS

AL(S)	AL(L)	AL	AL+	ALH	ALN(S)	ALN	ALO	ALO+	ALO-
ALOH+	ALOH-	ALO2	ALO2-	AL2O	AL2O+	AL2O2	AL2O2+	AL2O3(S)	AL6O13SI2(S)
ALS	AR+	C(S)	C	C+	C-	CAL	C3-	C2H-	CH
CH+	CH2	CH2O	CH3	CH4	CN	CN+	CN-	CNN	CN2
CO5-	CO2-	CO3-	CO4-	CP	CS-	CS2	C2	C2-	C2H
C2H2	C2H4	C2H6	C2N	C2N2	C2O	C3	C3O2	C4	C5
CA(S)	CA(S)	CA(L)	CA+	CACO3(S)	CACO3(S)	CAO(L)	CAO	CAOH+	CAO2H2(S)
CAS(S)	CASO4(S)	E	FE(S)	FE(S)	FE(S)	FE(L)	FE+	FEO(S)	FEO(L)
FEO-	FEO2	FEO2-	FEO2H2(S)	FEO3H3(S)	FES(S)	FES(S)	FES(S)	FESO4(S)	FES2(S)
FE2O3(S)	FE2O3(L)	FE3O4(S)	FE2S3O12(S)	H+	H-	HALO	HCO+	HCO3-	HCP
HK	HNCO	HNO	HNO2	HNO3	HO2	HPO2	H2O(S)	H2O(L)	H2O2
H2P	H2SO4(L)	H2SO4	H3O+	HP-	HSI-	K(S)	K(L)	K+	K-
KALO2(S)	KALSI3O8(S)	KCN	K2CO3(S)	K2CO3(L)	KO	KO+	KO-	KOH(S)	KOH(S)
KOH(L)	KOH+	K2	K2O(S)	K2O(L)	K2O2H2	K2SO4(S)	K2SO4(S)	K2SO4(L)	K2SIO3(L)
MG(S)	MG(L)	MG+	M3CO3(S)	MGN	MGO(S)	MGO(L)	MGOH+	MGS(S)	MGS
MGSO4(S)	MGSO4(L)	MG2SIO4(S)	N	NCO	NH	NO-	NO+	NO2	NO2-
NO3	NO3-	N2H4	N2O	N2O+	N2O4	N2O5	N3	NA(S)	NA(L)
NAALSI3O8(S)	NA-	NAO	NAO-	NAOH(S)	NAOH(L)	NAOH+	NA2	NA2CO3(S)	NA2CO3(S)
NA2CO3(L)	NA2O(S)	NA2O(S)	NA2O(L)	NA2O2H2	NA2SO4(S)	NA2SO4(S)	NA2SO4(S)	NA2SO4(L)	NA2SO4
NA2SIO3(S)	NA2SIO3(L)	NA2SIO5(S)	NA2SIO5(L)	O+	O-	OH+	OH-	O2-	O3
P	P(S)	P+	P-	PH	PH3	PO-	PO2-	PO3	PO3-
P2	P4	S(S)	S(L)	S+	S-	SO-	SO2-	SO3	SO3-
S2-	S8	SI(S)	SI(L)	SI	SI+	SI-	SIC(S)	SIC	SIC2
SIH	SIH+	SIH1	SIN	SIO2(S)	SIO2(S)	SIO2(S)	SIO2H2	SI2	SI2C
SI2N	SI3	TI(S)A	TI(S)B	TI(L)	TI	TI+	TIO(S)A	TIO(S)B	TIO(L)
TIO	TIO2(S)A	TIO2(S)B	TIO2(L)	TI2O3(S)	TI3O5(S)A	TI3O5(S)B	TI3O5(L)	TI5O7(S)	TI5O7(L)
TIC(S)	TIC(L)	TIN(S)	TIN(L)						

0NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

FIRST STAGE PROPERTIES AFTER 99.9 PERCENT SLAG REJECTION

ENTHALPY	HSUB0
(KG-MOL)/(DEG K)/KG	0.87570892E 02
KG-ATOMS/KG	B0(I)
C	0.11312936E-01
H	0.10662600E-01
N	0.43384515E-01
S	0.71367552E-04
O	0.14288655E-01
SI	0.57573715E-04
FE	0.26570925E-04

AL	#.83#68676E-#6											
MG	#.9551#163E-#5											
I'	#.15561#18E-#5											
CA	#.6#19674E-#5											
NA	#.35542885E-#5											
K	#.3168676#E-#7											
TI	#.345#6179E-#7											
AR	#.2771634#E-#3											
E	#.##000000#E ##											

#PT	C	H	N	S	O	SI	FE	AL	MG	P	CA	NA	K	TI
1	AR	E												
	-12.45#	-1#.44#	-13.259	-16.665	-21.3#5	-19.118	-9.375	-23.#53	-21.246	-21.332	-23.358	-23.731	-3#.692	-24.437
	-24.998	-2#.571	7.##											
P, ATM	4.5##													
T, DEG K	2321													
RHO, G/CC	6.#94#-4													
H, CAL/G	174.#													
S, CAL/(G)(K)	2.3438													
M, MJL WT	25.79#													
(DLV/DLP)T	-1.##1#9													
(DLV/DLT)P	1.#258													
CP, CAL/(G)(K)	#.4#21													
GAMMA (S)	1.25#9													
SON VEL,M/SEC	967.4													
ELEC DENS	#.## ##													
IONIC DENS)	#.## ##													
SIGMA (MHO/M)	#.## ##													
W/O IONS	#.## ##													
FREQ (1/SEC)	#.## ##													

MOLE FRACTIONS

ALOH	3.632#-7
ALO2H	8.1357-7
ALO2H2	1.7457-5
AL2O3(L)	2.1866-6
AR	7.148#-3
CO	2.6565-1
COS	6.856#-5
CO2	2.6#37-2
CS	3.7488-6
CA	3.425#-6
CAO(S)	1.7152-6
CAOH	1.#756-4
CAO2H2	4.2#38-5
FE	6.4699-4
FEO	1.4421-5
FEOH	8.753#-6
FE02H2	1.7596-5
H	1.4968-3
HCN	8.2669-7
HCO	3.3391-7
H2	8.7749-2
H2O	4.7941-2

H2S 5.8716-4
 HS- 1.2833-7
 K 4.5934-7
 KALO2(L) 1.8941-7
 KOH 1.1812-7
 K2SIO5(L) 4.9593-7
 MG 6.8923-5
 MGH 8.2546-7
 MGO 2.3468-7
 MGOH 1.7271-4
 MGO2H2 3.8323-6
 MG2SIO4(L) 2.9438-7
 NH2 2.8858-7
 NH3 1.1267-6
 NO 1.9158-5
 N2 5.5942-1
 NA 8.3233-5
 NA+ 1.7932-7
 NAH 4.5985-7
 NAOH 7.7781-6
 O 1.5835-6
 OH 1.3426-4
 O2 3.6531-7
 PN 1.8869-5
 PO 6.9875-6
 PO2 6.6171-7
 PS 2.1536-5
 S 1.8114-4
 SH 3.3512-4
 SN 1.3445-6
 SO 2.6824-4
 SO2 1.8911-4
 S2 1.1849-4
 SIO 1.4598-3
 SIO2(L) 5.6261-6
 SIO2 4.5285-6
 SIS 1.9671-5
 TIO2 7.7555-7

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SPECIES IN SOLUTION AT LAST STATION

AL2O3(L)	FE3O4(L)	KALO2(L)	KALSIO4(L)	KALSI2O6(L)	KALSI3O8(L)	K2CO3(L)	K2SO4(L)	K2SIO5(L)	SIO2(L)
SIO2(L)	TI2O3(L)								

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 8.18888E-86 FOR ALL ASSIGNED CONDITIONS

AL(S)	AL(L)	AL	AL+	ALH	ALN(S)	ALN	ALO	ALO+	ALO-
ALOH+	ALOH-	ALO2	ALO2-	AL2O	AL2O+	AL2O2	AL2O2+	AL2O3(S)	AL6O13SI2(S)
ALS	AR+	C(S)	C	C+	C-	CAL	C3-	C2H-	CH
CH+	CH2	CH2O	CH3	CH4	CN	CN+	CN-	CNN	CN2
COS-	CO2-	CO3-	CO4-	CP	CS-	CS2	C2	C2-	C2H
C2H2	C2H4	C2H6	C2N	C2N2	C2O	C3	C3O2	C4	C5
CA(S)	CA(S)	CA(L)	CA+	CACO3(S)	CACO3(S)	CAO(L)	CAO	CAOH+	CAO2H2(S)
CAS(S)	CASO4(S)	E	FE(S)	FE(S)	FE(S)	FE(L)	FE+	FE(S)	FE(L)
FEO-	FEO2	FEO2-	FEO2H2(S)	FEO3H3(S)	FES(S)	FES(S)	FES(S)	FES(S)	FES2(S)
FE2O3(S)	FE2O3(L)	FE3O4(S)	FE3O4(L)	FE2S3O12(S)	H+	H-	HALO	HCO+	HCO3-
HCP	HK	HNCO	HNO	HNO2	HNO3	HO2	HPO2	H2O(S)	H2O(L)
H2O2	H2P	H2SO4(L)	H2SO4	H3O+	HP-	HSI-	K(S)	K(L)	K+
K-	KALO2(S)	KALSIO4(L)	KALSI2O6(L)	KALSI3O8(S)	KALSI3O8(L)	KCN	K2CO3(S)	K2CO3(L)	KO

KO+	KO-	KOH(S)	KOH(S)	KOH(L)	KOH+	K2	K2O(S)	K2O(L)	K2O2H2
K2SO4(S)	K2SO4(S)	K2SO4(L)	K2SIO3(L)	MG(S)	MG(L)	MG+	MGCO3(S)	MGN	MGO(S)
MGO(L)	MGOH+	MGS(S)	MGS	MGSO4(S)	MGSO4(L)	MG2SIO4(S)	N	NCO	NH
NO-	NO+	NO2	NO2-	NO3	NO3-	N2H4	N2O	N2O+	N2O4
N2O5	N3	NA(S)	NA(L)	NAALSIO3(S)	NA-	NAO	NAO-	NAOH(S)	NAOH(L)
NAOH+	NA2	NA2CO3(S)	NA2CO3(S)	NA2CO3(L)	NA2O(S)	NA2O(S)	NA2O(L)	NA2O2H2	NA2SO4(S)
NA2SO4(S)	NA2SO4(S)	NA2SO4(L)	NA2SO4	NA2SIO3(S)	NA2SIO3(L)	NA2SIO5(S)	NA2SIO5(L)	O+	O-
OH+	O2-	O2-	O3	P	P(S)	P+	P-	PH	PH3
PO-	PO2-	PO3	PO3-	P2	P4	S(S)	S(L)	S+	S-
SO-	SO2-	SO3	SO3-	S2-	S8	SI(S)	SI(L)	SI	SI+
SI-	SIC(S)	SIC	SIC2	SIH	SIH+	SIH4	SIN	SIO2(S)	SIO2(S)
SIO2(S)	SIO2H2	SI2	SI2C	SI2N	SI3	TI(S)A	TI(S)B	TI(L)	TI
TI+	TIO(S)A	TIO(S)B	TIO(L)	TIO	TIO2(S)A	TIO2(S)B	TIO2(L)	TI2O3(S)	TI2O3(L)
TI3O5(S)A	TI3O5(S)B	TI3O5(L)	TI5O7(S)	TI5O7(L)	TIC(S)	TIC(L)	TIN(S)	TIN(L)	

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

SECOND STAGE ENTHALPY AND ELEMENTAL COMPOSITION

ENTHALPY	HSUB0
(KG-MOL)(DEG K)/KG	0.11639336E 03
KG-ATOMS/KG	B0(I)
C	0.62864255E-02
H	0.58426438E-02
N	0.47464646E-01
S	0.38941944E-04
O	0.14470125E-01
SI	0.31592706E-04
FE	0.14614512E-04
AL	0.45518038E-06
MG	0.52335436E-05
P	0.85267641E-06
CA	0.32888183E-05
NA	0.19475960E-05
K	0.17487092E-03
TI	0.18907894E-07
AR	0.30314707E-03
E	0.00000000E 00

REMOVE SOLUTION

SP	C	H	N	S	O	SI	FE	AL	MG	P	CA	NA	K	TI
AR	E													
1	-18.417	-12.090	-13.496	-23.267	-16.393	-23.615	-14.750	-26.686	-21.298	-27.291	-23.739	-25.796	-23.195	-33.018
	-25.205	-14.853	13.000											
REMOVE CAO(S)														
1	-18.409	-12.082	-13.498	-23.261	-16.392	-23.590	-14.775	-26.679	-21.261	-27.285	-26.434	-25.805	-23.202	-33.010
	-25.208	-14.836	5.000											
REMOVE MG2SIO4(L)														
1	-18.353	-12.060	-13.511	-23.214	-16.396	-24.409	-14.886	-26.607	-24.078	-27.239	-26.403	-25.841	-23.222	-32.953
	-25.222	-14.748	5.000											
ADD SOLUTION														
1	-18.353	-12.060	-13.511	-23.214	-16.396	-24.410	-14.887	-28.182	-24.030	-27.243	-26.403	-25.841	-23.224	-32.953
	-25.222	-14.740	6.000											

ION

DENS (M-3)

ION

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 1

DENS (M-3)

ION

DENS (M-3)

ION

DENS (M-3)

1	CAOH+	1.888E 16	2	K+	5.711E 28	3	KOH+	1.866E 16	4	NA+	3.288E 17
1	ALO-	1.593E 17	2	ALO2-	2.522E 18	3	CN-	3.275E 15	4	CO2-	7.789E 17
5	CO3-	8.471E 15	6	FEO-	3.481E 17	7	FEO2-	3.496E 19	8	H-	2.388E 17
9	HCO3-	6.424E 16	18	HS-	1.351E 17	11	K-	6.822E 16	12	KO-	6.857E 17
13	NO-	8.177E 16	14	NO2-	2.787E 17	15	NAO-	1.197E 15	16	NAO-	8.849E 15
17	O-	5.514E 18	18	OH-	2.877E 19	19	O2-	9.514E 17	28	PO-	4.237E 15
21	PO2-	9.571E 19	22	PO3-	2.419E 19	23	S-	5.586E 16	24	SO-	3.896E 17
25	SO2-	1.289E 18	26	SO3-	6.388E 15						

CONDUCTIVITY = 11.7835 (MHO/M)

2 -18.848 -12.324 -13.667 -23.515 -16.724 -24.674 -14.166 -29.867 -24.217 -27.585 -26.675 -25.944 -23.398 -33.386
 -25.627 -15.619 4.888
 PC/PT= 1.748718 T= 2651.89
 2 -18.841 -12.324 -13.668 -23.516 -16.724 -24.674 -14.164 -29.872 -24.218 -27.586 -26.676 -25.944 -23.398 -33.387
 -25.628 -15.622 2.888
 PC/PT= 1.743889 T= 2651.47

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 2											
ION	DENS (M-3)	ION	DENS (M-3)								
1	CAOH+	2.787E 15	2	K+	2.587E 28	3	KOH+	2.192E 15	4	NA+	1.195E 17
1	ALO-	1.528E 16	2	ALO2-	3.631E 17	3	CO2-	1.915E 17	4	CO3-	1.871E 15
5	FEO-	1.269E 17	6	FEO2-	2.885E 19	7	H-	4.688E 16	8	HCO3-	2.131E 16
9	HS-	3.388E 16	18	K-	1.994E 16	11	KO-	2.865E 17	12	NO-	1.392E 16
13	NO2-	6.443E 16	14	NAO-	2.488E 15	15	O-	1.148E 18	16	OH-	8.369E 18
17	O2-	1.941E 17	18	PO-	1.136E 15	19	PO2-	6.295E 19	28	PO3-	2.894E 19
21	S-	1.272E 16	22	SO-	7.566E 16	23	SO2-	4.668E 17	24	SO3-	2.135E 15

CONDUCTIVITY = 7.4387 (MHO/M)

3 -18.668 -12.229 -13.612 -23.414 -16.599 -24.584 -14.437 -29.217 -24.178 -27.418 -26.577 -25.918 -23.338 -33.187
 -25.483 -15.291 3.888

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 3											
ION	DENS (M-3)	ION	DENS (M-3)								
1	CAOH+	4.373E 15	2	K+	3.439E 28	3	KOH+	3.982E 15	4	NA+	1.786E 17
1	ALO-	3.771E 16	2	ALO2-	7.732E 17	3	CN-	1.886E 15	4	CO2-	3.213E 17
5	CO3-	3.287E 15	6	FEO-	1.829E 17	7	FEO2-	2.472E 19	8	H-	8.368E 16
9	HCO3-	3.288E 16	18	HS-	5.598E 16	11	K-	3.148E 16	12	KO-	3.226E 17
13	NO-	2.692E 16	14	NO2-	1.184E 17	15	NAO-	3.849E 15	16	O-	2.867E 18
17	OH-	1.327E 19	18	O2-	3.533E 17	19	PO-	1.843E 15	28	PO2-	7.347E 19
21	PO3-	2.214E 19	22	S-	2.174E 16	23	SO-	1.271E 17	24	SO2-	6.798E 17
25	SO3-	3.193E 15									

CONDUCTIVITY = 8.8776 (MHO/M)

*****CHANNEL INPUTS*****

NMPATH= 1
 IMPRNT= 2
 XXSTOP= 8.51888
 VEINI= 8.88888
 ITP= 1

INDEPENDENT VARIABLE				DEPENDENT VARIABLE										
0.00000				750.35083										
1.00000				750.35083										
4	-18.699	-12.247	-13.624	-23.433	-16.620	-24.603	-14.400	-29.306	-24.180	-27.435	-26.593	-25.921	-23.352	-33.209
	-25.512	-15.344	1.000											

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 4														
ION		DENS (M-3)	ION		DENS (M-3)	ION		DENS (M-3)	ION		DENS (M-3)			
1	CAOH+	4.040E 15	2	K+	3.276E 20	3	KOH+	3.535E 15	4	NA+	1.605E 17			
1	ALO-	3.309E 16	2	ALO2-	6.933E 17	3	CO2-	2.940E 17	4	CO3-	2.982E 15			
5	FEO-	1.715E 17	6	FEO2-	2.371E 19	7	H-	7.591E 16	8	HCO3-	2.973E 16			
9	HS-	5.139E 16	10	K-	2.909E 16	11	KO-	2.988E 17	12	NO-	2.415E 16			
13	NO2-	1.008E 17	14	NAO-	3.567E 15	15	O-	1.881E 18	16	OH-	1.229E 19			
17	O2-	3.205E 17	18	PO-	1.700E 15	19	PO2-	7.123E 19	20	PO3-	2.176E 19			
21	S-	1.990E 16	22	SO-	1.165E 17	23	SO2-	6.363E 17	24	SO3-	2.972E 15			
CONDUCTIVITY =		8.6842 (MHO/M)												
5	-18.730	-12.264	-13.636	-23.453	-16.641	-24.622	-14.361	-29.399	-24.191	-27.452	-26.609	-25.932	-23.366	-33.232
	-25.542	-15.397	1.000											

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 5												
ION		DENS (M-3)	ION		DENS (M-3)	ION		DENS (M-3)	ION		DENS (M-3)	
3-94	1	CAOH+	3.726E 15	2	K+	3.117E 20	3	KOH+	3.198E 15	4	NA+	1.509E 17
	1	ALO-	2.893E 16	2	ALO2-	6.196E 17	3	CO2-	2.686E 17	4	CO3-	2.700E 15
	5	FEO-	1.606E 17	6	FEO2-	2.273E 19	7	H-	6.878E 16	8	HCO3-	2.752E 16
	9	HS-	4.710E 16	10	K-	2.690E 16	11	KO-	2.763E 17	12	NO-	2.161E 16
	13	NO2-	9.180E 16	14	NAO-	3.301E 15	15	O-	1.708E 18	16	OH-	1.136E 19
	17	O2-	2.901E 17	18	PO-	1.565E 15	19	PO2-	6.901E 19	20	PO3-	2.139E 19
	21	S-	1.819E 16	22	SO-	1.066E 17	23	SO2-	5.948E 17	24	SO3-	2.762E 15
CONDUCTIVITY =		8.4886 (MHO/M)										

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THEORETICAL MHD CORE PERFORMANCE

OPC = 66.1 PSIA
CASE NO. 105

CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	C	5.46166	H	4.56349	N 0.07139	S 0.03431	O 0.90000	S	298.00	0.0000
FUEL	SI	0.80718	FE	0.09769	AL 0.43349	MG 0.11413	O 2.52526	S	298.00	0.0000
FUEL	P	2.00000	O	5.00000				S	298.00	0.0000
FUEL	CA	0.26213	NA	0.01290	K 0.01486	TI 0.01001	O 0.29604	S	298.00	0.0000
FUEL	K	2.00000	C	1.00000	O 3.00000			S	298.00	1.0000
FUEL	H	2.00000	O	1.00000				L	298.00	0.0000
OXIDANT	N	2.00000						G	1660.00	0.5000
OXIDANT	O	2.00000						G	1660.00	0.5000
OXIDANT	AR	1.00000						G	1660.00	0.5000
O/F= 6.6885						PERCENT FUEL= 13.0065	EQUIVALENC RATIO= 1.0870	REACTANT DENSITY=	0.0000	

AXIAL STATION (M)
CHAMBER THROAT 0.000 0.250 0.500

PC/P	1.0000	1.7431	1.4290	1.4831	1.5412
P, ATM	4.5000	2.5816	3.1513	3.0342	2.9198
T, DEG K	2824	2651	2713	2703	2693
RHO, G/CC	5.6336-4	3.4755-4	4.1327-4	3.9955-4	3.8609-4
H, CAL/G	232.3	128.6	165.0	159.4	153.7
S, CAL/(G)(K)	2.2250	2.2250	2.2250	2.2255	2.2260

M, MOL WT	29.006	29.290	29.192	29.206	29.220
(DLV/DLP)T	-1.01200	-1.00916	-1.01018	-1.01003	-1.00989
(DLV/DLT)P	1.2736	1.2221	1.2416	1.2390	1.2363
CP, CAL/(G)(K)	0.7822	0.7177	0.7434	0.7402	0.7369
GAMMA (S)	1.1495	1.1521	1.1507	1.1508	1.1510
VELOCITY,M/SEC			750.35	750.35	750.35
TOTAL H(CAL/G)			232.26	226.68	221.03
MAG FLD(TESLA)			6.00	6.00	6.00
BETA			1.62	1.68	1.74
SON VEL,M/SEC	964.6	931.2	942.9	941.0	939.1
ELEC DENS	3.744 20	1.435 20	2.053 20	1.940 20	1.830 20
IONIC DENS)	7.686 20	3.741 20	4.830 20	4.615 20	4.407 20
SIGMA (MHO/M)	11.7035	7.4307	8.8776	8.6842	8.4886
W/O IONS	12.7108	8.0514	9.6264	9.4173	9.2057
FREQ (1/SEC)	9.015 11	5.442 11	6.517 11	6.294 11	6.076 11
MACH NUMBER	0.0000	1.0000	0.7958	0.7974	0.7990

AE/AT		1.0000	1.0437	1.0795	1.1171
TOTAL MOL WT	29.006	29.290	29.191	29.206	29.220

CS
1
CS

MOLE FRACTIONS

ALO2	1.3351-7	2.4707-8	4.8052-8	4.4023-8	4.0207-8
ALO2-	2.1564-7	5.0808-8	9.0682-8	8.4151-8	7.7864-8
ALO2H	1.1512-6	3.2016-7	5.3346-7	4.9939-7	4.6630-7
ALO2H2	1.1627-6	3.7765-7	5.9180-7	5.5787-7	5.2467-7
AR	8.8104-3	8.8967-3	8.8668-3	8.8711-3	8.8755-3
CO	7.2253-2	5.9910-2	6.4280-2	6.3646-2	6.3004-2
CO2	1.1009-1	1.2422-1	1.1923-1	1.1995-1	1.2068-1
CA	1.3108-6	9.2448-7	1.0577-6	1.0418-6	1.0257-6
CAO	1.0945-6	6.8794-7	8.2115-7	8.0217-7	7.8317-7
CAOH	5.6055-5	5.2144-5	5.3685-5	5.3536-5	5.3382-5
CAO2H2	3.6926-5	4.2573-5	4.0442-5	4.0672-5	4.0908-5
E	3.2007-5	2.0081-5	2.4078-5	2.3541-5	2.3000-5
FE	1.9799-4	1.9192-4	1.9403-4	1.9395-4	1.9388-4
FEO	1.7284-4	1.7374-4	1.7388-4	1.7384-4	1.7378-4
FEOH	8.4052-6	8.4347-6	8.4166-6	8.3961-6	8.3756-6
FEO2	2.5508-5	2.7358-5	2.6813-5	2.6855-5	2.6894-5
FEO2-	2.9888-6	2.8059-6	2.8993-6	2.8781-6	2.8559-6
FEO2H2	1.6142-5	2.3758-5	2.0547-5	2.0874-5	2.1216-5
H	3.4121-3	2.1712-3	2.5736-3	2.5158-3	2.4580-3
HCO	1.0322-7	3.8517-8	5.5337-8	5.2203-8	4.9191-8
HK	3.8342-6	2.3794-6	2.8317-6	2.7531-6	2.6753-6
HNO	7.5600-7	3.3695-7	4.5574-7	4.3431-7	4.1346-7
HO2	2.7955-6	1.3074-6	1.7478-6	1.6718-6	1.5972-6
H2	6.7056-3	5.5334-3	5.9357-3	5.8784-3	5.8207-3
H2O	7.0003-2	7.4130-2	7.2730-2	7.2936-2	7.3144-2

H2O2	2.4667-7	1.2104-7	1.5833-7	1.5155-7	1.4492-7
K	2.8340-3	2.8147-3	2.8246-3	2.3280-3	2.8314-3
K+	4.8828-5	3.6199-5	4.0340-5	3.9756-5	3.9171-5
KALO2(L)	1.4036-5	1.2249-5	1.1842-5	1.1915-5	1.1985-5
KALSI2O6(L)	4.2271-8	1.9906-7	1.0236-7	1.1192-7	1.2256-7
KO	8.2263-5	5.4885-5	6.4020-5	6.2512-5	6.1004-5
KOH	2.0927-3	2.2011-3	2.1608-3	2.1620-3	2.1631-3
MG	2.4405-5	2.1412-5	2.2527-5	2.2429-5	2.2328-5
MGO	8.4504-6	5.7553-6	6.6705-6	6.5320-6	6.3928-6
MGOH	1.1526-4	1.2145-4	1.1930-4	1.1957-4	1.1985-4
MGO2H2	3.5804-6	4.6103-6	4.2006-6	4.2424-6	4.2856-6
N	1.6132-6	5.6521-7	8.3621-7	7.8902-7	7.4353-7
NO	9.5657-3	6.3150-3	7.4128-3	7.2422-3	7.0709-3
NO2	3.1085-6	1.5321-6	2.0099-6	1.9268-6	1.8452-6
N2	6.8359-1	6.9196-1	6.8907-1	6.8949-1	6.8992-1
N2O	9.5429-7	4.7753-7	6.1902-7	5.9344-7	5.6839-7
NA	4.2105-5	4.2702-5	4.2510-5	4.2581-5	4.2654-5
NAO	1.1361-6	7.8764-7	9.0549-7	8.8549-7	8.6544-7
NAOH	1.3147-5	1.3483-5	1.3360-5	1.3338-5	1.3315-5
O	3.3096-3	1.8100-3	2.2846-3	2.2141-3	2.1438-3
O-	4.7144-7	1.6062-7	2.4245-7	2.2833-7	2.1469-7
OH	1.0227-2	7.0738-3	8.1558-3	7.9958-3	7.8346-3
OH-	2.4595-6	1.1711-6	1.5561-6	1.4911-6	1.4272-6
O2	1.4115-2	1.0005-2	1.1507-2	1.1299-2	1.1087-2
PN	1.2668-7	8.5281-8	9.8025-8	9.5910-8	9.3815-8
PO	4.8791-6	3.8104-6	4.1708-6	4.1198-6	4.0685-6
PO2	9.3102-6	9.1756-6	9.2419-6	9.2349-6	9.2275-6
PO2-	8.1023-6	8.8083-6	8.6176-6	8.6450-6	8.6721-6
PO3	1.5568-7	1.5671-7	1.5704-7	1.5682-7	1.5657-7
PO3-	2.0678-6	2.9299-6	2.5963-6	2.6413-6	2.6876-6
S	2.9370-6	1.5190-6	1.9312-6	1.8653-6	1.8005-6
SH	7.3899-7	3.8781-7	4.8865-7	4.7138-7	4.5448-7
SO	1.1716-4	8.3541-5	9.4592-5	9.2900-5	9.1206-5
SO2	1.0081-3	1.0547-3	1.0393-3	1.0416-3	1.0440-3
SO2-	1.1020-7	6.5322-8	7.9734-8	7.7229-8	7.4744-8
SO3	2.8591-7	2.4516-7	2.6078-7	2.5787-7	2.5490-7
SIO	8.3157-4	8.2997-4	8.3114-4	8.3113-4	8.3111-4
SIO2(L)	1.1318-6	3.5079-6	2.0573-6	2.2099-6	2.3784-6
SIO2	8.4148-5	9.1516-5	8.9022-5	8.9293-5	8.9564-5
TIO2	5.4343-7	5.5074-7	5.4825-7	5.4862-7	5.4899-7

05-3
#SPECIES IN SOLUTION AT LAST STATION

AL2O3(L)	FE3O4(L)	KALO2(L)	KALSIO4(L)	KALSI2O6(L)	KALSI3O8(L)	K2CO3(L)	K2SO4(L)	K2SI2O5(L)	SIO2(L)
SIO2(L)	TI2O3(L)								

#ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-06 FOR ALL ASSIGNED CONDITIONS

AL(S)	AL(L)	AL	AL+	ALH	ALN(S)	ALN	ALO	ALO+	ALO-
ALOH	ALOH+	ALOH-	AL2O	AL2O+	AL2O2	AL2O2+	AL2O3(S)	AL2O3(L)	AL6O13SI2(S)
ALS	AR+	C(S)	C	C+	C-	CAL	C3-	C2H-	CH
CH+	CH2	CH2O	CH3	CH4	CN	CN+	CN-	CNN	CN2
COS	COS-	CO2-	CO3-	CO4-	CP	CS	CS-	CS2	C2
C2-	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2O	C3	C3O2
C4	C5	CA(S)	CA(S)	CA(L)	CA+	CACO3(S)	CACO3(S)	CAO(S)	CAO(L)
CAOH+	CAO2H2(S)	CAS(S)	CASO4(S)	FE(S)	FE(S)	FE(S)	FE(L)	FE+	FEO(S)
FE0(L)	FE0-	FE02H2(S)	FE03H3(S)	FES(S)	FES(S)	FES(S)	FES04(S)	FES2(S)	FE2O3(S)
FE2O3(L)	FE3O4(S)	FE3O4(L)	FE3O3O12(S)	H+	H-	HALO	HCN	HCO+	HCO3-
HCP	HNCO	HNO2	HNO3	HPO2	H2O(S)	H2O(L)	H2P	H2S	H2SO4(L)

H2SO4	H3O+	HP-	HS-	HSI-	K(S)	K(L)	K-	KALO2(S)	KALSIO4(L)
KALSI3O8(S)	KALSI3O8(L)	KCN	K2CO3(S)	K2CO3(L)	KO+	KO-	KOH(S)	KOH(S)	KOH(L)
KOH+	K2	K2O(S)	K2O(L)	K2O2H2	K2SO4(S)	K2SO4(S)	K2SO4(L)	K2SIO3(L)	K2SIO5(L)
MG(S)	MG(L)	MG+	MGCO3(S)	MGH	MGN	MGO(S)	MGO(L)	MGOH+	MGS(S)
MGS	MGSO4(S)	MGSO4(L)	MG2SIO4(S)	MG2SIO4(L)	NCO	NH	NH2	NH3	NO-
NO+	NO2-	NO3	NO3-	N2H4	N2O+	N2O4	N2O5	N3	NA(S)
NA(L)	NA+	NAALSI3O8(S)	NA-	NAH	NAO-	NAOH(S)	NAOH(L)	NAOH+	NA2
NA2CO3(S)	NA2CO3(S)	NA2CO3(L)	NA2O(S)	NA2O(S)	NA2O(L)	NA2O2H2	NA2SO4(S)	NA2SO4(S)	NA2SO4(S)
NA2SO4(L)	NA2SO4	NA2SIO3(S)	NA2SIO3(L)	NA2SIO5(S)	NA2SIO5(L)	O+	OH+	O2-	O3
P	P(S)	P+	P-	PH	PH3	PO-	PS	P2	P4
S(S)	S(L)	S+	S-	SN	SO-	SO3-	S2	S2-	S8
SI(S)	SI(L)	SI	SI+	SI-	SIC(S)	SIC	SIC2	SIH	SIH+
SIH4	SIN	SIO2(S)	SIO2(S)	SIO2(S)	SIO2H2	SIS	SI2	SI2C	SI2N
SI3	TI(S)A	TI(S)B	TI(L)	TI	TI+	TIO(S)A	TIO(S)B	TIO(L)	TIO
TIO2(S)A	TIO2(S)B	TIO2(L)	TI2O3(S)	TI2O3(L)	TI3O5(S)A	TI3O5(S)B	TI3O5(L)	TI5O7(S)	TI5O7(L)
TIC(S)	TIC(L)	TIN(S)	TIN(L)						

#NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

STOP 5 IS NORMAL CHANNEL STOP

IT OCCURS WHEN XPOSITION EXCEEDS INPUTTED XXSTOP VALUE

3.3 Partial Equilibrium/Partial Rate Controlled Channel Problems

In this subsection, we consider a sample problem which illustrates the INPUT/OUTPUT format for partial chemical rate controlled channel problems. These problems also show how to execute problems with profiles of area ratio, velocity, or pressure given along the channel. Four problems are considered. In the first three, the non-equilibrium chemistry begins from the channel entrance. In the fourth, it begins from the throat. The first three problems describe the same channel flow. In the first problem, the channel area ratio is specified, in the second, the channel velocity, and in the third, the channel pressure. These problems are designed to show the effects of all the source terms $\dot{w}_i$, F , and q appearing on the right hand side of Eqs. (1) - (4) of Section 1. To be more specific, MHD type channel problems are considered here which satisfy Eqs. (113) - (117) and (124) of Section 1. These are illustrative examples and have no practical value. In the following, the INPUT/OUTPUT data for these problems is described in more detail.

3.3.1 Input Data

For this type of problems, the REACTANTS, OMIT, SOLUTION and INSERT cards are similar to those described in Subsection 3.1.1. The INPT2, RKTINP, and CHNLIN input data are similar to the channel problems considered in Subsection 3.2.1. Four additional types of input data are required for this type of problems (see Subsection 2.1.6). These are DLIT cards which contain the name of rate controlled species, REACTANT cards, which specify the reactant side of a chemical reaction, PRODUCT cards, which specify the product side of a chemical reaction, and KFRR cards, which specify the rate constant for a given reaction. The input data for the four sample problems considered here is given below.

3.3.1.1 Input data for a channel problem with partial equilibrium/partial rate controlled chemistry, NEQPT=4, and channel area ratio specified

The input data for this problem is listed below: (Fortran Logical Unit 5)

```

REACTANTS
C 1.000000 2.000000      00      .641859  000000.0G 2600.00F
K 2.000000 0 1.000      00      0.25000 -86800.00S 2600.00F 0.0
AR1.0      00      .178141  0.0G 2600.00F
O 2.000000      00      3.79720  000.0G 2600.00F 0.0
N 2.000000      00      0.20230  00000.0G 2600.00F 0.0

```

NAMELISTS

```

$INPT2 KASE=300, P(1)=1.0, DXI=0.001, BZ=8.00, XK=0.8, MIX=1.05, RKT=T,
TRACE=1.0E-7, IONS=T, ACCURC=1.0E-3, HMIN=1.0E-30 $END
$RKTINP PCP(1)=4.0, HPATH=T, SPATH=F,
NEQPT=4, TCEST=3000.0, TCHFNL=700.0, IPRRKT=1 $END

```

NAME	TCR	D	CO	CS
1	1.000	1.000		
2	1.0000	1.000		
3	1.00E-10	0.0	3250.0	
4	1.0000	1.000		
5	1.000	1.000		
6	3.15E-11	0.0	2250.0	
7	1.0	1.000		
8	1.000	1.0		
9	1.0E-12	0.0	0.0	
10	1.0002	1.0		
11	1.000	1.000		
12	1.0E-11	0.0	950.0	
13	1.0000	1.000		
14	1.000	1.000		
15	1.0E-10	0.0	22000.0	
16	1.000	1.000		
17	1.000	1.0		
18	3.00E-10	0.0	1000.0	
19	1.000	1.000		
20	1.000	1.0		
21	1.0E-12	0.0	24000.0	
22	1.000	1.0		1.0THIRD BODY
23	1.0002	1.0THIRD BODY		
24	1.0E-10	0.0	900.0	
25	1.000	1.000		
26	1.000	1.0		
27	1.0E-11	0.0	6000.0	

STOP

For example, the first set:

REACTANT	1.0 SO	1.0 O2	
PRODUCT	1.0 SO2	1.0 O	
KFRR	5.8E-13	0.0	3250.0

means that $\text{SO} + \text{O}_2 \xrightleftharpoons{k_f} \text{SO}_2 + \text{O}$ has a rate constant given by (in units of molecule-cm³-sec)

$$k_f = 5.8\text{E-}13 \times T^{0.0} \times \text{EXP}(-3250.0/T)$$

Note: At least one of the species listed on the DLIT card must appear in each chemical equation. If a species appears in the DLIT card but not in any of the chemical equations, its concentration is assumed frozen. If a species appears in a chemical reaction but not on a DLIT card, it is not rate controlled.

DATA CARD 40 - A blank card to terminate the above input set.

DATA CARD 41 - A blank card.

DATA CARD 42 - A STOP card.

Channel input data appears on Fortran Logical Unit 11.

\$CHNLIN NMPATH=3, IMPRNT=2, XXSTOP=0.0202, \$END

DATA CARD 1 - CHNLIN namelist input is described in Table VI.

Note: NMPATH=3 implies a constant area ratio (value at channel entrance) specified channel problem

The following is a description of this data.

DATA CARD 1 - REACTANTS code card with the word REACTANTS in columns 1 - 9 and blank in columns 16-31 (which indicates this is not a two-stage problem). Note, since the THERMO data is to be input from a file described by Fortran Logical Unit 7, this is the first data card.

DATA CARDS 2 - 6 - This contains the REACTANTS data described by Table II.

DATA CARD 7 - A blank card to terminate the set of REACTANTS data.

DATA CARD 8 - NAMELISTS code card. Note that this problem does not have any SOLUTION, OMIT, or INSERT cards.

DATA CARD 9 - INPT2 namelist data is described in Table III. This is a RKT=T (i. e. channel) problem, thus DXI, ACCURC, and HMIN are required inputs. Note, BZ and XIC are required for MHD channel problems.

DATA CARD 10 - RKTINP namelist data is described in Table IV. It is recommended that all channel problems be run with HPATH=TRUE and SPATH=FALSE. TCHFNL is set equal to 700.0 (the program will stop executing any time the calculated temperature falls below this value). NEQPT=4 implies that finite rate chemistry begins at the channel entrance.

DATA CARD 11 - The DLIT code card contains the names of rate controlled species. See Subsection 2.1.6.1 for more detail.

DATA CARD 12 - A blank card to terminate DLIT card inputs.

DATA CARDS 13 - 39 - Contains the set of REACTANT, PRODUCT, KFRR cards for the 9 rate equations initiated at the channel entrance. These cards are described in Subsections 2.1.6.2 and 2.1.6.3.

3.3.1.2 Input data for a channel problem with partial equilibrium/partial rate controlled chemistry, NEQPT=4, and channel velocity specified

In this set of problems, the same channel flow is assumed. Therefore, the REACTANTS, INPT2, RKTINP, DLIT, REACTANT, PRODUCT, and KFRR input cards are identical to those of the previous problem. The channel input data is different, and is listed below:

\$CHNLIN NMPATH=1, IMPRNT=2, XXSTOP=0.02, \$END

0.0	1372.95264
0.001	1359.81196
0.002	1344.95654
0.003	1330.77808
0.004	1316.46582
0.005	1302.33879
0.006	1287.39453
0.007	1272.55786
0.008	1257.52612
0.009	1242.28027
0.01	1226.79614
0.011	1211.04492
0.012	1194.99219
0.013	1178.50197
0.014	1161.00566
0.015	1144.00206
0.016	1127.044859
0.017	1108.79248
0.018	1089.77197
0.019	1069.81592
0.020	1048.61841

DATA CARD 1 - CHNLIN namelist input is described in Table VI. NMPATH=1 implies velocity given channel problem.

DATA CARDS 2 - 21 - The first column is the axial position in the channel in meters. The second column is the corresponding specified velocity in meters/sec.

3.3.1.3 Input data for a channel problem with partial equilibrium/partial rate controlled chemistry, NEQPT=4, and channel pressure specified

In these set of problems, the same channel flow is assumed. Therefore, the REACTANTS, INPT2, RKTINP, DLIT, REACTANT, PRODUCT, and KFRR input cards are identical to those of the problem discussed in Subsection 3.3.1.1. The channel input data is different and is listed below:

\$CHNLIN NMPATH=2, IMPRNT=2, XXSTOP=0.0202, \$END

0.0	0.25
0.001	0.2529841
0.002	0.2560548
0.003	0.2592171
0.004	0.2624782
0.005	0.2659455
0.006	0.2693263
0.007	0.2729665
0.008	0.2767448
0.009	0.2806724
0.01	0.2847636
0.011	0.2890357
0.012	0.2935086
0.013	0.2982077
0.014	0.3031601
0.015	0.3083237
0.016	0.3138069
0.017	0.3196728
0.018	0.3260012
0.019	0.3328878
0.02	0.3405024

DATA CARD 1 - CHNLIN namelist input described in Table VI. NMPATH=2 implies pressure specified channel problem.

DATA CARDS 2 - 21 - The first column is the axial position in the channel in meters. The second column is the corresponding specified pressure in atm.

3.3.1.4 Input data for a channel problem with partial equilibrium/partial rate controlled chemistry, NEQPT=3, and channel area ratio specified

For this problem, the flow from the combustor to the throat is assumed to be the same as that of the channel problem 3.3.1.1. The only unique property of this flow is that rate controlled chemistry begins at the throat. Therefore, the REACTANTS, INPT2, DLIT, REACTANT, PRODUCT, and KFRR data cards are identical to those of problem 3.3.1.1. As shown below, the RKTINP and \$CHNLIN input data are different.

```
$RKTINP  PCP(1)=4.0, HPATH=T, SPATH=F,  
          NEQPT=3, TCEST=3000.0, TCHFNL=700.0, IPRRKT=1  $END  
Note that, for this problem, NEQPT=3 implies a constant area  
ratio specified channel problem (value used is channel entrance  
area ratio).
```

```
$CHNLIN  NMPATH=-3, IMPRNT=2, XXSTOP=0.0102, $END  
-0.1     0.25
```

DATA CARD 1 - CHNLIN namelist input is described in Table VI.

DATA CARD 2 - See discussion of SPECIAL CHANNEL PROFILE in Subsection 2.1.7.2. The first input, which is negative, flags the special iteration starting at the throat. In this case, -0.1 is the position of the throat (meters) relative to the channel entrance, and 0.25 is the pressure (atm) at the channel entrance.

3.3.2 Output Data

Major parts of the output data for the type of problems considered here have the same format as those described in Subsections 3.1.2 and 3.3.2. Additional

output is printed to give information about chemical reactions and rate controlled species. The chemical reactions and their rate constants are printed out just after output information about the channel input data appears. To distinguish the rate controlled species concentration, their mole fraction is listed under a separate heading and appear after the mole fraction of other species is printed out.

Output data for the sample problems considered here is described below.

3.3.2.1 Output data for a channel problem with partial equilibrium/partial rate controlled chemistry, NEQPT=4, and channel area specified

This output data is shown on Sample Output (7). The output data format for this set of problems is basically the same as those of other channel problems. It contains information about the contents of the REACTANT, INPT2, RKTNP and \$CHNLIN data cards. The chemical reactions and their rate constants are printed out after they are read by the program (see output pages 4 and 5). The mole fraction of the chemically rate controlled species are printed under a separate heading after those of nonrate controlled species (see output pages 9 and 13).

3.3.2.2 Output data for a channel problem with partial equilibrium/partial rate controlled chemistry, NEQPT=4, and channel velocity specified

This output data is shown on Sample Output (8). The output data format for this set of problem is identical to that of the previous sample problem. In this case, the velocity profile is printed out under the output associated with channel input data (see output page 4).

3.3.2.3 Output data for a channel problem with partial equilibrium/partial rate controlled chemistry, NEQPT=4, and channel pressure specified

This output data is shown on Sample Output (9). The output format for this problem is also identical to that of the first problem of this subsection. In this case, however, the pressure profile is printed out under the output corresponding to channel input data (see output page 4).

**Sample Output 7, Channel Problem
With Partial Equilibrium/Partial Rate
Controlled Chemistry and Channel
Area Ratio Specified**

(13 Output Pages)

1

Page 1

1

REACTANTS

C 1.0000 S 2.0000 0.0000 0.0000 00 0.0000 0.64186
 K 2.0000 O 1.0000 0.0000 0.0000 0.0000 0.25000
 AR 1.0000 0.0000 0.0000 0.0000 00 0.0000 0.10814
 O 2.0000 0.0000 0.0000 0.0000 00 0.0000 0.79720
 N 2.0000 0.0000 0.0000 0.0000 00 0.0000 0.20280

NAMELISTS

1

\$INPT2

KASE = 300,

T = 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,

P = 1.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,

PSIA = F,

MMHG = F,

NSQM = F,

V = 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,

3-109

RHO = 1.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,

ERATIO = F,

OXFL = F,

FPCT = F,

FA = F,

MIX = 1.050000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 ,

TP = F,

HP = F,

SP = F,

TV = F,

UV = F,

SV = F,

RKT = T,

SHOCK = F,

DETN = F,

OTTO = F,

CR = 0.000000 ,

SO = 0.000000000000

IONS = T,

0.00 G 2600.000 0 F 0.000000
 -86800.00 S 2600.000 0 F 0.000000
 0.00 G 2600.000 0 F 0.000000
 0.00 G 2600.000 0 O 0.000000
 0.00 G 2600.000 0 O 0.000000


```

IDEBUG=      0,
TRACE = 0.100000E-06,
SIUNIT= F,
DXI  = 0.100000E-02,
NITER =      0,
NSTOP =      0,
NEQL  = F,
BZ    = 8.000000 ,
XK    = 0.800000 ,
ACCURC= 0.100000E-02,
HMIN  = 0.100000E-29,
ALPH  = 0.000000 ,
EXIN  = 2400.00 ,
TWOESTG= F,
$END
LLMT =

```

C
S
K
O
AR
N

0SPECIES BEING CONSIDERED IN THIS SYSTEM

3-110	L 5/66	AR	L12/66	AR+	J 3/61	C(S)	J 3/61	C	L12/66	C+
	J 9/65	C-	3/3/7	C3-	J 6/69	CN	J12/70	CN+	J12/70	CN-
	J 6/66	CNN	J12/70	CN2	J 9/65	CO	J 3/61	COS	3/3/7	COS-
	J 9/65	CO2	4/12/7	CO2-	3/3/7	CO3-	3/7/7	CO4-	J12/62	CS
	3/3/7	CS-	J 6/61	CS2	J12/69	C2	J12/69	C2-	J 3/67	C2N
	J 3/61	C2N2	J 9/66	C2O	J12/69	C3	J 6/68	C3O2	J12/69	C4
	J12/69	C5	L02/67	E	J12/61	K(S)	J12/61	K(L)	J 6/62	K
	J 3/65	K+	3/3/7	K-	3/8/7	KCN	J 3/66	K2CO3(S)	J 3/66	K2CO3(L)
	J12/67	KO	7/29/8	KO+	J12/67	KO-	J12/61	K2	J 6/63	K2O(S)
	10/78	K2O(L)	J12/71	K2SO4(S)	J12/71	K2SO4(S)	J12/71	K2SO4(L)	J 3/61	N
	J12/70	NCO	J 6/63	NO	3/3/7	NO-	J 6/66	NO+	J 9/64	NO2
	J 6/72	NO2-	J12/64	NO3	3/3/7	NO3-	J 9/65	N2	J12/64	N2O
	J12/70	N2O+	J 9/64	N2O4	J12/64	N2O5	J12/70	N3	J 6/62	O
	L12/66	O+	J 6/65	O-	J 9/65	O2	J12/66	O2-	J 6/61	O3
	J12/65	S(S)	J12/65	S(L)	J 6/71	S	L12/66	S+	3/3/7	S-
	J 6/61	SN	J 6/71	SO	3/3/7	SO-	J 6/61	SO2	3/3/7	SO2-
J 9/65	SO3	3/3/7	SO3-	J12/65	S2	3/3/7	S2-	J6/64	S8	
85	7	12	6	0	5	755				

C
S
K
O
AR
N
E

\$RKTINP

```

EOL  = T,
FROZ = F,
SUBAR = 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
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0.000000 , 0.000000 , 0.000000 , 0.000000 ,

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NFZ = 1 ,
NEOPT = 4 ,
HTLOSS = 0.000000 ,
HPATH = T ,
SPATH = F ,
NUMHLS = 0 ,
CHNLEN = 1.000000 ,
CHNHLS = 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
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      0.000000 ,
TCHINP = 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
      0.000000 , 0.000000 , 0.000000 , 0.000000 ,
      0.000000 ,
TCHNL = 700.000 ,
IPRRT = 1 ,
$END
JOE = 1.050000

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3-111

ENTHALPY (KG-MOL)(DEG K)/KG	EFFECTIVE FUEL HFP(2)	EFFECTIVE OXIDANT HPP(1)	MIXTURE HSUB0					
0KG-ATOMS/KG	0.15592358E 03	0.31446185E 03	0.23712613E 03					
C	0.84300786E-02	0.00000000E 00	0.41122334E-02					
S	0.16360157E-01	0.00000000E 00	0.82244668E-02					
K	0.53076642E-02	0.00000000E 00	0.25891047E-02					
O	0.26538321E-02	0.49826868E-01	0.26815630E-01					
AR	0.27070437E-02	0.00000000E 00	0.13205092E-02					
N	0.00000000E 00	0.14478784E-01	0.74159624E-02					
E	0.00000000E 00	0.00000000E 00	0.00000000E 00					
OPT	C	S	K	O	AR	N	E	
1	-19.182	-18.444	-22.243	-16.467	-25.372	-15.414	-12.361	13.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 1								
ION	DENS (M-3)	ION	DENS (M-3)					
1 K+	5.860E 21	2 KO+	3.462E 16					
1 CN-	5.620E 15	2 COS-	1.444E 16					
5 K-	3.126E 18	6 KO-	1.255E 19					
9 O-	1.383E 20	10 O2-	1.081E 19					
13 SO2-	2.087E 20	14 SO3-	5.621E 17					
CONDUCTIVITY =	213.1110 (MHO/M)	15 S2-	3.262E 18					
2	-19.554	-18.694	-22.537	-16.661	-25.808	-15.597	-12.862	3.000
PC/PT=	1.721229	T=	3230.81					
2	-19.553	-18.693	-22.537	-16.660	-25.807	-15.596	-12.861	2.000
PC/PT=	1.718772	T=	3231.14					

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 2							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 K+	3.252E 21	2 KO+	1.029E 16				
1 CN-	1.609E 15	2 COS-	4.389E 15	3 CO2-	2.813E 17	4 CO3-	1.636E 15
5 K-	1.275E 18	6 KO-	5.026E 18	7 NO-	1.169E 17	8 NO2-	8.431E 16
9 O-	5.675E 19	10 O2-	4.237E 18	11 S-	5.840E 19	12 SO-	1.227E 20
13 SO2-	9.919E 19	14 SO3-	2.418E 17	15 S2-	1.116E 18		
CONDUCTIVITY = 194.4897 (MHO/M)							
3	-20.143	-19.106	-23.001	-16.971	-26.491	-15.887	-13.662
4.000							

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 3							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 K+	1.297E 21	2 KO+	1.530E 15				
1 CO2-	6.082E 16	2 K-	3.067E 17	3 KO-	1.176E 18	4 NO-	2.003E 16
5 NO2-	1.803E 16	6 O-	1.370E 19	7 O2-	9.528E 17	8 S-	1.358E 19
9 SO-	2.830E 19	10 SO2-	3.001E 19	11 SO3-	6.354E 16	12 S2-	1.978E 17
CONDUCTIVITY = 167.5795 (MHO/M)							

DLIT COS O CO CS
1 NON-EQUILIBRIUM REACTIONS

3-112

6 1.0 CS + 1.0 O = 1.0 CO + 1.0 S

CHEMICAL RATE - 3.9900E-10*T** 0.0000*EXP(- 1.0000E 03/T)

7 1.0 CO + 1.0 O2 = 1.0 CO2 + 1.0 O

CHEMICAL RATE - 4.2000E-12*T** 0.0000*EXP(- 2.4000E 04/T)

8 1.0 CO + 1.0 O + 1.0 THIRD BODY = 1.0 CO2 + 1.0 THIRD BODY

CHEMICAL RATE - 5.5000E-32*T** 0.0000*EXP(- 9.0000E 02/T)

9 1.0 CS + 1.0 O2 = 1.0 COS + 1.0 O

CHEMICAL RATE - 1.7000E-11*T** 0.0000*EXP(- 6.0000E 03/T)

*****CHANNEL INPUTS*****

3-113

NMPATH= 3
IMPRNT= 2
XXSTOP= 0.2000E-01
UEIMP= 0.00000
ITYPE= 1

INDEPENDENT VARIABLE	DEPENDENT VARIABLE
0.00000	1.36497
1.00000	1.36497

4 -20.129 -19.099 -22.998 -16.966 -26.483 -15.884 -13.647 2.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 4			
ION	DENS (M-3)	ION	DENS (M-3)
1 K+	1.318E 21	2 KO+	1.586E 15
1 CO2-	6.250E 16	2 K-	3.135E 17
5 NO2-	1.045E 16	6 O-	1.406E 19
9 SO-	2.900E 19	10 SO2-	3.050E 19
CONDUCTIVITY =	160.4161 (MHO/M)	11 SO3-	6.463E 16
		12 S2-	2.038E 17

5 -20.115 -19.093 -22.994 -16.962 -26.474 -15.880 -13.632 1.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 5			
ION	DENS (M-3)	ION	DENS (M-3)
1 K+	1.341E 21	2 KO+	1.644E 15

1	CO2-	6.425E 16	2	K-	3.206E 17	3	KO-	1.225E 18	4	NO-	2.129E 16
5	NO2-	1.889E 16	6	O-	1.443E 19	7	O2-	1.003E 18	8	S-	1.432E 19
9	SO-	2.972E 19	10	SO2-	3.101E 19	11	SO3-	6.576E 16	12	S2-	2.100E 17

CONDUCTIVITY = 169.2479 (MHO/M)

6 -20.101 -19.086 -22.989 -16.957 -26.465 -15.877 -13.617 1.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 6											
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1	K+	1.364E 21	2	KO+	1.705E 15						
1	CO2-	6.606E 16	2	K-	3.278E 17	3	KO-	1.251E 18	4	NO-	2.195E 16
5	NO2-	1.935E 16	6	O-	1.482E 19	7	O2-	1.029E 18	8	S-	1.471E 19
9	SO-	3.047E 19	10	SO2-	3.154E 19	11	SO3-	6.693E 16	12	S2-	2.165E 17

CONDUCTIVITY = 170.0756 (MHO/M)

7 -20.086 -19.079 -22.985 -16.952 -26.456 -15.873 -13.602 1.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 7											
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1	K+	1.387E 21	2	KO+	1.769E 15						
1	CO2-	6.794E 16	2	K-	3.354E 17	3	KO-	1.278E 18	4	NO-	2.265E 16
5	NO2-	1.982E 16	6	O-	1.522E 19	7	O2-	1.056E 18	8	S-	1.512E 19
9	SO-	3.125E 19	10	SO2-	3.208E 19	11	SO3-	6.815E 16	12	S2-	2.232E 17

CONDUCTIVITY = 170.8995 (MHO/M)

8 -20.072 -19.072 -22.980 -16.947 -26.446 -15.870 -13.587 1.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 8											
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1	K+	1.411E 21	2	KO+	1.835E 15						
1	CO2-	6.990E 16	2	K-	3.432E 17	3	KO-	1.306E 18	4	NO-	2.337E 16
5	NO2-	2.031E 16	6	O-	1.563E 19	7	O2-	1.084E 18	8	S-	1.553E 19
9	SO-	3.205E 19	10	SO2-	3.265E 19	11	SO3-	6.942E 16	12	S2-	2.303E 17

CONDUCTIVITY = 171.7201 (MHO/M)

9 -20.058 -19.065 -22.975 -16.942 -26.437 -15.866 -13.572 1.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 9											
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1	K+	1.436E 21	2	KO+	1.905E 15						
1	CO2-	7.194E 16	2	K-	3.514E 17	3	KO-	1.335E 18	4	NO-	2.412E 16
5	NO2-	2.083E 16	6	O-	1.606E 19	7	O2-	1.113E 18	8	S-	1.597E 19
9	SO-	3.289E 19	10	SO2-	3.324E 19	11	SO3-	7.075E 16	12	S2-	2.376E 17

CONDUCTIVITY = 172.5377 (MHO/M)

10 -20.043 -19.058 -22.970 -16.937 -26.427 -15.862 -13.557 1.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 10		ION		DENS (M-3)		
					DENS (M-3)		DENS (M-3)				
1	K+	1.461E 21	2	KO+	1.978E 15						
1	CO2-	7.408E 16	2	K-	3.600E 17	3	KO-	1.366E 18	4	NO-	2.492E 16
5	NO2-	2.137E 16	6	O-	1.651E 19	7	O2-	1.144E 18	8	S-	1.642E 19
9	SO-	3.377E 19	10	SO2-	3.386E 19	11	SO3-	7.215E 16	12	S2-	2.454E 17
CONDUCTIVITY =		173.3583 (MHO/M)									

11 -20.028 -19.051 -22.905 -16.932 -26.416 -15.858 -13.541 1.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 11		ION		DENS (M-3)		
					DENS (M-3)		DENS (M-3)				
1	K+	1.487E 21	2	KO+	2.055E 15						
1	CO2-	7.633E 16	2	K-	3.689E 17	3	KO-	1.399E 18	4	NO-	2.576E 16
5	NO2-	2.193E 16	6	O-	1.697E 19	7	O2-	1.176E 18	8	S-	1.690E 19
9	SO-	3.469E 19	10	SO2-	3.450E 19	11	SO3-	7.361E 16	12	S2-	2.535E 17
CONDUCTIVITY =		174.1782 (MHO/M)									

12 -20.014 -19.043 -22.959 -16.926 -26.406 -15.854 -13.525 1.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 12		ION		DENS (M-3)		
					DENS (M-3)		DENS (M-3)				
1	K+	1.515E 21	2	KO+	2.136E 15						
1	CO2-	7.869E 16	2	K-	3.783E 17	3	KO-	1.433E 18	4	NO-	2.663E 16
5	NO2-	2.253E 16	6	O-	1.746E 19	7	O2-	1.210E 18	8	S-	1.740E 19
9	SO-	3.565E 19	10	SO2-	3.518E 19	11	SO3-	7.515E 16	12	S2-	2.621E 17
CONDUCTIVITY =		174.9984 (MHO/M)									

13 -19.999 -19.036 -22.953 -16.921 -26.395 -15.850 -13.509 1.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 13		ION		DENS (M-3)		
					DENS (M-3)		DENS (M-3)				
1	K+	1.543E 21	2	KO+	2.222E 15						
1	CO2-	8.116E 16	2	K-	3.882E 17	3	KO-	1.468E 18	4	NO-	2.756E 16
5	NO2-	2.315E 16	6	O-	1.796E 19	7	O2-	1.245E 18	8	S-	1.791E 19
9	SO-	3.666E 19	10	SO2-	3.589E 19	11	SO3-	7.677E 16	12	S2-	2.711E 17
CONDUCTIVITY =		175.8202 (MHO/M)									

1

0PC = 14.7 PSIA

THEORETICAL MHD CORE PERFORMANCE

CASE NO. 300

CHEMICAL FORMULA

FUEL C 1.00000 S 2.00000
 FUEL K 2.00000 O 1.00000
 FUEL AR 1.00000
 OXIDANT O 2.00000
 OXIDANT N 2.00000

WT FRACTION ENERGY STATE TEMP DENSITY
 (SEE NOTE) CAL/MOL DEG K G/CC
 0.64186 60407.805 G 2600.00 0.0000
 0.25000 -36800.000 S 2600.00 0.0000
 0.10814 11435.389 G 2600.00 0.0000
 0.79720 19666.641 G 2600.00 0.0000
 0.20280 18637.500 G 2600.00 0.0000

O/F= 1.0500 PERCENT FUEL= 48.7805

EQUIVALENCE RATIO= 0.9684

REACTANT DENSITY= 0.0000

	AXIAL STATION (M)												
	CHAMBER	THROAT	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009	0.010
PC/P	1.0000	1.7188	4.0000	3.9528	3.9054	3.8578	3.8098	3.7616	3.7130	3.6635	3.6134	3.5629	3.5117
P, ATM	1.0000	0.5818	0.2500	0.2530	0.2561	0.2592	0.2625	0.2658	0.2693	0.2730	0.2767	0.2807	0.2848
T, DEG K	3362	3231	3044	3047	3051	3055	3059	3063	3067	3071	3075	3079	3083
RHO, G/CC	1.3889-4	8.5485-5	3.9984-5	4.0394-5	4.0817-5	4.1252-5	4.1700-5	4.2164-5	4.2643-5	4.3144-5	4.3664-5	4.4205-5	4.4768-5
H, CAL/G	471.2	379.4	245.9	248.3	250.7	253.1	255.5	258.0	260.4	263.0	265.6	268.3	271.0
S, CAL/(G)(K)	1.8840	1.8840	1.8840	1.8842	1.8843	1.8845	1.8847	1.8849	1.8850	1.8852	1.8853	1.8855	1.8857
M, MOL WT	38.316	38.956	39.942	39.927	39.911	39.896	39.880	39.863	39.846	39.829	39.811	39.793	39.774
(DLV/DLP)T	-1.06918	-1.06455	-1.05728	-1.05213	-1.04713	-1.04213	-1.03714	-1.03215	-1.02716	-1.02217	-1.01718	-1.01218	-1.00719
(DLV/DLP)P	2.3473	2.3120	2.2404	1.4908	1.4921	1.4934	1.4946	1.4958	1.4970	1.4982	1.4993	1.5004	1.5015
CP, CAL/(G)(K)	1.6374	1.6327	1.6033	0.8278	0.8289	0.8299	0.8309	0.8319	0.8328	0.8337	0.8346	0.8354	0.8362
GAMMA (S)	1.1177	1.1141	1.1092	1.1266	1.1267	1.1267	1.1267	1.1268	1.1268	1.1269	1.1269	1.1270	1.1271
VELOCITY, M/SEC			1372.95	1359.01	1344.96	1330.78	1316.47	1302.01	1287.39	1272.56	1257.53	1242.28	1226.80
TOTAL H(CAL/G)			471.21	469.00	466.83	464.70	462.60	460.54	458.51	456.53	454.59	452.68	450.82
MAG FLD(TESLA)			8.00	3.18	3.18	3.18	3.18	3.18	3.18	3.18	3.18	3.18	3.18
BETA			6.92	2.72	2.69	2.66	2.62	2.59	2.56	2.53	2.50	2.47	2.43
SON VEL, M/SEC	903.0	876.5	838.3	845.5	846.3	847.0	847.7	848.4	849.2	849.9	850.7	851.5	852.3
ELEC DENS	5.031 21	2.902 21	1.208 21	1.228 21	1.248 21	1.269 21	1.290 21	1.312 21	1.334 21	1.357 21	1.381 21	1.406 21	1.431 21
IONIC DENS	6.689 21	3.601 21	1.385 21	1.409 21	1.433 21	1.458 21	1.484 21	1.510 21	1.537 21	1.565 21	1.594 21	1.624 21	1.655 21
SIGMA (MHO/M)	213.1110	194.4897	167.5795	168.4161	169.2479	170.0756	170.8995	171.7201	172.5377	173.3583	174.1782	174.9984	175.8202
W/O IONS	427.9375	399.8962	355.1946	357.4567	359.6929	361.9034	364.0879	366.2472	368.3815	370.5021	372.6015	374.6802	376.7417
FREQ (1/SEC)	6.653 11	4.205 11	2.032 11	2.055 11	2.079 11	2.103 11	2.127 11	2.153 11	2.179 11	2.206 11	2.234 11	2.263 11	2.293 11
MACH NUMBER	0.0000	1.0000	1.6378	1.6073	1.5893	1.5712	1.5530	1.5346	1.5160	1.4972	1.4782	1.4589	1.4394
AE/AT		1.0000	1.3650	1.3650	1.3650	1.3650	1.3650	1.3650	1.3650	1.3650	1.3650	1.3650	1.3650
TOTAL MOL WT	38.316	38.956	39.942	39.927	39.911	39.896	39.880	39.863	39.847	39.829	39.811	39.793	39.775

MOLE FRACTIONS

AR	5.0596-2	5.1442-2	5.2744-2	5.2724-2	5.2703-2	5.2683-2	5.2661-2	5.2640-2	5.2618-2	5.2595-2	5.2571-2	5.2547-2	5.2523-2
CO2	3.7547-2	4.1767-2	4.9257-2	4.9238-2	4.9216-2	4.9192-2	4.9166-2	4.9138-2	4.9107-2	4.9073-2	4.9036-2	4.8995-2	4.8952-2
CO2-	3.3778-7	2.1286-7	1.0088-7	1.0258-7	1.0431-7	1.0608-7	1.0788-7	1.0973-7	1.1161-7	1.1356-7	1.1556-7	1.1761-7	1.1973-7
E	2.3045-3	2.1962-3	2.0043-3	2.0156-3	2.0268-3	2.0379-3	2.0488-3	2.0595-3	2.0700-3	2.0805-3	2.0907-3	2.1009-3	2.1109-3
K	9.3379-2	9.5877-2	9.9483-2	9.9421-2	9.9358-2	9.9294-2	9.9229-2	9.9163-2	9.9097-2	9.9029-2	9.8959-2	9.8888-2	9.8816-2
K+	2.6843-3	2.4606-3	2.1508-3	2.1639-3	2.1769-3	2.1897-3	2.2024-3	2.2149-3	2.2273-3	2.2397-3	2.2519-3	2.2640-3	2.2761-3
K-	1.4318-6	9.6442-7	5.0879-7	5.1456-7	5.2045-7	5.2644-7	5.3255-7	5.3880-7	5.4518-7	5.5178-7	5.5855-7	5.6551-7	5.7268-7
KO	3.1181-3	2.5096-3	1.7729-3	1.7829-3	1.7929-3	1.8032-3	1.8135-3	1.8241-3	1.8349-3	1.8459-3	1.8572-3	1.8688-3	1.8806-3
KO-	5.7504-6	3.8032-6	1.9502-6	1.9692-6	1.9887-6	2.0087-6	2.0291-6	2.0501-6	2.0717-6	2.0942-6	2.1174-6	2.1413-6	2.1662-6
K2	7.0063-6	4.6613-6	2.4504-6	2.4696-6	2.4895-6	2.5100-6	2.5311-6	2.5531-6	2.5758-6	2.5996-6	2.6244-6	2.6502-6	2.6771-6
N	4.0322-5	2.6614-5	1.3673-5	1.3921-5	1.4173-5	1.4427-5	1.4685-5	1.4946-5	1.5211-5	1.5481-5	1.5756-5	1.6037-5	1.6323-5
NO	2.1573-2	1.9166-2	1.5788-2	1.5874-2	1.5960-2	1.6046-2	1.6131-2	1.6215-2	1.6300-2	1.6385-2	1.6470-2	1.6555-2	1.6641-2
NO-	1.6253-7	8.8465-8	3.3222-8	3.3884-8	3.4562-8	3.5254-8	3.5962-8	3.6687-8	3.7431-8	3.8201-8	3.8993-8	3.9811-8	4.0656-8

NO2	6.2536-6	4.5923-6	2.8049-6	2.8325-6	2.8603-6	2.8884-6	2.9168-6	2.9456-6	2.9748-6	3.0047-6	3.0351-6	3.0660-6	3.0977-6
NO2-	1.0200-7	6.3797-8	2.9904-8	3.0285-8	3.0674-8	3.1070-8	3.1476-8	3.1890-8	3.2315-8	3.2755-8	3.3208-8	3.3674-8	3.4155-8
N2	1.3125-1	1.3481-1	1.4020-1	1.4010-1	1.4000-1	1.3990-1	1.3979-1	1.3969-1	1.3958-1	1.3948-1	1.3937-1	1.3926-1	1.3915-1
N2O	4.5609-7	3.1105-7	1.6963-7	1.7159-7	1.7353-7	1.7550-7	1.7751-7	1.7955-7	1.8163-7	1.8377-7	1.8596-7	1.8821-7	1.9052-7
O-	6.3361-5	4.2930-5	2.2723-5	2.3078-5	2.3436-5	2.3799-5	2.4166-5	2.4538-5	2.4915-5	2.5301-5	2.5693-5	2.6093-5	2.6502-5
O2	1.0993-1	1.0941-1	1.0781-1	1.0809-1	1.0835-1	1.0861-1	1.0885-1	1.0909-1	1.0931-1	1.0953-1	1.0974-1	1.0993-1	1.1012-1
O2-	4.9524-6	3.2058-6	1.5805-6	1.6041-6	1.6280-6	1.6523-6	1.6770-6	1.7020-6	1.7276-6	1.7538-6	1.7805-6	1.8080-6	1.8361-6
S	1.5589-2	1.2714-2	9.0029-3	9.1080-3	9.2133-3	9.3186-3	9.4241-3	9.5297-3	9.6357-3	9.7427-3	9.8503-3	9.9586-3	1.0068-2
S-	6.6262-5	4.4190-5	2.2528-5	2.2890-5	2.3256-5	2.3627-5	2.4004-5	2.4387-5	2.4776-5	2.5176-5	2.5584-5	2.6001-5	2.6428-5
SN	3.4597-5	2.2484-5	1.1151-5	1.1333-5	1.1517-5	1.1704-5	1.1894-5	1.2088-5	1.2285-5	1.2487-5	1.2694-5	1.2906-5	1.3123-5
SO	1.2182-1	1.1335-1	9.9126-2	9.9590-2	1.0007-1	1.0053-1	1.0099-1	1.0145-1	1.0190-1	1.0235-1	1.0281-1	1.0326-1	1.0371-1
SO-	1.4010-4	9.2825-5	4.6936-5	4.7591-5	4.8257-5	4.8932-5	4.9620-5	5.0320-5	5.1034-5	5.1769-5	5.2522-5	5.3293-5	5.4085-5
SO2	1.7628-1	1.9329-1	2.1974-1	2.1904-1	2.1833-1	2.1762-1	2.1692-1	2.1621-1	2.1551-1	2.1479-1	2.1408-1	2.1336-1	2.1264-1
SO2-	9.5589-5	7.5057-5	4.9772-5	5.0055-5	5.0345-5	5.0641-5	5.0943-5	5.1252-5	5.1570-5	5.1898-5	5.2237-5	5.2586-5	5.2946-5
SO3	3.5655-5	3.3857-5	3.0760-5	3.0743-5	3.0728-5	3.0714-5	3.0702-5	3.0692-5	3.0683-5	3.0677-5	3.0673-5	3.0671-5	3.0671-5
SO3-	2.5748-7	1.8294-7	1.0540-7	1.0607-7	1.0677-7	1.0748-7	1.0822-7	1.0898-7	1.0977-7	1.1059-7	1.1144-7	1.1233-7	1.1326-7
S2	5.2713-4	3.8803-4	2.3117-4	2.3415-4	2.3716-4	2.4020-4	2.4327-4	2.4638-4	2.4953-4	2.5275-4	2.5603-4	2.5937-4	2.6277-4
S2-	1.4940-6	8.4464-7	3.2809-7	3.3447-7	3.4099-7	3.4766-7	3.5449-7	3.6149-7	3.6867-7	3.7612-7	3.8379-7	3.9171-7	3.9990-7

MOLE FRACTIONS OF NEOL SPECIES

COS	8.6658-6	6.2416-6	3.6544-6	3.6683-6	3.7033-6	3.7508-6	3.8057-6	3.8648-6	3.9264-6	3.9898-6	4.0539-6	4.1187-6	4.1842-6
O	1.1289-1	1.0179-1	8.5487-2	8.5463-2	8.5455-2	8.5462-2	8.5486-2	8.5527-2	8.5585-2	8.5664-2	8.5762-2	8.5878-2	8.6012-2
CO	1.2001-1	1.1842-1	1.1499-1	1.1495-1	1.1491-1	1.1486-1	1.1482-1	1.1478-1	1.1475-1	1.1471-1	1.1467-1	1.1464-1	1.1461-1
CS	5.7010-7	3.2277-7	1.2843-7	1.3162-7	1.3522-7	1.3889-7	1.4260-7	1.4639-7	1.5024-7	1.5419-7	1.5821-7	1.6231-7	1.6652-7

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.100000E-06 FOR ALL ASSIGNED CONDITIONS

AR+	C(S)	C	C+	C-	C3-	CN	CN+	CN-	CNN
CN2	COS-	CO3-	CO4-	CS-	CS2	C2	C2-	C2N	C2N2
C2O	C3	C3O2	C4	C5	K(S)	K(L)	KCN	K2CO3(S)	K2CO3(L)
KO+	K2O(S)	K2O(L)	K2SO4(S)	K2SO4(S)	K(SO4(L)	NCO	NO+	NO3	NO3-
N2O+	N2O4	N2O;	N3	O+	O3	S(S)	S(L)	S+	S8

3	-19.983	-19.028	-22.947	-16.915	-26.383	-15.845	-13.492	1.000
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ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 3									
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 K+	1.572E 21	2 KO+	2.312E 15						
1 CO2-	8.377E 16	2 K-	3.986E 17	3 KO-	1.506E 18	4 NO-	2.854E 16		
5 NO2-	2.381E 16	6 O-	1.850E 19	7 O2-	1.281E 18	8 S-	1.846E 19		
9 SO-	3.772E 19	10 SO2-	3.663E 19	11 SO3-	7.848E 16	12 S2-	2.806E 17		
CONDUCTIVITY =		176.6454 (MHO/M)							

4	-19.968	-19.020	-22.940	-16.910	-26.372	-15.841	-13.476	1.000
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ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 4									
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 K+	1.603E 21	2 KO+	2.408E 15						
1 COS-	1.026E 15	2 CO2-	8.653E 16	3 K-	4.095E 17	4 KO-	1.546E 18		
5 NO-	2.957E 16	6 NO2-	2.451E 16	7 O-	1.906E 19	8 O2-	1.320E 18		

9 S- 1.983E 19 18 SO- 3.884E 19 11 SO2- 3.742E 19 12 SO3- 8.829E 16
 13 S2- 2.987E 17
 CONDUCTIVITY = 177.4753 (MHO/M)

5 -19.952 -19.811 -22.933 -16.984 -26.359 -15.836 -13.458 1.0000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 5		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.634E 21	2	KO+	2.511E 15						
1	COS-	1.878E 15	2	CO2-	3.945E 16	3	K-	4.211E 17	4	KO-	1.588E 18
5	NO-	3.867E 16	6	NO2-	2.525E 16	7	O-	1.965E 19	8	O2-	1.361E 18
9	S-	1.964E 19	18	SO-	4.882E 19	11	SO2-	3.825E 19	12	SO3-	8.221E 16
13	S2-	3.814E 17									
CONDUCTIVITY =		178.3132 (MHO/M)									

6 -19.936 -19.883 -22.926 -16.898 -26.347 -15.831 -13.441 1.0000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 6		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.668E 21	2	KO+	2.628E 15						
1	COS-	1.117E 15	2	CO2-	9.257E 16	3	K-	4.335E 17	4	KO-	1.634E 18
5	NO-	3.185E 16	6	NO2-	2.683E 16	7	O-	2.827E 19	8	O2-	1.485E 18
9	S-	2.828E 19	18	SO-	4.128E 19	11	SO2-	3.913E 19	12	SO3-	8.426E 16
13	S2-	3.129E 17									
CONDUCTIVITY =		179.1618 (MHO/M)									

7 -19.919 -18.994 -22.918 -16.892 -26.334 -15.825 -13.423 1.0000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 7		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.782E 21	2	KO+	2.736E 15						
1	COS-	1.168E 15	2	CO2-	9.585E 16	3	K-	4.465E 17	4	KO-	1.681E 18
5	NO-	3.389E 16	6	NO2-	2.686E 16	7	O-	2.893E 19	8	O2-	1.451E 18
9	S-	2.896E 19	18	SO-	4.268E 19	11	SO2-	4.886E 19	12	SO3-	8.642E 16
13	S2-	3.258E 17									
CONDUCTIVITY =		188.8124 (MHO/M)									

8 -19.982 -18.985 -22.918 -16.885 -26.328 -15.828 -13.484 1.0000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 8		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.739E 21	2	KO+	2.862E 15						
1	COS-	1.222E 15	2	CO2-	9.939E 16	3	K-	4.684E 17	4	KO-	1.733E 18
5	NO-	3.444E 16	6	NO2-	2.776E 16	7	O-	2.163E 19	8	O2-	1.588E 18

9 S- 2.168E 19 10 SO- 4.402E 19 11 SO2- 4.105E 19 12 SO3- 8.874E 16
 13 S2- 3.381E 17
 CONDUCTIVITY = 180.8803 (MHO/M)

9 -19.885 -18.975 -22.902 -16.878 -26.306 -15.814 -13.385 1.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 9		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.778E 21	2	KO+	2.998E 15						
1	COS-	1.282E 15	2	CO2-	1.032E 17	3	K-	4.755E 17	4	KO-	1.788E 18
5	NO-	3.590E 16	6	NO2-	2.873E 16	7	O-	2.238E 19	8	O2-	1.553E 18
9	S-	2.246E 19	10	SO-	4.554E 19	11	SO2-	4.211E 19	12	SO3-	9.125E 16
13	S2-	3.523E 17									
CONDUCTIVITY =		181.7721 (MHO/M)									

10 -19.867 -18.965 -22.892 -16.871 -26.290 -15.808 -13.364 1.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 10		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.820E 21	2	KO+	3.149E 15						
1	COS-	1.348E 15	2	CO2-	1.074E 17	3	K-	4.919E 17	4	KO-	1.849E 18
5	NO-	3.750E 16	6	NO2-	2.979E 16	7	O-	2.320E 19	8	O2-	1.611E 18
9	S-	2.331E 19	10	SO-	4.721E 19	11	SO2-	4.327E 19	12	SO3-	9.399E 16
13	S2-	3.679E 17									
CONDUCTIVITY =		182.6962 (MHO/M)									

11 -19.847 -18.955 -22.882 -16.863 -26.274 -15.801 -13.343 1.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 11		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.865E 21	2	KO+	3.316E 15						
1	COS-	1.421E 15	2	CO2-	1.120E 17	3	K-	5.100E 17	4	KO-	1.916E 18
5	NO-	3.928E 16	6	NO2-	3.096E 16	7	O-	2.410E 19	8	O2-	1.674E 18
9	S-	2.425E 19	10	SO-	4.905E 19	11	SO2-	4.455E 19	12	SO3-	9.702E 16
13	S2-	3.851E 17									
CONDUCTIVITY =		183.6026 (MHO/M)									

12 -19.827 -18.943 -22.871 -16.855 -26.256 -15.794 -13.319 1.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 12		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.915E 21	2	KO+	3.506E 15						
1	COS-	1.504E 15	2	CO2-	1.172E 17	3	K-	5.304E 17	4	KO-	1.991E 18
5	NO-	4.128E 16	6	NO2-	3.228E 16	7	O-	2.511E 19	8	O2-	1.746E 18

9 S- 2.529E 19 10 SO- 5.111E 19 11 SO2- 4.597E 19 12 SO3- 1.004E 17
 13 S2- 4.046E 17
 CONDUCTIVITY = 184.6907 (MHO/M)

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THEORETICAL MHD CORE PERFORMANCE

OPC = 14.7 PSIA
 CASE NO. 300

CHEMICAL FORMULA		WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	C 1.00000 S 2.00000	0.64186	60407.805	G	2600.00	0.0000
FUEL	K 2.00000 O 1.00000	0.25000	86800.000	S	2600.00	0.0000
FUEL	AR 1.00000	0.10814	11435.389	G	2600.00	0.0000
OXIDANT	O 2.00000	0.79720	19666.641	G	2600.00	0.0000
OXIDANT	N 2.00000	0.20280	18637.500	G	2600.00	0.0000

O/F= 1.0500 PERCENT FUEL= 48.7805 EQUIVALENC RATIO= 0.9684 REACTANT DENSITY= 0.0000

		AXIAL STATION (M)											
		0.011	0.012	0.013	0.014	0.015	0.016	0.017	0.018	0.019	0.020		
PC/P	1.00000	1.7188	3.4598	3.4071	3.3534	3.2986	3.2433	3.1867	3.1282	3.0675	3.0040	2.9368	
P, ATM	1.00000	0.5818	0.2890	0.2935	0.2982	0.3032	0.3083	0.3138	0.3197	0.3260	0.3329	0.3405	
T, DEG K	3362	3231	3087	3092	3096	3101	3105	3110	3115	3120	3125	3131	
RHO, G/CC	1.3889-4	8.5485-5	4.5356-5	4.5971-5	4.6617-5	4.7298-5	4.8008-5	4.8761-5	4.9566-5	5.0433-5	5.1376-5	5.2418-5	
H, CAL/G	471.2	379.4	273.7	276.6	279.5	282.4	285.5	288.6	291.9	295.4	299.0	302.9	
S, CAL/(G)(K)	1.8840	1.8340	1.8858	1.8860	1.8861	1.8862	1.8864	1.8865	1.8866	1.8868	1.8869	1.8870	
M, MOL WT	38.316	38.956	39.755	39.735	39.715	39.694	39.672	39.650	39.627	39.602	39.576	39.548	
(DLV/DLP)T	-1.06918	-1.06435	-1.02204	-1.02211	-1.02219	-1.02227	-1.02234	-1.02242	-1.02250	-1.02258	-1.02266	-1.02275	
(DLV/DLP)P	2.3473	2.3120	1.5025	1.5036	1.5046	1.5055	1.5065	1.5074	1.5084	1.5093	1.5102	1.5112	
CP, CAL/(G)(K)	1.6374	1.6327	0.8370	0.8377	0.8385	0.8391	0.8398	0.8404	0.8410	0.8416	0.8421	0.8426	
GAMMA (S)	1.1177	1.1141	1.1271	1.1272	1.1273	1.1273	1.1274	1.1275	1.1276	1.1277	1.1278	1.1279	
VELOCITY, M/SEC			1211.04	1194.99	1178.59	1161.81	1144.68	1127.05	1108.79	1089.77	1069.82	1048.62	
TOTAL H(CAL/G)			448.99	447.20	445.46	443.75	442.07	440.44	438.85	437.30	435.80	434.35	
MAG FLD(TESLA)			3.18	3.18	3.18	3.18	3.18	3.18	3.18	3.18	3.18	3.18	
BETA			2.40	2.37	2.34	2.30	2.27	2.23	2.19	2.16	2.12	2.08	
SON VEL, M/SEC	903.0	876.5	853.1	853.9	854.8	855.7	856.5	857.5	858.4	859.4	860.5	861.6	
ELEC DENS	5.031 21	2.902 21	1.457 21	1.484 21	1.513 21	1.543 21	1.574 21	1.606 21	1.641 21	1.678 21	1.719 21	1.763 21	
IONIC DENS	6.689 21	3.601 21	1.687 21	1.721 21	1.756 21	1.793 21	1.831 21	1.872 21	1.915 21	1.961 21	2.012 21	2.068 21	
SIGMA (MHO/M)	213.1110	194.4397	176.6454	177.4753	178.3132	179.1610	180.0124	180.8803	181.7721	182.6962	183.6626	184.6907	
W/O IONS	427.9375	399.8962	378.7831	380.8228	382.8513	384.8775	386.8872	388.9085	390.9553	393.0456	395.2001	397.4611	
FRLO (1/SEC)	6.653 11	4.205 11	2.325 11	2.357 11	2.391 11	2.427 11	2.464 11	2.503 11	2.544 11	2.589 11	2.637 11	2.690 11	
MACH NUMBER	0.0000	1.0130	1.4196	1.3994	1.3788	1.3578	1.3364	1.3144	1.2917	1.2680	1.2433	1.2170	
AE/AT		1.0300	1.3650	1.3650	1.3650	1.3650	1.3650	1.3650	1.3650	1.3650	1.3650	1.3650	
TOTAL MOL WT	38.316	38.956	39.755	39.736	39.715	39.694	39.673	39.650	39.627	39.602	39.576	39.548	

MOLE FRACTIONS

AR	5.0596-2	5.1442-2	5.2497-2	5.2471-2	5.2444-2	5.2416-2	5.2380-2	5.2358-2	5.2327-2	5.2295-2	5.2261-2	5.2224-2
CO2	3.7547-2	4.1767-2	4.8905-2	4.8854-2	4.8800-2	4.8741-2	4.8679-2	4.8611-2	4.8539-2	4.8460-2	4.8374-2	4.8279-2
CO2-	3.3778-7	2.1286-7	1.2192-7	1.2418-7	1.2654-7	1.2899-7	1.3153-7	1.3419-7	1.3702-7	1.4004-7	1.4329-7	1.4687-7
E	2.3045-3	2.1962-3	2.1207-3	2.1105-3	2.1102-3	2.1498-3	2.1594-3	2.1689-3	2.1784-3	2.1882-3	2.1982-3	2.2086-3
K	9.3379-2	9.5877-2	9.2742-2	9.8666-2	9.8588-2	9.8508-2	9.8426-2	9.8341-2	9.8253-2	9.8160-2	9.8062-2	9.7957-2
K+	2.6843-3	2.4600-3	2.2881-3	2.3001-3	2.3120-3	2.3240-3	2.3359-3	2.3480-3	2.3602-3	2.3728-3	2.3858-3	2.3995-3

K-	1.4318-6	9.6442-7	5.8809-7	5.8776-7	5.9574-7	6.0405-7	6.1263-7	6.2165-7	6.3120-7	6.4139-7	6.5238-7	6.6441-7
KO	3.1181-3	2.5890-3	1.8929-3	1.9054-3	1.9185-3	1.9320-3	1.9459-3	1.9605-3	1.9758-3	1.9921-3	2.0097-3	2.0288-3
KO-	5.7504-6	3.8032-6	2.1920-6	2.2189-6	2.2470-6	2.2765-6	2.3071-6	2.3394-6	2.3738-6	2.4108-6	2.4508-6	2.4948-6
K2	7.0063-6	4.6613-6	2.7052-6	2.7346-6	2.7656-6	2.7983-6	2.8323-6	2.8684-6	2.9071-6	2.9487-6	2.9940-6	3.0439-6
N	4.0322-5	2.6614-5	1.6615-5	1.6915-5	1.7223-5	1.7541-5	1.7867-5	1.8205-5	1.8560-5	1.8936-5	1.9337-5	1.9773-5
NO	2.1573-2	1.9165-2	1.6727-2	1.6814-2	1.6902-2	1.6992-2	1.7082-2	1.7174-2	1.7270-2	1.7369-2	1.7474-2	1.7586-2
NO-	1.6253-7	8.8465-8	4.1531-8	4.2440-8	4.3308-8	4.4381-8	4.5410-8	4.6496-8	4.7651-8	4.8892-8	5.0236-8	5.1720-8
NO2	6.2536-6	4.5923-6	3.1301-6	3.1634-6	3.1977-6	3.2332-6	3.2696-6	3.3075-6	3.3474-6	3.3898-6	3.4351-6	3.4846-6
NO2-	1.0208-7	6.3797-8	3.4654-8	3.5172-8	3.5712-8	3.6276-8	3.6861-8	3.7478-8	3.8133-8	3.8836-8	3.9597-8	4.0434-8
N2	1.3125-1	1.3484-1	1.3903-1	1.3891-1	1.3879-1	1.3867-1	1.3855-1	1.3842-1	1.3828-1	1.3814-1	1.3799-1	1.3783-1
N2O	4.5609-7	3.1106-7	1.9290-7	1.9535-7	1.9790-7	2.0055-7	2.0327-7	2.0613-7	2.0915-7	2.1237-7	2.1584-7	2.1963-7
O-	6.3361-5	4.2938-5	2.6920-5	2.7349-5	2.7790-5	2.8246-5	2.8713-5	2.9200-5	2.9710-5	3.0251-5	3.0830-5	3.1460-5
O2	1.0993-1	1.0944-1	1.1030-1	1.1048-1	1.1064-1	1.1080-1	1.1095-1	1.1109-1	1.1123-1	1.1136-1	1.1150-1	1.1164-1
O2-	4.9524-6	3.2053-6	1.8649-6	1.8947-6	1.9255-6	1.9575-6	1.9905-6	2.0250-6	2.0613-6	2.1001-6	2.1418-6	2.1874-6
S	1.5589-2	1.2714-2	1.0178-2	1.0289-2	1.0402-2	1.0517-2	1.0633-2	1.0752-2	1.0875-2	1.1003-2	1.1137-2	1.1280-2
S-	6.6262-5	4.4197-5	2.6866-5	2.7317-5	2.7783-5	2.8265-5	2.8760-5	2.9276-5	2.9819-5	3.0395-5	3.1011-5	3.1682-5
SN	3.4597-5	2.2482-5	1.3345-5	1.3575-5	1.3812-5	1.4058-5	1.4311-5	1.4575-5	1.4853-5	1.5149-5	1.5465-5	1.5810-5
SO	1.2182-1	1.1335-1	1.0415-1	1.0460-1	1.0506-1	1.0551-1	1.0597-1	1.0643-1	1.0690-1	1.0739-1	1.0790-1	1.0843-1
SO-	1.4010-4	9.2825-5	5.4900-5	5.5742-5	5.6613-5	5.7519-5	5.8452-5	5.9429-5	6.0460-5	6.1558-5	6.2737-5	6.4025-5
SO2	1.7628-1	1.9323-1	2.1192-1	2.1118-1	2.1044-1	2.0969-1	2.0893-1	2.0815-1	2.0736-1	2.0653-1	2.0566-1	2.0474-1
SO2-	9.5589-5	7.5057-5	5.3319-5	5.3706-5	5.4109-5	5.4529-5	5.4964-5	5.5421-5	5.5906-5	5.6423-5	5.6980-5	5.7589-5
SO3	3.5655-5	3.3857-5	3.0673-5	3.0678-5	3.0686-5	3.0696-5	3.0709-5	3.0725-5	3.0745-5	3.0769-5	3.0798-5	3.0832-5
SO3-	2.5748-7	1.8294-7	1.1422-7	1.1523-7	1.1630-7	1.1741-7	1.1858-7	1.1981-7	1.2113-7	1.2255-7	1.2409-7	1.2579-7
S2	5.2713-4	3.8803-4	2.6624-4	2.6981-4	2.7347-4	2.7724-4	2.8110-4	2.8510-4	2.8928-4	2.9369-4	2.9837-4	3.0343-4
S2-	1.4940-6	8.4464-7	4.0838-7	4.1720-7	4.2640-7	4.3602-7	4.4600-7	4.5651-7	4.6768-7	4.7966-7	4.9260-7	5.0684-7

MOLE FRACTIONS OF NEQL SPECIES

3-COS	8.6658-6	6.2416-6	4.2502-6	4.3170-6	4.3846-6	4.4533-6	4.5229-6	4.5940-6	4.6671-6	4.7430-6	4.8226-6	4.9076-6
O	1.1289-1	1.0179-1	8.6165-2	8.6338-2	8.6531-2	8.6744-2	8.6973-2	8.7224-2	8.7499-2	8.7799-2	8.8125-2	8.8480-2
CO	1.2001-1	1.1842-1	1.1457-1	1.1454-1	1.1451-1	1.1449-1	1.1446-1	1.1443-1	1.1441-1	1.1439-1	1.1437-1	1.1435-1
CS	5.7010-7	3.2277-7	1.7082-7	1.7524-7	1.7979-7	1.8451-7	1.8934-7	1.9439-7	1.9969-7	2.0531-7	2.1136-7	2.1796-7

#ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-06 FOR ALL ASSIGNED CONDITIONS

AR+	C(S)	C	C+	C-	C3-	CN	CN+	CN-	CNN
CN2	COS-	CO3-	CO4-	CS-	CS2	C2	C2-	C2N	C2N2
C2O	C3	C3O2	C4	C5	K(S)	K(L)	KCN	K2CO3(S)	K2CO3(L)
KO+	K2O(S)	K2O(L)	K2SO4(S)	K2SO4(S)	K2SO4(L)	NCO	NO+	NO3	NO3-
N2O+	N2O4	N2O5	N3	O+	O3	S(S)	S(L)	S+	S8

STOP 5 IS NORMAL CHANNEL STOP

IT OCCURS WHEN XPOSITION EXCEEDS INPUTTED XXSTOP VALUE

**Sample Output 8, Channel Problem
With Partial Equilibrium/Partial Rate
Controlled Chemistry and Channel Velocity Specified
(14 Output Pages)**

1

REACTANTS

C	1.0000	S	2.0000	0.0000	0.0000	0.0000	0.0000	0.64186
K	2.0000	O	1.0000	0.0000	0.0000	0.0000	0.0000	0.25000
AR	1.0000		0.0000	0.0000	0.0000	0.0000	0.0000	0.10814
O	2.0000		0.0000	0.0000	0.0000	0.0000	0.0000	0.79720
N	2.0000		0.0000	0.0000	0.0000	0.0000	0.0000	0.20280

0.00	G	2600.000	S	F	0.00000
-86800.00	S	2600.000	F	F	0.00000
0.00	G	2600.000	F	F	0.00000
0.00	G	2600.000	O	O	0.00000
0.00	G	2600.000	O	O	0.00000

NAMELISTS

1

\$INPT2

KASE = 300,

T	= 0.000000	, 0.000000	, 0.000000	, 0.000000	, 0.000000	, 0.000000	, 0.000000
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P	= 1.000000	, 0.000000	, 0.000000	, 0.000000	, 0.000000	, 0.000000	, 0.000000
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PSIA = F,

MMHG = F,

NSQM = F,

V	= 0.000000	, 0.000000	, 0.000000	, 0.000000	, 0.000000	, 0.000000	, 0.000000
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RHO	= 1.000000	, 0.000000	, 0.000000	, 0.000000	, 0.000000	, 0.000000	, 0.000000
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ERATIO = F,

OXFL = F,

FPCT = F,

FA = F,

MIX	= 1.050000	, 0.000000	, 0.000000	, 0.000000	, 0.000000	, 0.000000	, 0.000000
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0.000000	, 0.000000	, 0.000000	, 0.000000	, 0.000000	, 0.000000	, 0.000000	, 0.000000

TP = F,

HP = F,

SP = F,

TV = F,

UV = F,

SV = F,

RKT = T,

SHOCK = F,

DETN = F,

OTTO = F,

CR = 0.000000

S0 = 0.0000000000

IONS = T,

```

IDEBUG=          0,
TRACE  = 0.1000000E-06,
SIUNIT = F,
DXI    = 0.1000000E-02,
NITER  =          0,
NSTOP  =          0,
NEOL   = F,
BZ     = 0.000000,
XK     = 0.800000,
ACCURC = 0.1000000E-02,
HMIN   = 0.1000000E-29,
ALPH   = 0.000000,
EXIN   = 2400.00,
TWOSTG = F,
$END
LLMT =

```

CSK
OAR
N

SPECIES BEING CONSIDERED IN THIS SYSTEM

SPECIES BEING CONSIDERED IN THIS STUDY											
3-126	L 5/66	AR	L12/66	AR+	J 3/61	C(S)	J 3/61	C	L12/66	C+	
	J 9/65	C-	3/3/7	C3-	J 6/69	CN	J12/78	CN+	J12/78	CN-	
	J 6/66	CNN	J12/78	CN2	J 9/65	CO	J 3/61	COS	3/3/7	COS-	
	J 9/65	CO2	4/12/7	CO2-	3/3/7	CO3-	3/7/7	CO4-	J12/62	CS	
	3/3/7	CS-	J 6/61	CS2	J12/69	C2	J12/69	C2-	J 3/67	C2N	
	J 3/61	C2N2	J 9/66	C2O	J12/69	C3	J 6/68	C3O2	J12/69	C4	
	J12/69	C5	L82/67	E	J12/61	K(S)	J12/61	K(L)	J 6/62	K	
	J 3/65	K+	3/3/7	K-	3/8/7	KCN	J 3/66	K2CO3(S)	J 3/66	K2CO3(L)	
	J12/67	KO	7/29/8	KO+	J12/67	KO-	J12/61	K2	J 6/63	K2O(S)	
	18/78	K2O(L)	J12/71	K2SO4(S)	J12/71	K2SO4(S)	J12/71	K2SO4(L)	J 3/61	N	
	J12/78	NCO	J 6/63	NO	3/3/7	NO-	J 6/66	NO+	J 9/64	NO2	
	J 6/72	NO2-	J12/64	NO3	3/3/7	NO3-	J 9/65	N2	J12/64	N2O	
	J12/78	N2O+	J 9/64	N2O4	J12/64	N2O5	J12/78	N3	J 6/62	O	
	L12/66	O+	J 6/65	O-	J 9/65	O2	J12/66	O2-	J 6/61	O3	
	J12/65	S(S)	J12/65	S(L)	J 6/71	S	L12/66	S+	3/3/7	S-	
J 6/61	SN	J 6/71	SO	3/3/7	SO-	J 6/61	SO2	3/3/7	SO2-		
J 9/65	SO3	3/3/7	SO3-	J12/65	S2	3/3/7	S2-	J6/64	S8		
85	7	12	6	8	5	755					

CSK
OAR
NE

\$RKTINP

```

EOL      = T,
FROZ     = F,
SUBAR    = 0.00000000, 0.00000000, 0.00000000, 0.00000000,
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0.00000000, 0.00000000, 0.00000000,

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NFZ = 1 ,
NEOPT = 4 ,
HTLOSS= 0.000000 ,
HPATH = T ,
SPATH = F ,
NUMHLS= 0 ,
CHNLEN= 1.000000 ,
CHNHLS= 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
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0.000000 ,
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0.000000 ,
TCHFNL= 700.000 ,
IPRRKT= 1 ,
$END
$OF = 1.050000

```

ENTHALPY (KG-MOL)(DEG K)/KG		EFFECTIVE FUEL HPP(2)		EFFECTIVE OXIDANT HPP(1)		MIXTURE HSUB0	
\$KG-ATOMS/KG		BJP(I,2)		BOP(I,1)		BO(I)	
C	0.84300786E-02	0.00000000E 00	0.41122334E-02				
S	0.16860157E-01	0.00000000E 00	0.82244668E-02				
K	0.53076642E-02	0.00000000E 00	0.25891047E-02				
O	0.26538321E-02	0.49326863E-01	0.26815630E-01				
AR	0.27070437E-02	0.00000000E 00	0.13205092E-02				
N	0.00000000E 00	0.14478784E-01	0.74159624E-02				
E	0.00000000E 00	0.00000000E 00	0.00000000E 00				
\$PT	C S K O AR N E						
1	-19.182 -18.444 -22.243 -16.467 -25.372 -15.414 -12.361 13.000						

ION				ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 1			
DENS (M-3)		DENS (M-3)		DENS (M-3)		DENS (M-3)	
1 K+	5.860E 21	2 KO+	3.462E 16				
1 CN-	5.620E 15	2 COS-	1.444E 16	3 CO2-	7.374E 17	4 CO3-	4.754E 15
5 K-	3.126E 18	6 KO-	1.255E 19	7 NO-	3.548E 17	8 NO2-	2.228E 17
9 O-	1.383E 20	10 O2-	1.081E 19	11 S-	1.447E 20	12 SO-	3.059E 20
13 SO2-	2.087E 20	14 SO3-	5.621E 17	15 S2-	3.262E 18		
CONDUCTIVITY = 213.1110 (MHO/M)							

```

2 -19.554 -18.694 -22.537 -16.661 -25.808 -15.597 -12.862 3.000
PC/PT= 1.721229 T= 3230.81
2 -19.553 -18.693 -22.537 -16.660 -25.807 -15.596 -12.861 2.000
PC/PT= 1.718772 T= 3231.14

```


ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 2		ION		DENS (M-3)		
1	K+	3.252E 21	2	KO+	1.029E 16						
1	CN-	1.609E 15	2	COS-	4.389E 15	3	CO2-	2.813E 17	4	CO3-	1.636E 15
5	K-	1.275E 18	6	KO-	5.026E 18	7	NO-	1.169E 17	8	NO2-	8.431E 16
9	O-	5.675E 19	10	O2-	4.237E 18	11	S-	5.840E 19	12	SO-	1.227E 20
13	SO2-	9.919E 19	14	SO3-	2.418E 17	15	S2-	1.116E 18			
CONDUCTIVITY =		194.4897 (MHO/M)									

*****CHANNEL INPUTS*****

NMPATH= 1
 IMPRNT= 2
 XXSTOP= 0.20200E-01
 UEINP= 0.00000
 ITYPE= 1

INDEPENDENT VARIABLE

0.00000
 0.00100
 0.00200
 0.00300
 0.00400
 0.00500
 0.00600
 0.00700
 0.00800
 0.00900
 0.01000
 0.01100
 0.01200
 0.01300
 0.01400
 0.01500
 0.01600
 0.01700
 0.01800
 0.01900
 0.02000

DEPENDENT VARIABLE

1372.95264
 1359.01172
 1344.95630
 1330.77808
 1316.46558
 1302.00879
 1287.39429
 1272.55762
 1257.52588
 1242.28003
 1226.79590
 1211.04468
 1194.99219
 1178.50488
 1161.80542
 1144.68262
 1127.04468
 1108.79224
 1089.77173
 1069.01592
 1048.61841

3-128

3 -20.143 -19.106 -23.001 -16.971 -26.491 -15.887 -13.662 4.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 3		ION		DENS (M-3)		
1	K+	1.297E 21	2	KO+	1.530E 15						
1	CO2-	6.002E 16	2	K-	3.067E 17	3	KO-	1.176E 18	4	NO-	2.003E 16
5	NO2-	1.803E 16	6	O-	1.370E 19	7	O2-	9.528E 17	8	S-	1.358E 19
9	SO-	2.830E 19	10	SO2-	3.001E 19	11	SO3-	6.354E 16	12	S2-	1.978E 17
CONDUCTIVITY =		167.5795 (MHO/M)									

DLIT

COS

O

CO

CS

NON-EQUILIBRIUM REACTIONS

1 1.0 SO + 1.0 O2 = 1.0 SO2 + 1.0 O
 CHEMICAL RATE - 5.8000E-13*T** 0.0000*EXP(- 3.2500E 03/T)

2 1.0 COS + 1.0 O = 1.0 CO + 1.0 SO
 CHEMICAL RATE - 3.1500E-11*T** 0.0000*EXP(- 2.2500E 03/T)

3 1.0 S + 1.0 O2 = 1.0 SO + 1.0 O
 CHEMICAL RATE - 1.7000E-12*T** 0.0000*EXP(- 0.0000E-01/T)

4 1.0 CS2 + 1.0 O = 1.0 CS + 1.0 SO
 CHEMICAL RATE - 8.3000E-11*T** 0.0000*EXP(- 9.5000E 02/T)

5 1.0 CS2 + 1.0 O2 = 1.0 SO2 + 1.0 CS
 CHEMICAL RATE - 1.7000E-12*T** 0.0000*EXP(- 2.2000E 04/T)

3-129 6 1.0 CS + 1.0 O = 1.0 CO + 1.0 S
 CHEMICAL RATE - 3.9900E-10*T** 0.0000*EXP(- 1.0000E 03/T)

7 1.0 CO + 1.0 O2 = 1.0 CO2 + 1.0 O
 CHEMICAL RATE - 4.2000E-12*T** 0.0000*EXP(- 2.4000E 04/T)

8 1.0 CO + 1.0 O + 1.0 THIRD BODY = 1.0 CO2 + 1.0 THIRD BODY
 CHEMICAL RATE - 5.5000E-32*T** 0.0000*EXP(- 9.0000E 02/T)

9 1.0 CS + 1.0 O2 = 1.0 COS + 1.0 O
 CHEMICAL RATE - 1.7000E-11*T** 0.0000*EXP(- 6.0000E 03/T)

4 -20.129 -19.099 -22.998 -16.966 -26.483 -15.834 -13.647 2.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 4		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.318E 21	2	KO+	1.586E 15						
1	CO2-	6.250E 16	2	K-	3.135E 17	3	KO-	1.200E 18	4	NO-	2.065E 16
5	NO2-	1.845E 16	6	O-	1.406E 19	7	O2-	9.774E 17	8	S-	1.395E 19
9	SO-	2.900E 19	10	SO2-	3.050E 19	11	SO3-	6.463E 16	12	S2-	2.038E 17
CONDUCTIVITY =		168.4155 (MHO/M)									

***** KFLAG= -4

5 -20.115 -19.093 -22.994 -16.962 -26.474 -15.880 -13.632 2.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 5		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.341E 21	2	KO+	1.644E 15						
1	CO2-	6.425E 16	2	K-	3.205E 17	3	KO-	1.225E 18	4	NO-	2.129E 16
5	NO2-	1.889E 16	6	O-	1.443E 19	7	O2-	1.003E 18	8	S-	1.432E 19
9	SO-	2.972E 19	10	SO2-	3.101E 19	11	SO3-	6.576E 16	12	S2-	2.100E 17
CONDUCTIVITY =		169.2473 (MHO/M)									

***** KFLAG= -4

6 -20.101 -19.086 -22.989 -16.957 -26.465 -15.877 -13.617 1.000

3-130

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 6		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.364E 21	2	KO+	1.705E 15						
1	CO2-	6.606E 16	2	K-	3.278E 17	3	KO-	1.251E 18	4	NO-	2.195E 16
5	NO2-	1.935E 16	6	O-	1.482E 19	7	O2-	1.029E 18	8	S-	1.471E 19
9	SO-	3.047E 19	10	SO2-	3.154E 19	11	SO3-	6.693E 16	12	S2-	2.165E 17
CONDUCTIVITY =		170.0741 (MHO/M)									

7 -20.086 -19.079 -22.985 -16.952 -26.456 -15.873 -13.602 2.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 7		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.387E 21	2	KO+	1.769E 15						
1	CO2-	6.794E 16	2	K-	3.354E 17	3	KO-	1.278E 18	4	NO-	2.265E 16
5	NO2-	1.982E 16	6	O-	1.522E 19	7	O2-	1.056E 18	8	S-	1.512E 19
9	SO-	3.125E 19	10	SO2-	3.208E 19	11	SO3-	6.816E 16	12	S2-	2.233E 17
CONDUCTIVITY =		170.8973 (MHO/M)									

***** KFLAG= -4

***** KFLAG= -4

***** KFLAG= -4

8 -20.072 -19.072 -22.930 -16.947 -26.446 -15.870 -13.587 2.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 8		ION		DENS (M-3)		
					DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)		
1	K+	1.411E 21	2	KO+	1.835E 15						
1	CO2-	6.998E 16	2	K-	3.432E 17	3	KO-	1.386E 18	4	NO-	2.337E 16
5	NO2-	2.832E 16	6	O-	1.563E 19	7	O2-	1.884E 18	8	S-	1.554E 19
9	SO-	3.286E 19	10	SO2-	3.265E 19	11	SO3-	6.943E 16	12	S2-	2.383E 17
CONDUCTIVITY =		171.7175 (MHO/M)									
9	-23.858	-19.865	-22.975	-16.942	-26.437	-15.866	-13.572	2.888			

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 9		ION		DENS (M-3)		
					DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)		
1	K+	1.436E 21	2	KO+	1.985E 15						
1	CO2-	7.194E 16	2	K-	3.514E 17	3	KO-	1.335E 18	4	NO-	2.413E 16
5	NO2-	2.883E 16	6	O-	1.686E 19	7	O2-	1.114E 18	8	S-	1.597E 19
9	SO-	3.289E 19	10	SO2-	3.324E 19	11	SO3-	7.875E 16	12	S2-	2.376E 17
CONDUCTIVITY =		172.5347 (MHO/M)									
10	-28.843	-19.858	-22.978	-16.937	-26.427	-15.862	-13.557	2.888			

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 10		ION		DENS (M-3)		
					DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)		
1	K+	1.461E 21	2	KO+	1.978E 15						
1	CO2-	7.489E 16	2	K-	3.688E 17	3	KO-	1.366E 18	4	NO-	2.492E 16
5	NO2-	2.137E 16	6	O-	1.651E 19	7	O2-	1.144E 18	8	S-	1.642E 19
9	SO-	3.377E 19	10	SO2-	3.386E 19	11	SO3-	7.215E 16	12	S2-	2.454E 17
CONDUCTIVITY =		173.3552 (MHO/M)									

***** KFLAG= -4
***** KFLAG= -4

11 -28.828 -19.851 -22.965 -16.932 -26.416 -15.858 -13.541 2.888

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 11		ION		DENS (M-3)		
					DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)		
1	K+	1.487E 21	2	KO+	2.855E 15						
1	CO2-	7.633E 16	2	K-	3.689E 17	3	KO-	1.399E 18	4	NO-	2.576E 16
5	NO2-	2.194E 16	6	O-	1.697E 19	7	O2-	1.176E 18	8	S-	1.698E 19
9	SO-	3.469E 19	10	SO2-	3.458E 19	11	SO3-	7.362E 16	12	S2-	2.535E 17
CONDUCTIVITY =		174.1752 (MHO/M)									
12	-28.814	-19.843	-22.959	-16.926	-26.486	-15.854	-13.525	2.888			

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 12											
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 K+	1.515E 21	2 KO+	2.136E 15								
1 CO2-	7.868E 16	2 K-	3.783E 17	3 KO-	1.433E 18	4 NO-	2.663E 16				
5 NO2-	2.253E 16	6 O-	1.746E 19	7 O2-	1.210E 18	8 S-	1.739E 19				
9 SO-	3.565E 19	10 SO2-	3.518E 19	11 SO3-	7.515E 16	12 S2-	2.620E 17				
CONDUCTIVITY = 174.9953 (MHO/M)											
13	-19.999	-19.036	-22.953	-16.921	-26.395	-15.850	-13.509	2.000			

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 13											
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 K+	1.543E 21	2 KO+	2.221E 15								
1 CO2-	8.116E 16	2 K-	3.882E 17	3 KO-	1.468E 18	4 NO-	2.756E 16				
5 NO2-	2.315E 16	6 O-	1.796E 19	7 O2-	1.245E 18	8 S-	1.791E 19				
9 SO-	3.666E 19	10 SO2-	3.589E 19	11 SO3-	7.677E 16	12 S2-	2.710E 17				
CONDUCTIVITY = 175.8167 (MHO/M)											

1

THEORETICAL MHD CORE PERFORMANCE

SPC = 14.7 PSIA
CASE NO. 300

CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	C	1.00000	S	2.00000	0.64186	60407.805	G	2600.00
FUEL	K	2.00000	O	1.00000	0.25000	-86800.000	S	2600.00
FUEL	AR	1.00000			0.10814	11435.389	G	2600.00
OXIDANT	O	2.00000			0.79720	19666.641	G	2600.00
OXIDANT	N	2.00000			0.20280	18637.500	G	2600.00
O/F= 1.0500 PERCENT FUEL= 48.7805 EQUIVALENCE RATIO= 0.9684 REACTANT DENSITY= 0.0000								

AXIAL STATION (M)													
	CHAMBER	THROAT	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009	0.010
PC/P	1.0000	1.7188	4.0000	3.9528	3.9054	3.8577	3.8097	3.7614	3.7127	3.6635	3.6134	3.5630	3.5118
P, ATM	1.0000	0.5018	0.2500	0.2530	0.2561	0.2592	0.2625	0.2659	0.2693	0.2730	0.2767	0.2807	0.2848
T, DEG K	3362	3231	3044	3047	3051	3055	3059	3063	3067	3071	3075	3079	3083
RHO, G/CC	1.3889-4	8.5485-5	3.9984-5	4.0394-5	4.0817-5	4.1252-5	4.1702-5	4.2166-5	4.2645-5	4.3146-5	4.3664-5	4.4204-5	4.4767-5
H, CAL/G	471.2	379.4	245.9	248.3	250.7	253.1	255.5	258.0	260.5	263.0	265.6	268.2	270.9
S, CAL/(G)(K)	1.8840	1.8840	1.8840	1.8842	1.8843	1.8845	1.8847	1.8848	1.8850	1.8851	1.8853	1.8855	1.8856
M, MOL WT	38.316	38.956	39.942	39.927	39.911	39.896	39.880	39.863	39.846	39.820	39.812	39.793	39.775
(DLV/DLP)T	-1.06918	-1.06455	-1.05728	-1.05213	-1.05131	-1.052139	-1.052148	-1.052156	-1.052164	-1.052172	-1.052180	-1.052188	-1.052196
(DLV/DLP)P	2.3473	2.3120	2.2404	1.4908	1.4921	1.4934	1.4946	1.4958	1.4970	1.4982	1.4993	1.5004	1.5015
CP, CAL/(G)(K)	1.6374	1.6327	1.6033	0.8278	0.8289	0.8299	0.8309	0.8319	0.8328	0.833	0.8346	0.8354	0.8362
GAMMA (S)	1.1177	1.1141	1.1092	1.1266	1.1267	1.1267	1.1267	1.1267	1.1268	1.1269	1.1269	1.1270	1.1271
VELOCITY, M/SEC			1372.95	1359.01	1344.96	1330.78	1316.47	1302.01	1287.39	1272.50	1257.53	1242.28	1226.80
TOTAL H(CAL/G)			471.21	469.00	466.84	464.70	462.60	460.54	458.52	456.54	454.57	452.65	450.77
MAG FLD(TESLA)			8.00	3.18	3.18	3.18	3.18	3.18	3.18	3.18	3.18	3.18	3.18
BETA			6.92	2.72	2.69	2.66	2.63	2.60	2.56	2.53	2.50	2.47	2.44
SON VEL, M/SEC	903.0	875.5	838.3	845.5	846.3	847.0	847.7	848.4	849.2	849.9	850.7	851.5	852.3
ELEC DENS	5.031 21	2.902 21	1.208 21	1.228 21	1.248 21	1.269 21	1.290 21	1.312 21	1.334 21	1.357 21	1.381 21	1.405 21	1.431 21

IONIC DENS)	6.689	21	3.601	21	1.385	21	1.409	21	1.433	21	1.458	21	1.484	21	1.510	21	1.537	21	1.565	21	1.594	21	1.624	21	1.655	21
SIGMA (MHO/M)	213.1110		194.4897		167.5795		168.4155		169.2473		170.0741		170.8973		171.7175		172.5347		173.3552		174.1752		174.9953		175.8167	
W/O IONS	427.9375		399.8962		355.1946		357.4544		359.6899		361.8976		364.0771		366.2350		368.3664		370.4876		372.5887		374.6689		376.7303	
FREQ (1/SEC)	6.653	11	4.205	11	2.032	11	2.055	11	2.079	11	2.103	11	2.128	11	2.153	11	2.179	11	2.206	11	2.234	11	2.263	11	2.293	11
MACH NUMBER	0.0000		1.0000		1.6378		1.6073		1.5893		1.5712		1.5530		1.5346		1.5160		1.4972		1.4782		1.4589		1.4394	
AE/AT			1.0000		1.3650		1.3650		1.3649		1.3649		1.3649		1.3649		1.3648		1.3647		1.3646		1.3645		1.3644	
TOTAL MOL WT	38.316		38.956		39.942		39.927		39.911		39.896		39.880		39.863		39.847		39.829		39.812		39.794		39.775	

MOLE FRACTIONS

AR	5.0596-2	5.1442-2	5.2744-2	5.2724-2	5.2703-2	5.2683-2	5.2661-2	5.2640-2	5.2618-2	5.2595-2	5.2572-2	5.2548-2	5.2523-2
CO2	3.7547-2	4.1767-2	4.9257-2	4.9238-2	4.9216-2	4.9192-2	4.9166-2	4.9138-2	4.9107-2	4.9073-2	4.9037-2	4.8997-2	4.8955-2
CO2-	3.3778-7	2.1286-7	1.0088-7	1.0258-7	1.0431-7	1.0608-7	1.0789-7	1.0973-7	1.1161-7	1.1356-7	1.1556-7	1.1761-7	1.1973-7
E	2.3045-3	2.1962-3	2.0043-3	2.0156-3	2.0268-3	2.0379-3	2.0487-3	2.0594-3	2.0699-3	2.0804-3	2.0907-3	2.1008-3	2.1108-3
K	9.3379-2	9.5877-2	9.9483-2	9.9421-2	9.9358-2	9.9294-2	9.9229-2	9.9163-2	9.9097-2	9.9029-2	9.8960-2	9.8889-2	9.8817-2
K+	2.6843-3	2.4606-3	2.1508-3	2.1639-3	2.1769-3	2.1897-3	2.2023-3	2.2149-3	2.2272-3	2.2396-3	2.2519-3	2.2640-3	2.2761-3
K-	1.4318-6	9.6442-7	5.0879-7	5.1456-7	5.2044-7	5.2644-7	5.3256-7	5.3880-7	5.4519-7	5.5178-7	5.5854-7	5.6550-7	5.7266-7
KO	3.1181-3	2.5096-3	1.7729-3	1.7829-3	1.7929-3	1.8032-3	1.8136-3	1.8241-3	1.8349-3	1.8460-3	1.8572-3	1.8688-3	1.8807-3
KO-	5.7504-6	3.8032-6	1.9502-6	1.9693-6	1.9887-6	2.0087-6	2.0292-6	2.0502-6	2.0718-6	2.0943-6	2.1174-6	2.1414-6	2.1662-6
K2	7.0063-6	4.6618-6	2.4504-6	2.4696-6	2.4895-6	2.5100-6	2.5313-6	2.5532-6	2.5760-6	2.5998-6	2.6244-6	2.6502-6	2.6770-6
N	4.0322-5	2.6614-5	1.3673-5	1.3921-5	1.4173-5	1.4427-5	1.4684-5	1.4945-5	1.5210-5	1.5480-5	1.5756-5	1.6036-5	1.6322-5
NO	2.1573-2	1.9166-2	1.5788-2	1.5874-2	1.5960-2	1.6045-2	1.6130-2	1.6215-2	1.6300-2	1.6385-2	1.6470-2	1.6556-2	1.6641-2
NO-	1.6253-7	8.8465-8	3.3222-8	3.3884-8	3.4561-8	3.5253-8	3.5962-8	3.6687-8	3.7431-8	3.8201-8	3.8993-8	3.9818-8	4.0654-8
NO2	6.2536-6	4.5923-6	2.8049-6	2.8324-6	2.8603-6	2.8884-6	2.9168-6	2.9456-6	2.9748-6	3.0047-6	3.0351-6	3.0661-6	3.0978-6
NO2-	1.0200-7	6.3797-8	2.9904-8	3.0285-8	3.0674-8	3.1070-8	3.1476-8	3.1891-8	3.2316-8	3.2756-8	3.3208-8	3.3674-8	3.4156-8
N2	1.3125-1	1.3484-1	1.4020-1	1.4010-1	1.4000-1	1.3990-1	1.3979-1	1.3969-1	1.3958-1	1.3948-1	1.3937-1	1.3926-1	1.3915-1
N2O	4.5609-7	3.1106-7	1.6968-7	1.7159-7	1.7353-7	1.7550-7	1.7751-7	1.7957-7	1.8163-7	1.8378-7	1.8596-7	1.8821-7	1.9052-7
O-	6.3361-5	4.2938-5	2.2723-5	2.3077-5	2.3436-5	2.3798-5	2.4166-5	2.4537-5	2.4915-5	2.5300-5	2.5693-5	2.6093-5	2.6501-5
O2	1.0993-1	1.0944-1	1.0781-1	1.0809-1	1.0835-1	1.0861-1	1.0885-1	1.0909-1	1.0931-1	1.0953-1	1.0974-1	1.0994-1	1.1013-1
O2-	4.9524-6	3.2058-6	1.5805-6	1.6041-6	1.6280-6	1.6523-6	1.6770-6	1.7020-6	1.7276-6	1.7538-6	1.7805-6	1.8080-6	1.8361-6
S	1.5589-2	1.2714-2	9.0029-3	9.1080-3	9.2131-3	9.3184-3	9.4238-3	9.5294-3	9.6353-3	9.7422-3	9.8497-3	9.9579-3	1.0067-2
S-	6.6262-5	4.4190-5	2.2528-5	2.2889-5	2.3255-5	2.3627-5	2.4004-5	2.4387-5	2.4776-5	2.5175-5	2.5583-5	2.5999-5	2.6426-5
SN	3.4597-5	2.2482-5	1.1151-5	1.1332-5	1.1517-5	1.1704-5	1.1894-5	1.2088-5	1.2285-5	1.2487-5	1.2693-5	1.2905-5	1.3121-5
SO	1.2182-1	1.1335-1	9.9126-2	9.9598-2	1.0007-1	1.0053-1	1.0099-1	1.0145-1	1.0190-1	1.0235-1	1.0280-1	1.0325-1	1.0370-1
SO-	1.4010-4	9.2825-5	4.6936-5	4.7591-5	4.8256-5	4.8932-5	4.9620-5	5.0321-5	5.1035-5	5.1769-5	5.2520-5	5.3290-5	5.4081-5
SO2	1.7628-1	1.9328-1	2.1974-1	2.1904-1	2.1833-1	2.1762-1	2.1692-1	2.1621-1	2.1551-1	2.1480-1	2.1409-1	2.1337-1	2.1265-1
SO2-	9.5589-5	7.5057-5	4.9772-5	5.0056-5	5.0345-5	5.0641-5	5.0944-5	5.1254-5	5.1571-5	5.1900-5	5.2238-5	5.2586-5	5.2946-5
SO3	3.5655-5	3.3857-5	3.0760-5	3.0743-5	3.0728-5	3.0714-5	3.0703-5	3.0693-5	3.0684-5	3.0678-5	3.0674-5	3.0672-5	3.0673-5
SO3-	2.5748-7	1.8294-7	1.0540-7	1.0607-7	1.0677-7	1.0748-7	1.0822-7	1.0898-7	1.0977-7	1.1060-7	1.1145-7	1.1234-7	1.1326-7
S2	5.2713-4	3.8808-4	2.3117-4	2.3415-4	2.3716-4	2.4019-4	2.4327-4	2.4637-4	2.4952-4	2.5274-4	2.5601-4	2.5934-4	2.6273-4
S2-	1.4940-6	8.4464-7	3.2809-7	3.3147-7	3.3499-7	3.3866-7	3.4249-7	3.4649-7	3.5067-7	3.5500-7	3.5948-7	3.6409-7	3.6884-7

MOLE FRACTIONS OF NEOL SPECIES

COS	8.6658-6	6.2416-6	3.6544-6	3.6690-6	3.7037-6	3.7510-6	3.8061-6	3.8647-6	3.9260-6	3.9886-6	4.0529-6	4.1175-6	4.1830-6
O	1.1289-1	1.0179-1	8.5487-2	8.5463-2	8.5455-2	8.5463-2	8.5489-2	8.5530-2	8.5588-2	8.5664-2	8.5756-2	8.5866-2	8.5996-2
CO	1.2001-1	1.1842-1	1.1499-1	1.1495-1	1.1491-1	1.1486-1	1.1482-1	1.1479-1	1.1475-1	1.1471-1	1.1467-1	1.1464-1	1.1460-1
CS	5.7010-7	3.2277-7	1.2843-7	1.3150-7	1.3505-7	1.3879-7	1.4251-7	1.4634-7	1.5020-7	1.5402-7	1.5818-7	1.6217-7	1.6645-7

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-06 FOR ALL SIGNED CONDITIONS

AR+	C(S)	C	C+	C-	C3-	CN	CN+	CN-	CNN
CN2	CUS-	CO3-	CO4-	CS-	CS2	C2	C2-	C2N	C2N2
C2O	C3	C3O2	C4	C5	K(S)	K(L)	KCN	K(CO3(S))	K2CO3(L)

KO+	K2O(S)	K2O(L)	K2SO4(S)	K2SO4(S)	K2SO4(L)	NCO	NO+	NO3	NO3-
N2O+	N2O4	N2O5	N3	O+	O3	S(S)	S(L)	3+	S8

1
***** KFLAG= -4
3 -19.983 -19.828 -22.947 -16.915 -26.383 -15.845 -13.492 1.888

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 3		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.572E 21	2	KO+	2.312E 15						
1	CO2-	8.376E 16	2	K-	3.985E 17	3	KO-	1.586E 18	4	NO-	2.853E 16
5	NO2-	2.381E 16	6	O-	1.849E 19	7	O2-	1.281E 18	8	S-	1.846E 19
9	SO-	3.771E 19	10	SO2-	3.663E 19	11	SO3-	7.848E 16	12	S2-	2.885E 17
CONDUCTIVITY =		176.6488 (MHO/M)									
4	-19.968	-19.828	-22.948	-16.918	-26.372	-15.841	-13.476	2.888			

3-134

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 4		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.682E 21	2	KO+	2.488E 15						
1	COS-	1.826E 15	2	CO2-	8.652E 16	3	K-	4.895E 17	4	KO-	1.546E 18
5	NO-	2.957E 16	6	NO2-	2.458E 16	7	O-	1.985E 19	8	O2-	1.328E 18
9	S-	1.983E 19	10	SO-	3.883E 19	11	SO2-	3.742E 19	12	SO3-	8.828E 16
13	S2-	2.986E 17									
CONDUCTIVITY =		177.4789 (MHO/M)									
5	-19.952	-19.811	-22.933	-16.984	-26.359	-15.836	-13.458	2.888			

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 5		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.635E 21	2	KO+	2.511E 15						
1	COS-	1.878E 15	2	CO2-	8.948E 16	3	K-	4.212E 17	4	KO-	1.589E 18
5	NO-	3.868E 16	6	NO2-	2.525E 16	7	O-	1.965E 19	8	O2-	1.362E 18
9	S-	1.964E 19	10	SO-	4.883E 19	11	SO2-	3.826E 19	12	SO3-	8.223E 16
13	S2-	3.814E 17									
CONDUCTIVITY =		178.3161 (MHO/M)									
6	-19.936	-19.883	-22.927	-16.898	-26.348	-15.831	-13.441	2.888			

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 6		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.667E 21	2	KO+	2.618E 15						
1	COS-	1.116E 15	2	CO2-	9.243E 16	3	K-	4.328E 17	4	KO-	1.638E 18
5	NO-	3.188E 16	6	NO2-	2.598E 16	7	O-	2.825E 19	8	O2-	1.483E 18
9	S-	2.827E 19	10	SO-	4.122E 19	11	SO2-	3.986E 19	12	SO3-	8.486E 16

13 S2- 3.125E 17
CONDUCTIVITY = 179.2277 (MHO/M)

7 -19.919 -18.994 -22.918 -16.891 -26.334 -15.825 -13.423 2.0000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 7		ION		DENS (M-3)		
					DENS (M-3)	ION	DENS (M-3)				
1	K+	1.702E 21	2	KO+	2.736E 15						
1	COS-	1.168E 15	2	CO2-	9.585E 16	3	K-	4.464E 17	4	KO-	1.681E 18
5	NO-	3.309E 16	6	NO2-	2.686E 16	7	O-	2.092E 19	8	O2-	1.451E 18
9	S-	2.005E 19	10	SO-	4.259E 19	11	SO2-	4.006E 19	12	SO3-	8.642E 16
13	S2-	3.249E 17									
CONDUCTIVITY =		180.0047 (MHO/M)									

8 -19.902 -18.985 -22.900 -16.885 -26.320 -15.820 -13.404 2.0000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 8		ION		DENS (M-3)		
					DENS (M-3)	ION	DENS (M-3)				
1	K+	1.739E 21	2	KO+	2.862E 15						
1	COS-	1.222E 15	2	CO2-	9.940E 16	3	K-	4.604E 17	4	KO-	1.733E 18
5	NO-	3.444E 16	6	NO2-	2.776E 16	7	O-	2.163E 19	8	O2-	1.500E 18
9	S-	2.168E 19	10	SO-	4.401E 19	11	SO2-	4.105E 19	12	SO3-	8.875E 16
13	S2-	3.380E 17									
CONDUCTIVITY =		180.8713 (MHO/M)									

9 -19.885 -18.976 -22.901 -16.878 -26.306 -15.814 -13.385 1.0000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 9		ION		DENS (M-3)		
					DENS (M-3)	ION	DENS (M-3)				
1	K+	1.778E 21	2	KO+	2.998E 15						
1	COS-	1.282E 15	2	CO2-	1.032E 17	3	K-	4.755E 17	4	KO-	1.788E 18
5	NO-	3.590E 16	6	NO2-	2.873E 16	7	O-	2.238E 19	8	O2-	1.553E 18
9	S-	2.246E 19	10	SO-	4.554E 19	11	SO2-	4.212E 19	12	SO3-	9.127E 16
13	S2-	3.522E 17									
CONDUCTIVITY =		181.7614 (MHO/M)									

10 -19.867 -18.965 -22.892 -16.871 -26.290 -15.808 -13.364 2.0000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 10		ION		DENS (M-3)		
					DENS (M-3)	ION	DENS (M-3)				
1	K+	1.820E 21	2	KO+	3.150E 15						
1	COS-	1.348E 15	2	CO2-	1.075E 17	3	K-	4.922E 17	4	KO-	1.850E 18
5	NO-	3.752E 16	6	NO2-	2.981E 16	7	O-	2.321E 19	8	O2-	1.612E 18
9	S-	2.332E 19	10	SO-	4.723E 19	11	SO2-	4.330E 19	12	SO3-	9.406E 16

13 S2- 3.688E 17
CONDUCTIVITY = 182.6888 (MHO/M)

***** KFLAG= -4

11 -19.847 -18.955 -22.882 -16.863 -26.274 -15.801 -13.342 2.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 11							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 K+	1.866E 21	2 KO+	3.318E 15				
1 COS-	1.422E 15	2 CO2-	1.121E 17	3 K-	5.103E 17	4 KO-	1.918E 18
5 NO-	3.930E 16	6 NO2-	3.098E 16	7 O-	2.411E 19	8 O2-	1.676E 18
9 S-	2.425E 19	10 SO-	4.907E 19	11 SO2-	4.458E 19	12 SO3-	9.710E 16
13 S2-	3.853E 17						
CONDUCTIVITY = 183.6460 (MHO/M)							

12 -19.827 -18.943 -22.871 -16.855 -26.256 -15.794 -13.319 1.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 12							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 K+	1.916E 21	2 KO+	3.508E 15				
1 COS-	1.505E 15	2 CO2-	1.173E 17	3 K-	5.307E 17	4 KO-	1.993E 18
5 NO-	4.131E 16	6 NO2-	3.230E 16	7 O-	2.512E 19	8 O2-	1.747E 18
9 S-	2.530E 19	10 SO-	5.113E 19	11 SO2-	4.600E 19	12 SO3-	1.005E 17
13 S2-	4.047E 17						
CONDUCTIVITY = 184.6726 (MHO/M)							

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THEORETICAL MHD CORE PERFORMANCE

0PC = 14.7 PSIA
CASE NO. 300

CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	C	1.00000	S 2.00000	0.64186	60407.805	G	2600.00	0.0000
FUEL	K	2.00000	O 1.00000	0.25000	-86800.000	S	2600.00	0.0000
FUEL	AR	1.00000		0.10814	11435.389	G	2600.00	0.0000
OXIDANT	O	2.00000		0.79720	19666.641	G	2600.00	0.0000
OXIDANT	N	2.00000		0.20280	18637.500	G	2600.00	0.0000
O/F= 1.0500 PERCENT FUEL= 48.7805 EQUIVALENCE RATIO= 0.9684 REACTANT DENSITY= 0.0000								

	AXIAL STATION (M)											
	CHAMBER	THROAT	0.011	0.012	0.013	0.014	0.015	0.016	0.017	0.018	0.019	0.020
PC/P	1.0000	1.7188	3.4601	3.4074	3.3531	3.3023	3.2436	3.1867	3.1281	3.0666	3.0029	2.9357
P, ATM	1.0000	0.5818	0.2890	0.2935	0.2982	0.3028	0.3083	0.3138	0.3197	0.3261	0.3330	0.3406
T, DEG K	3362	3231	3087	3092	3096	3101	3105	3110	3115	3120	3125	3131
RHO, G/CC	1.3839-4	8.5485-5	4.5353-5	4.5967-5	4.6621-5	4.7244-5	4.8006-5	4.8762-5	4.9569-5	5.0449-5	5.1396-5	5.2439-5
H, CAL/G	471.2	379.4	273.7	276.5	279.4	282.5	285.4	288.6	291.8	295.3	298.9	302.9
S, CAL/(G)(K)	1.8840	1.8340	1.8858	1.8859	1.8861	1.8863	1.8863	1.8865	1.8866	1.8867	1.8868	1.8870
M, MOL WT	38.316	38.956	39.756	39.736	39.716	39.694	39.673	39.651	39.628	39.603	39.577	39.549
(DLV/DLP)T	-1.06918	-1.06455	-1.02204	-1.02211	-1.02219	-1.02227	-1.02234	-1.02242	-1.02250	-1.02258	-1.02266	-1.02275

(DLV/DLT)P	2.3473	2.3120	1.5025	1.5035	1.5046	1.5057	1.5065	1.5074	1.5084	1.5097	1.5102	1.5112
CP, CAL/(G)(K)	1.6374	1.6327	0.8370	0.8377	0.8384	0.8393	0.8398	0.8404	0.8410	0.8415	0.8420	0.8426
GAMMA (S)	1.1177	1.1141	1.1271	1.1272	1.1273	1.1273	1.1274	1.1275	1.1276	1.1277	1.1278	1.1279
VELOCITY,M/SEC			1211.04	1194.99	1178.50	1161.81	1144.68	1127.04	1108.79	1089.77	1069.82	1048.62
TOTAL H(CAL/G)			448.93	447.13	445.38	443.76	441.98	440.35	438.76	437.22	435.72	434.27
MAG FLD(TESLA)			3.18	3.18	3.18	3.18	3.18	3.18	3.18	3.18	3.18	3.18
BETA			2.40	2.37	2.34	2.30	2.27	2.23	2.20	2.16	2.12	2.08
SON VEL,M/SEC	903.0	876.5	853.1	853.9	854.8	855.7	856.5	857.5	858.4	859.4	860.5	861.6
ELEC DENS	5.031 21	2.902 21	1.457 21	1.484 21	1.513 21	1.542 21	1.574 21	1.606 21	1.641 21	1.679 21	1.719 21	1.763 21
IONIC DENS)	6.689 21	3.601 21	1.687 21	1.721 21	1.756 21	1.792 21	1.831 21	1.872 21	1.915 21	1.962 21	2.012 21	2.068 21
SIGMA (MHO/M)	213.1110	194.4897	176.6408	177.4709	178.3161	179.2277	180.0047	180.8713	181.7614	182.6800	183.6460	184.6726
W/O IONS	427.9375	399.8962	378.7770	380.8111	382.8550	385.1749	386.8617	388.8737	390.9130	392.9700	395.1173	397.3732
FREQ (1/SEC)	6.653 11	4.205 11	2.324 11	2.357 11	2.391 11	2.425 11	2.463 11	2.503 11	2.544 11	2.589 11	2.638 11	2.691 11
MACH NUMBER	0.0000	1.0000	1.4196	1.3994	1.3787	1.3578	1.3364	1.3144	1.2917	1.2680	1.2433	1.2170
AE/AT		1.0000	1.3643	1.3641	1.3638	1.3652	1.3636	1.3635	1.3633	1.3620	1.3628	1.3627
TOTAL MOL WT	38.316	38.956	39.756	39.736	39.716	39.695	39.674	39.651	39.628	39.600	39.577	39.549

MOLE FRACTIONS

AR	5.0596-2	5.1442-2	5.2498-2	5.2472-2	5.2445-2	5.2417-2	5.2389-2	5.2360-2	5.2329-2	5.2296-2	5.2262-2	5.2225-2
CO2	3.7547-2	4.1767-2	4.8909-2	4.8859-2	4.8805-2	4.8747-2	4.8685-2	4.8618-2	4.8545-2	4.8466-2	4.8379-2	4.8284-2
CO2-	3.3778-7	2.1286-7	1.2192-7	1.2418-7	1.2656-7	1.2895-7	1.3153-7	1.3420-7	1.3703-7	1.4007-7	1.4334-7	1.4691-7
SE	2.3045-3	2.1962-3	2.1207-3	2.1305-3	2.1403-3	2.1514-3	2.1593-3	2.1687-3	2.1783-3	2.1879-3	2.1978-3	2.2082-3
K	9.3379-2	9.5877-2	9.8743-2	9.8668-2	9.8590-2	9.8508-2	9.8429-2	9.8344-2	9.8256-2	9.8163-2	9.8065-2	9.7960-2
K+	2.6843-3	2.4606-3	2.2881-3	2.3000-3	2.3121-3	2.3255-3	2.3359-3	2.3479-3	2.3601-3	2.3725-3	2.3855-3	2.3992-3
K-	1.4318-6	9.6442-7	5.8006-7	5.8772-7	5.9579-7	6.0376-7	6.1261-7	6.2165-7	6.3121-7	6.4150-7	6.5252-7	6.6455-7
KO	3.1181-3	2.5096-3	1.8929-3	1.9055-3	1.9187-3	1.9313-3	1.9460-3	1.9606-3	1.9760-3	1.9926-3	2.0101-3	2.0292-3
KO-	5.7504-6	3.8032-6	2.1920-6	2.2188-6	2.2473-6	2.2743-6	2.3071-6	2.3396-6	2.3741-6	2.4116-6	2.4518-6	2.4959-6
K2	7.0053-6	4.6613-6	2.7051-6	2.7345-6	2.7659-6	2.7950-6	2.8323-6	2.8686-6	2.9074-6	2.9497-6	2.9952-6	3.0451-6
N	4.0322-5	2.6614-5	1.6614-5	1.6913-5	1.7225-5	1.7555-5	1.7865-5	1.8203-5	1.8558-5	1.8933-5	1.9334-5	1.9770-5
NO	2.1573-2	1.9165-2	1.6728-2	1.6815-2	1.6904-2	1.6996-2	1.7083-2	1.7175-2	1.7270-2	1.7370-2	1.7475-2	1.7586-2
NO-	1.6253-7	8.8465-8	4.1528-8	4.2437-8	4.3396-8	4.4371-8	4.5408-8	4.6496-8	4.7652-8	4.8901-8	5.0248-8	5.1732-8
NO2	6.2536-6	4.5923-6	3.1302-6	3.1635-6	3.1982-6	3.2326-6	3.2698-6	3.3078-6	3.3478-6	3.3905-6	3.4360-6	3.4854-6
NO2-	1.0208-7	6.3797-8	3.4654-8	3.5172-8	3.5719-8	3.6249-8	3.6863-8	3.7482-8	3.8139-8	3.8850-8	3.9614-8	4.0451-8
N2	1.3125-1	1.3484-1	1.3903-1	1.3892-1	1.3880-1	1.3867-1	1.3855-1	1.3842-1	1.3829-1	1.3814-1	1.3799-1	1.3783-1
N2O	4.5609-7	3.1106-7	1.9289-7	1.9535-7	1.9792-7	2.0048-7	2.0328-7	2.0614-7	2.0917-7	2.1242-7	2.1589-7	2.1968-7
O-	6.3361-5	4.2938-5	2.6919-5	2.7348-5	2.7794-5	2.8256-5	2.8712-5	2.9199-5	2.9710-5	3.0252-5	3.0831-5	3.1461-5
O2	1.0993-1	1.0944-1	1.1031-1	1.1049-1	1.1065-1	1.1084-1	1.1096-1	1.1110-1	1.1124-1	1.1137-1	1.1150-1	1.1164-1
O2-	4.9524-6	3.2058-6	1.8649-6	1.8947-6	1.9259-6	1.9573-6	1.9905-6	2.0251-6	2.0615-6	2.1005-6	2.1423-6	2.1879-6
S	1.5589-2	1.2714-2	1.0177-2	1.0288-2	1.0402-2	1.0526-2	1.0632-2	1.0750-2	1.0873-2	1.1000-2	1.1134-2	1.1272-2
S-	6.6262-5	4.4190-5	2.6863-5	2.7313-5	2.7783-5	2.8273-5	2.8755-5	2.9271-5	2.9814-5	3.0391-5	3.1008-5	3.1679-5
SN	3.4597-5	2.2482-5	1.3344-5	1.3573-5	1.3812-5	1.4062-5	1.4308-5	1.4573-5	1.4851-5	1.5147-5	1.5464-5	1.5809-5
SO	1.2182-1	1.1335-1	1.0415-1	1.0460-1	1.0506-1	1.0555-1	1.0596-1	1.0642-1	1.0690-1	1.0738-1	1.0789-1	1.0842-1
SO-	1.4010-4	9.2820-5	5.4395-5	5.5736-5	5.6617-5	5.7510-5	5.8447-5	5.9425-5	6.0457-5	6.1562-5	6.2744-5	6.4032-5
SO2	1.7628-1	1.9328-1	2.1193-1	2.1120-1	2.1045-1	2.0965-1	2.0894-1	2.0817-1	2.0737-1	2.0655-1	2.0568-1	2.0476-1
SO2-	9.5589-5	7.5057-5	5.3318-5	5.3705-5	5.4113-5	5.4491-5	5.4966-5	5.5425-5	5.5911-5	5.6437-5	5.6996-5	5.7605-5
SO3	3.5655-5	3.3857-5	3.0675-5	3.0680-5	3.0689-5	3.0677-5	3.0713-5	3.0730-5	3.0751-5	3.0778-5	3.0807-5	3.0841-5
SO3-	2.5748-7	1.8294-7	1.1422-7	1.1524-7	1.1631-7	1.1720-7	1.1859-7	1.1983-7	1.2115-7	1.2260-7	1.2415-7	1.2585-7
S2	5.2713-4	3.8803-4	2.6620-4	2.6976-4	2.7345-4	2.7734-4	2.8103-4	2.8503-4	2.8921-4	2.9362-4	2.9831-4	3.0337-4
S2-	1.4940-6	8.4464-7	4.0830-7	4.1710-7	4.2638-7	4.3594-7	4.4587-7	4.5641-7	4.6758-7	4.7962-7	4.9259-7	5.0683-7

MOLE FRACTIONS OF NEOL SPECIES

COS 8.6658-6 6.2416-6 4.2497-6 4.3161-6 4.3846-6 4.4486-6 4.5227-6 4.5937-6 4.6665-6 4.7429-6 4.8222-6 4.9080-6
 O 1.1219-1 1.0179-1 8.6144-2 8.6312-2 8.6501-2 8.6692-2 8.6940-2 8.7193-2 8.7468-2 8.7772-2 8.8099-2 8.8456-2
 CO 1.2001-1 1.1842-1 1.1457-1 1.1454-1 1.1451-1 1.1448-1 1.1446-1 1.1443-1 1.1441-1 1.1439- 1.1437-1 1.1435-1
 CS 5.7010-7 3.2277-7 1.7076-7 1.7504-7 1.7985-7 1.8414-7 1.8926-7 1.9432-7 1.9962-7 2.0516-7 2.1116-7 2.1787-7
 #ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-06 FOR ALL ASSIGNED CONDITIONS

AR+	C(S)	C	C+	C-	C3-	CN	CN+	CN-	CNN
CN2	COS-	CO3-	CO4-	CS-	CS2	C2	C2-	C2N	C2N2
C2O	C3	C3O2	C4	C5	K(S)	K(L)	KCN	K2CO3(S)	K2CO3(L)
KO+	K2O(S)	K2O(L)	K2SO4(S)	K2SO4(S)	K2SO4(L)	NCO	NO+	NO3	NO3-
N2O+	N2O4	N2O5	N3	O+	O3	S(S)	S(L)	S+	S8

STOP 5 IS NORMAL CHANNEL STOP

IT OCCURS WHEN XPOSITION EXCEEDS INPUTTED XXSTOP VALUE

Sample Output 9, Channel Problem
With Partial Equilibrium/Partial Rate Controlled
Chemistry and Channel Pressure Specified
(14 Output Pages)


```

IDEBUG=      0,
TRACE = 0.100000E-06,
SIUNIT= F,
DXI  = 0.100000E-02,
NITER =      0,
NSTOP =      0,
NEQL  = F,
BZ    = 8.000000 ,
XK     = 0.800000 ,
ACCURC= 0.100000E-02,
HMIN  = 0.100000E-29,
ALPH  = 0.000000 ,
EXIN  = 2400.00 ,
TWOBTG= F,
$END
LLMT =

```

C
S
K
O
AR
N

8SPECIES BEING CONSIDERED IN THIS SYSTEM

3-142	L 5/66	AR	L12/66	AR+	J 3/61	C(S)	J 3/61	C	L12/66	C+
	J 9/65	C-	3/3/7	C3-	J 6/69	CN	J12/70	CN+	J12/70	CN-
	J 6/66	CNN	J12/70	CN2	J 9/65	CO	J 3/61	COS	3/3/7	COS-
	J 9/65	CO2	4/12/7	CO2-	3/3/7	CO3-	3/7/7	CO4-	J12/62	C5
	3/3/7	CS-	J 6/61	CS2	J12/69	C2	J12/69	C2-	J 3/67	C2N
	J 3/61	C2N2	J 9/66	C2O	J12/69	C3	J 6/68	C3O2	J12/69	C4
	J12/69	C5	L02/67	E	J12/61	K(S)	J12/61	K(L)	J 6/62	K
	J 3/65	K+	3/3/7	K-	3/8/7	KCN	J 3/66	K2CO3(S)	J 3/66	K2CO3(L)
	J12/67	KO	7/29/8	KO+	J12/67	KO-	J12/61	K2	J 6/63	K2O(S)
	10/78	K2O(L)	J12/71	K2SO4(S)	J12/71	K2SO4(S)	J12/71	K2SO4(L)	J 3/61	N
	J12/70	NCO	J 6/63	NO	3/3/7	NO-	J 6/66	NO+	J 9/64	NO2
	J 6/72	NO2-	J12/64	NO3	3/3/7	NO3-	J 9/65	N2	J12/64	N2O
	J12/70	N2O+	J 9/64	N2O4	J12/64	N2O5	J12/70	N3	J 6/62	O
	L12/66	O+	J 6/65	O-	J 9/65	O2	J12/66	O2-	J 6/61	O3
	J12/65	S(S)	J12/65	S(L)	J 6/71	S	L12/66	S+	3/3/7	S-
J 6/61	SN	J 6/71	SO	3/3/7	SO-	J 6/61	SO2	3/3/7	SO2-	
J 9/65	SO3	3/3/7	SO3-	J12/65	S2	3/3/7	S2-	J6/64	S8	
85		7	12	6	0	5	755			

C
S
K
O
AR
N
E

\$RKTNP

```

EOL  = T,
FROZ = F,
SUBAR = 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 ,
SUPAR = 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,

```

ENTHALPY (KG-MOL) (DEG K)/KG			EFFECTIVE FUEL HPP(2)		EFFECTIVE OXIDANT HPP(1)			MIXTURE HSUB0	
ØKG-ATOMS/KG			Ø.15592358E Ø3		Ø.31446185E Ø3			Ø.23712613E Ø3	
			BØP(I,2)		BØP(I,1)			BØ(I)	
3-143	C		Ø.8430Ø786E-Ø2		Ø.ØØØØØØØØE ØØ		Ø.41122334E-Ø2		
	S		Ø.1686Ø157E-Ø1		Ø.ØØØØØØØØE ØØ		Ø.82244668E-Ø2		
	K		Ø.53076642E-Ø2		Ø.ØØØØØØØØE ØØ		Ø.25891Ø47E-Ø2		
	O		Ø.26538321E-Ø2		Ø.49826868E-Ø1		Ø.2681563ØE-Ø1		
	AR		Ø.27Ø7Ø437E-Ø2		Ø.ØØØØØØØØE ØØ		Ø.132Ø5Ø92E-Ø2		
	N		Ø.ØØØØØØØØE ØØ		Ø.14473784E-Ø1		Ø.74159624E-Ø2		
	E		Ø.ØØØØØØØØE ØØ		Ø.ØØØØØØØØE ØØ		Ø.ØØØØØØØØE ØØ		
ØPT	C	S	K	O	AR	N	E		
1	-19.182	-18.444	-22.243	-16.467	-25.372	-15.414	-12.361	13.ØØØ	

						ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 1									
ION		DENS (M-3)		ION		DENS (M-3)		ION		DENS (M-3)		ION		DENS (M-3)	
1	K+		5.860E 21	2	KO+		3.462E 16								
1	CN-		5.620E 15	2	COS-		1.444E 16	3	CO2-		7.374E 17	4	CO3-		4.754E 15
5	K-		3.126E 18	6	KO-		1.255E 19	7	NO-		3.548E 17	8	NO2-		2.228E 17
9	O-		1.383E 20	10	O2-		1.081E 19	11	S-		1.447E 20	12	SO-		3.059E 20
13	SO2-		2.087E 20	14	SO3-		5.621E 17	15	S2-		3.262E 18				
CONDUCTIVITY =		213.1110 (MHO/M)													
2	-19.554	-18.694	-22.537	-16.661	-25.808	-15.597	-12.862	3.000							
PC/PT=		1.71229	T=	3230.81											
2	-19.553	-18.693	-22.537	-16.660	-25.807	-15.596	-12.861	2.000							
PC/PT=		1.718772	T=	3231.14											

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 2		ION		DENS (M-3)		
				DENS (M-3)		DENS (M-3)					
1	K+	3.252E 21	2	KO+	1.029E 16						
1	CN-	1.609E 15	2	COS-	4.389E 15	3	CO2-	2.813E 17	4	CO3-	1.636E 15
5	K-	1.275E 18	6	KO-	5.026E 18	7	NO-	1.169E 17	8	NO2-	8.431E 16
9	O-	5.675E 19	10	O2-	4.237E 18	11	S-	5.840E 19	12	SO-	1.227E 20
13	SO2-	9.919E 19	14	SO3-	2.418E 17	15	S2-	1.116E 18			
CONDUCTIVITY =		194.4897 (MHO/M)									

*****CHANNEL INPUTS*****

NMPATH= 2
 IMPRNT= 2
 XXSTOP= 0.20200E-01
 UEINP= 0.00000
 ITYPE= 1

INDEPENDENT VARIABLE

DEPENDENT VARIABLE

0.00000	0.25000
0.00100	0.25298
0.00200	0.25605
0.00300	0.25922
0.00400	0.26248
0.00500	0.26585
0.00600	0.26933
0.00700	0.27297
0.00800	0.27674
0.00900	0.28067
0.01000	0.28476
0.01100	0.28904
0.01200	0.29351
0.01300	0.29821
0.01400	0.30316
0.01500	0.30832
0.01600	0.31381
0.01700	0.31967
0.01800	0.32600
0.01900	0.33289
0.02000	0.34050

3 -144

3 -20.143 -19.106 -23.001 -16.971 -26.491 -15.887 -13.662 4.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 3		ION		DENS (M-3)		
				DENS (M-3)		DENS (M-3)					
1	K+	1.297E 21	2	KO+	1.530E 15						
1	CO2-	6.082E 16	2	K-	3.067E 17	3	KO-	1.176E 18	4	NO-	2.003E 16
5	NO2-	1.803E 16	6	O-	1.370E 19	7	O2-	9.528E 17	8	S-	1.358E 19
9	SO-	2.830E 19	10	SO2-	3.001E 19	11	SO3-	6.354E 16	12	S2-	1.978E 17
CONDUCTIVITY =		167.5795 (MHO/M)									

DLIT COS O CO CS

1 NON-EQUILIBRIUM REACTIONS

1 1.0 SO + 1.0 O2 = 1.0 SO2 + 1.0 O

CHEMICAL RATE - 5.8000E-13*T** 0.0000*EXP(- 3.2500E 03/T)

2 1.0 COS + 1.0 O = 1.0 CO + 1.0 SO

CHEMICAL RATE - 3.1500E-11*T** 0.0000*EXP(- 2.2500E 03/T)

3 1.0 S + 1.0 O2 = 1.0 SO + 1.0 O

CHEMICAL RATE - 1.7000E-12*T** 0.0000*EXP(- 0.0000E-01/T)

4 1.0 CS2 + 1.0 O = 1.0 CS + 1.0 SO

CHEMICAL RATE - 8.3000E-11*T** 0.0000*EXP(- 9.5000E 02/T)

5 1.0 CS2 + 1.0 O2 = 1.0 SO2 + 1.0 CS

CHEMICAL RATE - 1.7000E-12*T** 0.0000*EXP(- 2.2000E 04/T)

3-146 1.0 CS + 1.0 O = 1.0 CO + 1.0 S

CHEMICAL RATE - 3.9900E-10*T** 0.0000*EXP(- 1.0000E 03/T)

7 1.0 CO + 1.0 O2 = 1.0 CO2 + 1.0 O

CHEMICAL RATE - 4.2000E-12*T** 0.0000*EXP(- 2.4000E 04/T)

8 1.0 CO + 1.0 O + 1.0 THIRD BODY = 1.0 CO2 + 1.0 THIRD BODY

CHEMICAL RATE - 5.5000E-32*T** 0.0000*EXP(- 9.0000E 02/T)

9 1.0 CS + 1.0 O2 = 1.0 COS + 1.0 O

CHEMICAL RATE - 1.7000E-11*T** 0.0000*EXP(- 6.0000E 03/T)

4 -20.129 -19.099 -22.998 -16.966 -26.483 -15.884 -13.647 2.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 4							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 K+	1.318E 21	2 KO+	1.586E 15				
1 CO2-	6.250E 16	2 K-	3.135E 17	3 KO-	1.200E 18	4 NO-	2.065E 16
5 NO2-	1.845E 16	6 O-	1.406E 19	7 O2-	9.774E 17	8 S-	1.395E 19
9 SO-	2.900E 19	10 SO2-	3.050E 19	11 SO3-	6.463E 16	12 S2-	2.038E 17
CONDUCTIVITY = 168.4170 (MHO/M)							
5	-20.115	-19.093	-22.994	-16.962	-26.474	-15.880	-13.632 2.0000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 5							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 K+	1.341E 21	2 KO+	1.644E 15				
1 CO2-	6.425E 16	2 K-	3.205E 17	3 KO-	1.225E 18	4 NO-	2.129E 16
5 NO2-	1.889E 16	6 O-	1.443E 19	7 O2-	1.003E 18	8 S-	1.432E 19
9 SO-	2.972E 19	10 SO2-	3.101E 19	11 SO3-	6.576E 16	12 S2-	2.100E 17
CONDUCTIVITY = 169.2513 (MHO/M)							
6	-20.101	-19.086	-22.989	-16.957	-26.465	-15.877	-13.617 2.0000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 6							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 K+	1.364E 21	2 KO+	1.705E 15				
1 CO2-	6.606E 16	2 K-	3.278E 17	3 KO-	1.251E 18	4 NO-	2.195E 16
5 NO2-	1.935E 16	6 O-	1.482E 19	7 O2-	1.029E 18	8 S-	1.471E 19
9 SO-	3.047E 19	10 SO2-	3.153E 19	11 SO3-	6.693E 16	12 S2-	2.165E 17
CONDUCTIVITY = 170.0835 (MHO/M)							
7	-20.086	-19.079	-22.985	-16.952	-26.456	-15.873	-13.602 2.0000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 7							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 K+	1.387E 21	2 KO+	1.769E 15				
1 CO2-	6.794E 16	2 K-	3.354E 17	3 KO-	1.278E 18	4 NO-	2.265E 16
5 NO2-	1.982E 16	6 O-	1.522E 19	7 O2-	1.056E 18	8 S-	1.512E 19
9 SO-	3.125E 19	10 SO2-	3.208E 19	11 SO3-	6.814E 16	12 S2-	2.233E 17
CONDUCTIVITY = 170.9127 (MHO/M)							
8	-20.072	-19.072	-22.980	-16.947	-26.446	-15.870	-13.587 1.0000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 8							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)

1	K+	1.411E 21	2	KO+	1.836E 15						
1	CO2-	6.990E 16	2	K-	3.432E 17	3	KO-	1.306E 18	4	NO-	2.337E 16
5	NO2-	2.031E 16	6	O-	1.563E 19	7	O2-	1.084E 18	8	S-	1.554E 19
9	SO-	3.206E 19	10	SO2-	3.265E 19	11	SO3-	6.941E 16	12	S2-	2.303E 17
CONDUCTIVITY =		171.7366	(MHO/M)								

9 -20.058 -19.065 -22.976 -16.942 -26.437 -15.866 -13.572 2.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 9		ION		DENS (M-3)		
ION		DENS (M-3)	ION		DENS (M-3)		ION		DENS (M-3)		
1	K+	1.436E 21	2	KO+	1.905E 15						
1	CO2-	7.194E 16	2	K-	3.514E 17	3	KO-	1.335E 18	4	NO-	2.413E 16
5	NO2-	2.083E 16	6	O-	1.606E 19	7	O2-	1.114E 18	8	S-	1.597E 19
9	SO-	3.290E 19	10	SO2-	3.323E 19	11	SO3-	7.073E 16	12	S2-	2.377E 17
CONDUCTIVITY =		172.5641	(MHO/M)								

10 -20.043 -19.058 -22.970 -16.937 -26.427 -15.862 -13.556 2.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 10		ION		DENS (M-3)		
ION		DENS (M-3)	ION		DENS (M-3)		ION		DENS (M-3)		
1	K+	1.461E 21	2	KO+	1.979E 15						
1	CO2-	7.409E 16	2	K-	3.600E 17	3	KO-	1.366E 18	4	NO-	2.493E 16
5	NO2-	2.137E 16	6	O-	1.651E 19	7	O2-	1.144E 18	8	S-	1.643E 19
9	SO-	3.378E 19	10	SO2-	3.385E 19	11	SO3-	7.213E 16	12	S2-	2.455E 17
CONDUCTIVITY =		173.3893	(MHO/M)								

11 -20.028 -19.051 -22.965 -16.932 -26.416 -15.858 -13.541 1.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 11		ION		DENS (M-3)		
ION		DENS (M-3)	ION		DENS (M-3)		ION		DENS (M-3)		
1	K+	1.488E 21	2	KO+	2.056E 15						
1	CO2-	7.635E 16	2	K-	3.690E 17	3	KO-	1.398E 18	4	NO-	2.577E 16
5	NO2-	2.193E 16	6	O-	1.698E 19	7	O2-	1.176E 18	8	S-	1.691E 19
9	SO-	3.470E 19	10	SO2-	3.450E 19	11	SO3-	7.359E 16	12	S2-	2.536E 17
CONDUCTIVITY =		174.2188	(MHO/M)								

12 -20.013 -19.043 -22.959 -16.926 -26.406 -15.854 -13.525 2.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 12		ION		DENS (M-3)		
ION		DENS (M-3)	ION		DENS (M-3)		ION		DENS (M-3)		
1	K+	1.515E 21	2	KO+	2.138E 15						
1	CO2-	7.871E 16	2	K-	3.784E 17	3	KO-	1.432E 18	4	NO-	2.665E 16
5	NO2-	2.253E 16	6	O-	1.747E 19	7	O2-	1.210E 18	8	S-	1.741E 19

9 SO- 3.567E 19 10 SO2- 3.518E 19 11 SO3- 7.513E 16 12 S2- 2.622E 17
CONDUCTIVITY = 175.0508 (MHO/M)

13 -19.998 -19.035 -22.954 -16.921 -26.395 -15.850 -13.508 1.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 13		ION		DENS (M-3)	ION		DENS (M-3)
1	K+	1.544E 21	2	KO+	2.224E 15							
1	CO2-	8.119E 16	2	K-	3.883E 17	3	KO-	1.468E 18	4	NO-	2.757E 16	
5	NO2-	2.315E 16	6	O-	1.798E 19	7	O2-	1.245E 18	8	S-	1.793E 19	
9	SO-	3.668E 19	10	SO2-	3.588E 19	11	SO3-	7.674E 16	12	S2-	2.713E 17	
CONDUCTIVITY =		175.8839 (MHO/M)										

1

THEORETICAL MHD CORE PERFORMANCE

OPC = 14.7 PSIA
CASE NO. 300

CHEMICAL FORMULA		WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	C 1.000000 S 2.000000	0.64186	60407.805	G	2600.00	0.0000
FUEL	K 2.000000 O 1.000000	0.25000	-86800.000	S	2600.00	0.0000
FUEL	AR 1.000000	0.10814	11435.389	G	2600.00	0.0000
OXIDANT	O 2.000000	0.79720	19666.641	G	2600.00	0.0000
OXIDANT	N 2.000000	0.20280	18637.500	G	2600.00	0.0000
O/F = 1.0500		PERCENT FUEL = 48.7805	EQUIVALENCE RATIO = 0.9684	REACTANT DENSITY = 0.0000		

	AXIAL STATION (M)												
	CHAMBER	THROAT	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009	0.010
PC/P	1.0000	1.7188	4.0000	3.9528	3.9054	3.8578	3.8098	3.7616	3.7130	3.6635	3.6134	3.5629	3.5117
P, ATM	1.0000	0.5818	0.2500	0.2530	0.2561	0.2592	0.2625	0.2658	0.2693	0.2730	0.2767	0.2807	0.2848
T, DEG K	3362	3231	3044	3047	3051	3055	3059	3063	3067	3071	3075	3079	3083
RHO, G/CC	1.3889-4	8.5485-5	3.9984-5	4.0394-5	4.0816-5	4.1251-5	4.1699-5	4.2163-5	4.2641-5	4.3142-5	4.3661-5	4.4201-5	4.4764-5
H, CAL/G	471.2	379.4	245.9	248.3	250.7	253.1	255.5	258.0	260.5	263.1	265.7	268.4	271.1
S, CAL/(G)(K)	1.8840	1.8840	1.8840	1.8842	1.8843	1.8845	1.8847	1.8849	1.8850	1.8852	1.8854	1.8856	1.8857
M, MOL WT	38.316	38.956	39.942	39.927	39.911	39.895	39.879	39.863	39.846	39.828	39.810	39.792	39.773
(DLV/DLP)T	-1.06918	-1.06455	-1.05728	-1.05213	-1.04713	-1.04214	-1.03715	-1.03216	-1.02717	-1.02218	-1.01719	-1.01220	-1.00721
(DLV/DLT)P	2.3473	2.3120	2.2404	1.4908	1.4921	1.4934	1.4946	1.4959	1.4971	1.4982	1.4994	1.5005	1.5016
CP, CAL/(G)(K)	1.6374	1.6327	1.6033	0.8278	0.8289	0.8299	0.8309	0.8319	0.8329	0.8338	0.8347	0.8355	0.8364
GAMMA (S)	1.1177	1.1141	1.1092	1.1266	1.1267	1.1267	1.1267	1.1268	1.1268	1.1269	1.1269	1.1270	1.1271
VELOCITY, M/SEC			1372.95	1359.00	1344.93	1330.71	1316.34	1301.85	1287.10	1272.22	1257.10	1241.74	1226.12
TOTAL H(CAL/G)			471.21	469.00	466.84	464.71	462.61	460.55	458.51	456.53	454.58	452.67	450.80
MAG FLD(TESLA)			8.00	3.18	3.18	3.18	3.18	3.18	3.18	3.18	3.18	3.18	3.18
BETA			6.92	2.72	2.69	2.66	2.63	2.59	2.56	2.53	2.50	2.48	2.43
SON VEL, M/SEC	903.0	876.5	838.3	845.5	846.3	847.0	847.7	848.5	849.2	850.0	850.7	851.5	852.3
ELEC DENS	5.031 21	2.902 21	1.208 21	1.228 21	1.248 21	1.269 21	1.290 21	1.312 21	1.334 21	1.358 21	1.381 21	1.406 21	1.432 21
IONIC DENS	6.689 21	3.601 21	1.385 21	1.409 21	1.433 21	1.458 21	1.484 21	1.510 21	1.537 21	1.565 21	1.594 21	1.624 21	1.656 21
SIGMA (MHO/M)	213.1110	194.4097	167.5795	168.4170	169.2513	170.0835	170.9127	171.7366	172.5641	173.3893	174.2188	175.0508	175.8839
W/O IONS	427.9375	399.8962	355.1946	357.4594	359.7039	361.9299	364.1332	366.3060	368.4731	370.6098	372.7437	374.8630	376.9653
FREQ (1/SEC)	6.653 11	4.205 11	2.032 11	2.055 11	2.079 11	2.103 11	2.127 11	2.153 11	2.179 11	2.206 11	2.234 11	2.263 11	2.294 11
MACH NUMBER	0.0000	1.0000	1.6378	1.6073	1.5893	1.5711	1.5528	1.5344	1.5157	1.4968	1.4777	1.4582	1.4385
AE/AT		1.0000	1.3650	1.3650	1.3650	1.3650	1.3651	1.3651	1.3653	1.3652	1.3652	1.3652	1.3652

TOTAL MOL WT	38.316	38.956	39.942	39.927	39.911	39.895	39.879	39.863	39.846	39.828	39.810	39.792	39.773
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MOLE FRACTIONS

AR	5.0596-2	5.1442-2	5.2744-2	5.2724-2	5.2703-2	5.2682-2	5.2661-2	5.2639-2	5.2617-2	5.2594-2	5.2570-2	5.2546-2	5.2521-2
CO2	3.7547-2	4.1767-2	4.9257-2	4.9238-2	4.9216-2	4.9192-2	4.9165-2	4.9136-2	4.9105-2	4.9071-2	4.9033-2	4.8993-2	4.8948-2
CO2-	3.3778-7	2.1286-7	1.0088-7	1.0258-7	1.0431-7	1.0608-7	1.0789-7	1.0974-7	1.1163-7	1.1358-7	1.1559-7	1.1765-7	1.1978-7
E	2.3045-3	2.1962-3	2.0043-3	2.0156-3	2.0269-3	2.0380-3	2.0490-3	2.0598-3	2.0705-3	2.0810-3	2.0914-3	2.1017-3	2.1119-3
K	9.3379-2	9.5877-2	9.9483-2	9.9420-2	9.9357-2	9.9293-2	9.9228-2	9.9162-2	9.9094-2	9.9026-2	9.8955-2	9.8884-2	9.8811-2
K+	2.6843-3	2.4676-3	2.1508-3	2.1640-3	2.1770-3	2.1898-3	2.2026-3	2.2152-3	2.2278-3	2.2402-3	2.2526-3	2.2650-3	2.2772-3
K-	1.4318-6	9.6442-7	5.0879-7	5.1457-7	5.2045-7	5.2645-7	5.3257-7	5.3882-7	5.4522-7	5.5183-7	5.5862-7	5.6560-7	5.7280-7
KO	3.1181-3	2.5096-3	1.7729-3	1.7829-3	1.7929-3	1.8031-3	1.8135-3	1.8240-3	1.8348-3	1.8459-3	1.8572-3	1.8687-3	1.8806-3
KO-	5.7504-6	3.8032-6	1.9502-6	1.9692-6	1.9887-6	2.0086-6	2.0290-6	2.0500-6	2.0716-6	2.0940-6	2.1172-6	2.1411-6	2.1660-6
K2	7.0063-6	4.6618-6	2.4504-6	2.4696-6	2.4894-6	2.5099-6	2.5310-6	2.5529-6	2.5755-6	2.5993-6	2.6240-6	2.6497-6	2.6765-6
N	4.0322-5	2.6614-5	1.3673-5	1.3922-5	1.4174-5	1.4429-5	1.4688-5	1.4950-5	1.5217-5	1.5489-5	1.5767-5	1.6050-5	1.6340-5
NO	2.1573-2	1.9166-2	1.5788-2	1.5875-2	1.5960-2	1.6046-2	1.6131-2	1.6216-2	1.6301-2	1.6387-2	1.6473-2	1.6559-2	1.6645-2
NO-	1.6253-7	8.8465-8	3.3222-8	3.3885-8	3.4562-8	3.5256-8	3.5965-8	3.6692-8	3.7439-8	3.8211-8	3.9008-8	3.9831-8	4.0680-8
NO2	6.2536-6	4.5923-6	2.8049-6	2.8325-6	2.8603-6	2.8884-6	2.9168-6	2.9456-6	2.9749-6	3.0049-6	3.0354-6	3.0665-6	3.0982-6
NO2-	1.0208-7	6.3797-8	2.9904-8	3.0205-8	3.0674-8	3.1070-8	3.1475-8	3.1890-8	3.2315-8	3.2755-8	3.3208-8	3.3675-8	3.4157-8
N2	1.3125-1	1.3484-1	1.4020-1	1.4010-1	1.4000-1	1.3989-1	1.3979-1	1.3969-1	1.3958-1	1.3947-1	1.3936-1	1.3925-1	1.3914-1
N2O	4.5609-7	3.1106-7	1.6968-7	1.7159-7	1.7353-7	1.7551-7	1.7751-7	1.7956-7	1.8164-7	1.8379-7	1.8599-7	1.8825-7	1.9056-7
O-	6.3361-5	4.2938-5	2.2723-5	2.3078-5	2.3437-5	2.3801-5	2.4169-5	2.4542-5	2.4922-5	2.5309-5	2.5705-5	2.6108-5	2.6520-5
O2	1.0993-1	1.0944-1	1.0781-1	1.0809-1	1.0835-1	1.0861-1	1.0885-1	1.0909-1	1.0932-1	1.0954-1	1.0975-1	1.0995-1	1.1014-1
O2-	4.9524-6	3.2058-6	1.5805-6	1.6041-6	1.6280-6	1.6524-6	1.6770-6	1.7022-6	1.7278-6	1.7541-6	1.7810-6	1.8086-6	1.8368-6
S	1.5589-2	1.2714-2	9.0029-3	9.1081-3	9.2137-3	9.3196-3	9.4259-3	9.5322-3	9.6394-3	9.7470-3	9.8560-3	9.9657-3	1.0077-2
S-	6.6262-5	4.4190-5	2.2528-5	2.2890-5	2.3257-5	2.3629-5	2.4008-5	2.4393-5	2.4785-5	2.5186-5	2.5598-5	2.6018-5	2.6450-5
SN	3.4597-5	2.2482-5	1.1151-5	1.1333-5	1.1517-5	1.1705-5	1.1897-5	1.2091-5	1.2289-5	1.2492-5	1.2701-5	1.2914-5	1.3133-5
SO	1.2182-1	1.1335-1	9.9126-2	9.9598-2	1.0007-1	1.0053-1	1.0100-1	1.0146-1	1.0192-1	1.0237-1	1.0283-1	1.0328-1	1.0374-1
SO-	1.4010-4	9.2825-5	4.6936-5	4.7591-5	4.8257-5	4.8935-5	4.9625-5	5.0327-5	5.1044-5	5.1781-5	5.2538-5	5.3313-5	5.4110-5
SO2	1.7628-1	1.9329-1	2.1974-1	2.1903-1	2.1832-1	2.1761-1	2.1690-1	2.1619-1	2.1548-1	2.1477-1	2.1404-1	2.1332-1	2.1259-1
SO2-	9.5589-5	7.5057-5	4.9772-5	5.0055-5	5.0344-5	5.0640-5	5.0941-5	5.1250-5	5.1566-5	5.1895-5	5.2232-5	5.2580-5	5.2939-5
SO3	3.5655-5	3.3857-5	3.0760-5	3.0743-5	3.0727-5	3.0712-5	3.0699-5	3.0688-5	3.0678-5	3.0671-5	3.0665-5	3.0661-5	3.0659-5
SO3-	2.5748-7	1.8294-7	1.0540-7	1.0607-7	1.0676-7	1.0748-7	1.0821-7	1.0897-7	1.0975-7	1.1057-7	1.1142-7	1.1230-7	1.1322-7
S2	5.2713-4	3.8808-4	2.3117-4	2.3415-4	2.3717-4	2.4022-4	2.4331-4	2.4644-4	2.4962-4	2.5285-4	2.5616-4	2.5953-4	2.6297-4
S2-	1.4940-6	8.4464-7	3.2809-7	3.3447-7	3.4101-7	3.4769-7	3.5455-7	3.6158-7	3.6880-7	3.7627-7	3.8400-7	3.9196-7	4.0022-7

MOLE FRACTIONS OF NEOL SPECIES

COS	8.6658-6	6.2416-6	3.6544-6	3.6684-6	3.7046-6	3.7522-6	3.8068-6	3.8660-6	3.9277-6	3.9907-6	4.0550-6	4.1193-6	4.1848-6
O	1.1289-1	1.0179-1	8.5487-2	8.5463-2	8.5456-2	8.5467-2	8.5495-2	8.5539-2	8.5599-2	8.5675-2	8.5773-2	8.5890-2	8.6025-2
CO	1.2001-1	1.1842-1	1.1499-1	1.1495-1	1.1490-1	1.1486-1	1.1482-1	1.1478-1	1.1475-1	1.1471-1	1.1467-1	1.1464-1	1.1460-1
CS	5.7010-7	3.2277-7	1.2843-7	1.3159-7	1.3523-7	1.3884-7	1.4262-7	1.4643-7	1.5031-7	1.5427-7	1.5834-7	1.6242-7	1.6672-7

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-06 FOR ALL ASSIGNED CONDITIONS

AR+	C(S)	C	C+	C-	C3-	CN	CN+	CN-	CNN
CN2	COS-	CO3-	CO4-	CS-	CS2	C2	C2-	C2N	C2N2
C2O	C3	C3O2	C4	C5	K(S)	K(L)	KCN	K2CO3(S)	K2CO3(L)
KO+	K2O(S)	K2O(L)	K2SO4(S)	K2SO4(S)	K2SO4(L)	NCO	NO+	NO3	NO3-
N2O+	N2O4	N2O5	N3	O+	O3	S(S)	S(L)	S+	S8

1

	3	-19.983	-19.028	-22.947	-16.915	-26.384	-15.845	-13.492	1.000
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ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 K+	1.573E 21	2 KO+	2.315E 15				
1 CO2-	8.388E 16	2 K-	3.986E 17	3 KO-	1.586E 18	4 NO-	2.855E 16
5 NO2-	2.381E 16	6 O-	1.851E 19	7 O2-	1.282E 18	8 S-	1.848E 19
9 SO-	3.774E 19	10 SO2-	3.663E 19	11 SO3-	7.844E 16	12 S2-	2.888E 17
CONDUCTIVITY = 176.7198 (MHO/M)							
4	-19.967	-19.828	-22.941	-16.918	-26.372	-15.841	-13.475 2.888

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 4							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 K+	1.684E 21	2 KO+	2.412E 15				
1 COS-	1.827E 15	2 CO2-	8.657E 16	3 K-	4.896E 17	4 KO-	1.546E 18
5 NO-	2.968E 16	6 NO2-	2.451E 16	7 O-	1.987E 19	8 O2-	1.321E 18
9 S-	1.985E 19	10 SO-	3.886E 19	11 SO2-	3.741E 19	12 SO3-	8.825E 16
13 S2-	2.918E 17						
CONDUCTIVITY = 177.5694 (MHO/M)							
5	-19.951	-19.811	-22.934	-16.984	-26.368	-15.836	-13.458 2.888

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 5							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 K+	1.636E 21	2 KO+	2.515E 15				
1 COS-	1.871E 15	2 CO2-	8.958E 16	3 K-	4.212E 17	4 KO-	1.588E 18
5 NO-	3.878E 16	6 NO2-	2.525E 16	7 O-	1.967E 19	8 O2-	1.362E 18
9 S-	1.966E 19	10 SO-	4.885E 19	11 SO2-	3.824E 19	12 SO3-	8.216E 16
13 S2-	3.818E 17						
CONDUCTIVITY = 178.4188 (MHO/M)							
6	-19.935	-19.883	-22.927	-16.898	-26.347	-15.831	-13.448 2.888

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 6							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 K+	1.669E 21	2 KO+	2.625E 15				
1 COS-	1.119E 15	2 CO2-	9.263E 16	3 K-	4.336E 17	4 KO-	1.633E 18
5 NO-	3.188E 16	6 NO2-	2.883E 16	7 O-	2.829E 19	8 O2-	1.486E 18
9 S-	2.831E 19	10 SO-	4.131E 19	11 SO2-	3.912E 19	12 SO3-	8.428E 16
13 S2-	3.133E 17						
CONDUCTIVITY = 179.2781 (MHO/M)							
7	-19.918	-18.994	-22.919	-16.892	-26.334	-15.826	-13.422 2.888

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 7							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)

1	K+	1.704E 21	2	KO+	2.742E 15						
1	COS-	1.170E 15	2	CO2-	9.592E 16	3	K-	4.466E 17	4	KO-	1.681E 18
5	NO-	3.313E 16	6	NO2-	2.686E 16	7	O-	2.095E 19	8	O2-	1.452E 18
9	S-	2.099E 19	10	SO-	4.263E 19	11	SO2-	4.004E 19	12	SO3-	8.634E 16
13	S2-	3.255E 17									

CONDUCTIVITY = 180.1426 (MHO/M)

8 -19.901 -18.985 -22.911 -16.885 -26.320 -15.820 -13.403 2.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 8											
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)				
1	K+	1.741E 21	2	KO+	2.868E 15						
1	COS-	1.225E 15	2	CO2-	9.946E 16	3	K-	4.606E 17	4	KO-	1.732E 18
5	NO-	3.448E 16	6	NO2-	2.776E 16	7	O-	2.166E 19	8	O2-	1.501E 18
9	S-	2.172E 19	10	SO-	4.405E 19	11	SO2-	4.103E 19	12	SO3-	8.865E 16
13	S2-	3.387E 17									

CONDUCTIVITY = 181.0280 (MHO/M)

9 -19.884 -18.975 -22.903 -16.878 -26.306 -15.814 -13.384 2.000

3-151	ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 9											
	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)				
	1	K+	1.780E 21	2	KO+	3.006E 15						
	1	COS-	1.285E 15	2	CO2-	1.033E 17	3	K-	4.757E 17	4	KO-	1.787E 18
	5	NO-	3.594E 16	6	NO2-	2.872E 16	7	O-	2.242E 19	8	O2-	1.554E 18
	9	S-	2.251E 19	10	SO-	4.559E 19	11	SO2-	4.209E 19	12	SO3-	9.114E 16
13	S2-	3.530E 17										

CONDUCTIVITY = 181.9407 (MHO/M)

10 -19.865 -18.965 -22.893 -16.871 -26.291 -15.808 -13.363 2.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 10											
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)				
1	K+	1.822E 21	2	KO+	3.158E 15						
1	COS-	1.351E 15	2	CO2-	1.075E 17	3	K-	4.921E 17	4	KO-	1.848E 18
5	NO-	3.755E 16	6	NO2-	2.978E 16	7	O-	2.324E 19	8	O2-	1.612E 18
9	S-	2.336E 19	10	SO-	4.726E 19	11	SO2-	4.325E 19	12	SO3-	9.387E 16
13	S2-	3.686E 17									

CONDUCTIVITY = 182.8816 (MHO/M)

11 -19.846 -18.954 -22.834 -16.864 -26.275 -15.801 -13.341 1.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 11										
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)			

1 K+	1.868E 21	2 KO+	3.328E 15				
1 COS-	1.425E 15	2 CO2-	1.121E 17	3 K-	5.103E 17	4 KO-	1.915E 18
5 NO-	3.935E 16	6 NO2-	3.095E 16	7 O-	2.415E 19	8 O2-	1.676E 18
9 S-	2.431E 19	10 SO-	4.912E 19	11 SO2-	4.451E 19	12 SO3-	9.687E 16
13 S2-	3.861E 17						

CONDUCTIVITY = 183.8924 (MHO/M)

12 -19.825 -18.943 -22.873 -16.855 -26.257 -15.794 -13.318 1.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 12							
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 K+	1.918E 21	2 KO+	3.518E 15				
1 COS-	1.508E 15	2 CO2-	1.174E 17	3 K-	5.306E 17	4 KO-	1.990E 18
5 NO-	4.136E 16	6 NO2-	3.227E 16	7 O-	2.516E 19	8 O2-	1.748E 18
9 S-	2.535E 19	10 SO-	5.118E 19	11 SO2-	4.593E 19	12 SO3-	1.003E 17
13 S2-	4.056E 17						

CONDUCTIVITY = 184.9222 (MHO/M)

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THEORETICAL MHD CORE PERFORMANCE

SPC = 14.7 PSIA
 CAS' NO. 300

CHEMICAL FORMULA				WT FRACTION	ENERGY	STATE	TEMP	DENSITY	
				(SEE NOTE)	CAL/MOL		DEG K	G/CC	
FUEL	C	1.00000	S	2.00000	0.64186	60407.805	G	2600.00	0.0000
FUEL	K	2.00000	O	1.00000	0.25000	-86800.000	S	2600.00	0.0000
FUEL	AR	1.00000			0.10814	11435.389	G	2600.00	0.0000
OXIDANT	O	2.00000			0.79720	19666.641	G	2600.00	0.0000
OXIDANT	N	2.00000			0.20280	18637.500	G	2600.00	0.0000

O/F= 1.0500 PERCENT FUEL= 48.7805 EQUIVALENC RATIO= 0.9684 REACTANT DENSITY= 0.0000

AXIAL STATION (M)												
	CHAMBER	THROAT	0.011	0.012	0.013	0.014	0.015	0.016	0.017	0.018	0.019	0.020
PC/P	1.0000	1.7188	3.4598	3.4071	3.3534	3.2986	3.2433	3.1867	3.1282	3.0675	3.0040	2.9368
P, ATM	1.0000	0.5818	0.2890	0.2935	0.2982	0.3032	0.3083	0.3138	0.3197	0.3260	0.3329	0.3405
T, DEG K	3362	3231	3038	3092	3096	3101	3105	3110	3115	3120	3126	3131
RHO, G/CC	1.3889-4	8.5485-5	4.5351-5	4.5965-5	4.6610-5	4.7290-5	4.7998-5	4.8750-5	4.9552-5	5.0418-5	5.1358-5	5.2399-5
H, CAL/G	471.2	370.4	273.9	276.8	279.7	282.8	285.9	289.1	292.4	295.9	299.7	303.7
S, CAL/(G)(K)	1.8840	1.8840	1.8859	1.8860	1.8862	1.8863	1.8865	1.8866	1.8868	1.8869	1.8871	1.8872

M, MOL WT	38.316	38.956	39.753	39.733	39.713	39.691	39.669	39.646	39.622	39.597	39.570	39.541
(DLV/DLP)T	-1.06918	-1.06455	-1.02204	-1.02212	-1.02220	-1.02228	-1.02236	-1.02244	-1.02252	-1.02260	-1.02268	-1.02277
(DLV/DLT)P	2.3473	2.3120	1.5027	1.5037	1.5047	1.5057	1.5067	1.5077	1.5086	1.5096	1.5106	1.5116
CP, CAL/(G)(K)	1.6374	1.6327	0.8371	0.8379	0.8386	0.8393	0.8400	0.8406	0.8413	0.8419	0.8425	0.8430
GAMMA (S)	1.1177	1.1141	1.1271	1.1272	1.1273	1.1273	1.1274	1.1275	1.1276	1.1277	1.1278	1.1279
VELOCITY, M/SEC			1210.27	1193.96	1177.44	1160.51	1143.23	1125.38	1106.87	1087.62	1067.17	1045.76
TOTAL H(CAL/G)			448.97	447.17	445.42	443.71	442.05	440.43	438.85	437.31	435.82	434.37
MAG FLD(TESLA)			3.18	3.18	3.18	3.18	3.18	3.18	3.18	3.18	3.18	3.18
FIELD			2.40	2.39	2.34	2.30	2.27	2.23	2.20	2.16	2.12	2.08
ION VELOCITY, M/SEC	903.0	870.5	853.2	854.0	854.9	855.7	856.6	857.6	858.5	859.6	860.6	861.8
ION DENS	5.031 21	2.902 21	1.453 21	1.435 21	1.514 21	1.544 21	1.575 21	1.608 21	1.643 21	1.680 21	1.721 21	1.766 21

IONIC DENS)	6.689	21	3.681	21	1.688	21	1.722	21	1.757	21	1.794	21	1.833	21	1.873	21	1.917	21	1.964	21	2.015	21	2.071	21
SYGMA (MPO/M)	213.1118		194.4897		176.7198		177.5694		178.4180		179.2781		180.1426		181.0280		181.9407		182.8816		183.8924		184.9222	
W/ONS	427.9375		399.8962		379.8499		381.1520		383.2192		385.2889		387.3459		389.4283		391.5489		393.6988		396.0107		398.2786	
FREQ (1/SEC)	6.653	11	4.205	11	2.325	11	2.357	11	2.391	11	2.427	11	2.464	11	2.503	11	2.545	11	2.589	11	2.638	11	2.691	11
MACH NUMBER	0.0000		1.0000		1.4136		1.3981		1.3774		1.3562		1.3346		1.3123		1.2893		1.2653		1.2400		1.2135	
AE/AT			1.0000		1.3652		1.3654		1.3654		1.3654		1.3655		1.3658		1.3662		1.3665		1.3672		1.3674	
TOTAL MOL WT	38.316		38.956		39.754		39.733		39.713		39.691		39.669		39.646		39.622		39.597		39.570		39.542	

MOLE FRACTIONS

AR	5.0596-2	5.1442-2	5.2495-2	5.2768-2	5.2441-2	5.2413-2	5.2384-2	5.2353-2	5.2322-2	5.2288-2	5.2253-2	5.2215-2
CO2	3.7547-2	4.1767-2	4.8901-2	4.8850-2	4.8795-2	4.8735-2	4.8671-2	4.8601-2	4.8525-2	4.8444-2	4.8354-2	4.8256-2
CO2-	3.3778-7	2.1286-7	1.2198-7	1.2426-7	1.2662-7	1.2909-7	1.3163-7	1.3431-7	1.3715-7	1.4018-7	1.4347-7	1.4704-7
E	2.3045-3	2.1962-3	2.1220-3	2.1321-3	2.1420-3	2.1518-3	2.1616-3	2.1713-3	2.1813-3	2.1913-3	2.2020-3	2.2124-3
K	9.3379-2	9.5877-2	9.8736-2	9.8658-2	9.8580-2	9.8499-2	9.8415-2	9.8329-2	9.8239-2	9.8144-2	9.8043-2	9.7936-2
K+	2.6843-3	2.4606-3	2.2894-3	2.3017-3	2.3139-3	2.3261-3	2.3383-3	2.3506-3	2.3632-3	2.3761-3	2.3899-3	2.4036-3
K-	1.4318-6	9.6442-7	5.8023-7	5.8794-7	5.9594-7	6.0428-7	6.1288-7	6.2193-7	6.3152-7	6.4174-7	6.5283-7	6.6485-7
KO	3.1181-3	2.5096-3	1.8928-3	1.9054-3	1.9184-3	1.9319-3	1.9458-3	1.9603-3	1.9756-3	1.9919-3	2.0093-3	2.0283-3
KO-	5.7504-6	3.8032-6	2.1917-6	2.2186-6	2.2466-6	2.2760-6	2.3065-6	2.3387-6	2.3730-6	2.4099-6	2.4497-6	2.4936-6
K2	7.0063-6	4.6618-6	2.7045-6	2.7337-6	2.7646-6	2.7971-6	2.8310-6	2.8669-6	2.9053-6	2.9467-6	2.9915-6	3.0413-6
N	4.0322-5	2.6614-5	1.6635-5	1.6940-5	1.7252-5	1.7574-5	1.7904-5	1.8248-5	1.8609-5	1.8990-5	1.9405-5	1.9843-5
NO	2.1573-2	1.9166-2	1.6732-2	1.6820-2	1.6909-2	1.6999-2	1.7090-2	1.7183-2	1.7280-2	1.7380-2	1.7487-2	1.7599-2
NO-	1.6253-7	8.8465-8	4.1560-8	4.2478-8	4.3431-8	4.4430-8	4.5464-8	4.6558-8	4.7723-8	4.8971-8	5.0337-8	5.1822-8
NO2	6.2536-6	4.5923-6	3.1308-6	3.1643-6	3.1987-6	3.2343-6	3.2707-6	3.3087-6	3.3488-6	3.3912-6	3.4369-6	3.4862-6
NO2-	1.0208-7	6.3797-8	3.4656-8	3.5175-8	3.5715-8	3.6280-8	3.6864-8	3.7480-8	3.8135-8	3.8837-8	3.9599-8	4.0434-8
N2	1.3125-1	1.3484-1	1.3902-1	1.3890-1	1.3878-1	1.3866-1	1.3853-1	1.3840-1	1.3826-1	1.3812-1	1.3796-1	1.3780-1
N2O	4.5609-7	3.1106-7	1.9295-7	1.9542-7	1.9797-7	2.0063-7	2.0336-7	2.0623-7	2.0926-7	2.1249-7	2.1598-7	2.1977-7
O-	6.3361-5	4.2933-5	2.6941-5	2.7377-5	2.7821-5	2.8281-5	2.8753-5	2.9244-5	2.9761-5	3.0308-5	3.0901-5	3.1531-5
O2	1.0993-1	1.0944-1	1.1032-1	1.1050-1	1.1067-1	1.1082-1	1.1097-1	1.1112-1	1.1126-1	1.1140-1	1.1154-1	1.1167-1
O2-	4.9524-6	3.2058-6	1.8659-6	1.8959-6	1.9269-6	1.9590-6	1.9921-6	2.0268-6	2.0634-6	2.1023-6	2.1446-6	2.1901-6
S	1.5589-2	1.2714-2	1.0180-2	1.0302-2	1.0417-2	1.0534-2	1.0652-2	1.0773-2	1.0899-2	1.1030-2	1.1171-2	1.1315-2
S-	6.6262-5	4.4197-5	2.6892-5	2.7349-5	2.7819-5	2.8306-5	2.8806-5	2.9329-5	2.9880-5	3.0463-5	3.1097-5	3.1770-5
SN	3.4597-5	2.2482-5	1.3358-5	1.3590-5	1.3830-5	1.4078-5	1.4334-5	1.4601-5	1.4884-5	1.5183-5	1.5508-5	1.5854-5
SO	1.2182-1	1.1335-1	1.0419-1	1.0465-1	1.0511-1	1.0557-1	1.0604-1	1.0651-1	1.0699-1	1.0749-1	1.0801-1	1.0855-1
SO-	1.4010-4	9.2824-5	5.4930-5	5.5779-5	5.6656-5	5.7568-5	5.8506-5	5.9491-5	6.0531-5	6.1636-5	6.2835-5	6.4125-5
SO2	1.7628-1	1.9328-1	2.1185-1	2.1110-1	2.1035-1	2.0959-1	2.0881-1	2.0802-1	2.0720-1	2.0636-1	2.0546-1	2.0453-1
SO2-	9.5589-5	7.5057-5	5.3310-5	5.3695-5	5.4097-5	5.4516-5	5.4948-5	5.5402-5	5.5883-5	5.6397-5	5.6948-5	5.7554-5
SO3	3.5655-5	3.3857-5	3.0659-5	3.0661-5	3.0666-5	3.0674-5	3.0684-5	3.0697-5	3.0712-5	3.0732-5	3.0752-5	3.0784-5
SO3-	2.5748-7	1.8291-7	1.1418-7	1.1518-7	1.1623-7	1.1734-7	1.1849-7	1.1971-7	1.2101-7	1.2242-7	1.2393-7	1.2562-7
S2	5.2713-4	3.8803-4	2.6640-4	2.7010-4	2.7381-4	2.7762-4	2.8153-4	2.8559-4	2.8985-4	2.9433-4	2.9917-4	3.0426-4
S2-	1.4940-6	8.4404-7	4.0876-7	4.1767-7	4.2694-7	4.3664-7	4.4670-7	4.5733-7	4.6864-7	4.8073-7	4.9396-7	5.0825-7

MOLE FRACTIONS OF NEOL SPECIES

COS	8.6658-6	6.2416-6	4.2520-6	4.3163-6	4.3866-6	4.4570-6	4.5277-6	4.5997-6	4.6736-6	4.7503-6	4.8313-6	4.9132-6
O	1.1289-1	1.0179-1	8.6179-2	8.6355-2	8.6548-2	8.6764-2	8.7003-2	8.7261-2	8.7550-2	8.7859-2	8.8195-2	8.8567-2
CO	1.2001-1	1.1842-1	1.1457-1	1.1454-1	1.1451-1	1.1448-1	1.1445-1	1.1443-1	1.1441-1	1.1438-1	1.1436-1	1.1434-1
CS	5.1010-7	3.2277-7	1.7106-7	1.7536-7	1.8018-7	1.8496-7	1.8984-7	1.9497-7	2.0034-7	2.0606-7	2.1227-7	2.1812-7

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-06 FOR ALL ASSIGNED CONDITIONS

AR+	C(S)	C	C+	C-	C3-	CN	CN+	CN-	CNN
CN2	COS-	CO3-	CO4-	CS-	CS2	C2	C2-	C2N	C2N2
C2O	C3	C3O2	C4	C5	K(S)	K(L)	KCN	K2CO3(S)	K2CO3(L)

KO+	K20(S)	K20(L)	K2504(S)	K2504(S)	K2504(L)	NCO	NO+	NO3	NO3-
N20+	N204	N205	N3	O+	O3	S(S)	S(L)	S+	S8

STOP 5 IS NORMAL CHANNEL STOP
IT OCCURS WHEN XPOSITION EXCEEDS INPUTTED XXSTOP VALUE

3.3.2.4 Output data for a channel problem with partial equilibrium/partial rate controlled chemistry, NEQPT=3, and channel area specified

This output data is shown on Sample Output 10. This output format is again identical to that of other sample problems of this subsection. In this case, the linear pressure profile from the throat to the channel entrance is printed. The channel area profile downstream of the entrance is printed out under the output CHNLIN with other channel input data. This problem can also be executed with velocity or pressure specified downstream of the channel entrance. Only a linear pressure profile can be specified between the throat and the channel entrance.

Sample Output 10, Channel Problem
With Partial Equilibrium/Partial Rate
Controlled Chemistry Starting From the Throat
and Channel Area Ratio Specified
(9 Output Pages)

1

REACTANTS

C 1.00000 S 2.00000 0.00000 0.00000 00 0.00000 0.64186
 K 2.00000 O 1.00000 0.00000 0.00000 00 0.00000 0.25000
 AR 1.00000 0.00000 0.00000 0.00000 00 0.00000 0.10814
 O 2.00000 0.00000 0.00000 0.00000 00 0.00000 0.79720
 N 2.00000 0.00000 0.00000 0.00000 00 0.00000 0.20280

NAMELISTS

1

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 0.00 G 2600.000 0 O 0.000000
 0.00 G 2600.000 0 O 0.000000

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ALPH  = 0.000000 ,
EXIN  = 2400.00 ,
TWOBTG= F,
$END
LLMT =

```

C
S
K
O
AR
N

#SPECIES BEING CONSIDERED IN THIS SYSTEM

3-160	L 5/66	AR	L12/66	AR+	J 3/61	C(S)	J 3/61	C	L12/66	C+
	J 9/65	C-	3/3/7	C3-	J 6/69	CN	J12/70	CN+	J12/70	CN-
	J 6/66	CNN	J12/70	CN2	J 9/65	CO	J 3/61	COS	3/3/7	COS-
	J 9/65	CO2	4/12/7	CO2-	3/3/7	CO3-	3/7/7	CO4-	J12/62	CS
	3/3/7	CS-	J 6/61	CS2	J12/69	C2	J12/69	C2-	J 3/67	C2N
	J 3/61	C2N2	J 9/66	C2O	J12/69	C3	J 6/68	C3O2	J12/69	C4
	J12/69	C5	L02/67	E	J12/61	K(S)	J12/61	K(L)	J 6/62	K
	J 3/65	K+	3/3/7	K-	3/8/7	KCN	J 3/66	K2CO3(S)	J 3/66	K2CO3(L)
	J12/67	KO	7/29/8	KO+	J12/67	KO-	J12/61	K2	J 6/63	K2O(S)
	10/78	K2O(L)	J12/71	K2SO4(S)	J12/71	K2SO4(S)	J12/71	K2SO4(L)	J 3/61	N
	J12/70	NCO	J 6/63	NO	3/3/7	NO-	J 6/66	NO+	J 9/64	NO2
	J 6/72	NO2-	J12/64	NO3	3/3/7	NO3-	J 9/65	N2	J12/64	N2O
	J12/70	N2O+	J 9/64	N2O4	J12/64	N2O5	J12/70	N3	J 6/62	O
	L12/66	O+	J 6/65	O-	J 9/65	O2	J12/66	O2-	J 6/61	O3
	J12/65	S(S)	J12/65	S(L)	J 6/71	S	L12/66	S+	3/3/7	S-
J 6/61	SN	J 6/71	SO	3/3/7	SO-	J 6/61	SO2	3/3/7	SO2-	
J 9/65	SO3	3/3/7	SO3-	J12/65	S2	3/3/7	S2-	J6/64	S8	
85		7	12	6	0	5	755			

C
S
K
O
AR
N
E

\$RKTINP

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ENTHALPY (KG-MOL) (DEG K)/KG			EFFECTIVE FUEL HPP(2)		EFFECTIVE OXIDANT HPP(1)			MIXTURE HSUB0	
#KG-ATOMS/KG			#3 BOP(I,2)		#3 BOP(I,1)			#3 BOP(I)	
3-161	C		0.84300786E-02		0.00000000E 00		0.41122334E-02		
	S		0.16860157E-01		0.00000000E 00		0.82244668E-02		
	K		0.53076642E-02		0.00000000E 00		0.25891047E-02		
	J		0.26538321E-02		0.49826868E-01		0.26815630E-01		
	AR		0.27070437E-02		0.00000000E 00		0.13205092E-02		
	N		0.00000000E 00		0.14478784E-01		0.74159624E-02		
E		0.00000000E 00		0.00000000E 00		0.00000000E 00			
SPT	C	S	K	O	AR	N	E		
1	-19.182	-18.444	-22.243	-16.467	-25.372	-15.414	-12.361	13.000	

ION		DENS (M-3)		ION		DENS (M-3)		ION		DENS (M-3)		ION		DENS (M-3)	
1	K+	5.866E	21	2	KO+	3.462E	16								
1	CN-	5.628E	15	2	COS-	1.444E	16	3	CO2-	7.374E	17	4	CO3-	4.754E	15
5	K-	3.126E	18	6	KO-	1.255E	19	7	NO-	3.548E	17	8	NO2-	2.228E	17
9	O-	1.383E	28	10	O2-	1.081E	19	11	S-	1.447E	28	12	SO-	3.059E	28
13	SO2-	2.087E	28	14	SO3-	5.621E	17	15	S2-	3.262E	18				
CONDUCTIVITY =		213.1110 (MHO/M)													
2	-19.554	-18.604	-22.537	-16.661	-25.808	-15.597	-12.862	3.0000							
PC/PT=	1.721229	T=	3230.81												
2	-19.553	-18.693	-22.537	-16.660	-25.807	-15.596	-12.861	2.0000							
PC/PT=	1.718772	T=	3231.11												

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 2									
ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)	ION	DENS (M-3)
1 K+	3.252E 21	2 KO+	1.029E 16						
1 CN-	1.609E 15	2 COS-	4.389E 15	3 CO2-	2.813E 17	4 CO3-	1.636E 15		
5 K-	1.275E 18	6 KO-	5.026E 18	7 NO-	1.169E 17	8 NO2-	8.431E 16		
9 O-	5.675E 19	10 O2-	4.237E 18	11 S-	5.840E 19	12 SO-	1.227E 20		
13 SO2-	9.919E 19	14 SO3-	2.418E 17	15 S2-	1.116E 18				
CONDUCTIVITY =		194.4897 (MHO/M)							

DLIT COS O CO CS
1 NON-EQUILIBRIUM REACTIONS

1 1.0 SO + 1.0 O2 = 1.0 SO2 + 1.0 O
CHEMICAL RATE - 5.8000E-13*T** 0.0000*EXP(- 3.2500E 03/T)

2 1.0 COS + 1.0 O = 1.0 CO + 1.0 SO
CHEMICAL RATE - 3.1500E-11*T** 0.0000*EXP(- 2.2500E 03/T)

3 1.0 S + 1.0 O2 = 1.0 SO + 1.0 O
CHEMICAL RATE - 1.7000E-12*T** 0.0000*EXP(- 0.0000E-01/T)

4 1.0 CS2 + 1.0 O = 1.0 CS + 1.0 SO
CHEMICAL RATE - 8.3000E-11*T** 0.0000*EXP(- 9.5000E 02/T)

5 1.0 CS2 + 1.0 O2 = 1.0 SO2 + 1.0 CS
CHEMICAL RATE - 1.7000E-12*T** 0.0000*EXP(- 2.2000E 04/T)

6 1.0 CS + 1.0 O = 1.0 CO + 1.0 S
CHEMICAL RATE - 3.9900E-10*T** 0.0000*EXP(- 1.0000E 03/T)

7 1.0 CO + 1.0 O2 = 1.0 CO2 + 1.0 O
CHEMICAL RATE - 4.2000E-12*T** 0.0000*EXP(- 2.4000E 04/T)

8 1.0 CO + 1.0 O + 1.0 THIRD BODY = 1.0 CO2 + 1.0 THIRD BODY

CHEMICAL RATE - 5.5000E-32*T** 0.0000*EXP(- 9.0000E 02/T)

9 1.0 CS + 1.0 O2 = 1.0 COS + 1.0 O

CHEMICAL RATE - 1.7000E-11*T** 0.0000*EXP(- 6.0000E 03/T)

3 -20.261 -19.116 -22.976 -16.972 -26.483 -15.879 -13.694 2.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 3			
ION	DENS (M-3)	ION	DENS (M-3)
1 K+	1.249E 21	2 KO+	1.398E 15
1 CO2-	5.422E 16	2 K-	3.008E 17
5 NO2-	1.781E 16	6 O-	1.294E 19
9 SO-	2.722E 19	10 SO2-	3.016E 19
CONDUCTIVITY = 162.9631 (MHO/M)		3 KO-	1.178E 18
		7 O2-	9.162E 17
		11 SO3-	6.472E 16
		4 NO-	1.900E 16
		8 S-	1.277E 19
		12 S2-	1.862E 17

*****CHANNEL INPUTS*****

3-163
 MPPATH= 3
 IMPRNT= 2
 XXSTOP= 0.10200E-01
 UEINP= 0.00000
 ITYPE= 1

INDEPENDENT VARIABLE	DEPENDENT VARIABLE
0.00000	1.36391
1.00000	1.36391

4 -20.246 -19.109 -22.973 -16.967 -26.475 -15.876 -13.679 2.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 4			
ION	DENS (M-3)	ION	DENS (M-3)
1 K+	1.271E 21	2 KO+	1.454E 15
1 CO2-	5.580E 16	2 K-	3.075E 17
5 NO2-	1.824E 16	6 O-	1.331E 19
9 SO-	2.792E 19	10 SO2-	3.065E 19
CONDUCTIVITY = 163.9248 (MHO/M)		3 KO-	1.201E 18
		7 O2-	9.412E 17
		11 SO3-	6.579E 16
		4 NO-	1.962E 16
		8 S-	1.313E 19
		12 S2-	1.920E 17

5 -20.230 -19.103 -22.970 -16.952 -26.467 -15.873 -13.663 1.000

ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 5			
ION	DENS (M-3)	ION	DENS (M-3)
1 K+	1.294E 21	2 KO+	1.511E 15

1	CO2-	5.744E 16	2	K-	3.145E 17	3	KO-	1.226E 18	4	NO-	2.026E 16
5	NO2-	1.868E 16	6	O-	1.368E 19	7	O2-	9.669E 17	8	S-	1.351E 19
9	SO-	2.864E 19	10	SO2-	3.115E 19	11	SO3-	6.690E 16	12	S2-	1.980E 17

CONDUCTIVITY = 164.8788 (MHO/M)

6 -20.215 -19.096 -22.967 -16.957 -26.458 -15.870 -13.648 1.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 6		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.317E 21	2	KO+	1.572E 15						
1	CO2-	5.913E 16	2	K-	3.217E 17	3	KO-	1.252E 18	4	NO-	2.092E 16
5	NO2-	1.914E 16	6	O-	1.407E 19	7	O2-	9.936E 17	8	S-	1.389E 19
9	SO-	2.938E 19	10	SO2-	3.167E 19	11	SO3-	6.805E 16	12	S2-	2.043E 17

CONDUCTIVITY = 165.8284 (MHO/M)

7 -20.200 -19.090 -22.964 -16.952 -26.449 -15.867 -13.632 2.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 7		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.341E 21	2	KO+	1.634E 15						
1	CO2-	6.090E 16	2	K-	3.292E 17	3	KO-	1.279E 18	4	NO-	2.161E 16
5	NO2-	1.961E 16	6	O-	1.448E 19	7	O2-	1.021E 18	8	S-	1.429E 19
9	SO-	3.015E 19	10	SO2-	3.220E 19	11	SO3-	6.925E 16	12	S2-	2.108E 17

CONDUCTIVITY = 166.7737 (MHO/M)

** ***** KFLAG= -4
 3-164 -20.184 -19.083 -22.960 -16.947 -26.440 -15.863 -13.616 1.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 8		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.365E 21	2	KO+	1.700E 15						
1	CO2-	6.274E 16	2	K-	3.370E 17	3	KO-	1.306E 18	4	NO-	2.234E 16
5	NO2-	2.011E 16	6	O-	1.489E 19	7	O2-	1.050E 18	8	S-	1.470E 19
9	SO-	3.095E 19	10	SO2-	3.276E 19	11	SO3-	7.050E 16	12	S2-	2.176E 17

CONDUCTIVITY = 167.7145 (MHO/M)

9 -20.168 -19.076 -22.956 -16.942 -26.431 -15.860 -13.600 1.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 9		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.391E 21	2	KO+	1.769E 15						
1	CO2-	6.467E 16	2	K-	3.451E 17	3	KO-	1.336E 18	4	NO-	2.310E 16
5	NO2-	2.063E 16	6	O-	1.533E 19	7	O2-	1.080E 18	8	S-	1.513E 19
9	SO-	3.179E 19	10	SO2-	3.334E 19	11	SO3-	7.181E 16	12	S2-	2.248E 17

CONDUCTIVITY = 168.6553 (MHO/M)

10 -20.152 -19.069 -22.952 -16.936 -26.422 -15.857 -13.584 1.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 10		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.417E 21	2	KO+	1.842E 15						
1	CO2-	6.668E 16	2	K-	3.536E 17	3	KO-	1.366E 18	4	NO-	2.389E 16
5	NO2-	2.117E 16	6	O-	1.578E 19	7	O2-	1.111E 18	8	S-	1.558E 19
9	SO-	3.267E 19	10	SO2-	3.395E 19	11	SO3-	7.318E 16	12	S2-	2.323E 17

CONDUCTIVITY = 169.5931 (MHO/M)

11 -20.137 -19.062 -22.947 -16.931 -26.412 -15.853 -13.567 1.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 11		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.443E 21	2	KO+	1.918E 15						
1	CO2-	6.879E 16	2	K-	3.624E 17	3	KO-	1.398E 18	4	NO-	2.472E 16
5	NO2-	2.174E 16	6	O-	1.625E 19	7	O2-	1.143E 18	8	S-	1.605E 19
9	SO-	3.357E 19	10	SO2-	3.459E 19	11	SO3-	7.462E 16	12	S2-	2.402E 17

CONDUCTIVITY = 170.5278 (MHO/M)

12 -20.120 -19.054 -22.943 -16.926 -26.402 -15.849 -13.550 1.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 12		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.471E 21	2	KO+	1.998E 15						
1	CO2-	7.099E 16	2	K-	3.717E 17	3	KO-	1.432E 18	4	NO-	2.559E 16
5	NO2-	2.233E 16	6	O-	1.674E 19	7	O2-	1.177E 18	8	S-	1.654E 19
9	SO-	3.452E 19	10	SO2-	3.525E 19	11	SO3-	7.613E 16	12	S2-	2.484E 17

CONDUCTIVITY = 171.4623 (MHO/M)

13 -20.104 -19.047 -22.938 -16.920 -26.391 -15.845 -13.534 2.000

ION		DENS (M-3)	ION		ION NUMBER DENSITY AND CONDUCTIVITY AT POINT 13		ION		DENS (M-3)		
					DENS (M-3)						
1	K+	1.499E 21	2	KO+	2.082E 15						
1	CO2-	7.331E 16	2	K-	3.814E 17	3	KO-	1.467E 18	4	NO-	2.651E 16
5	NO2-	2.296E 16	6	O-	1.725E 19	7	O2-	1.212E 18	8	S-	1.705E 19
9	SO-	3.552E 19	10	SO2-	3.594E 19	11	SO3-	7.771E 16	12	S2-	2.571E 17

CONDUCTIVITY = 172.3965 (MHO/M)

GPC = 14.7 PSIA
CASE NO. 301

CHEMICAL FORMULA
FUEL C 1.00000 S 2.00000
FUEL K 2.00000 O 1.00000
FUEL AR 1.00000
OXIDANT O 2.00000
OXIDANT N 2.00000

WT FRACTION (SEE NOTE) ENERGY CAL/MOL STATE TEMP DEG K DENSITY G/CC
0.64186 60407.805 G 2600.00 0.0000
0.25000 -86800.000 S 2600.00 0.0000
0.10814 11435.389 G 2600.00 0.0000
0.79728 19666.641 G 2600.00 0.0000
0.20280 18637.500 G 2600.00 0.0000

O/F= 1.0500 PERCENT FUEL= 48.7805

EQUIVALENCE RATIO= 0.9684 REACTANT DENSITY= 0.0000

	AXIAL STATION (M)													
	CHAMBER	THROAT	0.0000	0.0001	0.0002	0.0003	0.0004	0.0005	0.0006	0.0007	0.0008	0.0009	0.0010	
PC/P	1.0000	1.7188	4.0000	3.9538	3.9074	3.8607	3.8137	3.7663	3.7182	3.6696	3.6206	3.5710	3.5209	
P, ATM	1.0000	0.5818	0.2500	0.2529	0.2559	0.2590	0.2622	0.2655	0.2690	0.2725	0.2762	0.2800	0.2840	
T, DEG K	3362	3231	3030	3034	3039	3043	3047	3051	3056	3060	3064	3069	3073	
RHO, G/CC	1.3889-4	8.5485-5	4.0096-5	4.0495-5	4.0905-5	4.1328-5	4.1764-5	4.2215-5	4.2685-5	4.3173-5	4.3677-5	4.4202-5	4.4748-5	
H, CAL/G	471.2	379.4	246.9	249.1	251.4	253.8	256.2	258.6	261.0	263.5	266.0	268.6	271.3	
S, CAL/(G)(K)	1.8840	1.8340	1.8843	1.8844	1.8846	1.8848	1.8849	1.8851	1.8853	1.8854	1.8856	1.8857	1.8859	
M, MOL WT	38.316	38.956	39.877	39.864	39.951	39.838	39.824	39.810	39.795	39.780	39.765	39.749	39.732	
(DLV/DLP)T	-1.06918	-1.06155	-1.02058	-1.02069	-1.02079	-1.02089	-1.02099	-1.02109	-1.02118	-1.02128	-1.02138	-1.02147	-1.02156	
(DLV/DLP)P	2.3473	2.3120	1.4787	1.4804	1.4820	1.4837	1.4853	1.4868	1.4883	1.4898	1.4913	1.4927	1.4941	
CP, CAL/(G)(K)	1.6374	1.6327	0.8173	0.8137	0.8202	0.8215	0.8228	0.8241	0.8254	0.8266	0.8278	0.8289	0.8300	
GAMMA (S)	1.1177	1.1141	1.1271	1.1271	1.1271	1.1271	1.1271	1.1271	1.1272	1.1272	1.1272	1.1273	1.1273	
VELOCITY,M/SEC			1370.18	1356.67	1343.05	1329.30	1315.40	1301.35	1287.10	1272.66	1258.04	1243.20	1228.13	
TOTAL H(CAL/G)			471.21	469.09	467.01	464.95	462.93	460.93	458.98	457.06	455.17	453.32	451.51	
MAC FLD(TESLA)			0.00	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	3.16	
BETA			0.00	2.73	2.70	2.67	2.64	2.61	2.58	2.54	2.51	2.48	2.45	
SON VEL,M/SEC	903.0	876.5	843.8	844.6	845.3	846.0	846.8	847.5	848.3	849.1	849.9	850.7	851.5	
ELEC DENS	5.031 21	2.902 21	1.163 21	1.183 21	1.204 21	1.225 21	1.247 21	1.269 21	1.292 21	1.315 21	1.340 21	1.364 21	1.390 21	
IONIC DENS	6.689 21	3.601 21	1.335 21	1.359 21	1.384 21	1.409 21	1.435 21	1.462 21	1.489 21	1.518 21	1.547 21	1.577 21	1.609 21	
SIGMA (MHO/M)	213.1110	194.4897	162.9631	163.9248	164.8788	165.8284	166.7737	167.7145	168.6553	169.5931	170.5278	171.4623	172.3965	
W/O IONS	427.9375	399.8962	339.5926	342.2484	344.8746	347.4764	350.0540	352.6064	355.1407	357.6519	360.1377	362.6039	365.0490	
FREQ (1/SEC)	6.653 11	4.205 11	2.011 11	2.034 11	2.058 11	2.082 11	2.107 11	2.132 11	2.159 11	2.186 11	2.214 11	2.243 11	2.272 11	
MACH NUMBER	0.0000	1.0100	1.6238	1.6064	1.5889	1.5712	1.5534	1.5355	1.5173	1.4989	1.4803	1.4614	1.4423	
AE/AT		1.0000	1.3639	1.3639	1.3639	1.3639	1.3639	1.3639	1.3639	1.3639	1.3639	1.3639	1.3639	
TOTAL MOL WT	38.316	38.956	39.877	39.864	39.851	39.838	39.824	39.810	39.795	39.780	39.765	39.749	39.732	

MOLE FRACTIONS

AR	5.0596-2	5.1442-2	5.2658-2	5.2641-2	5.2624-2	5.2606-2	5.2588-2	5.2570-2	5.2550-2	5.2530-2	5.2510-2	5.2488-2	5.2467-2
CO2	3.7547-2	4.1767-2	4.5564-2	4.5575-2	4.5583-2	4.5590-2	4.5594-2	4.5597-2	4.5598-2	4.5596-2	4.5592-2	4.5585-2	4.5576-2
CO2-	3.3778-7	2.1286-7	8.9536-8	9.1208-8	9.2911-8	9.4649-8	9.6423-8	9.8239-8	1.0011-7	1.0202-7	1.0398-7	1.0600-7	1.0808-7
E	2.3045-3	2.1962-3	1.9203-3	1.9340-3	1.9475-3	1.9608-3	1.9740-3	1.9870-3	1.9998-3	2.0125-3	2.0250-3	2.0374-3	2.0496-3
K	9.3379-2	9.5877-2	9.9416-2	9.9357-2	9.9297-2	9.9236-2	9.9174-2	9.9112-2	9.9047-2	9.8982-2	9.8915-2	9.8847-2	9.8778-2
K+	2.6843-3	2.4606-3	2.0620-3	2.0775-3	2.0928-3	2.1080-3	2.1230-3	2.1379-3	2.1527-3	2.1674-3	2.1819-3	2.1963-3	2.2107-3
K-	1.4318-6	9.6442-7	4.9675-7	5.0271-7	5.0877-7	5.1494-7	5.2122-7	5.2764-7	5.3425-7	5.4100-7	5.4791-7	5.5501-7	5.6229-7
KO	3.1181-3	2.5096-3	1.7609-3	1.7715-3	1.7822-3	1.7930-3	1.8040-3	1.8151-3	1.8265-3	1.8381-3	1.8499-3	1.8620-3	1.8743-3
KO-	5.7504-6	3.8032-6	1.9446-6	1.9639-6	1.9836-6	2.0038-6	2.0245-6	2.0457-6	2.0677-6	2.0903-6	2.1136-6	2.1376-6	2.1625-6
K2	7.0063-6	4.6613-6	2.4709-6	2.4891-6	2.5079-6	2.5274-6	2.5475-6	2.5684-6	2.5903-6	2.6130-6	2.6365-6	2.6611-6	2.6868-6
N	4.0322-5	2.6614-5	1.2562-5	1.2825-5	1.3091-5	1.3361-5	1.3635-5	1.3912-5	1.4195-5	1.4483-5	1.4775-5	1.5072-5	1.5375-5
NO	2.1573-2	1.9166-2	1.5392-2	1.5493-2	1.5593-2	1.5692-2	1.5792-2	1.5890-2	1.5989-2	1.6088-2	1.6186-2	1.6285-2	1.6383-2

NO-	1.6253-7	8.8465-8	3.1379-8	3.2068-8	3.2770-8	3.3488-8	3.4223-8	3.4975-8	3.5752-8	3.6548-8	3.7366-8	3.8210-8	3.9079-8
NO2	6.2536-6	4.5925-6	2.7358-6	2.7661-6	2.7966-6	2.8274-6	2.8585-6	2.8900-6	2.9220-6	2.9545-6	2.9874-6	3.0209-6	3.0549-6
NO2-	1.0208-7	6.3797-8	2.9406-8	2.9807-8	3.0215-8	3.0631-8	3.1056-8	3.1490-8	3.1937-8	3.2395-8	3.2864-8	3.3347-8	3.3844-8
N2	1.3125-1	1.3484-1	1.4015-1	1.4006-1	1.3996-1	1.3986-1	1.3976-1	1.3966-1	1.3955-1	1.3945-1	1.3934-1	1.3923-1	1.3912-1
N2O	4.5609-7	3.1105-7	1.6530-7	1.6732-7	1.6937-7	1.7145-7	1.7357-7	1.7572-7	1.7793-7	1.8017-7	1.8247-7	1.8481-7	1.8722-7
O-	6.3361-5	4.2938-5	2.1369-5	2.1750-5	2.2135-5	2.2525-5	2.2920-5	2.3320-5	2.3728-5	2.4142-5	2.4562-5	2.4990-5	2.5426-5
O2	1.0993-1	1.0944-1	1.0578-1	1.0617-1	1.0655-1	1.0693-1	1.0729-1	1.0764-1	1.0797-1	1.0830-1	1.0861-1	1.0892-1	1.0921-1
O2-	4.9524-6	3.2058-6	1.5131-6	1.5385-6	1.5642-6	1.5903-6	1.6168-6	1.6437-6	1.6712-6	1.6993-6	1.7278-6	1.7570-6	1.7869-6
S	1.5589-2	1.2714-2	8.4013-3	8.5159-3	8.6306-3	8.7455-3	8.8607-3	8.9763-3	9.0928-3	9.2098-3	9.3272-3	9.4454-3	9.5644-3
S-	6.6262-5	4.4190-5	2.1091-5	2.1467-5	2.1847-5	2.2232-5	2.2624-5	2.3022-5	2.3429-5	2.3844-5	2.4266-5	2.4697-5	2.5138-5
SN	3.4597-5	2.2482-5	1.0441-5	1.0629-5	1.0820-5	1.1014-5	1.1211-5	1.1412-5	1.1617-5	1.1826-5	1.2040-5	1.2258-5	1.2481-5
SO	1.2102-1	1.1335-1	9.6220-2	9.6766-2	9.7307-2	9.7843-2	9.8374-2	9.8902-2	9.9428-2	9.9951-2	1.00047-1	1.00099-1	1.00150-1
SO-	1.4010-4	9.2825-5	4.4949-5	4.5632-5	4.6324-5	4.7027-5	4.7742-5	4.8470-5	4.9216-5	4.9977-5	5.0754-5	5.1549-5	5.2364-5
SO2	1.7628-1	1.9323-1	2.2275-1	2.2198-1	2.2121-1	2.2044-1	2.1967-1	2.1890-1	2.1813-1	2.1736-1	2.1658-1	2.1581-1	2.1503-1
SO2-	9.5589-5	7.5057-5	4.9808-5	5.0094-5	5.0386-5	5.0683-5	5.0986-5	5.1297-5	5.1618-5	5.1946-5	5.2283-5	5.2630-5	5.2987-5
SO3	3.5655-5	3.3857-5	3.1376-5	3.1350-5	3.1326-5	3.1304-5	3.1283-5	3.1264-5	3.1247-5	3.1231-5	3.1218-5	3.1207-5	3.1198-5
SO3-	2.5748-7	1.8293-7	1.0688-7	1.0754-7	1.0822-7	1.0892-7	1.0964-7	1.1039-7	1.1116-7	1.1197-7	1.1280-7	1.1367-7	1.1457-7
S2	5.2713-4	3.8808-4	2.1755-4	2.2063-4	2.2373-4	2.2687-4	2.3004-4	2.3326-4	2.3653-4	2.3986-4	2.4322-4	2.4666-4	2.5015-4
S2-	1.4940-6	8.4464-7	3.0744-7	3.1382-7	3.2033-7	3.2699-7	3.3381-7	3.4080-7	3.4803-7	3.5546-7	3.6308-7	3.7096-7	3.7908-7

MOLE FRACTIONS OF NEOL SPECIES

COS	8.6658-6	6.2416-6	3.4278-6	3.4159-6	3.4394-6	3.4852-6	3.5435-6	3.6096-6	3.6800-6	3.7524-6	3.8263-6	3.9012-6	3.9770-6
O	1.1289-1	1.0179-1	8.9085-2	8.8884-2	8.8701-2	8.8537-2	8.8390-2	8.8264-2	8.8162-2	8.8079-2	8.8015-2	8.7973-2	8.7951-2
CO	1.2001-1	1.1842-1	1.1842-1	1.1835-1	1.1829-1	1.1823-1	1.1817-1	1.1811-1	1.1805-1	1.1799-1	1.1793-1	1.1787-1	1.1781-1
CS	5.7010-7	3.2277-7	1.1254-7	1.1558-7	1.1936-7	1.2322-7	1.2718-7	1.3122-7	1.3535-7	1.3958-7	1.4390-7	1.4835-7	1.5287-7

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-06 FOR ALL ASSIGNED CONDITIONS

AR+	C(S)	C	C+	C-	C3-	CN	CN+	CN-	CNN
CN2	COS-	CO3-	CO4-	CS-	CS2	C2	C2-	C2N	C2N2
C2O	C3	C3O2	C4	C5	K(S)	K(L)	KCN	K2CO3(S)	K2CO3(L)
KO+	K2O(S)	K2O(L)	K2SO4(S)	K2SO4(S)	K2SO4(L)	NCO	NO+	NO3	NO3-
N2O+	N2O4	N2O5	N3	O+	O3	S(S)	S(L)	S+	S8

1

STOP 5 IS NORMAL CHANNEL STOP

IT OCCURS WHEN XPOSITION EXCEEDS INPUTTED XXSTOP VALUE

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3.4 Channel Problems With Fully Rate Controlled Chemistry and Heat Loss

In this subsection, we consider sample problems where rate controlled chemistry is assumed at all points of the flowfield. An example is the combustion of premixed reactants in a flow tube. In such a case, rate controlled chemistry can be used to determine where the combustion is initiated and whether an equilibrium state is reached. In its present mode, the program can only solve fully rate controlled problems for a constant area channel. A sample problem using the simple channel heat loss model (see Subsection 1.6.4.1) is also considered.

3.4.1 Input Data

For this type of problem, the REACTANTS, OMIT, and INSERT cards are similar to those described in Subsection 3.1.1. No liquid solution model is allowed, hence, SOLUTION cards are not used. All the reactants must be classified either fuel or oxidizer. No mixed classification is allowed. The INPT2, RKTNP, and CHNLIN input data are similar to those of channel problems considered in Subsection 3.2.1. An initial value of flow velocity (meters/sec) must be specified in the CHNLIN input. The DLIT, REACTANT, PRODUCT, and KFRR input data have the same format as those described in Subsection 3.3.1. Two additional types of input data are required, however. These are: One SPEC card, which contains the initial flow velocity (same as the one in CHNLIN), and flags the reading of reactant species which participate in the initiation of chemical reactions (see Subsection 2.1.5), and a set of input cards containing the name(s) of the reactant species on the REACTANT input cards (see Subsection 2.1.5). The DLIT cards must follow the two types of cards just described. This will be clarified through the examples given below.

3.4.1.1 Input data for a fully rate controlled channel problem without heat loss

The following data cards are required for this sample problem:

```

REACTANTS
C 1.000000 2.0000 00 .441859 000000.0G 1000.04 F 0.0
AR1.0 00 .000001 0.0G 1000.44 F 0.0
O 2.000000 00 .558140 000.0G 1000.00 F 0.0

```

NAMELISTS

```

$INPT2 KASE=201, p(1)=.01, DXI=.05, MIX=.0., RKT=T,
TRACE=1.0E-7, IONS=F, ACCURC=1.0E-3,
HMIN=1.0E-30 $END
$RKTINP PCP(1)=.01
NEQPT=1, TCEST=3000.0, TCHFNL=1100.0, IPRRKT=1 $END

```

```

SPEC      1.
O2         3      CS2      1

DLIT       SO      CO      SO2      O2
DLIT       COS      O      CS2      CS
DLIT       S      CO2

REACTANT   1.0SO      1.0O2
PRODUCT    1.0SO2     1.0O
KERR       5.8E-13    0.0    3250.0
REACTANT   1.0COS     1.0O
PRODUCT    1.0CO      1.0SO
KERR       3.15E-11    0.0    2250.0
REACTANT   1.0S      1.0O2
PRODUCT    1.0SO      1.0O
KERR       1.7E-12    0.0    0.0
REACTANT   1.0CS2     1.0O
PRODUCT    1.0CS      1.0SO
KERR       9.3E-11    0.0    950.0
REACTANT   1.0TS2     1.0O2
PRODUCT    1.0SO2     1.0CS
KERR       1.7E-12    0.0    22500.0
REACTANT   1.0CS      1.0O
PRODUCT    1.0CO      1.0S
KERR       3.99E-10    0.0    1000.0
REACTANT   1.0CO      1.0O2
PRODUCT    1.0CO2     1.0O
KERR       4.2E-12    0.0    24000.0
REACTANT   1.0CO      1.0O      1.0THIRD BODY
PRODUCT    1.0CO2     1.0THIRD BODY
KERR       0.5E-32    0.0    900.0
REACTANT   1.0CS      1.0O2
PRODUCT    1.0COS     1.0O
KERR       1.7E-11    0.0    6000.0

```

STOP

A description of these data cards follows:

DATA CARD 1 - REACTANTS code card with the word REACTANTS in Columns 1 - 9 and blank in Columns 16 - 21, indicating this is not a two-stage problem. Note, this is the first data card, as the THERMO data is to be read from file unit 7.

- DATA CARDS 2 - 4 - This contains the REACTANTS data described by Table II. Note, the entry in column 72 is an F for all three species. This has no effect on HP or TP problems, but is important for the fully finite rate chemical problems.
- DATA CARD 5 - A blank card to terminate the set of REACTANTS data.
- DATA CARD 6 - Since this problem does not have any OMIT or INSERT cards associated with it, NAMELISTS code card appears next.
- DATA CARD 7 - INPT2 namelist data is described in Table III. The variables DXI, ACCURC, and HMIN are required, as well as RKT=TRUE, for this channel problem.
- DATA CARD 8 - RKTINP namelist data is described in Table IV. It is recommended that all channel problems be run with HPATH=TRUE and SPATH=FALSE. Note, PCP(1) is a required input, while the rest are optional. NEQPT=1 is necessary to initiate a fully finite rate chemical problem.
- DATA CARD 9 - SPEC code card (see Subsection 2.1.5) includes SPEC in columns 1 - 4 and the initial flow velocity (meters/sec) in columns 13 - 23. This card is required, in this position, for all NEQPT=1 problems.
- DATA CARD 10 - A SPEC data card, which contains names of certain species appearing in the REACTANTS input cards. These are species which are driven by finite rate chemistry. Note, the species names appear in columns 1 - 12, 24 - 35, and 47 - 58, while their position on the REACTANTS cards (Data cards 2 - 4) is indicated by placing an integer in columns 15, 38, and 61. For this example, CS₂ is the first REACTANTS species, while O₂ is the third REACTANTS species. This data card is needed to determine the starting concentration (i. e. number of moles per kilogram of reactants) of CS₂ and O₂. Note: There must be at least one reactant species whose name does not appear on SPEC data cards. To achieve this in this problem, a trace amount of Ar is included as a reactant.

DATA CARD 11 - A blank card to terminate SPEC data input.

DATA CARDS 12 - 14 - A set of DLIT cards containing the names of rate controlled species. All species appearing on the SPEC data cards, as well as all species which will appear on the following REACTANT, PRODUCT cards, must be placed on a DLIT card for NEQPT=1 problems.

DATA CARD 15 - A blank card to terminate DLIT card inputs.

DATA CARDS 16 - 42 - Contains the set of REACTANT, PRODUCT, KFRR cards for the 9 rate equations considered here. These cards are described in Subsections 2.1.6.2 and 2.1.6.3. For example, the first set:

REACTANT	1.0SO	1.0O2
PRODUCT	1.0SO2	1.0O
KFRR	$5.8E-13 \times T^{0.0} \times \exp(-3250.0/T)$	

has been described in Subsection 3.3.1.1.

DATA CARD 43 - A blank card to terminate the above input set.

DATA CARD 44 - A blank card.

DATA CARD 45 - A STOP card.

The following channel input file (Logical Unit 11) is used for this problem.

\$CHNLIN NMPATH=3, IMPRNT=2, XXSTOP=3.02, UEINP=1.0, \$END

0.0 1.000

1.0 1.000

DATA CARD 1 - CHNLIN namelist input is described in Table VI.

Note, the value of UEINP, the initial channel velocity, must be the same as that appearing on the SPEC card.

DATA CARD 2 - 3 - These cards contain the area ratio profiles. Since the area is a constant, only two data points are required (see Table VII).

3.4.1.2 Input data for a fully rate controlled channel problem with heat loss

Except for the RKTINP, all input data for this sample problem is the same as that of the previous problem. The RKTINP namelist for this case is given below:

```
$RKTINP  PCP(1)=0.01    HPATH=T, SPATH=F,  
          NUMHLS=1, TCHINP=1100.,  
          CHNHLS=-1204.9,  
          NEQPT=1, TCEST=3000.0, TCHFNL=1100.0, IPRRKT=1  $END
```

RKTINP namelist data is described in Table IV. The variables required for a channel heat loss problem are: NUMHLS, which must be set equal to one; TCHINP, which is the value of T_w defined in Subsection 1.6.4.1; and CHNHLS, which is the value of gas enthalpy at temperature T_w and pressure p_{av} specified by the user. Note that p_{av} is not a required input parameter. The value of CHNHLS can be determined using the TP mode of the code. An additional variable to be specified in RKTINP is CHNLEN which is the effective folding length, Z , defined in Subsection 1.6.4.1. This variable is left out here because, for this problem, we have assumed $Z = 1.0$ meter, which is the default value of CHNLEN.

3.4.2 Output Data

For this type of channel problem, the output data format associated with REACTANTS, INPT2, RKIINP, REACTANT, PRODUCT, KFRR, and CHNLIN input data is the same as those described in Subsections 3.2.2 and 3.3.2. Additional data containing the following information is also printed out. These are: chemical formula and concentration (in moles/kg) of species which appear on the REACTANTS input cards and are rate controlled; the rate controlled chemical species; chemical elements which only exist in the rate controlled chemical species; species, comprised of chemical elements which only exist in the rate controlled species, which are considered by the system but do not appear in the DLIT cards; and the mixture maximum temperature together with the channel location, flow velocity, molecular weight, and species mole fraction at the point where the temperature is maximum. The output data for the sample problems considered in this subsection are given below.

3.4.2.1 Output data for a fully chemical rate controlled channel problem without heat loss

This data is shown in Sample Output 11. The output unique to this type of problem begins on output page 3. The two lines beginning with the words DLIT SPEC contain the names and the initial concentration of rate controlled species which appear on the REACTANTS input cards. The three lines beginning with the word DLIT contain the names of the rate controlled species. For this problem, there are no species which are composed of elements C, S, and O and are not rate controlled. These elements are shown in the output under the heading "Eliminated the Following 3 Elements in Equilibrium Calculations." Species which contain these elements and are being considered by the system (see page 2 of the sample output) but do not appear on the DLIT cards are removed from consideration. A list of these species is printed out under the heading "Removed Following Species From Consideration." On page 10 of this sample output is the heading "Output at Maximum Temperature." This is followed by the mixture flow velocity and certain thermodynamic parameters at that point in the channel where the temperature is a maximum. These are useful information which may be lost if the maximum temperature does not occur at an axial station, which is a multiple of the printout increment, DXI, assigned by the user. Note that, for this sample problem, the flow parameters remain effectively unchanged beyond 1.2 meters. This indicates that the combustion has reached equilibrium. The same equilibrium results will be obtained if the HP mode of the code is run.

3.4.2.2 Output data for a fully chemical rate controlled channel problem with heat loss

This output data is shown in Output Sample 12. The Output format for this problem is identical to that of the previous one and requires no additional discussion.

**Sample Output 11, Channel Problem
With Fully Rate Controlled Chemistry
Without Heat Loss
(12 Output Pages)**

Page 1

REACTANTS														
C	1.0000	S	2.0000	0.0000	0.0000	00	0.0000	0.44186	0.00	G	1000.000	0	F	0.000000
AR	1.0000		0.0000	0.0000	0.0000	00	0.0000	0.10000E-05	0.00	G	1000.000	0	F	0.000000
O	2.0000		0.0000	0.0000	0.0000	00	0.0000	0.55814	0.00	G	1000.000	0	F	0.000000
NAMELISTS														

```
$INPT2
KASE =      201,
T = 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
P = 0.100000E-01, 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000
```

```

PSIA = F,
MMHG = F,
NSQM = F,
V = 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000,
RHO = 0.100000E-01, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000,
3-177

```

```

ERATIO= F,
OXFL   = F,
FPCT   = F,
FA      = F,
MIX     = 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000,

```

```

TP      = F,
HP      = F,
SP      = F,
TV      = F,
UV      = F,
SV      = F,
RKT     = T,
SHOCK   = F,
DETN    = F,
OTTO    = F,
CR      = 0.000000,
SO      = 0.000000000000,
ICIS    = T,
JL      = F,
TRACE   = 0.100000E-06,

```

```

SIUMIT= F,
DXI = 0.500000E-01,
NITER = 0,
NSTOP = 0,
NEQL = F,
BZ = 0.000000,
XK = 0.650000,
ACCURC= 0.100000E-02,
HMIN = 0.100000E-29,
ALPH = 0.000000,
EXIN = 2400.00,
TWOBTG= F,
$END
LLMT =

```

C
S
AR
O

NO INPT2 VALUE GIVEN FOR OF, EORAT, FA, OR FPCT
SPECIES BEING CONSIDERED IN THIS SYSTEM

L 5/66	AR	L12/66	AR+	J 3/61	C(S)	J 3/61	C	L12/66	C+
J 9/65	C-	3/3/7	C3-	J 9/65	CO	J 3/61	COS	3/3/7	COS-
J 9/65	CO2	4/12/7	CO2-	3/3/7	CO3-	3/7/7	CO4-	J12/62	CS
3/3/7	CS-	J 6/61	CS2	J12/69	C2	J12/69	C2-	J 9/66	C20
J12/69	C3	J 6/68	C302	J12/69	C4	J12/69	C5	L02/67	E
J 6/62	O	L12/66	O+	J 6/65	O-	J 9/65	O2	J12/66	O2-
J 6/61	O3	J12/65	S(S)	J12/65	S(L)	J 6/71	S	L12/66	S+
3/3/7	S-	J 6/71	SO	3/3/7	SO-	J 6/61	SO2	3/3/7	SO2-
J 9/65	SO3	3/3/7	SO3-	J12/65	S2	3/3/7	S2-	J6/64	S8
45	5	3	2	0	3	755			

3-178
C
S
AR
O
E

\$RKTINP

```

EOL = T,
FRCZ = F,
SUBAR = 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000,
SUPAR = 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000,
PCP = 0.100000E-01, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000, 0.000000,
0.000000, 0.000000, 0.000000,
TCEST = 3000.00,
NFZ = 1,
NEQPT = 1,
HTLASS= 0.000000,
HPATH = T,
SPATH = F,
NUMHLS= 0,

```

```

CHNLEN= 1.000000 ,
CHNHLS= 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 ,
TCHINP= 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 ,
TCHFNL= 1100.00 ,
IPRRKT= 1,
$END
BOF = 0.000000

```

ENTHALPY (KG-MOL)(DEG K)/KG 0KG-ATOMS/KG	EFFECTIVE FUEL HPP(2) BOP(I,2)	EFFECTIVE OXIDANT HPP(1) BOP(I,1)	MIXTURE HSUB0 BOP(I)
C	0.58033103E-02	0.00000000E 00	0.58033103E-02
S	0.11606621E-01	0.00000000E 00	0.11606621E-01
AR	0.25032541E-07	0.00000000E 00	0.25032541E-07
O	0.34885056E-01	0.00000000E 00	0.34885056E-01
E	0.00000000E 00	0.00000000E 00	0.00000000E 00
DLIT SPEC= O2	CONCENTRATION(MOLES/KG)=	0.1744E-01 NO. 29	
DLIT SPEC= CS2	CONCENTRATION(MOLES/KG)=	0.5803E-02 NO. 17	
DLIT SO	CO	SO2	O2
DLIT COS	O	CS2	CS
DLIT S	CO2		

ELIMINATED THE FOLLOWING 4 ELEMENTS IN EQUILIBRIUM CALCULATION

3-179
C
S
O
E

REMOVED FOLLOWING SPECIES FROM CONSIDERATION

AR+
C(S)
C
C+
C-
C3-
COS-
CO2-
CO3-
CO4-
CS-
C2
C2-
C2O
C3
C3O2
C4
C5
E
O+
O-
O2-
O3
S(S)

S(L)
S+
S-
SO-
SO2-
SO3
SO3-
S2
S2-
S8

1

NON-EQUILIBRIUM REACTIONS

1 1.0 SO + 1.0 O2 = 1.0 SO2 + 1.0 O
CHEMICAL RATE - 5.8000E-13*T** 0.0000*EXP(- 3.2500E 03/T)

2 1.0 COS + 1.0 O = 1.0 CO + 1.0 SO
CHEMICAL RATE - 3.1500E-11*T** 0.0000*EXP(- 2.2500E 03/T)

3 1.0 S + 1.0 O2 = 1.0 SO + 1.0 O
CHEMICAL RATE - 1.7000E-12*T** 0.0000*EXP(- 0.0000E-01/T)

3-180
4 1.0 CS2 + 1.0 O = 1.0 CS + 1.0 SO
CHEMICAL RATE - 8.3000E-11*T** 0.0000*EXP(- 9.5000E 02/T)

5 1.0 CS2 + 1.0 O2 = 1.0 SO2 + 1.0 CS
CHEMICAL RATE - 1.7000E-12*T** 0.0000*EXP(- 2.2000E 04/T)

6 1.0 CS + 1.0 O = 1.0 CO + 1.0 S
CHEMICAL RATE - 3.9900E-10*T** 0.0000*EXP(- 1.0000E 03/T)

7 1.0 CO + 1.0 O2 = 1.0 CO2 + 1.0 O
CHEMICAL RATE - 4.2000E-12*T** 0.0000*EXP(- 2.4000E 04/T)

CHEMICAL RATE - 5.5000E-32*T** 0.0000*EXP(- 9.0000E 02/T)

CHEMICAL RATE - $1.70000E-11 * T^{**} 0.00000 * \exp(-6.00000E 03 / T)$

```

NMPATH= 3
IMPRNT= 0
XXSTOP= 3.0200
UEINP= 1.0000
ITYPE= 1

```

DEPENDENT VARIABLE

1.000000

1.000000

1

THEORETICAL MHD CORE PERFORMANCE

CASE NO. 201

WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
0.44186	37066.000	G	1000.00	0.0000
0.00000	3486.729	G	1000.00	0.0000
0.55814	5427.000	G	1000.00	0.0000

O/F= 0.0000 PERCENT FUEL=100.0000 EQUIVALENCE RATIO= 0.9981 REACTANT DENSITY= 0.0000

[illegible]

MACH NUMBER	0.0000	0.0020	0.0020	0.0039	0.0037	0.0037	0.0036	0.0036	0.0036	0.0036	0.0036	0.0036	0.0036
AE/AT		1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
TOTAL MOL WT	43.018	43.018	43.018	40.877	39.916	39.516	39.315	39.200	39.128	39.079	39.045	39.021	39.002

MOLE FRACTIONS

AR	1.0769-6	1.0769-6	1.0769-6	1.0233-6	9.9920-7	9.8918-7	9.8415-7	9.8127-7	9.7946-7	9.7825-7	9.7740-7	9.7679-7	9.7633-7
----	----------	----------	----------	----------	----------	----------	----------	----------	----------	----------	----------	----------	----------

MOLE FRACTIONS OF NEOL SPECIES

SO	0.0000	0.0000	0.4302-11	1.698 -1	1.765 -1	1.795 -1	1.815 -1	1.830 -1	1.841 -1	1.850 -1	1.857 -1	1.863 -1	1.867 -1
CO	0.0000	0.0000	0.4302-11	2.344 -1	2.238 -1	2.158 -1	2.095 -1	2.045 -1	2.006 -1	1.975 -1	1.951 -1	1.932 -1	1.917 -1
SO2	0.0000	0.0000	0.4302-11	2.861 -1	2.635 -1	2.533 -1	2.472 -1	2.431 -1	2.402 -1	2.380 -1	2.363 -1	2.350 -1	2.340 -1
O2	7.5035-1	7.5035-1	7.5035-1	1.5544-1	1.4428-1	1.3757-1	1.3326-1	1.3030-1	1.2818-1	1.2661-1	1.2543-1	1.2455-1	1.2385-1
COS	0.0000	0.0000	0.4302-11	2.564 -5	9.297 -6	5.624 -6	4.245 -6	3.566 -6	3.174 -6	2.925 -6	2.755 -6	2.638 -6	2.550 -6
O	0.0000	0.0000	0.4302-11	1.329 -1	1.608 -1	1.745 -1	1.823 -1	1.872 -1	1.906 -1	1.930 -1	1.948 -1	1.961 -1	1.971 -1
CS2	2.496 -1	2.496 -1	2.496 -1	1.542 -9	2.689-10	1.141-10	7.141-11	5.385-11	4.482-11	3.950-11	3.607-11	3.378-11	3.212-11
CS	0.0000	0.0000	0.4302-11	1.539 -6	5.237 -7	3.054 -7	2.269 -7	1.894 -7	1.683 -7	1.551 -7	1.462 -7	1.401 -7	1.356 -7
S	0.0000	0.0000	0.4302-11	1.842 -2	2.319 -2	2.585 -2	2.762 -2	2.890 -2	2.986 -2	3.060 -2	3.116 -2	3.160 -2	3.195 -2
CO2	0.0000	0.0000	0.4302-11	2.841 -3	7.833 -3	1.348 -2	1.864 -2	2.298 -2	2.649 -2	2.930 -2	3.152 -2	3.325 -2	3.465 -2

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-06 FOR ALL ASSIGNED CONDITIONS

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THEORETICAL MHD CORE PERFORMANCE

SPC = 0.1 PSIA

CASE NO. 201

	CHEMICAL FORMULA	WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	C 1.00000 S 2.00000	0.44186	37066.000	G	1000.00	0.0000
FUEL	AR 1.00000	0.00000	3486.729	G	1000.00	0.0000
FUEL	O 2.00000	0.55814	5427.000	G	1000.00	0.0000
O/F=	0.0000	PERCENT FUEL=100.0000	EQUIVALENCE RATIO= 0.9981	REACTANT DENSITY=	0.0000	

	CHAMBER	THROAT	0.550	0.600	0.650	0.700	0.750	0.800	0.850	0.900	0.950	1.000	1.050
PC/P	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
P, ATM	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100
T, DEG K	1000	1000	2836	2832	2829	2826	2824	2823	2822	2821	2820	2820	2819
RHO, G/CC	5.2426-6	5.2426-6	1.6756-6	1.6775-6	1.6789-6	1.6800-6	1.6809-6	1.6816-6	1.6821-6	1.6825-6	1.6829-6	1.6832-6	1.6834-6
H, CAL/G	309.8	309.8	309.8	309.8	309.8	309.8	309.8	309.8	309.8	309.8	309.8	309.8	309.8
S, CAL/(G)(K)	1.6722	1.6722	2.0922	2.0922	2.0922	2.0922	2.0922	2.0922	2.0922	2.0922	2.0922	2.0922	2.0922
M, MOL WT	43.018	43.018	38.988	38.977	38.969	38.962	38.957	38.953	38.950	38.948	38.946	38.944	38.943
(DLV/DLP)T	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000
(DLV/DLT)P	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
CP, CAL/(G)(K)	0.2268	0.2268	0.2478	0.2478	0.2478	0.2478	0.2479	0.2479	0.2479	0.2479	0.2479	0.2479	0.2479
GAMMA (S)	1.2557	1.2557	1.2589	1.2590	1.2590	1.2591	1.2591	1.2591	1.2592	1.2592	1.2592	1.2592	1.2592
VELOCITY, M/SEC			3.13	3.13	3.12	3.12	3.12	3.12	3.12	3.12	3.12	3.11	3.11
TOTAL H(CAL/G)			309.76	309.76	309.76	309.76	309.76	309.76	309.76	309.76	309.76	309.76	309.76
MAG FLD(TESLA)			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
BETA			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SON VEL, M/SEC	492.6	492.6	872.5	872.0	871.7	871.4	871.2	871.0	870.9	870.8	870.7	870.6	870.6

MOLE FRACTIONS

MOLE FRACTIONS OF NEQL SPECIES

00ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.100000E-06 FOR ALL ASSIGNED CONDITIONS

THEORETICAL MHD CORE PERFORMANCE

O/F= 0.0000 PERCENT FUEL=100.0000

WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
0.44186	37066.000	G	1000.00	0.0000
0.00000	3486.729	G	1000.00	0.0000
0.55814	5427.000	G	1000.00	0.0000
0.9981	REACTANT DENSITY=		0.0000	

[illegible]

VELOCITY,M/SEC			3.11	3.11	3.11	3.11	3.11	3.11	3.11	3.11	3.11	3.11	3.11
TOTAL H(CAL/G)			309.76	309.76	309.76	309.76	309.76	309.76	309.76	309.76	309.76	309.76	309.76
MAG FLD(TESLA)			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
BETA			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SON VEL,M/SEC	492.6	492.6	870.5	870.5	870.5	870.5	870.4	870.4	870.4	870.4	870.4	870.4	870.4
ELEC DENS	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
IONIC DENS	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
SIGMA (MHO/M)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
W/O IONS	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
FREQ (1/SEC)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
MACH NUMBER	0.00000	0.00000	0.00036	0.00036	0.00036	0.00036	0.00036	0.00036	0.00036	0.00036	0.00036	0.00036	0.00036
AE/AT	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
TOTAL MOL WT	43.018	43.018	38.942	38.941	38.940	38.940	38.939	38.939	38.939	38.939	38.938	38.938	38.938

MOLE FRACTIONS

AR 1.0769-6 1.0769-6 9.7481-7 9.7479-7 9.7478-7 9.7476-7 9.7475-7 9.7474-7 9.7474-7 9.7473-7 9.7473-7 9.7473-7 9.7472-7

MOLE FRACTIONS OF NEQL SPECIES

so	0.0000	0.0000	0.0000	1.8824-1	1.8826-1	1.8828-1	1.8829-1	1.8830-1	1.8831-1	1.8832-1	1.8832-1	1.8833-1	1.8833-1	1.8833-1
co	0.0000	0.0000	0.0000	1.8622-1	1.8614-1	1.8603-1	1.8603-1	1.8599-1	1.8596-1	1.8594-1	1.8592-1	1.8590-1	1.8589-1	1.8588-1
so2	0.0000	0.0000	0.0000	2.3053-1	2.3048-1	2.3044-1	2.3041-1	2.3039-1	2.3037-1	2.3035-1	2.3034-1	2.3033-1	2.3032-1	2.3032-1
o2	7.5035-1	7.5035-1	1.2139-1	1.2139-1	1.2136-1	1.2133-1	1.2131-1	1.2129-1	1.2128-1	1.2127-1	1.2126-1	1.2125-1	1.2125-1	1.2124-1
cos	0.0000	0.0000	0.0000	2.2719-6	2.2682-6	2.2654-6	2.2632-6	2.2614-6	2.2600-6	2.2588-6	2.2580-6	2.2572-6	2.2567-6	2.2562-6
184	0.0000	0.0000	0.0000	2.0063-1	2.0068-1	2.0072-1	2.0075-1	2.0078-1	2.0079-1	2.0081-1	2.0082-1	2.0083-1	2.0084-1	2.0085-1
cs2	2.496	-1	2.496	-1	2.714-11	2.707-11	2.703-11	2.699-11	2.696-11	2.693-11	2.691-11	2.689-11	2.688-11	2.687-11
cs	0.0000	0.0000	0.0000	1.2139-7	1.2120-7	1.2106-7	1.2095-7	1.2086-7	1.2078-7	1.2073-7	1.2068-7	1.2065-7	1.2062-7	1.2059-7
s	0.0000	0.0000	0.0000	3.3209-2	3.3227-2	3.3241-2	3.3253-2	3.3262-2	3.3269-2	3.3275-2	3.3279-2	3.3283-2	3.3286-2	3.3288-2
co2	0.0000	0.0000	0.0000	3.9768-2	3.9841-2	3.9900-2	3.9946-2	3.9983-2	4.0013-2	4.0036-2	4.0055-2	4.0070-2	4.0082-2	4.0091-2

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN $0.10000E-06$ FOR ALL ASSIGNED CONDITIONS

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THEORETICAL MHD CORE PERFORMANCE

OPC = 0.1 PSIA

C-5 NO. 201

CHEMICAL FORMULA		
FUEL	C	1.00000 S 2.00000
FUEL	AR	1.00000
FUEL	O	2.00000

WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
0.44186	37066.000	G	1000.00	0.0000
0.00000	3486.729	G	1000.00	0.0000
0.55814	5427.000	G	1000.00	0.0000
0.9981	REACTANT DENSITY=		0.0000	

[illegible]

M, MOL WT	43.018	43.018	38.938	38.938	38.938	38.938	38.938	38.938	38.938	38.938	38.938	38.938	38.938
(DLV/DLP)T	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000
(DLV/DLT)P	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
CP, CAL/(G)(K)	0.2268	0.2268	0.2479	0.2479	0.2479	0.2479	0.2479	0.2479	0.2479	0.2479	0.2479	0.2479	0.2479
GAMMA (S)	1.2557	1.2557	1.2592	1.2592	1.2592	1.2592	1.2592	1.2592	1.2592	1.2592	1.2592	1.2592	1.2592
VELOCITY,M/SEC			3.11	3.11	3.11	3.11	3.11	3.11	3.11	3.11	3.11	3.11	3.11
TOTAL H(CAL/G)			309.76	309.76	309.76	309.76	309.76	309.76	309.76	309.76	309.76	309.76	309.76
MAG FLD(TESLA)			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
BETA			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SON VEL,M/SEC	492.6	492.6	870.4	870.4	870.4	870.4	870.4	870.4	870.4	870.4	870.4	870.4	870.4
ELEC DENS	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
IONIC DENS	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
SICMA (MHG/M)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
W/O IONS	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
FREQ (1/SEC)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
MACH NUMBER	0.00000	0.00000	0.0036	0.0036	0.0036	0.0036	0.0036	0.0036	0.0036	0.0036	0.0036	0.0036	0.0036
AE/AT		1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
TOTAL MOL WT	43.018	43.018	38.938	38.938	38.938	38.938	38.938	38.938	38.938	38.938	38.938	38.938	38.938

MOLE FRACTIONS

AR 1.0769-6 1.0769-6 9.7472-7 9.7472-7 9.7472-7 9.7472-7 9.7472-7 9.7472-7 9.7472-7 9.7472-7 9.7471-7 9.7471-7 9.7471-7 9.7471-7

MOLE FRACTIONS OF NEOL SPECIES

SO	0.00000	0.00000	0.00000	1.8834-1	1.8834-1	1.8834-1	1.8834-1	1.8834-1	1.8834-1	1.8834-1	1.8834-1	1.8834-1	1.8835-1
CO	0.00000	0.00000	0.00000	1.8587-1	1.8586-1	1.8586-1	1.8585-1	1.8585-1	1.8585-1	1.8584-1	1.8584-1	1.8584-1	1.8584-1
SO2	0.00000	0.00000	0.00000	2.3031-1	2.3031-1	2.3030-1	2.3030-1	2.3030-1	2.3030-1	2.3030-1	2.3029-1	2.3029-1	2.3029-1
O2	7.5035-1	7.5035-1	1.2124-1	1.2124-1	1.2124-1	1.2123-1	1.2123-1	1.2123-1	1.2123-1	1.2123-1	1.2123-1	1.2123-1	1.2123-1
COS	0.00000	0.00000	0.00000	2.2558-6	2.2556-6	2.2553-6	2.2551-6	2.2550-6	2.2548-6	2.2547-6	2.2546-6	2.2545-6	2.2545-6
O	0.00000	0.00000	0.00000	2.0085-1	2.0085-1	2.0086-1	2.0086-1	2.0086-1	2.0086-1	2.0087-1	2.0087-1	2.0087-1	2.0087-1
CS2	2.496 -1	2.496 -1	2.686-11	2.686-11	2.685-11	2.685-11	2.685-11	2.684-11	2.684-11	2.684-11	2.684-11	2.684-11	2.684-11
CS	0.00000	0.00000	0.00000	1.2058-7	1.2056-7	1.2055-7	1.2054-7	1.2053-7	1.2053-7	1.2052-7	1.2051-7	1.2051-7	1.2051-7
S	0.00000	0.00000	0.00000	3.3290-2	3.3291-2	3.3292-2	3.3293-2	3.3294-2	3.3295-2	3.3295-2	3.3296-2	3.3296-2	3.3297-2
CO2	0.00000	0.00000	0.00000	4.0099-2	4.0105-2	4.0110-2	4.0114-2	4.0117-2	4.0120-2	4.0122-2	4.0123-2	4.0125-2	4.0127-2

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-06 FOR ALL ASSIGNED CONDITIONS

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THEORETICAL MHD CORE PERFORMANCE

OPC = 0.1 PSIA
CASE NO. 201

	CHEMICAL FORMULA	WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	C 1.00000 S 2.00000	0.44186	37066.000	G	1000.00	0.0000
FUEL	AR 1.00000	0.00000	3486.729	G	1000.00	0.0000
FUEL	O 2.00000	0.55814	5427.000	G	1000.00	0.0000
O/F=	0.0000	PERCENT FUEL=100.0000	EQUIVALENC RATIO=	0.9981	REACTANT DENSITY=	0.0000
AXIAL STATION (M)						
CHAMBER	THROAT	2.200	2.250	2.300	2.350	2.400
P, ATM		1.0000	1.0000	1.0000	1.0000	1.0000
P, ATM		0.0100	0.0100	0.0100	0.0100	0.0100

3-186

[illegible]

SO	0.00000	0.00000	0.00000	1.8835-1	1.8835-1	1.8835-1	1.8835-1	1.8835-1	1.8835-1	1.8835-1	1.8835-1	1.8835-1	1.8835-1	1.8835-1
CO	0.00000	0.00000	0.00000	1.8584-1	1.8584-1	1.8584-1	1.8584-1	1.8584-1	1.8584-1	1.8584-1	1.8584-1	1.8584-1	1.8584-1	1.8584-1
SO2	0.00000	0.00000	0.00000	2.3029-1	2.3029-1	2.3029-1	2.3029-1	2.3029-1	2.3029-1	2.3029-1	2.3029-1	2.3029-1	2.3029-1	2.3029-1
O2	7.5035-1	7.5035-1	1.2123-1	1.2123-1	1.2123-1	1.2123-1	1.2123-1	1.2123-1	1.2123-1	1.2123-1	1.2123-1	1.2123-1	1.2123-1	1.2123-1
COS	0.00000	0.00000	0.00000	2.2545-6	2.2544-6	2.2544-6	2.2544-6	2.2544-6	2.2544-6	2.2544-6	2.2544-6	2.2544-6	2.2544-6	2.2543-6
O	0.00000	0.00000	0.00000	2.0087-1	2.0087-1	2.0087-1	2.0087-1	2.0087-1	2.0087-1	2.0087-1	2.0087-1	2.0087-1	2.0087-1	2.0087-1
CS2	2.496 -1	2.496 -1	2.684-11	2.684-11	2.684-11	2.684-11	2.684-11	2.684-11	2.684-11	2.684-11	2.684-11	2.684-11	2.684-11	2.684-11
CS	0.00000	0.00000	0.00000	1.2050-7	1.2050-7	1.2050-7	1.2050-7	1.2050-7	1.2050-7	1.2050-7	1.2050-7	1.2050-7	1.2050-7	1.2050-7
S	0.00000	0.00000	0.00000	3.3297-2	3.3297-2	3.3297-2	3.3297-2	3.3297-2	3.3297-2	3.3297-2	3.3297-2	3.3297-2	3.3297-2	3.3297-2
CO2	0.00000	0.00000	0.00000	4.0127-2	4.0128-2	4.0128-2	4.0129-2	4.0129-2	4.0129-2	4.0129-2	4.0130-2	4.0130-2	4.0130-2	4.0130-2

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN $0.10000E-06$ FOR ALL ASSIGNED CONDITIONS

*****OUTPUTS AT MAXIMUM TEMPERATURE*****

```
*****TMAX=      4016.      AT X=      0.12933E-01  VEL=      4.0337      MOLES/KG=      0.23350E-01
SPECIES      MOLE FRACTION
AR      0.10720E-05
S J      0.18580
CO      0.24715
SO2      0.30444
O2      0.19500
COS      0.47369E-03
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O 0.59833E-01
 CS2 0.32374E-07
 CS 0.60399E-05
 S 0.63505E-02
 CO2 0.90726E-03

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THEORETICAL MHD CORE PERFORMANCE

OPC = 0.1 PSIA
 CASE NO. 201

CHEMICAL FORMULA		WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC		
FUEL	C 1.00000 S 2.00000	0.44186	37066.000	G	1000.00	0.0000		
FUEL	AR 1.00000	0.00000	3486.729	G	1000.00	0.0000		
FUEL	O 2.00000	0.55814	5427.000	G	1000.00	0.0000		
O/F= 0.0000 PERCENT FUEL=100.0000 EQUIVALENCE RATIO= 0.9981 REACTANT DENSITY= 0.0000								
AXIAL STATION (M)								
	CHAMBER	THROAT	2.750	2.800	2.850	2.900	2.950	3.000
PC/P	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
P, ATM	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100
T, DEG K	1000	1000	2817	2817	2817	2817	2817	2817
RHO, G/CC	5.2426-6	5.2426-6	1.6842-6	1.6842-6	1.6842-6	1.6842-6	1.6842-6	1.6842-6
H, CAL/G	309.8	309.8	309.8	309.8	309.8	309.8	309.8	309.8
S, CAL/(G)(K)	1.6722	1.6722	2.0922	2.0922	2.0922	2.0922	2.0922	2.0922
M, MOL WT								
(DLV/DLP)T	43.018	43.018	38.938	38.938	38.938	38.938	38.938	38.938
(DLV/DLT)P	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000
CP, CAL/(G)(K)	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
GAMMA (S)	0.2268	0.2268	0.2479	0.2479	0.2479	0.2479	0.2479	0.2479
VELOCITY, M/SEC	1.2557	1.2557	1.2592	1.2592	1.2592	1.2592	1.2592	1.2592
TOTAL H(CAL/G)			3.11	3.11	3.11	3.11	3.11	3.11
MAG -LD(TESLA)			309.76	309.76	309.76	309.76	309.76	309.76
BETA			0.00	0.00	0.00	0.00	0.00	0.00
SON VEL, M/SEC			0.00	0.00	0.00	0.00	0.00	0.00
ELEC DENS	492.6	492.6	870.4	870.4	870.4	870.4	870.4	870.4
IONIC DENS	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SIGMA (MHO/M)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
W/O IONS	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
FREQ (1/SEC)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MACH NUMBER	0.0000	0.0000	0.0036	0.0036	0.0036	0.0036	0.0036	0.0036
AE/AT			1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
TOTAL MOL WT	43.018	43.018	38.938	38.938	38.938	38.938	38.938	38.938

MOLE FRACTIONS

AR 1.0769-6 1.0769-6 9.7471-7 9.7471-7 9.7471-7 9.7471-7 9.7471-7 9.7471-7

MOLE FRACTIONS OF NEQL SPECIES

SO 0.0000 0.0000 0.0000 1.8835-1 1.8835-1 1.8835-1 1.8835-1 1.8835-1 1.8835-1
 CO 0.0000 0.0000 0.0000 1.8584-1 1.8584-1 1.8584-1 1.8584-1 1.8584-1 1.8584-1
 SO2 0.0000 0.0000 0.0000 2.3029-1 2.3029-1 2.3029-1 2.3029-1 2.3029-1 2.3029-1

O2	7.5035-1	7.5035-1	1.2123-1	1.2123-1	1.2123-1	1.2123-1	1.2123-1	1.2123-1	1.2123-1
COS	0.0000	0.0000	2.2544-6	2.2543-6	2.2543-6	2.2543-6	2.2543-6	2.2543-6	2.2543-6
O	0.0000	0.0000	2.0087-1	2.0087-1	2.0087-1	2.0087-1	2.0087-1	2.0087-1	2.0087-1
CS2	2.496	-1	2.684-11	2.684-11	2.684-11	2.684-11	2.684-11	2.684-11	2.684-11
CS	0.0000	0.0000	1.2050-7	1.2050-7	1.2050-7	1.2050-7	1.2050-7	1.2050-7	1.2050-7
S	0.0000	0.0000	3.3297-2	3.3297-2	3.3297-2	3.3297-2	3.3297-2	3.3297-2	3.3297-2
CO2	0.0000	0.0000	4.0130-2	4.0130-2	4.0130-2	4.0130-2	4.0130-2	4.0130-2	4.0130-2

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-06 FOR ALL ASSIGNED CONDITIONS

STOP 5 IS NORMAL CHANNEL STOP

IT OCCURS WHEN XPOSITION EXCEEDS INPUTTED XXSTOP VALUE

**Sample Output 12, Channel Problem
With Fully Rate Controlled Chemistry
With Heat Loss
(7 Output Pages)**

1

REACTANTS

C 1.0000 S 2.0000 0.0000 0.0000 00 0.0000 0.44186
 AR 1.0000 0.0000 0.0000 0.0000 00 0.0000 0.10000E-05
 O 2.0000 0.0000 0.0000 0.0000 00 0.0000 0.55814

0.00 G 1000.000 0 F 0.00000
 0.00 G 1000.000 0 F 0.00000
 0.00 G 1000.000 0 F 0.00000

NAMELISTS

1

\$INPT2

KASE = 202,

T = 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 ,

P = 0.100000E-01, 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 ,

PSIA = F,

MMHG = F,

NSOM = F,

V = 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 ,

RHO = 0.100000E-01, 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 ,

ERATIO = F,

OXFL = F,

FPCT = F,

FA = F,

MIX = 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 ,
 0.000000 ,

TP = F,

HP = F,

SP = F,

TV = F,

UV = F,

SV = F,

RKT = T,

SHOCK = F,

DOWN = F,

OTTO = F,

CR = 0.000000 ,

SO = 0.000000000000

IO = T,

INDIC = 0,

TRACE = 0.100000E-06,

SIUNIT= F,
 DXI = 0.500000E-01,
 NITER = 0,
 NCTOP = 0,
 NEOL = F,
 BZ = 0.000000,
 XK = 0.650000,
 ACCURC= 0.100000E-02,
 HMIN = 0.100000E-29,
 ALPH = 0.000000,
 EXIN = 2400.00,
 TLOSTG= F,
 \$END
 LLMF =

C
 S
 AR
 O

NO INPT2 VALUE GIVEN FOR OF, EORAT, FA, OR FPCT
 SPECIES BEING CONSIDERED IN THIS SYSTEM

L 5/66	AR	L12/66	AR+	J 3/61	C(S)	J 3/61	C	L12/66	C+
J 9/65	C-	3/3/7	C3-	J 9/65	CO	J 3/61	COS	3/3/7	COS-
J 9/65	CO2	4/12/7	CO2-	3/3/7	CO3-	3/7/7	CO4-	J12/62	CS
3/3/7	CS-	J 6/61	CS2	J12/69	C2	J12/69	C2-	J 9/66	C2O
J12/69	C3	J 6/68	C3O2	J12/69	C4	J12/69	C5	L02/67	E
J 6/62	O	L12/66	O+	J 6/65	O-	J 9/65	O2	J12/66	O2-
J 6/61	O3	J12/65	S(S)	J12/65	S(L)	J 6/71	S	L12/66	S+
3/3/7	S-	J 6/71	SO	3/3/7	SO-	J 6/61	SO2	3/3/7	SO2-
J 9/65	SO3	3/3/7	SO3-	J12/65	S2	3/3/7	S2-	J6/64	S8
45	5	3	2	0	3	755			

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C
 S
 AR
 O
 E

\$RKTINP

EOL = T,
 FROZ = F,
 SUBAR = 0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
 0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
 0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
 SUPAP = 0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
 0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
 0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
 PCP = 0.100000E-01, 0.000000, 0.000000, 0.000000, 0.000000,
 0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
 0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
 0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
 0.000000, 0.000000, 0.000000, 0.000000, 0.000000,
 TCEST = 3000.00,
 NP = 1,
 NLOPT = 1,
 HTLOSS = 0.000000,
 HPAIH = T,
 SPATH = F,
 NUMMLS = 1,

```

CHNLEN= 1.000000 , 0.000000 , 0.000000 , 0.000000 ,
CHNHLS= -1204.90 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 ,
TCHINP= 1100.00 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 , 0.000000 , 0.000000 , 0.000000 ,
0.000000 ,
TCHFNL= 1100.00
IPRRKT= 1
$END
$OF = 0.200000

```

ENTHALPY (KG-MOL)(DEG K)/KG JKG-ATOMS/KG	EFFECTIVE FUEL HPP(2) BPP(I,2)	EFFECTIVE OXIDANT HPP(1) BPP(I,1)	MIXTURE HSUB0 R0(I)
C	0.15588345E 03	0.00000000E 00	0.15588345E 03
S	0.58033103E-02	0.00000000E 00	0.58033103E-02
AR	0.11606621E-01	0.00000000E 00	0.11606621E-01
O	0.25032541E-07	0.00000000E 00	0.25032541E-07
E	0.34885056E-01	0.00000000E 00	0.34885056E-01
	0.00000000E 00	0.00000000E 00	0.00000000E 00
DLIT SPEC= O2	CONCENTRATION(MOLES/KG)=	0.1744E-01 NO. 29	
DLIT SPEC= CS2	CONCENTRATION(MOLES/KG)=	0.5803E-02 NO. 17	
DLIT SO	CO	SO2	O2
DLIT COS	O	CS2	CS
DLIT S	CO2		

ELIMINATED THE FOLLOWING 4 ELEMENTS IN EQUILIBRIUM CALCULATION

3-193

REMOVED FOLLOWING SPECIES FROM CONSIDERATION

C
 S
 O
 E
 AR+
 C(S)
 C
 C+
 C-
 C3-
 COS-
 CO2-
 CO3-
 CO4-
 CS-
 C2
 C2-
 C2O
 C3
 C3O2
 C4
 C5
 E
 O+
 O-
 O2-
 O3
 S(S)

S(L)
S+
S-
SO-
SO2-
SO3
SO3-
S2
S2-
S3

1

NON-EQUILIBRIUM REACTIONS

1 1.0 SO + 1.0 O2 = 1.0 SO2 + 1.0 O
CHEMICAL RATE - 5.8000E-13*T** 0.0000*EXP(- 3.2500E 03/T)

2 1.0 COS + 1.0 O = 1.0 CO + 1.0 SO
CHEMICAL RATE - 3.1500E-11*T** 0.0000*EXP(- 2.2500E 03/T)

3 1.0 S + 1.0 O2 = 1.0 SO + 1.0 O
CHEMICAL RATE - 1.7000E-12*T** 0.0000*EXP(- 0.0000E-01/T)

4 1.0 CS2 + 1.0 O = 1.0 CS + 1.0 SO
CHEMICAL RATE - 8.3000E-11*T** 0.0000*EXP(- 9.5000E 02/T)

5 1.0 CS2 + 1.0 O2 = 1.0 SO2 + 1.0 CS
CHEMICAL RATE - 1.7000E-12*T** 0.0000*EXP(- 2.2000E 04/T)

6 1.0 CS + 1.0 O = 1.0 CO + 1.0 S
CHEMICAL RATE - 3.9900E-10*T** 0.0000*EXP(- 1.0000E 03/T)

7 1.0 CO + 1.0 O2 = 1.0 CO2 + 1.0 O
CHEMICAL RATE - 4.2000E-12*T** 0.0000*EXP(- 2.4000E 04/T)

3-194

$$9 \quad 1.0 \text{ CS} \quad + \quad 1.0 \text{ O2} \quad = \quad 1.0 \text{ COS} \quad + \quad 1.0 \text{ O}$$

$$\text{CHEMICAL RATE} - \quad 1.70000\text{E-11} * \text{T}^{**} \quad 0.00000 * \text{EXP}(- \quad 6.00000\text{E} \text{ 03/T})$$

```

NMPATH= 3
IMPRNT= 0
XXSTOP= 0.60200
UEINP= 1.00000
ITYPE= 1

```

DEPENDENT VARIABLE

1.000000

1.000000

```
***** KFLAG= -4
***** KFLAG= -4
***** KFLAG= -4
***** KFLAG= -4
***** KFLAG= -4
```

THEORETICAL MHD CORE PERFORMANCE

OPC = 0.1 PSIA
CASE NO. 202

3-195

CHEMICAL FORMULA		
FUEL	C	1.00000 S 2.00000
FUEL	AR	1.00000
FUEL	O	2.00000

O/F= 0.0000 PERCENT FUEL=100.0000 EQUIVALENCE RATIO= 0.9981 REACTANT DENSITY= 0.0000

[illegible]

IONIC DENS)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
SIGMA (MHO/M)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
W/O IONG	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
FREQ (1/SEC)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
MACH NUMBER	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
AE/AT		1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
TOTAL MOL WT	43.018	43.018	43.018	41.287	40.940	41.206	41.686	42.252	42.853	43.461	44.066	44.658	45.233				

MOLE FRACTIONS

AR	1.0769-6	1.0769-6	1.0769-6	1.0335-6	1.0248-6	1.0315-6	1.0435-6	1.0577-6	1.0727-6	1.0879-6	1.1031-6	1.1179-6	1.1323-6
----	----------	----------	----------	----------	----------	----------	----------	----------	----------	----------	----------	----------	----------

MOLE FRACTIONS OF NEOL SPECIES

SO	0.0000	0.0000	0.0000	4.302-11	1.628 -1	1.633 -1	1.612 -1	1.590 -1	1.566 -1	1.540 -1	1.512 -1	1.482 -1	1.451 -1	1.418 -1
CO	0.0000	0.0000	0.0000	4.302-11	2.351 -1	2.224 -1	2.100 -1	1.979 -1	1.863 -1	1.753 -1	1.648 -1	1.549 -1	1.455 -1	1.365 -1
SO2	0.0000	0.0000	0.0000	4.302-11	2.997 -1	2.928 -1	2.975 -1	3.057 -1	3.153 -1	3.256 -1	3.362 -1	3.471 -1	3.579 -1	3.687 -1
O2	7.5035-1	7.5035-1	7.5035-1	1.5284-1	1.3922-1	1.3028-1	1.2371-1	1.1840-1	1.1377-1	1.0953-1	1.0550-1	1.0158-1	9.7741-2	
COS	0.0000	0.0000	0.0000	4.302-11	1.686 -5	4.358 -6	2.042 -6	1.251 -6	8.755 -7	6.564 -7	5.097 -7	4.024 -7	3.195 -7	2.534 -7
O	0.0000	0.0000	0.0000	4.302-11	1.284 -1	1.480 -1	1.523 -1	1.505 -1	1.460 -1	1.402 -1	1.338 -1	1.273 -1	1.209 -1	1.147 -1
CS2	2.496 -1	2.496 -1	2.496 -1	6.432-10	1.880-10	1.893-10	1.915-10	1.941-10	1.968-10	1.996-10	2.024-10	2.051-10	2.078-10	
CS	0.0000	0.0000	0.0000	4.302-11	8.411 -7	1.708 -7	6.644 -8	3.518 -8	2.178 -8	1.461 -8	1.021 -8	7.269 -9	5.211 -9	3.730 -9
S	0.0000	0.0000	0.0000	4.302-11	1.671 -2	1.907 -2	1.947 -2	1.919 -2	1.859 -2	1.784 -2	1.701 -2	1.615 -2	1.530 -2	1.447 -2
CO2	0.0000	0.0000	0.0000	4.302-11	4.445 -3	1.519 -2	2.913 -2	4.402 -2	5.891 -2	7.342 -2	8.739 -2	1.008 -1	1.137 -1	1.260 -1

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-06 FOR ALL ASSIGNED CONDITIONS

1

961-8 *****OUTPUTS AT MAXIMUM TEMPERATURE*****
 *****TMAX= 3943. AT X= 0.13874E-01 VEL= 3.9574 MOLES/KG= 0.23337E-01

SPECIES	MOLE FRACTION
AR	0.10726E-05
SO	0.18362
CO	0.24722
SO2	0.30694
O2	0.19322
COS	0.36934E-03
O	0.61141E-01
CS2	0.23410E-07
CS	0.49501E-05
S	0.64099E-02
CO2	0.10760E-02

1

THEORETICAL MHD CORE PERFORMANCE

OPC = 0.1 PSIA
 CASE NO. 202

	CHEMICAL FORMULA
FUEL	C 1.00000 S 2.00000
FUEL	AR 1.00000
FUEL	O 2.00000

O/F= 0.0000	PERCENT FUEL=100.0000	EQUIVALENCE RATIO= 0.9981	REACTANT DENSITY= 0.0000
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WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
0.44186	37066.000	G	1000.00	0.0000
0.00000	3486.729	G	1000.00	0.0000
0.55814	5427.000	G	1000.00	0.0000

	CHAMBER	THROAT	0.550	0.600
PC/P	1.0000	1.0000	1.0000	1.0000
P, ATM	0.0100	0.0100	0.0100	0.0100
T, DEG K	1000	1000	2280	2242
RHO, G/CC	5.2426-6	5.2426-6	2.4473-6	2.5175-6
H, CAL/G	309.8	309.8	-330.8	-373.4
S, CAL/(G)(K)	1.6722	1.6722	1.8525	1.8354
M, MOL WT	43.018	43.018	45.790	46.324
(DLV/DLP)T	-1.00000	-1.00000	-1.00000	-1.00000
(DLV/DLT)P	1.0000	1.0000	1.0000	1.0000
CP, CAL/(G)(K)	0.2268	0.2268	0.2456	0.2455
GAMMA (S)	1.2557	1.2557	1.2147	1.2118
VELOCITY,M/SEC			2.14	2.08
TOTAL H(CAL/G)			-330.79	-373.40
MAG FLD(TESLA)			0.00	0.00
BETA			0.00	0.00
SON VEL,M/SEC	492.6	492.6	709.2	698.4
ELEC DENS	0.0000 0	0.0000 0	0.0000 0	0.0000 0
IONIC DENS)	0.0000 0	0.0000 0	0.0000 0	0.0000 0
SIGMA (MHO/M)	0.0000	0.0000	0.0000	0.0000
W/O IONS	0.0000	0.0000	0.0000	0.0000
FREQ (1/SEC)	0.0000 0	0.0000 0	0.0000 0	0.0000 0
MACH NUMBER	0.0000	0.0000	0.0030	0.0030
AE/AT		1.0000	1.0000	1.0000
TOTAL MOL WT	43.018	43.018	45.790	46.324

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MOLE FRACTIONS

AR	1.0769-6	1.0769-6	1.1462-6	1.1596-6
----	----------	----------	----------	----------

MOLE FRACTIONS OF NEQL SPECIES

SO	0.0000 0	0.0000 0	1.3354-1	1.3519-1
CO	0.0000 0	0.0000 0	1.2783-1	1.1952-1
SO2	0.0000 0	0.0000 0	3.7923-1	3.8952-1
O2	7.5035-1	7.5035-1	9.3932-2	9.0147-2
COS	0.0000 0	0.0000 0	1.9997-7	1.5638-7
O	0.0000 0	0.0000 0	1.0887-1	1.0335-1
CS2	2.496 -1	2.496 -1	2.103-10	2.128-10
S	0.0000 0	0.0000 0	1.3690-2	1.2953-2
CO2	0.0000 0	0.0000 0	1.3790-1	1.4931-1

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-06 FOR ALL ASSIGNED CONDITIONS

CS

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

STOP 5 IS NORMAL CHANNEL STOP

IT OCCURS WHEN XPOSITION EXCEEDS INPUTTED XXSTOP VALUE

4. TABLES

Table I - Files Required in PACKAGE Code

FORTTRAN LOGICAL UNIT (FILE)	INPUT OR OUTPUT	CONTENTS	COMMENTS
5	INPUT	Program Data	Equivalent to Cards on Most Systems
11	INPUT	Channel Inputs	
6	OUTPUT	Contains Program Outputs, Iteration Outputs, and IDEBUG Flagged outputs	Equivalent to Printer on Most Systems
1	OUTPUT	Contains DEBUG Output Requested by IMPRNT of CHNLIN Input and IPRRKT of RKTINP Input	
7	INPUT/ OUTPUT	Contains Thermodynamic Data Taken From the JANAF Tables	Equivalent to Punch on Most Systems

Table II - REACTANTS Cards

ORDER	CONTENTS	FORMAT	CARD COLUMNS
First	REACTANTS TWOSTG ^(a)	3A4, 3X, 2A4	1 to 9 and 16 to 22
Any	One card for each reactant species (Maximum 30). Each card contains: (1) Atomic symbols and formula numbers (maximum 5 sets) ^(b) (2) Relative weight ^(c) or number of moles (3) Blank if (2) is relative weight or M if (2) is number of moles (4) Enthalpy ^(b) (cal/mole) (5) State: S, L, or G for solid, liquid, or gas, respectively (6) Temperature associated with enthalpy in (4) (7) F if fuel or O if oxidant ^(d) (8) Density in g/cm ³ (Optional) ^(e)	5(A2.F7.5) F7.5 A1 F9.5 A1 F8.5 A1 F8.5	1 to 45 46 to 52 53 54 to 62 63 64 to 71 72 73 to 80
Last	Blank		

(a) TWOSTG is required when TWOSTG = TRUE in namelist INPT2

(b) Program will calculate the enthalpy (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.)

(c) 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. Furthermore, if this value is $\phi.\phi$, follow this card input with an additional input card in Format (10X, E11.3) containing the correct value. If $\phi.\phi$ is the correct value, leave the second card blank.

(d) IF NEQPT = 1 REACTANTS must be designated either all F or all O.

(e) When TWOSTG = TRUE, DENS is fraction of the reactant which is added to the second stage.

TABLE III -- Variables in INPT2 NAMELIST

VARIABLE	DIMEN- SION	TYPE	VALUE BEFORE READ	DEFINITION AND COMMENTS
KASE	1	I	0	Optional assigned number associated with Problem Run
T	26	R	0.0	(a)Assigned Temperatures (Deg Kelvin)
P	26	R	0.0	(a)Assigned pressures; chamber pressures for rocket and channel problems; values in atm unless PSIA, NSQM or MMHG
NSQM	1	L	False	(b)Values in P array are in N/m^2
PSIA	1	L	False	(b)Values in P array are in psia units
MMHG	1	L	False	(b)Values in P array are in mmHg units
V	26	R	0	Volume, cm^3/g Not Used
RHO	26	R	0	Density, g/cm^3 Not Used
MIX	15	R	0	(a)Values of equivalence ratios if ERATIO = T: oxidant to fuel weight ratio if ERATIO = F; percent fuel by weight if FPCT = T: and fuel to air weight ratio if FA = T
ERATIO	1	L	False	(b)Equivalence ratios are given in MIX
OXFL	1	L	False	Not Used
FPCT	1	L	False	Percent fuel by weight are given in (b)MIX
FA	1	L	False	Fuel to air weight ratios are given in (b)MIX
TRACE	1	R	False	Option to print mole fractions TRACE in special E-format
TP	1	L	False	(b)Assigned temperature and pressure problem
HP	1	L	False	(b)Assigned enthalpy and pressure problem
(a) For channel problems, only a single value is allowed.				
(b) If variable is set to true.				

Table III (Cont'd)

VARIABLE	DIMEN- SION	TYPE	VALUE BEFORE READ	DEFINITION AND COMMENTS
SP	1	L	False	^(a) Assigned entropy ($S\phi$) and pressure problem
TV	1	L	False	Not used (volume can not be assigned)
SV	1	L	False	Not Used
UV	1	L	False	Not Used
SHOCK	1	L	False	Not Used
DETN	1	L	False	Not Used
OTTO	1	L	False	Not Used
$S\phi$	1	R*8	0.0	Assigned entropy cal/(g - K)
SIUNIT	1	L	False	^(a) International Units
NITER	1	I	0	Not Used
NSTOP	1	I	0	Not Used
NEQL	1	L	False	Not Used
EXIN	1	R	2400.0	Maximum axial electric field, V/m. Used as a criterion to change BZ for MHD calculations in the channel
CR	1	R	0.0	Not Used
TWOSTG	1	L	False	^(a) Indicates a two stage combustor
IONS	1	L	False	^(a) Consider ionic species and output results
IDDEBUG	1	I	0	Print intermediate output for all points indexed by this integer value
RKT	1	L	False	^(a) Channel problem
BZ	1	R	0.0	Magnetic field (TESLA) for an MHD problem
XK	1	R	0.0	Load factor for an MHD problem
DXI	1	R	0.05	Print increment for channel problems (Meters)
ACCURC	1	R	0.001	Relative accuracy obtained each integration step for channel problems
HMIN	1	R	1.0×10^{-15}	Smallest stepsize used to obtain the desired accuracy before aborting the program (for channel problems)

^(a)If variable is set to true

Table IV - Variables in RKTINP NAMELIST

VARIABLE	DIMEN- SION	Type	VALUE BEFORE READ	DEFINITIONS AND COMMENTS
EQL	1	L	True	Calculate channel performance assuming equilibrium composition (always true)
FROZ	1	L	False	Not Used
PCP	26	R	0	(a) Ratio of chamber pressure to exit pressure; list should not include values for the chamber and throat; storage allows for 26 values
NFZ	1	I	1	Not Used
SUBAR	13	R	0	(a) Subsonic area ratios
SUPAR	13	R	0	(a) Supersonic area ratios
TCEST	1	R	3000.0	Initial temperature estimate
NEQPT	1	I	100000	First station where finite rate chemistry applies
HTLOSS	1	R	0.0	Combustor heat loss (cal/g)
HPATH	1	L	False	After throat calculations set HP = HPATH
SPATH	1	L	True	After throat calculations set SP = SPATH
NUMHLS	1	I	0	Must be set to 1 when CHNHLS is used
CHNLEN	1	R	1.0	Characteristic length (meters)
CHNHLS	10	R	0.0	Assigned mixture enthalpy at the wall temperature in (cal/g)
TCHINP	10	R	0.0	Analogous to TCHFNL
TCHFNL	1	R	0.0	Wall temperature for which CHNHLS is assigned. Also used as minimum temperature to stop channel calculations
IPRRKT	1	I	0	Get extra debug output if greater than 0
(a) For channel problems, only a single value is allowed.				

Table V - DEBUG Output Generated by RKTINP Namelist Input IPRRKT

OUTPUT FROM SUBROUTINE	VALUE OF IPRRKT	NO. OUTPUTS	DBG OUTPUT NO.	VARIABLES (AND FORMAT IF NOT FROM DBGOUT)
ROCKET	0	2	--	CHCALC (F12.3) TCHFNL (F10.3) } These Variables described in Namelist RKTINP
ROCKET	0	4	--	HSUB0 HTLOSS (F10.3) HPATH (I2) } 0 if False or SPATH (I2) } 1 if True
MHD	0	4	--	"IN MHD" NPT (I3) PPP(NPT) (F10.3) SSUM(NPT) (F10.3) UE (F10.3) } Written on first call to MHD only
MHD	0	2	--	
ROCKET	1	No. of Chemical Elements	10	Each output is $\frac{B0(I) - B0N(I)}{B0(I)}$ for I = 1, ... No. of Elements This output results when NEQPT = 1
EQLBRM	1	4	6	1., CPSUM, ENNEMM, GAMMAS(NPT) Written when GAMMAS(NPT) ≤ 1. and FLAGED by C ... GROK1
EQLBRM	1	7	7	0.0, IQ1, NPT, X(IQ1), ENN, EMM, DLVPT(NPT) Written when DLVPT(NPT) ≥ 0. and FLAGED by C ... GROK0
EQLBRM	1	3	8	2., DLVPT(NPT), GAMMAS(NPT) Written when GAMMAS(NPT) ≤ 1. and FLAGED by C ... GROK2
EQLBRM	1	7	9	3., DLVPT(NPT), DLVTP(NPT), ENN, EMM, CPR(NPT), GAMMAS(NPT) Written when GAMMAS(NPT) ≤ 1. and FLAGED by C ... GROK3

Table V (Cont'd)

OUTPUT FROM SUBROUTINE	VALUE OF IPRRKT	NO. OUTPUTS	DBG OUTPUT NO.	VARIABLES (AND FORMAT IF NOT FROM DBGOUT)
ROCKET	2	NSK	11	LIST OF REORDERED SPECIES WHEN NEQPT=1
ROCKET	2	6	12	NSOLD, NS, NSKOLD, NSK, NLMOLD, NLM Printed When NEQPT=1
ROCKET	2	8	13	ENN, EMM, ENNL, ENDNW(1), ENDNW(2), EN(1,1), ENLN(1), SUMN Printed When NEQPT=1
ROCKET	2	NSK	14	(S(J)-H ϕ (J)) FOR J=1, NSK Printed When NEQPT=1
EQLBRM	2	No. Equations Plus 2	--	NPT, $\underbrace{(X(IL), IL=1, LE)}_{\text{PI's (Lagrange multipliers)}}$, TN
EQLBRM	2	3	--	"***** WARNING . . JLTQ =" (I4) "TT AND TBOT =" (G12.4, G12.4)
EQLBRM	3	3	--	NPT (I5) ITN (I5) NUMB (I5) } Written after basic convergence
EQLBRM	3	3	--	NPT (I5) KKKK (I5) NUMB (I5) } Condensed species added after basic convergence, try again. KKKK gives indicator of flow path
SETEQU	4	4	--	CHAN. LOSS = CHLOSS (G12.4) PASS = CHCALC (G12.4) LEN = CHNLEN (G12.4) HEAT = CHHEAT (G12.4) } Written only when there is heat loss in the channel

Table VI - Variables in CHNLIN Namelist

VARIABLE	DIMENSION	TYPE	VALUE BEFORE READ	DEFINITION AND COMMENTS
NMPATH	1	I	0	Channel profile which describes type of channel calculations (See Table VII)
IMPRNT	1	I	0	Debug output level described by Table VIII
XXSTOP	1	R	0.0	Axial stop position in the channel (meters)
UEINP	1	R	0.0	Initialize channel velocity. If this value is non-zero UEINP will override all other initial velocity calculations
ITYPE	1	I	0	ITYPE = 1 for MHD channel problems with a simple wall heat loss. ITYPE = 999 (or negative number) to set the force (FFF) and heat (QQQ) terms to 0.0. ITYPE = 0 defaults to ITYPE = 1

Table VII - Channel Profiles

NMPATH (Model Number)	INPUT VARIABLE	DIFFERENTIAL EQUATIONS- TO-SOLVE FOR
± 1	U	dP/dx and dH/dx for P and H
± 2	P	dU/dx and dH/dx for U and H
± 3	A	dP/dx , dU/dx , and dH/dx for P, U, and H
0	None	dP/dx and dH/dx for P and H

Model Number 0 assumes a constant velocity in the channel, which is equal to the channel entrance velocity. Negative values will generate a constant profile equal to the appropriate channel entrance parameter value. The following is a description of the terms used in the table.

P = channel pressure (atm)
 U = channel velocity (m/sec)
 H = channel enthalpy (J/kg)
 A = channel area ratio
 X = axial channel position with respect to the entrance (meters)

Table VIII - DEBUG Output Generated by CHNLIN Namelist Input IMPRNT

OUTPUT FROM SUBROUTINE	VALUE OF IMPRNT	NO. OUTPUTS	DBG OUTPUT NO.	VARIABLES (AND FORMAT IF NOT FROM DBGOUT)																								
MHD	0	4	--	"IN MHD" NPTM1 (I3) PPP(NPTM1) (F10.3) SSUM(NPTM1) (F10.3) UE (F10.3)																								
MHD	0	4	--	NMPATH (I3) XINDP(1) (F10.4) DUMMIN(1) (F10.4) PSLOPE (F10.4) } Written when user wishes to solve for conditions at the channel entrance																								
MHD	0	2	--	"REMOVE" (I3) "EQU VALUE=" (G13.5) Printed when the solution of a finite rate equation approaches zero downstream in the channel. The derivatives of this equation is subsequently set to zero.																								
MHD	0	5	--	"MHD FROM DIF" PP (F8.3) S0 (F8.3) UE (F8.3) ARINT (F8.3) HSUB0 (F8.3)																								
MHD	0	1 + ITE Where ITE= No. of Channel differential equations	--	NE, XMAX, ERROR FROM GEARS METHOD (I2) <table><tr><td><u>K</u></td><td><u>NE</u></td><td><u>XMAX</u></td><td><u>ERROR</u></td></tr><tr><td>1</td><td>'</td><td>'</td><td>'</td></tr><tr><td>'</td><td>'</td><td>'</td><td>'</td></tr><tr><td>'</td><td>'</td><td>'</td><td>'</td></tr><tr><td>'</td><td>'</td><td>'</td><td>'</td></tr><tr><td>ITE</td><td>'</td><td>'</td><td>'</td></tr></table> This message occurs when subroutine DIFSUB exhibits difficulties with the integration	<u>K</u>	<u>NE</u>	<u>XMAX</u>	<u>ERROR</u>	1	'	'	'	'	'	'	'	'	'	'	'	'	'	'	'	ITE	'	'	'
<u>K</u>	<u>NE</u>	<u>XMAX</u>	<u>ERROR</u>																									
1	'	'	'																									
'	'	'	'																									
'	'	'	'																									
'	'	'	'																									
ITE	'	'	'																									
DIFFUN	0	CHANNEL INPUT POINTS	--	INPUTS ARE FOR PATH (NMPATH) XINDP(K), VELIN(K) OR PRESIN(K) OR AREAIN(K) FOR K=1, NUMINV WHERE THE SECOND VECTOR DEPENDS ON THE VALUE OF NMPATH																								
GAUSS	0	IMAT	1	COEFX vector will be printed if a singularity occurs																								

Table VIII (Cont'd)

OUTPUT FROM SUBROUTINE	VALUE OF IMPRNT	NO. OF OUTPUTS	DBG OUTPUT NO.	VARIABLES (AND FORMAT IF NOT FROM DBGOUT)
EQLBRM	0	2* NO. OF ITERATIONS	2	X(IQ1) FOR K=1, ITN AMBDA FOR K=1, ITN
				Output after message "ITN ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREMENTS FOR THE POINT N"
EQLBRM	0	25+NLM	3	J, NPT, EN(NPT, J), TRACE, AMBDA, AMBDA1, SUM, SUM1, AA, TEM, TMELT FOR CONDENSED SPECIES FOR WHICH IAFLG=1 OR GARBAGE, UE, NLM, TSUM, EN(NPT, 1), EMM, ENN, IQ1, X(IQ1), DLNT, ENL, TT, TEMP0, TEMP1, NS, B0(I), FOR I=1, NLM. THE OUTPUT FOLLOWS PREVIOUS OUTPUT LISTED ABOVE.
MHD	1	4	--	TMAX= (G13.4) AT X= (G13.5) VEL= (G13.5) MOLE /KG= (G13.5)
				Outputted only when NEQPT=1
MHD	1	6	16	XN, XXSTOP, NEQPT, TTT(NPT), TMPSTP, KSAV outputted with normal STOP 5
DIFFUN	1	6	17	NMPATH (I3) XREG0 (F10.7) PPINT (F10.3) UE (F13.5) ARINT (F10.4) DINT (F10.2)
MHD	1	5	--	CHANNEL INPUTS NMPATH = (I3) IMPRNT = (I3) XXSTOP = (G13.5) UEINP = (G13.5) ITYPE = (I3)

Table VIII (Cont'd)

OUTPUT FROM SUBROUTINE	VALUE OF IMPRNT	NO. OUTPUTS	DBG OUTPUT NO.	VARIABLES (AND FORMAT IF NOT FROM DBGOUT)																	
MHD	2	2	--	'***, ... , *IPP=(I4) NEQPT=(I6)																	
MHD	2	4	--	'X0,XL,XN,XH' ALL IN (F8.5) BEFORE AND AFTER CALL TO DIFSUB																	
DIFFUN	2	8	--	<table><tr><td>K</td><td>(I3)</td><td rowspan="8">} One output for each reaction (if finite rate chemistry applies) where: ENR = (TSAV2-ENP*AKB)*AKF*((1.0-6 XAVN)**(RPOW-1.)) This output occurs upon entry into DIFFUN, for a new calculation point.</td></tr><tr><td>AKF</td><td>(G13.5)</td></tr><tr><td>AKB</td><td>(G13.5)</td></tr><tr><td>ENP</td><td>(G13.5)</td></tr><tr><td>TSAV2</td><td>(G13.5)</td></tr><tr><td>POW</td><td>(F9.5)</td></tr><tr><td>RPOW</td><td>(F9.5)</td></tr><tr><td>ENR</td><td>(G13.5)</td></tr></table>	K	(I3)	} One output for each reaction (if finite rate chemistry applies) where: ENR = (TSAV2-ENP*AKB)*AKF*((1.0-6 XAVN)**(RPOW-1.)) This output occurs upon entry into DIFFUN, for a new calculation point.	AKF	(G13.5)	AKB	(G13.5)	ENP	(G13.5)	TSAV2	(G13.5)	POW	(F9.5)	RPOW	(F9.5)	ENR	(G13.5)
K	(I3)	} One output for each reaction (if finite rate chemistry applies) where: ENR = (TSAV2-ENP*AKB)*AKF*((1.0-6 XAVN)**(RPOW-1.)) This output occurs upon entry into DIFFUN, for a new calculation point.																			
AKF	(G13.5)																				
AKB	(G13.5)																				
ENP	(G13.5)																				
TSAV2	(G13.5)																				
POW	(F9.5)																				
RPOW	(F9.5)																				
ENR	(G13.5)																				
DIFFUN	2	2	--	DIFFUN - X = , 1PE13.4 AVN/VLMI = , 1PE13.4 This output occurs upon entry into DIFFUN, for a new calculation point																	
MHD	3	12	15	NOMIT, NE(1, NOMIT) OR NE(1, 1) WHEN NOMIT=0, DUMMIN(1), ITE1, NE(1, ITE1), ITE2, NE(1, ITE2), ITE, ATEST, VARC, NJ1, ICASEC																	
DIFFUN	3	4	--	<table><tr><td>I</td><td>(I3)</td><td rowspan="4">} Written when there are rate equations (IPP ≥ NEQPT)</td></tr><tr><td>ENM</td><td>(G13.5)</td></tr><tr><td>TTT</td><td>(G13.5)</td></tr><tr><td>UE</td><td>(G13.5)</td></tr></table>	I	(I3)	} Written when there are rate equations (IPP ≥ NEQPT)	ENM	(G13.5)	TTT	(G13.5)	UE	(G13.5)								
I	(I3)	} Written when there are rate equations (IPP ≥ NEQPT)																			
ENM	(G13.5)																				
TTT	(G13.5)																				
UE	(G13.5)																				
DIFFUN	3	4	--	<table><tr><td>TSAV4</td><td>(G11.3)</td><td rowspan="4">} Nonequilibrium Finite Rate Contribution when Area Given</td></tr><tr><td>SAVEL</td><td>(G11.3)</td></tr><tr><td>SAVEH</td><td>(G11.3)</td></tr><tr><td>TTT</td><td>(G11.3)</td></tr></table>	TSAV4	(G11.3)	} Nonequilibrium Finite Rate Contribution when Area Given	SAVEL	(G11.3)	SAVEH	(G11.3)	TTT	(G11.3)								
TSAV4	(G11.3)	} Nonequilibrium Finite Rate Contribution when Area Given																			
SAVEL	(G11.3)																				
SAVEH	(G11.3)																				
TTT	(G11.3)																				
DIFFUN	3	4	--	<table><tr><td>BNEW</td><td>(G13.5)</td><td rowspan="4">} Nonequilibrium Finite Rate Contribution When Area Given</td></tr><tr><td>A11</td><td>(G13.5)</td></tr><tr><td>B11</td><td>(G13.5)</td></tr><tr><td>SAVELL</td><td>(G13.5)</td></tr></table>	BNEW	(G13.5)	} Nonequilibrium Finite Rate Contribution When Area Given	A11	(G13.5)	B11	(G13.5)	SAVELL	(G13.5)								
BNEW	(G13.5)	} Nonequilibrium Finite Rate Contribution When Area Given																			
A11	(G13.5)																				
B11	(G13.5)																				
SAVELL	(G13.5)																				

Table VIII (Cont'd)

OUTPUT FROM SUBROUTINE	VALUE OF IMPRNT	NO. OUTPUTS	DBG OUTPUT NO.	VARIABLES (AND FORMAT IF NOT FROM DBGOUT)
EQLBRM	3	6	--	(I3), SOLUTION SPECIES $\frac{1}{1}$ SUM2 SUMM H ϕ (J) S(J) TEST : : : : : : : : : : : : NSOL
EQLBRM	3	2	--	"MOMIT=" (I3) "DELTAB=" (G12.3) } Written when there are rate equations (IPP $\geq$ NEQPT)
EQLBRM	3	5	--	SMALB (G11.3) BIGB (G11.3) TSAV2 (G11.3) TSAV3 (G11.3) SIZE (G11.3) } Written when there are rate equations (IPP $\geq$ NEQPT)
EQLBRM	3	5	--	ENL (G11.3) ENN (G11.3) ENLS (G11.3) ENNS (G11.3) SIZE (G11.3) } Written when solution exists
SETEQU	4	4	--	X (F10.7) EXNEW (G13.5) BZ (G13.5) BETA (G13.5) } Written for Channel Problems When EXIN $\neq \emptyset$
EQLBRM	4	5	4	NLM, ENN, EMM, B ϕ (1), A(1, 1) Written when NEQPT=1
DIFFUN	9	6	23	NOMIT, NJ1, NOMSAV, NS, NSK, NSK1
DIFFUN	9	7	20	K, GSUM, ENP, TSAV2, TSAV1, TSAV3, TSAV5 Written when there is rate equations

Table VIII (Cont'd)

OUTPUT FROM SUBROUTINE	VALUE OF IMPRNT	NO. OUTPUTS	DBG OUTPUT NO.	VARIABLES (AND FORMAT IF NOT FROM DBGOUT)
DIFFUN	10X ^(a)	7	18	K, AX, NX, H0(NX), S(NX), GSUM, TT Written when there are rate equations (forward react.)
DIFFUN	10X ^(a)	7	19	-K, AX, NX, H0(NX), S(NX), GSUM, TT Written when there are rate equations (backward react.)
DIFFUN	10X ^(a)	51 +2* No. of Non- Eqlib. Equa- tions	21	N(1,1), SAVEL, SAVEH, ENM, AKF, AKB, ENP, SUM, UE, ENR, EMM, POW, RPOW, GSUM, AVN, XJY(I), TTT(I), EEN(1) THRU EEN(12), ENR OF REACTIONS 1 THRU 8, NOMIT, NS, NSK, EN(I, NSK1), VLMI, I, ENN, RR, R, TLN, CPSUM, S0, HSUB0, PP, EN(I, J) FOR J=NS1 to NSK, B0N(K) FOR K=1 to NOMIT Written when there are rate equations
DIFFUN	10X ^(a)	25*NJ1	22	L, AR(L, J), AP(L, J), NJR(L, J), NJP(L, J), MAR(L, J), MAP(L, J) FOR L=1, NJ1 AND J=1, 4 Written when there are rate equations
EQLBRM	10X ^(a)	11	5	TLN, AMBDA, DLNT, TT, TMELT, VLM(NPT), PP, NPT, ENN, EMM, SUMN
^(a) DIFFUN will change IMPRNT to IMPRNT-100 after the last set of this IMPRNT level is output. The new value = X.				

Table IX - Sample of Intermediate Output, Iteration Details

ITERATION		MATRIX							
0.775000E-01		0.375000E-01	0.375000E-01	0.175000E-01	0.525000E-01	0.748120E+00	-0.147251E+01		
0.375000E-01		0.272500E+00	0.475000E-01	0.500000E-02	0.825000E-01	0.960424E+00	-0.253541E+01		
0.375000E-01		0.175000E-01	0.750000E+00	0.625000E-01	0.110000E+00	0.225254E+01	-7.279447E+01		
0.175000E-01		0.500000E-02	0.625000E-01	0.180000E+00	0.700000E-01	-0.432496E+01	-7.360210E+01		
0.525000E-01		0.425000E-01	0.110000E+00	0.700000E-01	0.	0.129548E+01	-0.242170E+01		
0.748120E+00		0.960424E+00	0.225254E+01	-0.432496E-01	0.129548E+01	0.320091E+02	-0.220377E+02		
PI		A	M	C	F				
-0.114557E+02		-0.830788E+01	-0.670914E+01	-0.163577E+02	0.224937E+02	0.270547E+00			
T= 0.38001033E+04 LN= 0.05599999E+00 FNML=-0.23025851E+01 PP= 0.10000000E+03 LN P/N= 0.69077552E+01 AMPL= 0.245E+00									
		NJ		LN NJ		DEL LN NJ		HJ/RT	
C151		0.	0.	0.	0.	0.106756E-15	0.255670E+01	0.682244E+01	0.427214E+01
C1		0.250000E-02	-0.599146E+01	-0.192088E+00	0.249787E+02	0.249787E+02	0.249787E+02	0.249787E+02	0.445525E+01
C2		0.250000E-02	-0.599146E+01	0.375930E+01	0.121579E+02	0.363812E+02	0.363812E+02	0.363812E+02	0.242237E+02
C3		0.250000E-02	-0.599146E+01	0.457011E+01	0.424252E+00	0.449905E+02	0.449905E+02	0.449905E+02	0.445663E+02
C4		0.250000E-02	-0.599146E+01	0.226660E+01	-0.619178E+01	0.542188E+02	0.542188E+02	0.542188E+02	0.604101E+02
C5		0.250000E-02	-0.599146E+01	0.724818E+00	0.182767E+02	0.602191E+02	0.602191E+02	0.602191E+02	0.744954E+02
C6		0.250000E-02	-0.599146E+01	0.658594E+01	0.229680E+02	0.375235E+02	0.375235E+02	0.375235E+02	0.955544E+02
C7		0.250000E-02	-0.599146E+01	-0.877760E+00	0.182133E+02	0.364246E+02	0.364246E+02	0.364246E+02	0.182109E+02
C8		0.250000E-02	-0.599146E+01	0.489988E+00	0.122663E+02	0.417569E+02	0.417569E+02	0.417569E+02	0.294975E+02
C9		0.250000E-02	-0.599146E+01	-0.144617E+01	0.726030E+01	0.464770E+02	0.464770E+02	0.464770E+02	0.372167E+02
C10		0.250000E-02	-0.599146E+01	0.296569E+01	0.179497E+02	0.349345E+02	0.349345E+02	0.349345E+02	0.169847E+02
C11		0.250000E-02	-0.599146E+01	-0.423552E+01	0.248664E+02	0.442984E+02	0.442984E+02	0.442984E+02	0.194322E+02
C12		0.250000E-02	-0.599146E+01	-0.913843E+00	0.308414E+02	0.356863E+02	0.356863E+02	0.356863E+02	0.484694E+01
C13		0.250000E-02	-0.599146E+01	-0.993611E+00	0.978809E+01	0.529665E+02	0.529665E+02	0.529665E+02	0.431744E+02
C14		0.250000E-02	-0.599146E+01	-0.287405E+01	-0.707585E+01	0.716010E+02	0.716010E+02	0.716010E+02	0.786068E+02
C15		0.250000E-02	-0.599146E+01	0.266689E+01	0.214493E+02	0.407704E+02	0.407704E+02	0.407704E+02	0.193011E+02
C16		0.250000E-02	-0.599146E+01	0.200451E+01	0.127050E+02	0.500426E+02	0.500426E+02	0.500426E+02	0.373375E+02
C17		0.250000E-02	-0.599146E+01	0.304606E+01	0.158335E+02	0.453164E+02	0.453164E+02	0.453164E+02	0.294829E+02
C18		0.250000E-02	-0.599146E+01	-0.276457E+01	0.138135E+02	0.546480E+02	0.546480E+02	0.546480E+02	0.403456E+02
C19		0.250000E-02	-0.599146E+01	0.204201E+01	0.242775E+02	0.453558E+02	0.453558E+02	0.453558E+02	0.210783E+02
C20		0.250000E-02	-0.599146E+01	0.126559E+01	0.187255E+02	0.570291E+02	0.570291E+02	0.570291E+02	0.333033E+02
C21		0.250000E-02	-0.599146E+01	-0.131610E+01	0.314394E+02	0.424314E+02	0.424314E+02	0.424314E+02	0.109921E+02
C22		0.250000E-02	-0.599146E+01	-0.626311E+01	0.396707E+02	0.501980E+02	0.501980E+02	0.501980E+02	0.105273E+02
C23		0.250000E-02	-0.599146E+01	-0.713524E+01	0.424475E+02	0.580569E+02	0.580569E+02	0.580569E+02	0.156144E+02
C24		0.250000E-02	-0.599146E+01	0.507517E+01	0.403716E+01	0.756477E+02	0.756477E+02	0.756477E+02	0.209106E+02
C25		0.250000E-02	-0.599146E+01	0.303237E+01	0.754770E+01	0.438271E+02	0.438271E+02	0.438271E+02	0.362299E+02
C26		0.250000E-02	-0.599146E+01	-0.855432E+00	0.425524E+02	0.356504E+02	0.356504E+02	0.356504E+02	0.311951E+02
C27		0.250000E-02	-0.599146E+01	0.443924E+01	0.920306E+01	0.201468E+02	0.201468E+02	0.201468E+02	0.109437E+02
C28		0.250000E-02	-0.599146E+01	0.487249E+01	0.104405E+02	0.397061E+02	0.397061E+02	0.397061E+02	0.294566E+02
C29		0.250000E-02	-0.599146E+01	0.881067E+01	-0.450616E+01	0.305838E+02	0.305838E+02	0.305838E+02	0.344994E+02
C30		0.250000E-02	-0.599146E+01	0.541631E+01	0.376914E+01	0.254679E+02	0.254679E+02	0.254679E+02	0.214997E+02
C31		0.250000E-02	-0.599146E+01	0.140463E+01	0.172759E+02	0.248027E+02	0.248027E+02	0.248027E+02	0.752623E+01
C32		0.250000E-02	-0.599146E+01	-0.487857E+00	0.120067E+02	0.368143E+02	0.368143E+02	0.368143E+02	0.244076E+02
C33		0.250000E-02	-0.599146E+01	-0.409316E+01	0.754265E+01	0.463644E+02	0.463644E+02	0.463644E+02	0.388217E+02
C34		0.250000E-02	-0.599146E+01	0.103071E+02	0.465937E+01	0.543509E+02	0.543509E+02	0.543509E+02	0.496915E+02
C35		0.250000E-02	-0.599146E+01	0.614820E+00	0.145489E+02	0.317362E+02	0.317362E+02	0.317362E+02	0.171673E+02
C36		0.250000E-02	-0.599146E+01	0.273295E+00	0.107633E+02	0.368825E+02	0.368825E+02	0.368825E+02	0.261192E+02
C37		0.250000E-02	-0.599146E+01	-0.566411E+00	0.612052E+01	0.410080E+02	0.410080E+02	0.410080E+02	0.348874E+02
C38		0.250000E-02	-0.599146E+01	0.663143E+01	0.387959E+01	0.331472E+02	0.331472E+02	0.331472E+02	0.292676E+02
C39		0.250000E-02	-0.599146E+01	-0.519863E+00	0.202300E+02	0.446320E+02	0.446320E+02	0.446320E+02	0.244022E+02
C40		0.250000E-02	-0.599146E+01	-0.100827E+02	0.153115E+02	0.580936E+02	0.580936E+02	0.580936E+02	0.426922E+02
T DEPT. MATRIX									
0.255266E-01		0.666043E-03	0.199388E-02	0.865496E-04	0.136700E-01	0.715742E-01	0.		
0.666043E-03		0.384154E-01	0.189197E-02	0.320738E-01	0.368480E-01	-0.678687E-01	0.		
0.199388E-02		0.184197E-02	0.696977E-02	0.175341E-02	0.475402E-02	0.717455E-01	0.		
0.865496E-04		0.320738E-01	0.175341E-02	0.382665E-01	0.375972E-01	-0.789308E-01	0.		
0.136700E-01		0.368480E-01	0.475402E-02	0.375972E-01	0.	0.285781E-02	0.		
PI		A	M	C	F				
0.227109E+01		-0.412088E+00	0.105453E+02	-0.167927E+01	-0.531033E+01				
P DEPT. MATRIX									
0.256769E-01		0.666043E-03	0.199388E-02	0.865496E-04	0.136700E-01	0.136700E-01	0.		
0.666043E-03		0.384154E-01	0.189197E-02	0.320738E-01	0.368480E-01	0.368480E-01	0.		
0.199388E-02		0.184197E-02	0.696977E-02	0.175341E-02	0.475402E-02	0.475402E-02	0.		
0.865496E-04		0.320738E-01	0.175341E-02	0.382665E-01	0.375972E-01	0.375972E-01	0.		
0.136700E-01		0.368480E-01	0.475402E-02	0.375972E-01	0.	0.484072E-01	0.		
PI		A	M	C	F				
0.515006E+00		0.441740E+00	0.279995E+00	0.631931E+00	-0.342684E+01				
PCINT= 1 P= 0.100000E+03 T= 0.453457E+04 M/R= 0.129590E+02 S/R= 0.136009E+01									
PH= 0.206581E+02 CP/R= 0.636139E+00 DLVPI=-0.103427E+01 DLVTP= 0.153303E+01 GAMMA(S)= 0.116000E+01 W= 0.15017E+03									

Table X - Intermediate Output, Test for Condensed Phases

AL(S)	300.000	933.000	IUSE=	-1	0.
GO-SUM(AIJ*PII)	= 0.7170131E+02				MAX NEG DELTA G = 0.
AL(L)	933.000	3000.000	IUSE=	-1	0.
ALCL3(S)	300.000	465.700	IUSE=	-2	0.
ALCL3(L)	465.700	3000.000	IUSE=	-2	0.
GO-SUM(AIJ*PII)	= 0.3783759E+02				MAX NEG DELTA G = 0.
AL4(S)	300.000	3000.000	IUSE=	-3	0.
GO-SUM(AIJ*PII)	= 0.3137253E+02				MAX NEG DELTA G = 0.
AL203(S)	300.000	2315.000	IUSE=	4	0.1657809E-02
AL203(L)	2315.000	3000.000	IUSE=	-4	0.
C(S)	300.000	3000.000	IUSE=	-5	0.
GO-SUM(AIJ*PII)	= -0.1317053E+01				MAX NEG DELTA G = 0.
M20(S)	200.000	273.150	IUSE=	-6	0.
M20(L)	273.150	373.150	IUSE=	-6	0.
M3(S)	300.000	922.000	IUSE=	-7	0.
GO-SUM(AIJ*PII)	= 0.4137586E+02				MAX NEG DELTA G = -0.1317053E+01
M3(L)	922.000	3000.000	IUSE=	-7	0.
MGCL2(S)	300.000	387.000	IUSE=	-8	0.
GO-SUM(AIJ*PII)	= -0.1033547E+02				MAX NEG DELTA G = -0.1317053E+01
MGCL2(L)	387.000	3000.000	IUSE=	-8	0.
MGO(S)	300.000	3098.000	IUSE=	-9	0.
GO-SUM(AIJ*PII)	= -0.1368991E+02				MAX NEG DELTA G = -0.1033547E+02
MGO(L)	3098.000	3000.000	IUSE=	-9	0.
S(S)	300.000	388.360	IUSE=	-10	0.
S(L)	388.360	2000.000	IUSE=	-10	0.
GO-SUM(AIJ*PII)	= 0.1291119E+02				MAX NEG DELTA G = -0.1368991E+02

Table XI - Storage Requirement Per Variable

VARIABLE	EQUATION CALCULATING STORAGE	CURRENT VALUES	AMNT. OF K BYTES STORAGE (when var. = 1)	CURRENT K BYTES NEEDED
NSPCMX (No. Species)	$(31 \cdot 8 + 9 \cdot 4 + \text{NELMX} \cdot 4) \cdot \text{NSPCMX}$	NELMX = 30 (No. of Elem.) NSPCMX = 300 (No. of Species)	0.404K	121.2K
NCMAX (No. Condens. Species)	$8 \cdot \text{NCMAX}$	NCMAX = 175 (No. of Cond.)	0.008K	1.4K
NELMX (No. Elements)	$(16 + 4 \cdot \text{NSPCMX}) \cdot \text{NELMX}$	NSPCMX = 300 NELMX = 30	6.0K	40.8K
NUMIV (No. Channel Inputs)	$16 \cdot \text{NUMIV}$	NUMIV = 90	0.002K	1.44K
Total			6.414K	* 165.44K
<p>*NOTE, the A(NELMX, NSPCMX) term was represented twice in the above equations. Its total of 36K should be subtracted from the grand total.</p>				

**Table XII. Cross Reference of Input Description
and Examples**

INPUT TYPE	DESCRIBED IN SECTION	INPUT SAMPLES IN SECTION
THERMO DATA	2.1.1	NONE
REACTANTS CARDS	2.1.2	3.1.1, 3.2.1.3, 3.3.1.1, 3.4.1.1
OMIT CARDS	2.1.3, 2.1.3.1	3.1.1
SOLUTION CARDS	2.1.3, 2.1.3.2	3.1.1
INSERT CARDS	2.1.3, 2.1.3.3	3.1.1
INPT2 NAMELIST	2.1.4, 2.1.4.1	3.1.1.1, 3.1.1.2, 3.1.1.3, 3.2.1.1, 3.2.1.2, 3.2.1.3, 3.3.1.1, 3.4.1.1
RKTNP NAMELIST	2.1.4, 2.1.4.2	3.2.1.1, 3.2.1.2, 3.2.1.3, 3.3.1.1 3.3.1.4 (THROAT), 3.4.1.1, 3.4.1.2
SPEC CARDS	2.1.5	3.4.1.1
DLIT CARDS	2.1.6, 2.1.6.1	3.3.1.1, 3.4.1.1
REACTANT/ PRODUCT CARDS	2.1.6, 2.1.6.2	3.3.1.1, 3.4.1.1
KFRR CARDS	2.1.6, 2.1.6.3	3.3.1.1, 3.4.1.1
CHNLIN NAMELIST	2.1.7, 2.1.7.1	3.2.1.1, 3.2.1.2, 3.2.1.3, 3.3.1.1, 3.3.1.2, 3.3.1.3, 3.3.1.4 (THROAT), 3.4.1.1
CHANNEL PROFILE DATA	2.1.7, 2.1.7.2	3.3.1.2, 3.3.1.3, 3.3.1.4 (THROAT) 3.4.1.1

**Table XIII. Cross Reference of Description and
Examples of Problem Types**

PROBLEM TYPE	DESCRIBED IN SECTION	INPUT SAMPLES IN SECTION
TP	2.1.4.1	3.1.1.1
HP	2.1.4.1	3.1.1.2
SP	2.1.4.1	3.1.1.3
CHANNEL	2.1.4.1, 2.1.7	3.2.1.1, 3.2.1.2, 3.2.1.3, 3.3.1.1 3.3.1.2, 3.3.1.3, 3.4.1.1
CHANNEL HEAT LOSS	2.1.4.2	3.4.1.2
TWOSTAGE	2.1.2, 2.1.2.1, 2.1.2.3, 2.1.4.1	3.2.1.3
SUPERSONIC/ SUBSONIC	2.1.4.1	3.2.1.2
FULLY FINITE RATE	2.1.4.2, 2.1.5, 2.1.6	3.4.1.1, 3.4.1.2
PARTIAL FINITE RATE (FROM ENTRANCE)	2.1.4.2, 2.1.6	3.3.1.1
PARTIAL FINITE RATE (FROM THROAT)	2.1.4.2, 2.1.6	3.3.1.4

5. FIGURES

Figure 1. MAIN Routine

Figure 1. (Continued)

Figure 1. (Continued)

Figure 2. Subroutine Tree Diagram

Figure 3. Subroutine THERMP

Figure 4. Subroutine EQLBRM(FLAG)

Figure 4. (Continued)

Figure 4. (Continued)

Figure 4. (Continued)

Figure 4. (Continued)

SUBROUTINE ROCKET

Figure 5. Subroutine ROCKET

Figure 5. (Continued)

Figure 6. Subroutine MHD (JJPATH)

Figure 6. (Continued)

Figure 6. (Continued)

Figure 6. (Continued)
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Figure 7. Subroutine DIFFUN (X, N, EEN)

6. REFERENCES

1. Gordon, S., and McBride, B.J., "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouguet Detonations," Report No. NASA SP-2731, National Aeronautics and Space Administration, Washington, DC (1971).
2. Callen, H.B., Thermodynamics, John Wiley & Sons, Inc., New York (1960).
3. Chase, Jr., M.W., et al., JANAF Thermochemical Tables, Dow Chemical Co., Midland, Michigan, Revised Version (June 30, 1977).
4. McBride, Bonnie j., and Gordon, Sanford: FORTRAN IV Program for Calculation of Thermodynamic Data. NASA TN D-4097, 1967.
5. Gordon, Sanford: Calculation of Theoretical Equilibrium Nozzle Throat Conditions when Velocity of Sound is Discontinuous. AIAA J., vol. 9, no. 1, (1970), pp.179-182.
6. Gordon, Sanford, and Zeleznik, Frank J.: Thermodynamic Extrapolation of Rocket Performance Parameters. ARS J., vol. 32, no. 8, (1962), pp. 1195-1202.
7. Sutton, G.W., and Sherman, A., Engineering Magnetohydrodynamics, McGraw-Hill, New York (1965).
8. Cohen, H.D., Conductivity Code "CONDUCT", private communication (1977).
9. Gear, C.W., Numerical Initial Value Problems in Ordinary Differential Equations, Prentice-Hall, Englewood Cliffs, N.J. (1971).

APPENDIX A

DERIVATION OF dp/dx WHEN CHANNEL AREA IS SPECIFIED

When channel area is specified, instead of velocity or pressure, the solution of the conservation equations, i.e., Eqs. (1) - (4) of Section 1, becomes more complicated since the number of unknown derivatives increases by one. This requires an additional differential equation which can be derived from the continuity equation and is given by:

$$\frac{1}{\rho} \frac{d\rho}{dx} + \frac{1}{u} \frac{du}{dx} = - \frac{1}{A} \frac{dA}{dx} \quad . \quad (A.1)$$

The derivatives integrated by the PACKAGE code are dp/dx , du/dx , dh/dx , and dn_i/dx ($i > ME$). Therefore, $d\rho/dx$ must be eliminated from Eq. (A.1). To do this we use the two equations of state which are:

$$\left. \begin{aligned} \rho &= \rho(p, T, n_{ME+1}, \dots, n_{NT}) \\ \text{and} \\ h &= h(p, T, n_{ME+1}, \dots, n_{NT}) \end{aligned} \right\} \quad . \quad (A.2)$$

If the variation of rate controlled species concentration is due to chemical reactions then, changes in n_i ($i > ME$) are not, in general, independent of one another.

To show this we refer to the chemical reaction equations given below:

Here, A_i represents the i^{th} species. The increase in the rate controlled i^{th} species concentration due to r^{th} reaction is:

$$dn_{ir} = (\nu_{ri}' - \nu_{ri}) d\xi_r \quad (i > ME, r = 1, \dots, L) \quad , \quad (A.4)$$

where $d\xi_r$ is a factor of proportionality unique to each reaction. The net increase in n_i is, therefore, given by:

$$dn_i = \sum_{r=1}^L (\nu_{ri}' - \nu_{ri}) d\xi_r \quad (A.5)$$

Equation (A.5) implies that n_i is a function of $\xi_1, \dots, \xi_L$. Equation (A.1) can be written as:

$$\left. \begin{aligned} \rho &= \rho(p, T, \xi_1, \dots, \xi_L) \\ h &= h(p, T, \xi_1, \dots, \xi_L) \end{aligned} \right\} \quad (A.6)$$

These two state equations can be combined to yield $d\rho/dx$ in terms of dp/dx , dh/dx , and $d\xi_i/dx$ ($i = 1, \dots, L$). This is considered next.

From Eq. (A.5) we have

$$\frac{d\rho}{dx} = \left(\frac{\partial \rho}{\partial p} \right)_{T, NE} \frac{dp}{dx} + \left(\frac{\partial \rho}{\partial T} \right)_{p, NE} \frac{dT}{dx} + \sum_{r=1}^L \left(\frac{\partial \rho}{\partial \xi_r} \right)_{p, T, \overline{NE}} \frac{d\xi_r}{dx} \quad , \quad (A.7)$$

where subscript NE means keeping all ξ_r constant, which is the same as holding n_i ($i > ME$) constant, and $\overline{NE}$ means holding all but one ξ_r constant. To eliminate dT/dx we use the state equation for enthalpy which yields:

$$\frac{dh}{dx} = \left(\frac{\partial h}{\partial p} \right)_{T, NE} \frac{dp}{dx} + C_{p, NE} \frac{dT}{dx} + \sum_{r=1}^L \left(\frac{\partial h}{\partial \xi_r} \right)_{p, T, \overline{NE}} \frac{d\xi_r}{dx} \quad (A.8)$$

Here, we have used the definition of $C_{p, NE}$ to get the coefficient of dT/dx . Equations (A.7) and (A.8) can be combined to eliminate dT/dx . The result can be represented by the following equation:

$$\frac{d\rho}{dx} = C \frac{dp}{dx} + Q \frac{dh}{dx} + \sum_{r=1}^L O_r \frac{d\xi_r}{dr} \quad (A.9)$$

where

$$\left. \begin{aligned} C &\equiv \left(\frac{\partial \rho}{\partial p} \right)_{T, NE} - \frac{1}{C_{p, NE}} \left(\frac{\partial \rho}{\partial T} \right)_{p, NE} \left(\frac{\partial h}{\partial p} \right)_{T, NE} \\ Q &\equiv \frac{1}{C_{p, NE}} \left(\frac{\partial \rho}{\partial T} \right)_{p, NE} \\ \text{and} \\ O_r &\equiv \left(\frac{\partial \rho}{\partial \xi_r} \right)_{p, T, \overline{NE}} - \frac{1}{C_{p, NE}} \left(\frac{\partial \rho}{\partial T} \right)_{p, NE} \\ &\quad \times \left(\frac{\partial h}{\partial \xi_r} \right)_{p, T, \overline{NE}} \quad (r = 1, \dots, L) \end{aligned} \right\} \quad (A.10)$$

To evaluate these coefficients, we need the following thermodynamic relations:

$$\left. \begin{aligned} dh &= Tds + Vdp + \sum_{i=1}^{NT} \mu_i dn_i \\ dg &= -sdT + Vdp + \sum_{i=1}^{NT} \mu_i dn_i \end{aligned} \right\} \quad (A.11)$$

which in terms of $d\xi_r$ are:

$$\left. \begin{aligned} dh &= Tds + Vdp + \sum_{r=1}^L \eta_r d\xi_r \\ dg &= sdT + Vdp + \sum_{r=1}^L \eta_r d\xi_r \end{aligned} \right\} \quad (A.12)$$

where

$$\eta_r \equiv \sum_{i=1}^{NT} (\nu'_{ri} - \nu_{ri}) \mu_i \quad (A.13)$$

Equation (A.12) will be used to derive certain Maxwell relations in order to evaluate terms like $(\partial\rho/\partial\xi_i)$ in terms of other thermodynamic derivatives or parameters whose values are evaluated by the PACKAGE code. The required Maxwell relations are:

$$\begin{aligned}
\text{(I)} \quad & \left(\frac{\partial s}{\partial p} \right)_{T, NE} = - \left(\frac{\partial V}{\partial T} \right)_{p, NE} \\
\text{(II)} \quad & \left(\frac{\partial V}{\partial \xi_r} \right)_{p, T, \overline{NE}} = \left(\frac{\partial \eta_r}{\partial p} \right)_{T, NE} \quad (r = 1, \dots, L) \\
\text{(III)} \quad & \left(\frac{\partial s}{\partial \xi_r} \right)_{p, T, \overline{NE}} = - \left(\frac{\partial \eta_r}{\partial T} \right)_{p, NE} \quad (r = 1, \dots, L)
\end{aligned}
\quad \left. \vphantom{\begin{aligned} \text{(I)} \\ \text{(II)} \\ \text{(III)} \end{aligned}} \right\} \quad (\text{A.14})$$

Referring to Eq. (A.13), we note that to evaluate the derivatives of η_r we must evaluate the derivative of μ_i , the i^{th} species chemical potential. The chemical potentials are given by:

$$\mu_i = \begin{cases} RT \sum_{j=1}^{\ell} a_{ij} \pi_j & (i = 1, \dots, ME) \\ \mu_i^0 + RT \ln n_i - RT \ln n_g + RT \ln p_{\text{atm}} & (i = ME + 1, \dots, NG) \\ \mu_i^0 & (i = NG + 1, \dots, NT) \end{cases} \quad (\text{A.15})$$

We have used Eq. (14) of Section 1 with $\lambda_i = -RT \pi_i$ to get the chemical potentials for species with $i \leq ME$. The derivatives of μ_i with respect to pressure and temperature are:

$$\left(\frac{\partial \mu_i}{\partial p}\right)_{T,NE} = \begin{cases} \frac{RT}{p} \sum_{j=1}^{\ell} a_{ij} \left(\frac{\partial \pi_j}{\partial \ln p}\right)_{T,NE} & (i = 1, \dots, ME) \\ \frac{RT}{p} \left[1 - \frac{N}{N+M} \left(\frac{\partial \ln N}{\partial \ln p}\right)_{T,NE}\right] & (i = ME+1, \dots, NG) \\ 0 & (i = NG+1, \dots, NT) \end{cases} \quad (A.16)$$

and

$$\left(\frac{\partial \mu_i}{\partial T}\right)_{p,NE} = \begin{cases} \frac{\mu_i}{T} + R \sum_{j=1}^{\ell} a_{ij} \left(\frac{\partial \pi_j}{\partial \ln T}\right)_{p,NE} & (i = 1, \dots, ME) \\ \frac{\mu_i}{T} - \frac{(H_T^0)_i}{T} - R \frac{N}{N+M} \left(\frac{\partial \ln N}{\partial \ln T}\right)_{p,NE} & (i = ME+1, \dots, NG) \\ \frac{\mu_i}{T} - \frac{(H_T^0)_i}{T} & (i = NG+1, \dots, NT) \end{cases} \quad (A.17)$$

To derive the derivatives with respect to temperature we have used the following relations:

$$\left. \begin{aligned} \mu_i^0(T) &= (H_T^0)_i - T (S_T^0)_i \\ d(H_T^0)_i &= T d(S_T^0)_i \end{aligned} \right\} \quad (A.18)$$

Note that the derivatives appearing in Eqs. (A.16) and (A.17) are calculated by the PACAGE code through Eqs. (60) - (63) and (49) - (52) of Section 1.

As shown below, we can now reduce the coefficients given by Eq. (A.10) in terms of parameters which are evaluated by the code. To do this we first replace ρ by $1/V$ and rewrite the derivatives of ρ with respect to p and T in terms of logarithmic derivatives. This yields:

$$\left. \begin{aligned} \left(\frac{\partial \rho}{\partial p} \right)_{T, NE} &= - \frac{1}{pV} \left(\frac{\partial \ln V}{\partial \ln p} \right)_{T, NE} \\ \left(\frac{\partial \rho}{\partial T} \right)_{p, NE} &= - \frac{1}{TV} \left(\frac{\partial \ln V}{\partial \ln T} \right)_{p, NE} \end{aligned} \right\} \quad . \quad (A.19)$$

The logarithmic derivatives given by Eq. (A.19) are calculated by the code. Therefore, the coefficient, Q , of Eq. (A.10) can be evaluated. To evaluate the coefficient C , we must determine $(\partial h / \partial p)_{T, NE}$. This can be calculated using the relations (A.12) and the Maxwell relation (A.14 i). The result can be reduced to:

$$\begin{aligned} C = & - \frac{(\partial \ln V / \partial \ln p)_{T, NE}}{pV C_{p, NE}} \left[C_{p, NE} + \frac{(pV/T) (\partial \ln V / \partial \ln T)_{p, NE}^2}{(\partial \ln V / \partial \ln p)_{T, NE}} \right] \\ & + \frac{1}{T C_{p, NE}} \left(\frac{\partial \ln V}{\partial \ln T} \right)_{p, NE} \quad . \end{aligned} \quad (A.20)$$

From the definition of $C_{V, NE}$ and $\gamma_{S, NE}$ (see Eqs. (69) and (70) of Section 1), we get:

$$C = \frac{1}{pV \gamma_{S, NE}} + \frac{1}{T C_{p, NE}} \left(\frac{\partial \ln V}{\partial \ln T} \right)_{p, NE} \quad . \quad (A.21)$$

To determine the coefficient O_r we need to evaluate $(\partial \rho / \partial \xi_r)_{p, T, \overline{NE}}$ and $(\partial h / \partial \xi_r)_{p, T, \overline{NE}}$. Using the Maxwell relation (A.14II) and Eqs. (A.13) and (A.16) it can be shown that:

$$\begin{aligned} \left(\frac{\partial \rho}{\partial \xi_r} \right)_{p, T, \overline{NE}} &= -\frac{1}{V^2} \left(\frac{\partial V}{\partial \xi_r} \right)_{p, T, \overline{NE}} = -\frac{RT}{p V^2} \\ &\times \left\{ \sum_{i=1}^{ME} (\nu'_{ri} - \nu_{ri}) \sum_{j=1}^{\ell} a_{ij} \left(\frac{\partial \pi_j}{\partial \ln p} \right)_{T, NE} \right. \\ &\left. + \sum_{i=ME+1}^{NG} (\nu'_{ri} - \nu_{ri}) \left[1 - \frac{N}{N+M} \left(\frac{\partial \ln N}{\partial \ln p} \right)_{T, NE} \right] \right\} \end{aligned} \quad (A.22)$$

To evaluate $(\partial h / \partial \xi_r)_{p, T, \overline{NE}}$ we use Eqs. (A.12), (A.13), and the Maxwell relation (A.14III) and Eq. (A.17) to get:

$$\begin{aligned} \left(\frac{\partial h}{\partial \xi_r} \right)_{p, T, \overline{NE}} &= T \left(\frac{\partial s}{\partial \xi_r} \right)_{p, T, \overline{NE}} + \eta_r \\ &= RT \left\{ \sum_{i=1}^{ME} (\nu'_{ri} - \nu_{ri}) \left[- \sum_{j=1}^{\ell} a_{ij} \left(\frac{\partial \pi_j}{\partial \ln T} \right)_{p, NE} \right] \right. \\ &\quad + \sum_{i=ME+1}^{NG} (\nu'_{ri} - \nu_{ri}) \left[\frac{(H_T^0)_i}{RT} + \frac{N}{N+M} \left(\frac{\partial \ln N}{\partial \ln T} \right)_{p, NE} \right] \\ &\quad \left. + \sum_{i=NG+1}^{NT} (\nu'_{ri} - \nu_{ri}) \frac{(H_T^0)_i}{RT} \right\} \end{aligned} \quad (A.23)$$

Substitution of Eqs. (A.22) and (A.23) in the last of Eq. (A.10) will yield O_r . Referring to Eq. (A.9) we note that $d\rho/dx$ depends on the summation of $O_r d\xi_r/dx$ over $r = 1$ to L . Therefore, we also need to evaluate $d\xi_r/dx$. This is done by combining Eqs. (114), (123) of Section 1, and Eq. (A.5) which yield:

$$\frac{d\xi_r}{dx} = \frac{\dot{w}_{rl}}{\rho u(\nu'_{rl} - \nu_{rl})} \quad (A.24)$$

From Eqs. (A.22), (A.23), (A.24), and the equation of state, $pV = n_g RT$, we now get:

$$\begin{aligned} \sum_{r=1}^L O_r \frac{d\xi_r}{dx} = & -\frac{1}{u n_g} \\ & \times \left\{ \sum_{i=1}^{ME} \dot{w}_i \sum_{j=1}^{\ell} a_{ij} \left(\frac{\partial \pi_i}{\partial \ln p} \right)_{T, NE} \right. \\ & \left. + \left[1 - \frac{N}{N+M} \left(\frac{\partial \ln N}{\partial \ln p} \right)_{T, NE} \right] \sum_{i=ME+1}^{NG} \dot{w}_i \right\} \\ & + \frac{R}{u C_{p, NE}} \left(\frac{\partial \ln V}{\partial \ln T} \right)_{p, NE} \\ & \times \left\{ - \sum_{i=1}^{ME} \dot{w}_i \sum_{j=1}^{\ell} a_{ij} \left(\frac{\partial \pi_i}{\partial \ln T} \right)_{p, NE} \right. \\ & \left. + \left[\frac{N}{N+M} \left(\frac{\partial \ln N}{\partial \ln T} \right)_{p, NE} \right] \sum_{i=ME+1}^{NG} \dot{w}_i + \sum_{i=ME+1}^{NT} \dot{w}_i \frac{(H_T^0)_i}{RT} \right\} . \end{aligned} \quad (A.25)$$

where $n_g = N + M$ and $\dot{w}_1 = \sum_{r=1}^L \dot{w}_{r1}$. Note that Eq. (A.25) is identical to

Eq. (125) of Section 1.

Given the coefficients C , Q , and O_r we can use Eq. (A.7) to eliminate $d\rho/dx$ from Eq. (A.1). The result yields an equation in terms of dp/dx , du/dx , dh/dx , and $d\xi_r/dx$. Substituting for du/dx and dh/dx , using conservation equations (cf. Eqs. (3) and (4) of Section 1), we can derive an equation for dp/dx which in terms of C , Q , and O_r $d\xi_r/dx$ is given by:

$$\left[u^2 \left(C + \frac{Q}{\rho} \right) - 1 \right] \frac{dp}{dx} = - \frac{\rho u^2}{A} \frac{dA}{dx} + \frac{Qu}{\rho} (uF - q) - u^2 \sum_{r=1}^L O_r \frac{d\xi_r}{dx} - F \quad (A.26)$$

Using Eq. (A.21) for C and noting that:

$$Q = - \frac{1}{TVC_{p,NE}} \left(\frac{\partial \ln V}{\partial \ln T} \right)_{p,NE} \quad (A.27)$$

The coefficient of dp/dx in Eq. (A.26) reduces to:

$$\frac{u^2}{pV\gamma_{S,NE}} - 1 = \mathcal{M}^2 - 1, \quad (A.28)$$

where $\mathcal{M}^2$ is the flow Mach number.

Note that $pV\gamma_{S,NE} = n_g RT\gamma_{S,NE} = a^2$. Substitution of Eqs. (A.27) and (A.28) in Eq. (A.26) leads to Eq. (124) of Section 1.

APPENDIX B

COMMON VARIABLES

All common variables are given in this appendix except those with common label OUP.T. These latter variables are discussed in Subsection 2.4.17 (BLOCK DATA).

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
A	30,300	STOIC	SRCHCC MATRX EQLBRM HCALC ROCKET MHD DIFFUN	a_{ij} , stoichiometric coefficient of i^{th} element in j^{th} species.
AC	2	MISC	SAVE	Saves JSOL (AC(1)) and JLIQ (AC(2)).
AEAT	13	PERF	ROCKET RKTOUT DIFFUN	in RKTOUT, area ratios A_e/A_t to be printed out.
AM	2	MISC	REACT HCALC	$AM(k) M^{(k)}$, molecular weight of total oxidant ($k = 1$) or total fuel ($k = 2$).
ANUM	30,5	MISC	REACT HCALC OUT1	Stoichiometric coefficients of reactants. First subscript refers to the reactant, the second, the element on the card. (See section Subroutine REACT).
APP	13	PERF	ROCKET RKTOUT	P_c/P_e , ratio of chamber pressure to exit pressure.
AREA	1	PERF	ROCKET	Logical variable indicating (if true) area ratios have been assigned.
AI	26	MHDD	----	Not used
ACCURC	1	EQ	MHD	Sets accuracy requirements for Subroutine DIFSUB
ATERM	1	MIKE1	MHD DIFFUN	Either SSUM(NPT) or HSUM(NPT)

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
AMULT	1	MIKE1	MHD DIFFUN	Multiplier associated with ATERM
ATOM	3,101	MISC	REACT BLOCK DATA	For j^{th} atom: ATOM (1,j) = atomic symbol (H, HE, ...). ATOM (2,j) = atomic weight. ATOM (3,j) = atomic valence.
AWT	1	PERF	ROCKET	nT/Pu at throat. AWT is used in obtaining area ratios, eq. (106).
AREAIN	20	MIKE3	MHD DIFFUN SETEQU	Contains inputted area in the Channel if Model 3
AKF1 AKF2 AKF3	30 30 30	DIFEQ DIFEQ DIFEQ	{ ROCKET MHD DIFFUN }	Forward reaction rate of finite rate equation for each reaction = AKF where $AKF = AKF1 * TAKF2 * e^{-AKF3/T}$
AP AR	30, 4 30, 4	DIFEQ DIFEQ	{ ROCKET MHD DIFFUN }	Coefficients of the products and reactants of finite rate equations
ANE AIONS	15 15	SIGOUT SIGOUT	{ OUT2 CONDUCT }	Electron density and ions for each point calculated in CONDUCT and outputted in OUT3
B θ	30	MISC	NEWOF MATRIX	b_i^0 , assigned kg-atoms of element i per kg of total reactant.
B θ P	30, 2	MISC	MAIN REACT NEWOF	B θ P(i, 1) $b_i^{(1)}$, kg-atoms of i^{th} element per kg of total oxidant. B θ P(i, 2) $b_i^{(2)}$, kg-atoms of i^{th} element per kg of total fuel, eq. (187).
B θ N	30	NEQ	ROCKET MATRIX MHD EQLBRM DIFFUN	b_i^0 , assigned kg-atom of element i per kg of total reactant for finite rate equations.

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
BØP2	30, 2	MIKE4	REACT ROCKET NEWOF	Analogous to BØP but need if TWOSTG is TRUE
BETOUT	13	MIKE8	SETEQU OUT2	Stores β (Hall Parameter) for output at each report Station
BZ	1	MHDD	MHD DIFFUN ROCKET SETEQU	Magnetic field for MHD equations
BZOUT	13	MIKE8	SETEQU OUT2	Stores BZ for output at each report station
CPCVEQ	1	INDX	EQLBRM MATRIX	Equivalenced to LOGV in EQLBRM and MATRIX (see LOGV)
CPCVFR	1	INDX	-----	Temporary storage.
CPR	13	POINTS	EQLBRM OUT2 ROCKET	c_p/R , constant pressure specific heat, kg-mole/kg (eq. (59) or (121)).
CPSUM	1	MISC	EQLBRM CPHS MATRIX HCALC ROCKET	c_p/R , frozen constant pressure specific heat, kg-mole/kg, eq. (121).
CR	1	MISC	-----	Not used.
CHHEAT	1	SETUPS	DIFFUN SETEQU	Stores enthalpy at each point
CSTR	1	PERF	RKTOUT	c^* , characteristic velocity, ft/sec
CALCH	1	INDX	MAIN SAVE CHALC THERMP ROCKET	Logical variable indicating (if true) zeros were punched in card columns 37 and 38 of at least one REACTANTS card.

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
COEF	2, 7, 300	SPECES	SRCHCC	Constants in empirical equations for thermodynamic functions. COEF(i, j, k): i = 1 for upper temperature interval and i = 2 for the lower one; j = 1 . . . , 7, for the 7 coefficients, a _j ; k = 1 . . . 300 for the number of species, eqs. (90) to (92).
CHLOSS	1	SETUPS	SETEQU	Temporary storage of part of heat term
CONVG	1	INDX	EQLBRM MATRIX	Logical variable indicating convergence is true.
CHCALC	1	MIKE7	DIFFUN EQLBRM SETEQU	Calculated channel heat loss.
CHNLEN	1	MIKE7	DIFFUN EQLBRM SETEQU	Length of channel (meters).
DLVPT	13	POINTS	EQLBRM OUT2	$\left(\frac{\partial \ln V}{\partial \ln P}\right)_T$, eq. (51) or (123).
DLVTP	13	POINTS	EQLBRU OUT2 ROCKET	$\left(\frac{\partial \ln V}{\partial \ln T}\right)_P$, eq. (50) or (122).
DATA	30	MISC	MAIN HCALC REACT	Temporary storage.
DPITP	30	AREASU	{ EQLBRM DIFFUN }	Stores derivatives of π with respect to temperature and pressure, when CONVG = TRUE in EQLBRM. Used for finite rate chemistry, with area given, in DIFFUN.
DPIPT	30	AREASU		
DLNTP	1	AREASU	{ EQLBRM DIFFUN }	Stores derivatives of LN(N) with respect to temperature and pressure to be used in connection with DPITP and DPIPT.
DLNPT	1	AREASU		
DUMMIN	300	MIKE5	MAIN MHD	Contains the dependent variables corresponding to XINDP in the channel.

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
DELN	300	SPECE4	EQLBRM	In EQLBRM: Corrections to $\ln n_j$ for gases or n_j for condensed.
DENS	30	MISC	REACT OUT1	Density of reactant read from input card and used only when TWOSTG is TRUE.
DATE	2,300	SPECE9	SRCHCC	Store date when species generated for thermo tables
DXI	1	MHDD	{ MAIN MHD }	INPUT print increment in channel
DX	1	MHDD		Used as DX in MHD
DXOUTP	200	DBGVEC	ROCKET RKTOUT MATRIX MHD DIFFUN EQLBRM SAVE	Temporary storage vector used or debug output for calls to DBGOUT
EN	13,300	KGM	MAIN EQLBRM CPHS MATRIX SAVE OUT3 CONDUCT SRCHCC MHD HCALC RKTOUT DIFFUN ROCKET	n_j , kg-moles of j^{th} species/kg of mixture ($j \leq 300$). The first subscript is for point number for output.
EXIN	1	MIKE8	MAIN SETEQU	Maximum allowable axial electric field
ENLN	300	SPECE2	MHD ROCKET EQLBRM MATRIX SAVE DIFFUN	LN J (see EN).

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
ENLSAV	1	MISC	SAVE	Lnn, saved for a particular point (see ENN).
ENN	1	MISC	<div> <div>MAIN EQLBRM</div> <div>MATRIX</div> <div>SAVE ROCKET MHD DIFFUN</div> </div>	n, moles of mixture, kg-mole/kg eq. (79) for assigned pressure problems).
EMM	1	MISC		Where ENN is for equilibrium pool, EMM is for finite rate equations, and ENNS is for solution species. Note, ENN not in SAVE, MHD, or DIFFUN.
ENNS	1	SOLUT		
ENLS	1	SOLUT	MAIN ROCKET MATRIX EQLBRM	Ln ENNS (see ENNS)
ENNL	1	MISC	MAIN EQLBRM SAVE MHD DIFFUN	Ln n, (see ENN).
ENSAVE	1	MISC	SAVE	n, saved for a particular point (see ENN).
ENTH	30	MISC	REACT HCALC OUT1	For assigned pressure problems, $(H_T^O)_i$, assigned enthalpy of a reactant in calories per mole.
EQL	1	PERF	MAIN ROCKET OUT3 RKTOUT OUT2	Logical variable always set true

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
EQRAT	1	MISC	MAIN NEWOF OUT1	r, equivalence ratio (eq. (204)).
FAZ	30	MISC	MAIN REACT HCALC OUT1	Alphameric letter read from reactant cards. The letter G indicates gas; any other letter indicates condensed phase.
FOX	30	MISC	REACT	Alphameric letter, F or O, read from reactant cards indicating reactant is a fuel (F or blank) or oxidant (O).
FPCT	1	MISC	MAIN	Logical variable in namelist INPT2 (see Table VIII).
FNEL	4	SIGOUT	BLOCKD OUT2	Set as names for electron density, IONIC density, WO IONS, SIGMA, and frequency in BLOCKD and used for outputs in OUT2.
FIONS	3	SIGOUT		
FSTGWO	4	SIGOUT		
FSIG	4	SIGOUT		
FFREQ	4	SIGOUT		
FROZ	1	PERF	ROCKET	Logical variable in namelist RKTINP.
FIRST	1	START	ROCKET MHD	Logical variable indicating entry into MHD to input channel inputs.
G	60, 61	DOUBLE	EQLBRM MATRIX GAUSS	Matrix region.
GAMMAS	13	POINTS	EQLBRM OUT2 DIFFUN ROCKET RKTOUT	γ_S or $\gamma_{S,T}$ isentropic exponent (eq. (71), (73), or (84)).

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
HØ	300	SPECE3	EQLBRM CPHS MATRIX HCALC DIFFUN ROCKET MHD	$\mathcal{H}_j$, dimensionless enthalpy for species j.
HP	1	INDX	MAIN EQLBRM MATRIX THERMP MHD DIFFUN ROCKET	Logical variable indicating (if true) enthalpy and pressure has been assigned.
HPP	2	MISC	.REACT HCALC NEWOF	$\mathcal{H}^{(k)}_T$ or $\mathcal{U}^{(k)}_T$, enthalpy of total oxidant (k=1) and total fuel (k=2) (eqs. (192) and (194)).
HSUBØ	1	MISC	NEWOF HCALC MATRIX MHD DIFFUN EQLBRM THERMP	h_o/R or u_o'/R assigned enthalpy of total reactant (eqs. (193) and (195)).
HSUM	13	POINTS	EQLBRM MATRIX OUT2 MHD ROCKET RKTOUT	$\mathcal{H}$ in MATRIX and h/R at the end of EQLBRM and in the other routines (eqs. (29) and (14)).
HMIN	1	EQ	MAIN MHD	Minimum step size to be used in calls to DIFSUB. Inputted namelist INPT2 in MAIN.
HPATH	1	MIKE2	MAIN ROCKET MHD DIFFUN	Analogous to definition of HP. HP is set to HPATH once you begin channel calculations. Inputted in ROCKET by namelist RKTINP.

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
HPP	2	MISC	REACT HCALC NEWOF	Used to store energy for fuel and oxidant.
HPP2	2	MIKE4	REACT	Analogous to HPP, but used when TWOSTG = .TRUE.
IC	1	INDX	-----	Not used.
IDEBUG	1	INDX	MAIN EQLBRM ROCKET THERMP	When set to a value i (i > 0), intermediate output is printed for all points $\geq i$.
IMAT	1	INDX	EQLBRM MATRIX GAUSS	Number of rows in matrix setup.
IONS	1	INDX	MAIN EQLBRM SAVE	Logical variable indicating (if true) ionic species are to be considered.
IP	1	INDX	THERMP ROCKET	Index for pressure values
IQ1	1	INDX	MAIN EQLBRM SAVE MATRIX	Number of elements plus the number of condensed species included in matrix equations plus 1.
IQSAVE	1	INDX	SAVE	IQ1 saved for a particular point when ISV is negative.
ISUB	1	INDX	ROCKET	Index for SUBAR values (see SUBAR).
ISUP	1	INDX	ROCKET	Index for SUPAR values (see SUPAR).
ISV	1	INDX	SAVE THERMP ROCKET	ISV > 0: Use compositions from last point (numbered ISV) as estimates for current point (numbered NPT). ISV < 0: Store compositions in SLN array to use as estimates for future points. Make ISV positive and proceed as with ISV > 0. ISV = 0: Use compositions stored in SLN array as estimates for current point (numbered NPT).

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
IT	1	INDX	MAIN THERMP ROCKET RKTOUT	Index for T values (see T).
ITM	1	INDX	ROCKET	Integer = 1
ITNUM	1	INDX	ROCKET	Iteration number for converging to assigned area ratio.
IPP	1	MHDD	ROCKET RKTOUT MHD DIFFUN EQLBRM	Global point counter
ISOLN	3,16	SOLUT	MAIN	Contains the species to be placed in the solution model. Control setting of IUSE vector.
IUSE	300	SPECE5	MAIN EQLBRM CPHS MATRIX HCALC SAVE SRCHCC DIFFUN ROCKET	See section "IUSE array".
ITYPE	1	SETUPS	MHD SETEQU	Indicates type of channel problem where 1 indicates MHD problems and 2 adds the friction terms to MHD problems.
IPRRKT	1	MIKE7	MAIN ROCKET MHD EQLBRM DIFFUN SETEQU	One of the debug option controlling variables discussed in Subsection 2.1.4.2

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
IMPRNT	1	MIKEØ	ROCKET MHD EQLBRM DIFFUN SETEQU	One of the debug options controlling variables discussed in Subsection 2.1.7.1.
ITE1		MIKEØ	{ MHD DIFFUN }	Contains the information regarding channel equations. See comments in listing of Subroutine MHD.
ITE2		MIKEØ		
ITE3		MIKEØ		
JLIQ	1	INDX	EQLBRM SAVE	Index of condensed species which is included simultaneously with another condensed phase of the same species. JLIQ is the index for the phase in the higher temperature range; JSOL is the index for the phase in the lower temperature range. Otherwise JLIQ = JSOL = 0.
JS1	1	INDX	CPHS EQLBRM HCALC	Index for species for which thermodynamic functions are to be calculated in CPHS.
JSOL	1	INDX	EQLBRM ROCKET SAVE	See JLIQ.
KASE	1	INDX	MAIN OUT1	Optional identifying case number for a set of reactants. The variable is part of namelist INPT2.
KMAT	1	INDX	EQLBRM MATRIX	Number of columns in matrix setup. KMAT=IMAT + 1.
KKIJJ	1	SPNQPT	MHD DIFSUB	Used to control step sizes for NEQPT problems
LLMT	30	MISC	MAIN REACT SRCHCC HCALC EQLBRM SAVE NEWOF ROCKET	Alphameric symbols for elements in the chemical system being processed.

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
LOGV	1	INDX	EQLBRM MATRIX	Logical variable indicating (if true) calculate special derivatives. LOGV is equivalenced to CPCVEQ which appears in common INDX.
LSAVE	1	INDX	SAVE	LLMT(NLM), the last element symbol is saved in LSAVE for use at some future point. If IONS is true and LSAVE is not "E", then ionic species were removed.
MOLES	1	INDX	MAIN REACT OUT1 HCALC ROCKET	Logical variable indicating (if true) that the relative amounts of the reactants have been specified in terms of moles.
MOMIT	1	DIFEQ	ROCKET MHD DIFFUN	Contains the number of non-equilibrium (finite rate) equations. Variable named NOMIT in MHD and DIFFUN.
MAR	30, 4	DIFEQ	{ MHD DIFFUN }	Contains indices into locations of products and reactants of finite rate equations
MAR	30, 4	DIFEQ		
NJR	30, 4	DIFEQ		
NJP	30, 4	DIFEQ		
NITER	1	MHDD	-----	Not used
NSTOP	1	MHDD	-----	Not used
NLM1	1	TSTG	REACT SRCHCC ROCKET NEWOF	NLM-1
NSOL	1	SOLUT	MATRIX EQLBRM	Number of solution variables
NEWR	1	INDX	MAIN REACT SRCHCC	Logical variable indicating (if true) that the search of file 7 has not yet been made for thermodynamic data for species in a new chemical system.

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
NFZ	1	INDX	-----	Not used
NLM	1	INDX	MAIN REACT SRCHCC DIFFUN HCALC NEWOF EQLBRM MATRIX MHD	Number of elements in the chemical system.
NOF	1	INDX	MAIN THERMP ROCKET	Number of o/f values. Note: mixture values given in the form of equivalence ratio, percent fuel, or fuel-air ratio are converted to o/f values in the main program.
NOMIT	1	INDX	MAIN SRCHCC EQLBRM MATRIX REACT	Number of species to be omitted. (see NOMIT for subroutines MHD and DIFFUN) (see NNNNN for EQLBRM on page B-14)
NP	1	INDX	MAIN THERMP ROCKET	Number of pressure values in the P array in namelist INPT2.
NPP	1	INDX	ROCKET	Number of P_c/P_e values. This is equal to the number of PCP values in namelist RKTINP plus 2 to include chamber and throat.
NMPATH	1	MIKEØ	MHD DIFFUN SETEQU	Indicates channel model
NUMIV	1	MIKEØ	MHD DIFFUN	Indicates length of vector describing channel inputs.
NPT	1	INDX	All routines except MAIN, REACT, GAUSS, AND SRCHCC	Index for the data saved for output (1 ≤ NPT ≤ 13). Global counter is IPP

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
NREAC	1	INDX	MAIN REACT HCALC OUT1 ROCKET	Number of reactants.
NS	1	INDX	MAIN SRCHCC HCALC OUT3 EQLBRM CPHS MATRIX MHD DIFFUN RKTOUT SAVE	Number of species considered in a particular chemical system.
NSERT	1	INDX	MAIN	Number of condensed species listed on INSERT cards.
NSUB	1	INDX	ROCKET	Number of SUBAR values (see SUBAR).
NSUP	1	INDX	ROCKET	Number of SUPAR values (see SUPAR).
NT	1	INDX	MAIN THERMP ROCKET	Number of temperature values listed in T schedule in namelist INPT2. //
NEQL	1	EQ	-----	Not used
NNNNN	1	MIKE5	MHD EQLBRM	Stores value of number of reacting (finite rate) equations used as NOMIT in EQLBRM
NUMB1	1	NVMM	EQLBRM	Counts number of iterations to converge.
NAME	30, 5	MISC	MAIN REACT HCALC OUT1	Alphameric symbols for elements as given on the reactant cards. Allowance is made for up to 5 symbols and 30 reactants.

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
NC	1	INDX	MAIN SRCHCC	Number of condensed species in thermodynamic data for a particular system.
NSPCMX	1	SPECE1	{ MAIN SRCHCC }	Stores allowed numbers for number of species (NSPCMX), number of condensed species (NCMAX), number of elements (NELMX).
NCMAX	1	SPECE1		
NELMX	1	SPECE1		
NJ1	1	DIFEQ	MHD DIFFUN	Number of finite rate equations
NQ1	1	NEQ	MHD MATRIX	Counts number of condensed species in finite rate equations
NSK	1	NEQ	ROCKET RKTOUT CPHS MATRIX OUT3 MHD EQLBRM DIFFUN	Total number of species (equilibrium plus finite rate)
NEQPT	1	NEQ	ROCKET EQLBRM MATRIX RKTOUT MHD	Used to flag occurrences of finite rate equations
OF	1	MISC	-----	Not used
OMIT	3,300	SPECE8	MAIN SRCHCC	Contains names of species to be omitted from calculations.
OXF	30	MISC	MAIN THERMP ROCKET	o/f, oxidant to fuel weight ratios. In the main program, OXF is equivalent to MIX, and INPT2 namelist variable.
P	26	POINTS	MAIN THERMP ROCKET	Assigned pressure schedule in namelist INPT2. Values are converted to atmosphere units in the main program.

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
PCP	22	PERF	ROCKET	Pressure ratio read in with RKTINP namelist.
PRESIN	20	MIKE2	MHD DIFFUN	Stores channel input pressure if model 2.
PECWT	30	MISC	REACT HCALC OUT1 ROCKET	Relative weight or number of moles of reactants as read from card columns 46 to 52 on the reactant cards.
PP	1	MISC	HCALC EQLBRM THERMP MHD DIFFUN ROCKET	Assigned pressure in atmospheres for current point.
PRINTX	1	XPRINT	MHD DIFFUN	Turn on/off intermediate prints
PIPP	1	MHDD	-----	Not used
PCWFT	2	MIKE4	{ REACT ROCKET NEWOFF }	Relative weights and densities of oxidants and fuels used when TWOSTG = .TRUE.
PCWSD	2	MIKE4		
PPP	13	POINTS	EQLBRM OUT2 MHD DIFFUN RKTOUT	Static pressure in atmospheres stored for output.
R	1	MISC	MAIN REACT HCALC OUT2 THERMP	Universal gas constant, 1.987165 cal/(g-mole) (K).
RH	2	MISC	REACT NEWOFF	$\rho^{(1)}$, density of total oxidant and $\rho^{(2)}$, density of total fuel, eq. (198).

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
RHOP	1	MISC	MAIN OUT1 NEWOF	ρ_o , density of total reactant, eq. (199).
RHOUE	1	SETUPS	DIFFUN SETEQU	Stores product of density and velocity at each point.
RMW	15	MISC	REACT HCALC ROCKET	Molecular weight of individual reactants.
RR	1	MISC	MAIN OUT2 EQLBRM MHD DIFFUN ROCKET RKTOUT	Universal gas constant, 8314.3 J/(kg-mole) (K).
RTEMP	30	MISC	REACT HCALC OUT1	Temperatures read from reactant card columns 64 to 71.
S	300	SPECE1	HCALC EQLBRM CPHS MATRIX ROCKET MHD DIFFUN	S_T^o , R, dimensionless entropy calculated from coefficients for reaction species. See Appendix A for definition.
SHOCK	1	INDX	-----	Not used
SSUMW	1	MHDD	-----	Not used
SLN	300	SPECE6	SAVE EQLBRM	$\ln n_i$ for gases and n_i for condensed species for a particular point (see ISV with negative value).

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
S ϕ	1	MISC	MAIN EQLBRM MATRIX THERMP ROCKET MHD DIFFUN	In INPT2 namelist for SP problem, entropy in cal/(g) (K). For RKT problems, $S\phi = s/R$, eq. (16), for the combustion point (NPT = 1).
SONVEL	13	POINTS	OUT2 RKTOUT	a, velocity of sound, eq. (74), or $a_{S,T}$, eq. (85).
SP	1	INDX	MAIN EQLBRM MATRIX THERMP ROCKET MHD DIFFUN	Logical variable indicating (if true) entropy and pressure have been assigned. In namelist INPT2, SP indicates an SP problem.
SPIM	13	PERF	RKTOUT	in RKTOUT, I_{sp} , specific impulse with ambient and exit pressures equal, (lb-force) (sec)/lb-mass.
SS ϕ	1	PERF	-----	Not used.
SNEQ	1	NEQ	-----	Not used.
SFLG	1	SOLUT	ROCKET MATRIX EQLBRM OUT3	When true indicates solution model exists.
SSUM	13	POINTS	HCALC EQLBRM OUT2 ROCKET MHD DIFFUN	s/R , entropy of mixture, (kg-mole)/kg.

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
SUB	600, 3	SPECE1	MAIN SRCHCC EQLBRM OUT3 RKTOUT ROCKET MHD DIFFUN	Alphameric names of species read from THERMO data. Each name takes 3 words, 4 characters each.
SUBAR	13	PERF	ROCKET	In ROCKET and RKTINP namelist, subsonic area ratios.
SUMN	1	MISC	MAIN EQLBRM MATRIX	$\sum_{j=1}^m n_j$, moles of mixture, kg-mole/kg.
SUPAR	13	PERF	ROCKET	In ROCKET and RKTINP namelist, supersonic area ratios.
SUMSN	1	SOLUT	MATRIX	Corrections to energy and S for solution species with SP=TRUE.
SIZE	1	MISC	ROCKET EQLBRM DIFFUN MHD	Default value for LN (concentration) when concentration is zero.
SPECNM	100, 3	MIKE6	ROCKET MHD	Contains the species for the fully non-equilibrium finite rate problem (when NEQPT=1) read after SPEC card. Used later in MHD to read DLIT species for any NEQPT problem.
SPATH	1	MIKE2	MAIN	Analogous to definition of SP. SP is set to SPATH once you begin channel calculations. Inputted in ROCKET by namelist RKTINP.
SIG	26	MHDD	DIFFUN SETEQU	Used as temporary storage location of SIGMA.

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
SCONMX	300	SPECE7	MHD	Used to store concentrations at maximum temperature for NEQPT=1 problem
SIGM	15	SIGOUT	OUT2 CONDUCT	WO Ions for output
THIGH	1	MISC	MAIN SRCHCC HCALC EQLBRM	Highest temperature in temperature range of species in the THERMO data.
TLN	1	MISC	EQLBRM CPHS HCALC MHD DIFFUN ROCKET	Ln T.
TLOW	1	MISC	MAIN SRCHCC HCALC EQLBRM	Lowest temperature in temperature range of species in the THERMO data.
TOTAL	15	SIGOUT	OUT2 CONDUCT SETEQU	Contains frequency at each point
TM	1	MISC	HCALC EQLBRM MATRIX	Ln (P_{atm}/n).
TMID	1	MISC	MAIN SRCHCC CPHS	Common temperature of two temperature ranges of the THERMO data.
TOTN	13	POINTS	EQLBRM OUT3 RKTOUT	NS $\sum_{j=1} n_j$, used in the calculation of mole fractions.

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
TP	1	INDX	MAIN EQLBRM MATRIX THERMP ROCKET	Logical variable indicating (if true) temperature pressure have been assigned. The assignments may be for a complete problem (TP) or a particular point.
TWOSTG	1	TSTG	MAIN REACT SRCHCC ROCKET NEWOF	If true, flags two stage combustor.
TRACE	1	MISC	MAIN EQLBRM OUT3	If TRACE 0, print mole fraction TRACE in special E-format. TRACE is namelist INPT2 variable.
TT	1	MISC	NEWOF HCALC EQLBRM CPHS MATRIX THERMP MHD DIFFUN ROCKET	Current temperature.
TTT	13	POINTS	EQLBRM OUT2 MHD DIFFUN ROCKET RKTOUT SETEQU	Temperature stored for printout.
T	26	POINTS	MAIN THERMP ROCKET RKTOUT	T, assigned temperature schedule in namelist INPT2. Values are in degrees Kelvin.
TEMP	175,2	SPECE1	SRCHCC HCALL EQLBRM GAUSS	Temperature ranges of individual condensed species. The lower value is in TEMP(j,1).

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
TDIFUN	1	MIKE7	ROCKET DIFFUN	Set to TCHFNL+10. In ROCKET (TCHFNL inputted in namelist RKTINP). Minimum value allowed is 300. If calculated temperature in DIFFUN less than this, program will stop (all output printed)
TMPSTP	1	MIKE7	ROCKET MHD	Set to TCHFNL. If calculated temperature in MHD less than this, program stops (all output printed).
TEQLBM		MIKE7	ROCKET EQLBRM	Value is 500 or 1000 (when channel heat loss = 0) controls temperature pt. where phase changes are restricted.
UEDP	1	SETUPS	-----	Not used
UE	1	MHDD	ROCKET RKTOUT MHD DIFFUN SETEQU	Contains the current channel velocity
V	13	POINTS	MAIN REACT OUT2 OUT3 VARFMT THERMP RKTOUT EFMT	Temporary storage. Assigned volume INPT2 namelist. Not used anymore.
VLMI	1	DIFEQ	DIFFUN	Contains current VLMI(NPT) $\times 10^{-3}$.
VELIN	20	MIKE1	MHD DIFFUN	Contains velocity data from channel inputs under the conditions of MODEL 1. (Default model if NMPATH= 0.
VACI	13	PERF	RKTOUT	In RKTOUT, I_{vac} , (lb force) (sec)/ (lb mass).

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
VLM	13	POINTS	EQLBRM THERMP DIFFUN OUT2	Volume, cm ³ /g, stored for output.
VMIN	2	MISC	MAIN REACT NEWOF	$V^{-(k)}$, negative oxidation state of total oxidant (if k = 1) or total fuel (if K = 2) eq. (201).
VMOC	13	PERF	RKTOUT MHD	$\mathcal{M}$, Mach number. Used as temporary storage of velocity at each point in MHD.
VOL	1	INDX	MAIN HCALC NEWOF EQLBRM MATRIX THERMP	Logical variable indicating (if true) volume has been assigned. Not allowed
VPLS	2	MISC	MAIN REACT NEWOF	$V^{+(k)}$, positive oxidation state of total oxidant (if k = 1) or total fuel (if k = 2).
WM	13	POINTS	OUT2 EQLBRM ROCKET RKTOUT	M, molecular weight of the mixture, kg/kg-mole, eq. (2).
WP	2	MISC	MAIN	$WP(k) = \sum_{j=1}^{NREAC} w_j^{(k)}$
X	60	DOUBLE	EQLBRM GAUSS MATRIX	Answer region for matrix solution.
XJY	26	MHDD	DIFFUN	Temporarily stores: SIGMA (NPT) *UE*(XK-1.0)*BZ for solution of channel equations.

Appendix B (Cont'd)

<u>Variable</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
XINDP	20	MIKEØ	MHD DIFFUN	Contains the independent X position value of the channel inputs
XK	1	MHDD	ROCKET DIFFUN SETEQU	Inputted in ROCKET by namelist RKTINP and appears in channel equations as (XK-1. 0).
XELMC	30	TSTG	SRCHCC	Contains the molecular weights of the elements stored in LLMT.
XMWC	30	TSTG	SRCHCC ROCKET	Contains the molecular weights of the species contained in the SUB array.

APPENDIX C
PROGRAM LISTING

C	PROGRAM NEQMDH(INPUT,OUTPUT,TAPE7,TAPE5=INPUT,TAPE6=OUTPUT)	MAIN	10	PAGE 0001
C	PROGRAM NEQMDH(INPUT,OUTPUT,TAPE7,TAPE5=INPUT,TAPE6=OUTPUT)	MAIN	10	
C		MAIN	20	
C		MAIN	30	
C	THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR	MAIN	40	
C	NON-CDC MACHINES	MAIN	50	
C		MAIN	60	
C	DOUBLE PRECISION TTT,TM,PP,SIGMA,SIG,VLM,VLM	MAIN	70	
C	DOUBLE PRECISION ENN,EMM,SUMN,AWT	MAIN	80	
C	DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS,SS	MAIN	90	
C	DOUBLE PRECISION G,X,S,EN,ENLN,H0,DELN,ENLS,ATERM,AMULT	MAIN	100	
C	DOUBLE PRECISION X0CRIT,COEF,DXOUTP	MAIN	110	
C		MAIN	120	
C	REAL MIX(15)	MAIN	130	
C	INTEGER DATA, CMIT, ENSERT, REAC, BLANK, THRM, END, SUB, TWO	MAIN	140	
C	LOGICAL SHOCK,MMHG,UV,DETN,SUNIT,NSOM,CALCH	MAIN	150	
C	LOGICAL HP,SP,TP,NEWR,IONS,MOLES,PROZ,EOL,PSIA,RKT,VOL,TV,SV	MAIN	160	
C	LOGICAL FA,OXFL,ERATIO,FPCT,OTTO	MAIN	170	
C	LOGICAL NEOL,CONVG,LOGV,SFLG,AREA,HPTH,SPATH	MAIN	180	
C	LOGICAL TWOSTG	MAIN	190	
C		MAIN	200	
C	DIMENSION FHE(4),FHS(4),FSE(4),FSS(4),FCE(4),FCS(4),FPE(4),FPS(4)	MAIN	210	
C	DIMENSION FRE(4),FRS(4),FIE(4),FIS(4),FAE(4),PAS(4),RHE(4),RHS(4)	MAIN	220	
C	DIMENSION NCD(4),ENSERT(3,30),RHO(26),LVP(2),VM(2),	MAIN	230	
C	1 VL(26),DAT(30)	MAIN	240	
C	COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)	MAIN	250	
C	1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)	MAIN	260	
C	2 ,VLM(13),TOTN(13)	MAIN	270	
C	COMMON/SOLUT/NSOL,ISOLN(3,16),SFLG,SUMSN,ENNS,ENLS	MAIN	280	
C	COMMON/MISC/SS,ENN,SUMN,TT,ATCM(3,101),LLMT(30),B0(30),B0P(30,2)	MAIN	290	
C	1 ,TM,TLOW,TMID,THIGH,CPSUM,PP,OF,EORAT,FPCT,R,RR,HSUB0,AC(2),AM(2)	MAIN	300	
C	2 ,HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(30),NAME(30,5)	MAIN	310	
C	3 ,ANUM(30,5),PRCWT(30),ENTH(30),FAZ(30),RTEMP(30),FOX(30),DENS(30)	MAIN	320	
C	4 ,RHOP,RMW(30),TLN,CR,OXF(30),ENNL,ENSAVE,ENLSAV,TRACE,SIZE	MAIN	330	
C	COMMON /DOUBLE/ G(60,61), X(60)	MAIN	340	
C	COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,ISV, NPP, MOLES,NP,NT,NPT,NLM	MAIN	350	
C	1 ,NS,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,NSUB,NSUP,ITM,CPCVFR,CPCVEQ	MAIN	360	
C	2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NPZ,CALCH	MAIN	370	
C	3 ,IQSAVE,LSAVE,ISUP,ISUB,ITNUM	MAIN	380	
C	COMMON/PERF/PCP(22),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)	MAIN	390	
C	1 ,APP(13),AEAT(13),CSTR,EOL,PROZ,SS0,AREA,AWT	MAIN	400	
C	COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)	MAIN	410	
C	1 ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMT19,FA1,FA2	MAIN	420	
C	2 ,FR1,FC!,FN(4),FR(4),FF(4),FI(4),FMT9X,F0,FRHO(4)	MAIN	430	
C	COMMON/MHDD/SSUMW,DX,DXI,XJY(26),AI(26),UE,NITER,NSTOP,SIG(26),IPP	MAIN	440	
C	X ,BZ,XK,PPPP	MAIN	450	
C	COMMON/EQ/NEOL,ACCURC,HMIN	MAIN	460	
C	COMMON/NEQ/B0N(30),EMM,SNEQ,NQ1,NSK,NEQPT	MAIN	470	
C		MAIN	480	
C	COMMON/SPECE1/NSPCMX,NCMAX,NELMX,TEMP(175,2),SUB(600,3),S(600)	MAIN	490	
C	COMMON/SPECE2/FNLN(600)	MAIN	500	
C	COMMON/SPECE3/H0(600)	MAIN	510	
C	COMMON/SPECE4/DELN(600)	MAIN	520	
C	COMMON/SPECE5/IUSE(600)	MAIN	530	
C	COMMON/SPECE6/SLN(600)	MAIN	540	
C	COMMON/SPECE7/SCONMX(600)	MAIN	550	
C	COMMON/SPECE8/OMIT(3,600)	MAIN	560	

C	PROGRAM NEQMD(INPUT,OUTPUT,TAPE7,TAPE5-INPUT,TAPE6-OUTPUT)	MAIN 10	PAGE 0002
	COMMON/SPECES/DATE(2,600)	MAIN 570	
	COMMON/KC/EN(13,600)	MAIN 580	
	COMMON/THIF/COEF(2,7,600)	MAIN 590	
	COMMON/STOIC/A(30,600)	MAIN 600	
	COMMON/TSTG/TWOSTG,ALPH,NLM1,XELMC(30),XMWC(600)	MAIN 610	
C	COMMON/DBGVEC/DXOUTP(200)	MAIN 620	
C		MAIN 630	
C		MAIN 640	
C...	NSPCMX REFERS TO THE MAXIMUM NO. OF SPECIES ALLOWED	MAIN 650	
C	IF MORE IS NEEDED CHANGE THIS VARIABLE AS WELL	MAIN 660	
C	AS THE APPROPRIATE NO. DEFINING THE SIZE OF	MAIN 670	
C	S,ENLN,H0,DELN,IUSE,SLN,SCONMX,EN,COEF,A,XMWC	MAIN 680	
C...	NCMAX REFERS TO THE MAXIMUM NO. OF CONDENSED SPECIES ALLOWED	MAIN 690	
C	THIS IS FIXED AND REFERS TO THE SIZE OF TEMP(N,2) IN COMMON	MAIN 700	
C	SPECI.....MUST CHANGE THIS COMMON EVERYWHERE IF A LARGER	MAIN 710	
C	SIZE IS NEEDED	MAIN 720	
C...	NELMX REFERS TO THE MAXIMUM NO. OF ELEMENTS ALLOWED	MAIN 730	
C	THIS IS FIXED AND REFERS TO THE SIZE OF XELMC(N) AND	MAIN 740	
C	A(N,NSPCMX).....MUST CHANGE COMMON TSTG AND STOIC	MAIN 750	
C	EVERYWHERE IF A LARGER SIZE IS NEEDED	MAIN 760	
C		MAIN 770	
	COMMON/MIKE0/NNDUMY(3),IMPRNT,NMPATH,NUMIV,XINDP(90)	MAIN 780	
	COMMON/MIKE1/ATERM,AMULT,VELIN(90)	MAIN 790	
	COMMON/MIKE2/HPATH,SPATH,PRESIN(90)	MAIN 800	
	COMMON/MIKE3/AREAIN(90)	MAIN 810	
	COMMON/MIKE5/NNNNN,X0CRIT,DUMMIN(90)	MAIN 820	
	COMMON/MIKE7/CHCALC,CHNLEN,IPRRKT,TMPSTP,TDIFUN,TEQLBM	MAIN 830	
	COMMON/MIKE8/EXIN,BZOUT(13),BETOUT(13)	MAIN 840	
C...	NNDUMY(3) IS DEFINED IN MHD AS WELL AS IMPRNT AND NMPATH	MAIN 850	
C...	NUMIV IS THE MAX. NO. OF PTS. TO BE INPUTTED=90(SET LATTER)	MAIN 860	
C...	XINDP CONTAINS INDEPENDENT X-VARIABLE	MAIN 870	
C...	VELIN,PRESIN,AREAIN CONTAINS PRESSURE,VELOCITY,OR AREA TO BE INPUTTMAIN	MAIN 880	
	EQUIVALENCE (OXF(1),MIX(1)),(NLS,IC)	MAIN 890	
	1,(RHO(1),P(1),VL(1)),(DATA(1),DAT(1)),(OF,OXFL)	MAIN 900	
	EQUIVALENCE (OTTO,CPCVFR),(CPCVEQ,LOGV)	MAIN 910	
C		MAIN 920	
C	*****	MAIN 930	
C	SOME INFORMATION USED IN VARIABLE OUTPUT FORMAT	MAIN 940	
C		MAIN 950	
	DATA FPS/4HP, N,4H/SQ,1HM,1H /	MAIN 960	
	1,FHS/4HH, K,4HJ/KG,1H,1H / ,FSS/4HS, K,4HJ/(K,4HG)(K,1H) /	MAIN 970	
	2,FCS/4HCP, ,4HKJ/(,4HKG)(,2HK) / ,FRS/4HCSTA,4HR, M,4H/SEC,1H /	MAIN 980	
	3,FIS/4HISP, ,4H M/S,2HEC,1H / ,FAS/4HIVAC,4H, M/,3HSEC,1H /	MAIN 990	
	4,RHE/4HRHO, ,4H G/C,1HC,1H / ,RHS/4HRHO, ,4H KG/,4HCU M,1H /	MAIN1000	
	DATA FPE/4HP, A,2HTM,1H,1H /	MAIN1010	
	1,FHE/4HH, C,4HPL/G,2H,1H / , FSE/4HS, C,4HAL/(,4HG)(K,2H) /	MAIN1020	
	2,FCE/4HCP, ,4HCAL/,4H(G)(,2HK) /	MAIN1030	
	DATA FRE/4HCSTA,4HR, F,4HT/S,2HC / ,FAE/4HIVAC,4H LB-,4HSEC/,2HLB/	MAIN1040	
	DATA FIE/'HISP, ,4H LB-,4HSEC/,2HLB/	MAIN1050	
	DATA TWO/4HTWOS/	MAIN1060	
C		MAIN1070	
	DATA MIT/4HOMIT/,BLANK/1H / , REAC/4HREAC/,IZ/2H00/	MAIN1080	
	1 ,NMLT/4HNAME/,IE/1HE/,INSERT/4HINSE/,THRM/4HTHER/,END/3HEND/	MAIN1090	
	2 ,GAS/1HG/,LAST/4HLAST/,TSTOP/4HSTOP/,ISOLU/1HSOLU/	MAIN1100	
C		MAIN1110	
C		MAIN1120	

C PROGRAM: NLSMID INPUT,OUTPUT,TAPE7,TAPE5=INPUT,TAPE6=OUTPUT) MAIN 10 PAGE 0003

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C          NAMELIST COMMENTED OUT - SPECIAL FUNCTIONS ARE USED       MAIN1130
C          FOR THE PRIME       MAIN1140
C          NAMELIST/INPT2/KASE,T,P,PSIA,MMHG,NSQM,V,RHO,ERATIO,OXFL,FPCT,FA,       MAIN1150
*MX,TP,HP,SP,TV,UV,SV,RKT,SHOCK,DETN,OTTO,CR,S0,IONS,IDEBUG,       MAIN1160
* TRACE,SIGNIT,DXI,NITER,NSTOP,NEQL,BZ,XK,ACCURC,HMIN,       MAIN1170
* ALPH,EXIN,TWOSTG       MAIN1180
C       MAIN1190
C*****CONTROL SIZE INTEGERS       MAIN1200
C       NSPCMX=600       MAIN1210
C       NCMAX=175       MAIN1220
C       NELMX=30       MAIN1230
C       NUMIV=90       MAIN1240
C*****       MAIN1250
C       INITIALIZE OTHER VARIABLES IN COMMON       MAIN1260
C       EMM=0.0       MAIN1270
C       TEQLBM=1000.0       MAIN1280
C       TMPSTP=1.0       MAIN1290
C       SFLG=.FALSE.       MAIN1300
C       NEQPT=100000       MAIN1310
C       JSOL=0       MAIN1320
C       CONVG=.FALSE.       MAIN1330
C       NNNNN=0       MAIN1340
C       IPP=0       MAIN1350
C       IMPRNT=0       MAIN1360
C       NMPATH=0       MAIN1370
C       NLS=0       MAIN1380
C       JLIO =0       MAIN1390
C       NEWNR = .FALSE.       MAIN1400
C       DO 200 K=1,30       MAIN1410
C       B0(K)=0.0       MAIN1420
C       B0N(K)=0.0       MAIN1430
C       200 CONTINUE       MAIN1440
C       1 WRITE(6,400)       MAIN1450
C       400 FORMAT(1H1)       MAIN1460
C       NSOL=0       MAIN1470
C       RR = 8314.3       MAIN1480
C       R = RR/4184.       MAIN1490
C       203 READ (5,204) (DATA(I),I=1,15)       MAIN1500
C       204 FORMAT(5(3A4,3X))       MAIN1510
C       WRITE (6,2045) (DATA(I),I=1,15)       MAIN1520
C       2045 FORMAT(1X,5(3A4,3X))       MAIN1530
C       IF(DATA(1).EQ. JSOLU) GO TO 315       MAIN1540
C       IF(DATA(1).EQ.THRM) GO TO 90       MAIN1550
C       IF(DATA(1).EQ.REAC) GO TO 11       MAIN1560
C       IF (DATA(1).EQ.MIT) GO TO 205       MAIN1570
C       IF (DATA(1).EQ.INSERT) GO TO 180       MAIN1580
C       IF (DATA(1).EQ.WMLT) GO TO 210       MAIN1590
C       IF (DATA(1).EQ.BLANK) GO TO 203       MAIN1600
C       IF (DATA(1).EQ.ISTOP) STOP       MAIN1610
C       1023 WRITE(6,1024)       MAIN1620
C       1024 FORMATT(4040)ERROR IN ABOVE CARD. CONTENTS IGNORED. )       MAIN1630
C       GO TO 203       MAIN1640
C       11 NSERT = 0       MAIN1650
C       MAIN1660
C       MAIN1670
C       MAIN1680

```

```

      MOLES = .FALSE.
      IF(NLWR) NLS=0
      TWOSTG=.FALSE.
      IF(DATA(4).EQ.TWO)TWOSTG=.TRUE.
      CALL REACT
      IF(NLM.EQ.0) WRITE(6,52)
52  FORMAT(24H0ERROR IN REACTANT CARDS)
      CALCH = .FALSE.
      DO 755 N=1,NREAC
      IF(NAME(N,5).EQ.IZ) CALCH=.TRUE.
755  CONTINUE
      GO TO 203

C
C  READ THERMO DATA FROM CARDS AND STORE ON TAPE 7
C
      90 NEWR = .TRUE.
      REWIND 7
      READ(5,5) TLOW,TMID,THIGH
      5  FORMAT (3F10.3)
      WRITE (7,5) TLOW,TMID,THIGH
      97 READ (5,10)(DAT(I),I=1,15),NCD(1)
      10 FORMAT(3A4,6X,2A3,4(A2,F3.0),A1,2F10.3,I15)
      IF(DATA(1).EQ.BLANK) DATA(1)=END
      WRITE (7,10)(DAT(I),I=1,16)
      IF(DATA(1).NE.END) GO TO 18
      WRITE(7,10) LAST
      END FILE 7
      GO TO 203
      18 READ(5,20)(DAT(I),I=1,5),NCD(2),(DAT(J),J=6,10),NCD(3),(DAT(K),
      1K=11,14),NCD(4)
      20 FORMAT(5E15.8,I5/5E15.8,I5/4E15.8,18X,I2)
      WRITE (7,21)(DAT(I),I=1,14)
      21 FORMAT(5E15.8/5E15.8/4E15.8)
      DO 25 I=1,4
      IF(NCD(I).EQ.1) GO TO 25
      WRITE(6,22) (DATA(J),J=1,3)
      22 FORMAT(28H0ERROR IN ORDER OF CARDS FOR ,3A4)
      25 CONTINUE
      GO TO 97

C
C  CHECK INSERT CARDS
C
      180 DO 185 I=4,15,3
      IF (DATA(I).EQ.BLANK) GO TO 185
      NSERT = NSERT+1
      ENSERT(1,NSERT) = DATA(I)
      ENSERT(2,NSERT) = DATA(I+1)
      ENSERT(3,NSERT) = DATA(I+2)
      185 CONTINUE
      GO TO 203

C
C  CHECK OMIT CARDS
C
      205 DO 208 I=4,15,3
      IF(DATA(I).EQ.BLANK) GO TO 208
      NOMIT = NOMIT+1
```

```

MAIN1690
MAIN1700
MAIN1710
MAIN1720
MAIN1730
MAIN1740
MAIN1750
MAIN1760
MAIN1770
MAIN1780
MAIN1790
MAIN1800
MAIN1810
MAIN1820
MAIN1830
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MAIN1860
MAIN1870
MAIN1880
MAIN1890
MAIN1900
MAIN1910
MAIN1920
MAIN1930
MAIN1940
MAIN1950
MAIN1960
MAIN1970
MAIN1980
MAIN1990
MAIN2000
MAIN2010
MAIN2020
MAIN2030
MAIN2040
MAIN2050
MAIN2060
MAIN2070
MAIN2080
MAIN2090
MAIN2100
MAIN2110
MAIN2120
MAIN2130
MAIN2140
MAIN2150
MAIN2160
MAIN2170
MAIN2180
MAIN2190
MAIN2200
MAIN2210
MAIN2220
MAIN2230
MAIN2240
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      OMIT(1,NOMIT) = DATA(I)
      OMIT(2,NOMIT) = DATA(I+1)
      OMIT(3,NOMIT) = DATA(I+2)
208  CONTINUE
      NEWR=.TRUE.
      REWIND 7
      GO TO 203
C
C      CHECK SOLU CARDS
C
      315 DO 308 I=4,15,3
            IF(DATA(I) .EQ. BLANK) GO TO 308
            IF(NSOL .EQ. 16) GO TO 203
            NSOL=NSOL+1
            ISOLN(1,NSOL)=DATA(I)
            ISOLN(2,NSOL)=DATA(I+1)
            ISOLN(3,NSOL)=DATA(I+2)
      308  CONTINUE
            GO TO 203
C
C      BEGIN NAMELIST INPT2
C
      210 DO 300 I=1,26
            P(I) = 0.
            T(I) = 0.
            V(I) = 0.
      300  CONTINUE
            TRACE = 0.
            SS = 0.
            CR = 0.
            LSAVE=0
            PHOP = 0.
            KASE= 0
            TP = .FALSE.
            HP=.FALSE.
            SP=.FALSE.
            TV = .FALSE.
            UV = .FALSE.
            SV = .FALSE.
            OTTO = .FALSE.
            NEOL = .FALSE.
            RKT = .FALSE.
            SHOCK = .FALSE.
            DETN = .FALSE.
            VOL = .FALSE.
            MMHG = .FALSE.
            PSIA = .FALSE.
            NROM = .FALSE.
            SUNIT = .FALSE.
            IONS = .FALSE.
            HMIN=1.E-15
            ACCURC=1.E-3
            IDEBUG=0
            FA = .FALSE.
            TWOSTG=.FALSE.
            EXIN=2400.

```

```

MAIN2250
MAIN2260
MAIN2270
MAIN2280
MAIN2290
MAIN2300
MAIN2310
MAIN2320
MAIN2330
MAIN2340
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MAIN2380
MAIN2390
MAIN2400
MAIN2410
MAIN2420
MAIN2430
MAIN2440
MAIN2450
MAIN2460
MAIN2470
MAIN2480
MAIN2490
MAIN2500
MAIN2510
MAIN2520
MAIN2530
MAIN2540
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MAIN2560
MAIN2570
MAIN2580
MAIN2590
MAIN2600
MAIN2610
MAIN2620
MAIN2630
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MAIN2670
MAIN2680
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MAIN2700
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MAIN2740
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MAIN2770
MAIN2780
MAIN2790
MAIN2800

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      ALPH=0.
      OXFL= .FALSE.
      ERATIO = .FALSE.
      FPCT= .FALSE.
      DO 303 I=1,15
      MIX(I) = 0.
303  CONTINUE
C
      DXI=0.0
      BZ=0 0
      XK=0.0
      NITER=0
      NSTOP=0
C
      NT = 1
      EQL = .TRUE.
C
      READ(5,INPT2)
C++++ CALL NMLST('INPT2 ',0,5,KASE,T,P,PSIA,MMHG,NSQM,V,RHO,ERATIO,OXFL
C++++1,FPCT,FA,MIX,TP,HP,SP,TV,UV,SV,RKT,SHOCK,DETN,OTTO,CR,S0,IONS,
C++++2IDEBUG,TRACE,SIUNIT,DXI,NITER,NSTOP,NEQL,BZ,XK,ACCURC,
C++++3HMIN,ALPH,EXIN,TWOSTG)
      IF(RKT)GO TO 77
      IPRRKT=3
      IF(KASE.EQ.7777)IMPRNT=4
      CHNLIN=-1.0
77  CONTINUE
      WRITE(6,400)
      WRITE(6,INPT2)
C++++ CALL NMLST('INPT2 ',1,6,KASE,T,P,PSIA,MMHG,NSQM,V,RHO,ERATIO,OXFL
C++++1,FPCT,FA,MIX,TP,HP,SP,TV,UV,SV,RKT,SHOCK,DETN,OTTO,CR,S0,IONS,
C++++2IDEBUG,TRACE,SIUNIT,DXI,NITER,NSTOP,NEQL,BZ,XK,ACCURC,
C++++3HMIN,ALPH,EXIN,TWOSTG)
      IF(DXI.EQ.0.0)DXI=0.05
      IF(ACCURC.EQ.0.0)ACCURC=1.0E-3
      IF(HMIN.EQ.0.0)HMIN=1.0E-15
      DX=DXI
      IF (SIUNIT) GO TO 450
      DO 410 I =1,4
      FP(I) = FPE(I)
      FH(I) = FHE(I)
      FS(I) = FSE(I)
      FC(I) = FCE(I)
410  FRHO(I) = RHE(I)
      IF (.NOT.RKT) GO TO 490
      DO 420 I = 1,4
      FR(I) = FRE(I)
      FI(I) = FIE(I)
420  FF(I) = FAE(I)
      GO TO 490
450  R = RR/1000.
      DO 430 I = 1,4
      FP(I) = FPS(I)
      FH(I) = FHS(I)
      FS(I) = FSS(I)
      FC(I) = FCS(J)

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MAIN2810
MAIN2820
MAIN2830
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MAIN2850
MAIN2860
MAIN2870
MAIN2880
MAIN2890
MAIN2900
MAIN2910
MAIN2920
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MAIN2940
MAIN2950
MAIN2960
MAIN2970
MAIN2980
MAIN2990
MAIN3000
MAIN3010
MAIN3020
MAIN3030
MAIN3040
MAIN3050
MAIN3060
MAIN3070
MAIN3080
MAIN3090
MAIN3100
MAIN3110
MAIN3120
MAIN3130
MAIN3140
MAIN3150
MAIN3160
MAIN3170
MAIN3180
MAIN3190
MAIN3200
MAIN3210
MAIN3220
MAIN3230
MAIN3240
MAIN3250
MAIN3260
MAIN3270
MAIN3280
MAIN3290
MAIN3300
MAIN3310
MAIN3320
MAIN3330
MAIN3340
MAIN3350
MAIN3360

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430 FRHO(I) = RHS(I)                                MAIN3370
WRITE(6,9902)                                         MAIN3380
9902 FORMAT(14H CHECK POINT 2)                        MAIN3390
IF (.NOT.RKT) GO TO 490                               MAIN3400
DO 440 I = 1,4                                         MAIN3410
FR(I) = FRS(I)                                         MAIN3420
FI(I) = FIS(I)                                         MAIN3430
440 FF(I) = FAS(I)                                     MAIN3440
490 CONTINUE                                           MAIN3450
IF (.NOT.DETN.AND..NOT.SHOCK) GO TO 1303             MAIN3460
DO 1300 N=1,NREAC                                     MAIN3470
IF (FAZ(N).NE.GAS) GO TO 1301                         MAIN3480
1300 CONTINUE                                          MAIN3490
GO TO 1303                                             MAIN3500
1301 WRITE(6,1302)                                     MAIN3510
1302 FORMAT(60H0CONDENSED REACTANTS NOT PERMITTED IN DETN OR SHOCK PROBMAIN3520
1LEMS)
GO TO 1                                                MAIN3530
1303 IF (.NOT.TV.AND..NOT.UV.AND..NOT.SV) GO TO 304   MAIN3540
WRITE(6,9904)                                         MAIN3550
9904 FORMAT(35H1ERROR - VOLUME MAY NOT BE ASSIGNED ) MAIN3560
STOP                                                  MAIN3570
304 DO 305 I=1,26                                     MAIN3580
IF (P(I).EQ.0.) GO TO 322                             MAIN3590
NP = I                                                MAIN3600
IF (MMHG) P(NP) = P(NP)/760.                         MAIN3610
IF (PSIA) P(NP)=P(NP)/14.696006                     MAIN3620
IF (NSQM) P(NP)=P(NP)/101325.                       MAIN3630
305 CONTINUE                                          MAIN3640
322 KKSAV=0                                           MAIN3650
DO 307 IT = 1,26                                     MAIN3660
WRITE(6,9922)(LLMT(IOPG),IOPG=1,NLM)                MAIN3670
9922 FORMAT(8H LLMT = ,/, (10X,A10))                MAIN3680
IF (T(IT).EQ.0.) GO TO 722                           MAIN3690
NT = IT                                               MAIN3700
IF (IT.EQ.1) GO TO 307                               MAIN3710
IF (T(IT).GT.T(IT-1)) KKSAV=1                       MAIN3720
307 CONTINUE                                          MAIN3730
722 CONTINUE                                          MAIN3740
IF (NT.LE.1) GO TO 309                               MAIN3750
IF (KKSAV.EQ.0) GO TO 309                            MAIN3760
KKSAV=NT-1                                           MAIN3770
DO 306 III=1, KKSAV                                  MAIN3780
IIIP1=III+1                                           MAIN3790
DO 306 JJJ=IIIP1,NT                                  MAIN3800
IF (T(III).GE.T(JJJ)) GO TO 306                     MAIN3810
TTEMP=T(III)                                          MAIN3820
T(JJJ)=T(JJJ)                                         MAIN3830
T(JJJ)=TTEMP                                          MAIN3840
306 CONTINUE                                          MAIN3850
309 CONTINUE                                          MAIN3860
DO 625 IST=1,15                                       MAIN3870
IF (WP(1).EQ.0.) OXF(IST)=0.                         MAIN3880
IF (WIX(IST).NE.0.) GO TO 323                       MAIN3890
IF (IST.NE.1) GO TO 745                             MAIN3900
WRITE(6,724)                                          MAIN3910

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```
724 FORM=T(48#NO INPT2 VALUE GIVEN FOR OF, EORAT, FA, OR FPCT )
      IF ( F(2).NE.#.) OF = WP(1)/WP(2)
      GO TO 333
323 OF = MIX(IST)
      IF(FA) OF =1./ MIX(IST)
      IF(FPCT) OF =(100.- MIX(IST))/ MIX(IST)
      IF(.NOT.ERATIO) GO TO 333
      EORAT = MIX(IST)
      OF = (-EORAT*VMIN(2)-VPLS(2))/(VPLS(1)+EORAT*VMIN(1))
333 OXF(IST) = OF
      NOF = IST
625 CONTINUE
745 IF(.NOT.IONS) GO TO 746
      IF(LLMT(NLM).NE.IE) GO TO 744
      IF(NEWR) GO TO 748
      GO TO 750
744 NL=NLM
      NLM = NLM+1
      LLMT(NLM) = IE
      BOP(NLM,1) = #.
      BOP(NLM,2) = #.
      GO TO 747
746 IF(LLMT(NLM).EQ.IE) NLM=NLM-1
      NL=NLM
      NLM1 = NLM+1
      IF(LLMT(NLM1).EQ.IE) GO TO 743
      IF(.NOT.NEWR) GO TO 750
      IF(NLS.NE.#) GO TO 748
743 LLMT(NLM1) = #
747 NEWR = .TRUE.
      REWIND 7
748 CONTINUE
      CAIL SRCHCC
      NSK=NS
750 IF(NS.EQ.#) GO TO 1
      NOMIT=#

C
C INITIAL ESTIMATES
C
      S# = S#/R
      ENN = .1
      NLM1=NLM
      ENNL = -2.3025851
      SUMN = ENN
      XI = NS - NC
      IF(XI.EQ.#.)XI=1.
      XI = LNN/XI
      XLN = ALOG(XI)
      DO 432 J=1,NS
      IF(IUSE(J).GT.#) IUSE(J)=-IUSE(J)
      EN(1,J) = #.
      ENLN(J) = #.
      IF (IUSE(J).NE.#) GO TO 432
      EN(1,J) = XI
      ENLN(J) = XLN
432 CONTINUE
```

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MAIN3930
MAIN3940
MAIN3950
MAIN3960
MAIN3970
MAIN3980
MAIN3990
MAIN4000
MAIN4010
MAIN4020
MAIN4030
MAIN4040
MAIN4050
MAIN4060
MAIN4070
MAIN4080
MAIN4090
MAIN4100
MAIN4110
MAIN4120
MAIN4130
MAIN4140
MAIN4150
MAIN4160
MAIN4170
MAIN4180
MAIN4190
MAIN4200
MAIN4210
MAIN4220
MAIN4230
MAIN4240
MAIN4250
MAIN4260
MAIN4270
MAIN4280
MAIN4290
MAIN4300
MAIN4310
MAIN4320
MAIN4330
MAIN4340
MAIN4350
MAIN4360
MAIN4370
MAIN4380
MAIN4390
MAIN4400
MAIN4410
MAIN4420
MAIN4430
MAIN4440
MAIN4450
MAIN4460
MAIN4470
MAIN4480
```

```

      IQ1 = NLM+1
      IF (NC.EQ.0.OR.NSERT.EQ.0) GO TO 790
      DO 302 I=1,NSERT
      INC = 0
      DO 301 J=1,NS
      IF(IUSE(J).EQ.0) GO TO 301
      INC = INC+1
      IF(SUB(J,1).NE.INSERT(1,I)) GO TO 301
      IF(SUB(J,2).NE.INSERT(2,I)) GO TO 301
      IF(SUB(J,3).NE.INSERT(3,I)) GO TO 301
      IF(T(1).EQ.0.) GO TO 295
      IF(T(1).LT.TEMP(INC,1).OR.T(1).GT.TEMP(INC,2)) GO TO 301
295  IQ1 = IQ1+1
      IUSE(J) = -IUSE(J)
      GO TO 302
301  CONTINUE
302  CONTINUE
790  CONTINUE
      IF(NC.EQ.0.OR.NSOL.EQ.0) GO TO 792
      DO 402 I=1,NSOL
      DO 401 J=1,NS
      IF(IUSE(J).EQ.0) GO TO 401
      DO 403 JJ=1,3
      IF(SUB(J,JJ).NE.ISOLN(JJ,I)) GO TO 401
403  CONTINUE
      IUX=IUSE(J)
      IUSE(J)=-1000 + IUSE(J)
      DO 404 JJ=1,NS
      IF(IUSE(JJ).EQ.IUX) IUSE(JJ)=-2000+IUX
404  CONTINUE
      GO TO 402
401  CONTINUE
402  CONTINUE
      WRITE(6,4000)
4000  FORMAT(20H0SPECIES IN SOLUTION )
      DO 405 J=1,NSOL
      WRITE(6,4001) (ISOLN(JJ,J),JJ=1,3)
4001  FORMAT(2X,3A4)
405  CONTINUE
792  IF(.NOT.TP.AND..NOT.HP.AND..NOT.SP) GO TO 791
      CALL THERMP
      GO TO 800
791  CONTINUE
      IF(RKT) CALL ROCKET
800  NSERT = 0
      GO TO 1
      END
      SUBROUTINE ROCKET
C
C      ROCKET PERFORMANCE
C
C      THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR
C      NON-CDC MACHINES
C
      DOUBLE PRECISION TTT,TM,PP,SIGMA,SIG,VLM,EN
      DOUBLE PRECISION ENN,EMM,SUMN,AWT

```

```

MAIN4490
MAIN4500
MAIN4510
MAIN4520
MAIN4530
MAIN4540
MAIN4550
MAIN4560
MAIN4570
MAIN4580
MAIN4590
MAIN4600
MAIN4610
MAIN4620
MAIN4630
MAIN4640
MAIN4650
MAIN4660
MAIN4670
MAIN4680
MAIN4690
MAIN4700
MAIN4710
MAIN4720
MAIN4730
MAIN4740
MAIN4750
MAIN4760
MAIN4770
MAIN4780
MAIN4790
MAIN4800
MAIN4810
MAIN4820
MAIN4830
MAIN4840
MAIN4850
MAIN4860
MAIN4870
MAIN4880
MAIN4890
MAIN4900
MAIN4910
MAIN4920
MAIN4930
MAIN4940
MAIN4950
ROCK 10
ROCK 20
ROCK 30
ROCK 40
ROCK 50
ROCK 60
ROCK 70
ROCK 80
ROCK 90

```

C	PROGRAM NEQMDH(INPUT,OUTPUT,TAPE7,TAPE5=INPUT,TAPE6=OUTPUT)	MAIN 10	PAGE 0010
	DOUBLE PRECISION X0CRIT	ROCK 100	
	DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS,S0,COEF	ROCK 110	
	DOUBLE PRECISION USQ,S,ASO,ENLN,H0,ENLS,TSV1,DXOUTP	ROCK 120	
	DOUBLE PRECISION TSV2,TSV3,ENSPEC	ROCK 130	
C	INTEGER SUB,SPECNM	ROCK 140	
	INTEGER DDATA,SPEC,BLNK,ENDD	ROCK 150	
	INTEGER*2 NORDER(600),NORDCN(200)	ROCK 160	
	LOGICAL SHOCK,MMHG,UV,DETN,SIUNIT,NSOM,CALCH,SEQL,RKTO	ROCK 170	
	LOGICAL HP,SP,TP,NEW,IONS,MOLES,FROZ,EQL,PSIA,RKT,VOL,TV,SV	ROCK 180	
	LOGICAL FA,ERATIO,FPCT,O 'TO	ROCK 190	
	LOGICAL NEQL,CONVG,LOGV,SFLG,AREA,THI,FIRST,PFLAG	ROCK 200	
	LOGICAL TWOSTG,HPATH,SPATH	ROCK 210	
C	REAL INTERP	ROCK 220	
C	COMMON/SOLUT/NSOL,ISOLN(3,16),SFLG,SUMSN,ENNS,ENLS	ROCK 230	
	COMMON/DBGVEC/DXOUTP(1)	ROCK 240	
	DIMENSION CHNLS(10),TCHINP(10)	ROCK 250	
	DIMENSION DDATA(9),ENDD(7),ENDNW(30),SPECNM(30,3)	ROCK 260	
	COMMON/MIKE5/NVNNN,X0CRIT,DUMMIN(1)	ROCK 270	
	COMMON/MIKE6/SPECNM	ROCK 280	
	COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)	ROCK 290	
	1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)	ROCK 300	
	2 ,VLM(13),TOTN(13)	ROCK 310	
	COMMON/START/FIRST	ROCK 320	
	COMMON/MISC/S0,ENN,SUMN,TT,ATOM(3,101),LLMT(30),B0(30),B0P(30,2)	ROCK 330	
	1 ,TM,TLOW,TMID,THIGH,CPSUM,PP,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)	ROCK 340	
	2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(30),NAME(30,5)	ROCK 350	
	3 ,ANUM(30,5),PECWT(30),ENTH(30),FAZ(30),RTEMP(30),FOX(30),DENS(30)	ROCK 360	
	4 ,RHOP,RMW(30),TLN,CR,OX*(30),ENNL,ENSAVE,ENLSAV ,TRACE,SIZE	ROCK 370	
	COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,ISV, NPP, MOLES,NP,NT,NPT,NLM	ROCK 380	
	1 ,NS,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEW,NSUB,NSUP,ITM,CPCVFR,CPCVEQ	ROCK 390	
	2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCHROCK	ROCK 400	
	3 ,IOSAVE,LSAVE,ISUP,ISUB,TNUM	ROCK 410	
	COMMON/PERF/PCP(22),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)	ROCK 420	
	1 ,APP(13),AEAT(13),CSTR,EQL,FROZ,SS0,AREA,AWT	ROCK 430	
	COMMON/MHDD/SSUMW,DX,DXI,XJY(26),AI(26),UE,NITER,NSTOP,SIG(26),IPPROCK	ROCK 440	
	X ,BZ,XK,P1PP	ROCK 450	
	COMMON/NEQ/B0N(30),EMM,SNEQ,NQ1,NSK,NEQPT	ROCK 460	
	COMMON/MIKE0/ NNDUMY(4),XMPATH,NUMIV,XINDP(1)	ROCK 470	
	COMMON/MIKE2/HPATH,SPATH,PRESIN(1)	ROCK 480	
C****	ADD MIKE4 FOR TWOSTG CHANGE 1/2/79	ROCK 490	
	COMMON/MIKE4/PCWET(2),HPP2(2),PCWSD(2),B0P2(30,2)	ROCK 500	
	COMMON/MIKE7/CHCALC,CHNL6N,IPRKT,TMPSTP,TDIFUN,TEQLBM	ROCK 510	
	COMMON/NS1SPC/1RSPEC,ENSPEC,RKT	ROCK 520	
C	COMMON/SPECE1/NSPCMX,NCMAX,NELMX,TEMP(175,2),SUB(600,3),S(1)	ROCK 530	
	COMMON/SPECE2/ENLN(1)	ROCK 540	
	COMMON/SPECE3/P0(1)	ROCK 550	
	COMMON/SPECE5/IUSE(1)	ROCK 560	
	COMMON/KGM/EN(13,1)	ROCK 570	
	COMMON/THMF/COEF(2,7,1)	ROCK 580	
	COMMON/STOIC/A(30,1)	ROCK 590	
	COMMON/TSTG/TWOSTG,ALPH,NLM1,XELMC(30),XMC(1)	ROCK 600	
C...	NSPCMX REFERS TO THE MAXIMUM NO. OF SPECIES ALLOWED	ROCK 610	
		ROCK 620	
		ROCK 630	
		ROCK 640	
		ROCK 650	

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C... NCMAX REFERS TO THE MAXIMUM NO. OF CONDENSED SPECIES ALLOWED      ROCK 660
C      THIS IS FIXED AND REFERS TO THE SIZE OF TEMP(N,2) IN COMMON    ROCK 670
C      SPECE1.....MUST CHANGE THIS COMMON EVERYWHERE IF A LARGER S    ROCK 680
C      IS NEEDED                                                         ROCK 690
C... NELMX REFERS TO THE MAXIMUM NO. OF ELEMENTS ALLOWED                ROCK 700
C      THIS IS FIXED AND REFERS TO THE SIZE OF XELMC(N) AND A(N,NS     ROCK 710
C      .....MUST CHANGE COMMON TSTG AND STOIC EVERYWHERE IF           ROCK 720
C      A LARGER SIZE IS NEEDED                                          ROCK 730
C                                                                           ROCK 740
C      EQUIVALENCE (OTTO,CPCVFR),(CPCVEQ,LOGV)                          ROCK 750
C                                                                           ROCK 760
C      NAMELIST COMMENTED OUT - SPECIAL FUNCTIONS USED FOR THE        ROCK 770
C      PRIME                                                             ROCK 780
C                                                                           ROCK 790
C      NAMELIST/RKTINP/EQL,FROZ,SUBAR,SUPAR,PCP,TCEST,NFZ,NEQPT,        ROCK 800
C      *HTLOSS,HPATH,SPATH,NUMHLS,CHNLEN,CHNHLS,TCHINP,TCHFNL,IPRRKT    ROCK 810
C      DATA BLNK/4H /                                                  ROCK 820
C      DATA CHECK/4.E-5/,SPEC/4HSPEC/,MSPCMN/30/                      ROCK 830
C.....                                                                  ROCK 840
C      JJPATH=1                                                         ROCK 850
C      HTLOSS=.0.0                                                       ROCK 860
C      HPATH=.FALSE.                                                    ROCK 870
C      SPATH=.TRUE.                                                      ROCK 880
C      TCEST = 3000.                                                     ROCK 890
C      ENSPEC=.0.0                                                       ROCK 900
C      IRSPEC=.0                                                         ROCK 910
C      PCRT=.0.0                                                         ROCK 920
C      SFLG=.FALSE.                                                      ROCK 930
C      NPPP = 0                                                          ROCK 940
C      FIRST=.TRUE.                                                      ROCK 950
C      ITM = 1                                                           ROCK 960
C      NFZ = 1                                                           ROCK 970
C      APP(1) = 1.                                                       ROCK 980
C      DO 295 I=1,10                                                     ROCK 990
C      CHNHLS(I)=0.0                                                     ROCK1000
C      TCHINP(I)=0.0                                                     ROCK1010
295 CONTINUE                                                            ROCK1020
C      TCHFNL=0.0                                                        ROCK1030
C      NUMHLS=0                                                          ROCK1040
C      IPRRKT=0                                                          ROCK1050
C      CHNLEN=1.0                                                        ROCK1060
C      TEQLBM=1000.0                                                     ROCK1070
C      DO 300 I=1,26                                                     ROCK1080
C      PCP(I)= 0.                                                        ROCK1090
C      SUBAR(I) = 0.                                                     ROCK1100
300 CONTINUE                                                            ROCK1110
C      NEQPT=1000000                                                     ROCK1120
C      MOL = .TRUE.                                                      ROCK1130
C      FROZ = .FALSE.                                                    ROCK1140
C      RKTO = .FALSE.                                                    ROCK1150
C      READ (5,RKTINP)                                                  ROCK1160
C**** CALL NMLST('RK INP',0,5,EOL,FROZ,SUBAR,SUPAR,PCP,TCEST,NFZ,NEQPT ROCK1170
C**** ,HTLOSS,HPATH,SPATH,NUMHLS,CHNLEN,CHNHLS,TCHINP,TCHFNL,        ROCK1180
C**** IPRRKT)                                                           ROCK1190
C      IF(NEQPT.LE.0) NEQPT=1000000                                     ROCK1200
C      IF(NEQPT.EQ.2) NEQPT=1000000                                     ROCK1210

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      NPP = 0
      CHCALC=CHNHLS(1)
      TMPSTF=TCHFNL+10.
      TDIFUN=300.0
      IF(TDIFUN.GT.TCHFNL)TDIFUN=TCHFNL
      IF(CHCALC.NE.0.0)TEQLBM=500.0
C**** IF(TCHFNL.NE.0.0)PCRT=0.0
      IF(NUMHLS-1)301,302,303
303 CONTINUE
      CHCALC=INTERP(TCHFNL,TCHINP,CHNHLS,1,NUMHLS,DINT,IER)
302 CONTINUE
      CHCALC=CHCALC*8314.3/1.987165
      IF(IPRRTT.GE.0)WRITE(1,3999) CHCALC,TCHFNL
3999 FORMAT(1X,7HCHCALC=,F12.3,10X,7HTCHFNL=,F10.3)
301 CONTINUE
      IF(NUMHLS.LE.0)CHCALC=0.0
      NPP = 500
CCCC IF(RKTO.AND.PCP(1).NE.0.) NPP=4
      IF(PCP(1).EQ.0.0)RKTO=.TRUE.
      NSUB = 0
      NSUP = 0
      IF(RKTO) GO TO 6
      IF(PCP(1).NE.0.) NPPP = 1
      DO 320 I=1,13
6        IF(SUBAR(I).NE.0.) NSUB=NSUB+1
          IF(SUPAR(I).NE.0.) NSUP=NSUP+1
320 CONTINUE
          IF(NSUB.GT.0)NPP=2
          IF(NSUP.GT.0)NPP=2
          WRITE (6,RKTINP)
C++++ CALL NMLST('RKTINP',1,6,EQL,FROZ,SUBAR,SUPAR,PCP,TCEST,NFZ,NEQPT
C++++ ,HTLOSS,HPATH,SPATH,NUMHLS,CHNLN,CHNHLS,TCHINP,TCHFNL,
C++++ IPRRTT)
          NFZS = NFZ
          SEQL = EQL
          IOF = 0
          TT = TCEST
C
C      LOOP FOR EACH O/F
C
321 IT = 1
      IOF = IOF + 1
      OF = OXF(IOF)
C***** DELETE NEXT LINE FOR TWOSTG FIX
C*** IF(TWOSTG)OF=(1.-BETH)*OF
      IF(TWOSTG) WRITE(6,90)
90 FORMAT(/,35X,4'HFIRST STAGE PROPERTIES BEFORE SLAG REJECTION)
C***** KKKK=22
C**** WRITE(1,9876) KKKK
      CALL NEWOF
      HSUB0=HSUB0-HTLOSS/1.987165
      IJH=0
      IJS=1
      IF(HPATH)IJH=1
      IF(.NOT.SPATH)IJS=0
      IF(IPRRTT.GE.0)WRITE(1,50000) HSUB0,HTLOSS,IJH,IJS

```

ROCK1220
 ROCK1230
 ROCK1240
 ROCK1250
 ROCK1260
 ROCK1270
 ROCK1280
 ROCK1290
 ROCK1300
 ROCK1310
 ROCK1320
 ROCK1330
 ROCK1340
 ROCK1350
 ROCK1360
 ROCK1370
 ROCK1380
 ROCK1390
 ROCK1400
 ROCK1410
 ROCK1420
 ROCK1430
 ROCK1440
 ROCK1450
 ROCK1460
 ROCK1470
 ROCK1480
 ROCK1490
 ROCK1500
 ROCK1510
 ROCK1520
 ROCK1530
 ROCK1540
 ROCK1550
 ROCK1560
 ROCK1570
 ROCK1580
 ROCK1590
 ROCK1600
 ROCK1610
 ROCK1620
 ROCK1630
 ROCK1640
 ROCK1650
 ROCK1660
 ROCK1670
 ROCK1680
 ROCK1690
 ROCK1700
 ROCK1710
 ROCK1720
 ROCK1730
 ROCK1740
 ROCK1750
 ROCK1760
 ROCK1770


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5000 FORMAT(1X,10(1H*),27HHSUB0 HTLOSS HPATH SPATH,/,3X,
*2(F10.3,1X),2(I2,3X))
IF(CALCH.AND.TT.EQ.0.) PETERN
IF(T(1).EQ.0.) GO TO 322
TT = T(1)
C
C LOOP FOR CHAMBER PRESSURES
322 DO 923 IP = 1,NP
NFZ = NFZS
ITNUM = 0
AREA = .FALSE.
IF(T(1).EQ.0.) HP=.TRUE.
IF(T(1).NE.0.) TP=.TRUE.
SP = .FALSE.
EQL = .TRUE.
ISUB = 1
ISUP = 1
PP = P(IP)
C**** KKKK=23
C**** WRITE(1,9876) KKKK
IPP = 1
ITROT = 3
ISUPSV = 1
C
C LOOP FOR PRESSURE RATIOS
C
C***** CODE ADDED TO CHANGE PROGRAM MEANING FOR W.VIRG. 11/27/78
IF(NEOPT.NE.1)GO TO 331
PCRT=0.0
INC=0
IITEM=0
JITEM=0
C**** INITIALIZE VARIABLES TO 0
DO 973 I=1,NS
CCCC IF(IUSE(I).NE.0)GO TO 973
EN(1,I)=0.0
ENLN(I)=0.0
973 CONTINUE
JJPATH=-10
HP=.TRUE.
C***** INPUT SPEC IN COLUMNS 1-4 AND FLOW VELOCITY(INITIAL) IN COLUMNS
C 13-23 IN E11.4 FORMAT
C.....SPECIAL INPUT IRSPEC CONTAINS THE POSITION OF THE REACTANTS
C SPECIES WHICH WILL BECOME THE NS=1 SPECIES(NOT AN ELEMENT)
C POSITION ENTERED IN I3 FORMAT ENDING IN COLUMN 30.....
READ(5,986) (DDATA(I),I=1,3),UEINP,IRSPEC
986 FORMAT(3A4,E11.4,4X,I3)
989 FORMAT(3(3A4,I3,8X))
IF(DDATA(1).EQ.SPEC)GO TO 909
980 WRITE(6,903)
988 FORMAT(1X,10(1H*),40HERROR..INCORRECT SPEC CARD FOR NEOPT=1 PROB)
STOP 2
909 CONTINUE
C... CALCULATE VARIABLES NEEDED TO DETERMINE CONCENTRATIONS OF
C SPEC SPECIES
TSAV1=0.0

```

ROCK1780
 ROCK1790
 ROCK1800
 ROCK1810
 ROCK1820
 ROCK1830
 ROCK1840
 ROCK1850
 ROCK1860
 ROCK1870
 ROCK1880
 ROCK1890
 ROCK1900
 ROCK1910
 ROCK1920
 ROCK1930
 ROCK1940
 ROCK1950
 ROCK1960
 ROCK1970
 ROCK1980
 ROCK1990
 ROCK2000
 ROCK2010
 ROCK2020
 ROCK2030
 ROCK2040
 ROCK2050
 ROCK2060
 ROCK2070
 ROCK2080
 ROCK2090
 ROCK2100
 ROCK2110
 ROCK2120
 ROCK2130
 ROCK2140
 ROCK2150
 ROCK2160
 ROCK2170
 ROCK2180
 ROCK2190
 ROCK2200
 ROCK2210
 ROCK2220
 ROCK2230
 ROCK2240
 ROCK2250
 ROCK2260
 ROCK2270
 ROCK2280
 ROCK2290
 ROCK2300
 ROCK2310
 ROCK2320
 ROCK2330

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      NLMOLD=NLM
      NLM=NPOS
      IO1='Q1-KOUNT
C... REORDER NO. OF ELEMENTS AND REMOVE APPROPRIATE A(I,J),B(I)
      DO 4010 I=1,NLM
      K=NORDER(I)
      IF(I.EQ.K)GO TO 4010
      LLMT(I)=LLMT(K)
      B(I)=B(K)
      B(N(I)=B(N(K)
      DO 4005 J=1,NSK
      A(I,J)=A(K,J)
4005 CONTINUE
4010 CONTINUE
C... SEARCH SPECIES TABLE FOR OCCURRENCES OF ALL B COEFFICIENTS
C FLAG THOSE SPECIES FOR REMOVAL AND RECORD THE NEW ORDER
      WRITE(6,4097)
4097 FORMAT(1X,44HREMOVED FOLLOWING SPECIES FROM CONSIDERATION)
      NPOS=N
      DO 4030 I=1,NS
C... RECORD POSITION OF CONDENSED SPECIES
      IF(IUSE(I).EQ.0)GO TO 4019
      INC=INC+1
      NORDCN(INC)=I
4019 CONTINUE
      DO 4020 J=1,NLM
      IF(A(J,I).NE.0.0)GO TO 4026
4020 CONTINUE
C... OUTPUT THE REMOVED SPECIES
      WRITE(6,4098) (SUB(I,K),K=1,3)
      GO TO 4030
4026 NPOS=NPOS+1
      NORDER(NPOS)=I
4030 CONTINUE
      NSOLD=NS
      NS=NPOS
      NSK1=NSK+1
C... PLACE NON-EQUIL TERMS (FROM DLIT) AT END OF LIST
      DO 4031 I=NS1,NSK1
      NPOS=NPOS+1
      NORDER(NPOS)=I
4031 CONTINUE
      NSKOLD=NSK
      NSK1=NPOS
      NSK=NSK1-1
      NS1OLD=NS1
      NS1=NS+1
C... REORDER SPECIES...SHIFT APPROPRIATE VARIABLES
      DO 4040 I=1,NSK1
      NPOS=NORDER(I)
C**** DEBUG
      DXOUTP(I)=NPOS
C**** DEBUG
      IF(I.NE.NPOS)GO TO 4035
      IF(IUSE(I).NE.0)IITEM=IITEM+1
      GO TO 4040

```

```

      ROCK3460
      ROCK3470
      ROCK3480
      ROCK3490
      ROCK3500
      ROCK3510
      ROCK3520
      ROCK3530
      ROCK3540
      ROCK3550
      ROCK3560
      ROCK3570
      ROCK3580
      ROCK3590
      ROCK3600
      ROCK3610
      ROCK3620
      ROCK3630
      ROCK3640
      ROCK3650
      ROCK3660
      ROCK3670
      ROCK3680
      ROCK3690
      ROCK3700
      ROCK3710
      ROCK3720
      ROCK3730
      ROCK3740
      ROCK3750
      ROCK3760
      ROCK3770
      ROCK3780
      ROCK3790
      ROCK3800
      ROCK3810
      ROCK3820
      ROCK3830
      ROCK3840
      ROCK3850
      ROCK3860
      ROCK3870
      ROCK3880
      ROCK3890
      ROCK3900
      ROCK3910
      ROCK3920
      ROCK3930
      ROCK3940
      ROCK3950
      ROCK3960
      ROCK3970
      ROCK3980
      ROCK3990
      ROCK4000
      ROCK4010

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```
4035 CONTINUE
C... SHIFT IUSE
      IUSE(I)=IUSE(NPOS)
      IF(IUSE(I).EQ.0)GO TO 4039
C... RESET TEMPERATURES OF SAVED COND. SPECIES
      IITEM=IITEM+1
      KITEM=JITEM
      DO 4036 JJ=JITEM,INC
      IF(NORDCN(JJ).NE.NPOS)GO TO 4036
      TEMP(IITEM,1)=TEMP(JJ,1)
      TEMP(IITEM,2)=TEMP(JJ,2)
      KITEM=JJ+1
      GO TO 4037
4036 CONTINUE
4037 JITEM=KITEM
4039 CONTINUE
C... SHIFT MOLECULAR WTS.
      XMWC(I)=XMWC(NPOS)
C... SHIFT NAME
      DO 4032 J=1,3
4032 SUB(I,J)=SUB(NPOS,J)
C... SHIFT COEFFICIENTS
      DO 4033 J=1,7
      COEF(1,J,I)=COEF(1,J,NPOS)
4033 COEF(2,J,I)=COEF(2,J,NPOS)
C... SHIFT REMAINING A(I,J)
      DO 4034 J=1,NLM
4034 A(J,I)=A(J,NPOS)
C... SPECIAL CONSIDERATIONS FOR NS1 TO NSK TERMS
C      IF(I.LT.NS1)GO TO 4040
C... SHIFT EN(1,I) AND ENLN(I)
      EN(1,I)=EN(1,NPOS)
      ENLN(I)=0.0
4040 CONTINUE
C*****DEBUG
      IF(IPRRKT.LE.1)GO TO 977
      NUMOUT=NSK
      NUMDBG=11
      CALL DBGOUT(NUMOUT,HP,SP,DXOUTP,NUMDBG)
C**** DEBUG
C***** DEBGS
      DXOUTP(1)=NSOLD
      DXOUTP(2)=NS
      DXOUTP(3)=NSKOLD
      DXOUTP(4)=NSK
      DXOUTP(5)=NLMOLD
      DXOUTP(6)=NLM
      NUMOUT=6
      NUMDBG=12
      CALL DBGOUT(NUMOUT,HP,SP,DXOUTP,NUMDBG)
      DO 4041 I=1,NSK
4041 WRITE(1,4098) (SUB(I,J),J=1,3)
C***** END DEBUG STATEMENTS
      977 CONTINUE
      IF(NS-1)4042,972,979
C....EPROR...NS=0 MEANS NO SPECIES IN EQUILIBRIUM POOL...STOP 30
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```
ROCK4020
ROCK4030
ROCK4040
ROCK4050
ROCK4060
ROCK4070
ROCK4080
ROCK4090
ROCK4100
ROCK4110
ROCK4120
ROCK4130
ROCK4140
ROCK4150
ROCK4160
ROCK4170
ROCK4180
ROCK4190
ROCK4200
ROCK4210
ROCK4220
ROCK4230
ROCK4240
ROCK4250
ROCK4260
ROCK4270
ROCK4280
ROCK4290
ROCK4300
ROCK4310
ROCK4320
ROCK4330
ROCK4340
ROCK4350
ROCK4360
ROCK4370
ROCK4380
ROCK4390
ROCK4400
ROCK4410
ROCK4420
ROCK4430
ROCK4440
ROCK4450
ROCK4460
ROCK4470
ROCK4480
ROCK4490
ROCK4500
ROCK4510
ROCK4520
ROCK4530
ROCK4540
ROCK4550
ROCK4560
ROCK4570
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      IF(.NOT.TWOSTG)GO TO 1334
C**** KFKK=0
C**** WRITE(1,9876) KKKK
9876 FORMAT(1X,25(1H*),5HKKKK=,I3)
      CALL OUT2
      CALL OUT3
      SENCA=1.
      NC=0
      DO 1020 IA=1,NS
      IF(IUSE(IA).NE.0)NC=NC+1
      IF(IUSE(IA).LE.0)GO TO 1020
      TSAV1=EN(1,IA)*ALPH
      SENCA=SENCA-TSAV1*XMWC(IA)
      HSUB0=HSUB0-TSAV1*H0(IA)*TT
      DO 1030 JA=1,NLM1
      B0(JA)=B0(JA)-TSAV1*A(JA,IA)
1030 CONTINUE
1020 CONTINUE
      HSUB0=HSUB0/SENCA
      DO 1040 IA=1,NLM1
      B0(IA)=B0(IA)/SENCA
1040 CONTINUE
      XPERC=100.0*ALPH
      WRITE(6,5001) XPERC
5001 FORMAT(/10X,29HFIRST STAGE PROPERTIES AFTER ,F5.1,
*23H PERCENT SLAG REJECTION)
      WRITE(6,91)
91 FORMAT(9H ENTHALPY,21X,5HHSUB0)
      WRITE(6,92) HSUB0
92 FORMAT(19H (KG-MOL)(DEG K)/KG,E21.8)
      WRITE(6,93)
93 FORMAT(12H KG-ATOMS/KG,17X,5HB0(I))
      WRITE(6,94)(LLMT(I),B0(I),I=1,NLM1)
94 FORMAT(7X,A4,4X,E25.8)
      DO 1050 IA=1,NS
      IF(IUSE(IA))1050,1044,1045
1044 IF(EN(1,IA).EQ.0.0D0)GO TO 1050
      EN(1,IA)=EN(1,IA)/SENCA
      ENLN(IA)=DLOG(EN(1,IA))
      GO TO 1050
1045 IF(IUSE(IA).LT.1000) EN(1,IA)=EN(1,IA)*(1.-ALPH)/SENCA
1050 CONTINUE
      ENNS=(1.-ALPH)*ENNS/SENCA
      ENN=ENN/SENCA
      CALL EQLBRM(.TRUE.)
      CALL OUT2
      CALL OUT3
C**** DELETE NEXT 6 LINES FOR TWOSTG FIX
C**** REPLACED BY THE PRECEDING 7 LINES 1/2/79
C*** TSAV1=(1.+OF)*SENCA
C*** TSAV2=(BETH*OF)/(1.-BETH)
C*** AXW=TSAV1+TSAV2
C*** HSUB0=(TSAV1*HSUB0+TSAV2*HPP(1))/AXW
C*** DO 1055 I=1,NLM1
C1055 B0(I)=(TSAV1*B0(I)+TSAV2*B0P(I,1))/AXW
      TSAV1=(PCWFT(2)+OF*PCWFT(1))*SENCA

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ROCK5700
ROCK5710
ROCK5720
ROCK5730
ROCK5740
ROCK5750
ROCK5760
ROCK5770
ROCK5780
ROCK5790
ROCK5800
ROCK5810
ROCK5820
ROCK5830
ROCK5840
ROCK5850
ROCK5860
ROCK5870
ROCK5880
ROCK5890
ROCK5900
ROCK5910
ROCK5920
ROCK5930
ROCK5940
ROCK5950
ROCK5960
ROCK5970
ROCK5980
ROCK5990
ROCK6000
ROCK6010
ROCK6020
ROCK6030
ROCK6040
ROCK6050
ROCK6060
ROCK6070
ROCK6080
ROCK6090
ROCK6100
ROCK6110
ROCK6120
ROCK6130
ROCK6140
ROCK6150
ROCK6160
ROCK6170
ROCK6180
ROCK6190
ROCK6200
ROCK6210
ROCK6220
ROCK6230
ROCK6240
ROCK6250

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      TSAV2=TSAV1*HSUB0+HPP2(2)+OF*HPP2(1)
      TSAV3=TSAV1+PCWSD(2)+OF*PCWSD(1)
      HSUB0=TSAV2/TSAV3
      DO 1055 I=1,NLM1
      TSAV2=TSAV1*B0(I)+B0P2(I,2)+OF*B0P2(I,1)
1055 B0(I)=TSAV2/TSAV3
C***** END OF TOSTG CHANGES
      WRITE(6,5002)
5002 FORMAT(/10X,47HSECOND STAGE ENTHALPY AND ELEMENTAL COMPOSITION)
      WRITE(6,91)
      WRITE(6,92)HSUB0
      WRITE(6,93)
      WRITE(6,94)(LLMT(I),B0(I),I=1,NLM1)
      BIGB=B0(1)
      SMALB=B0(1)
      IF(NLM1.LE.1)GO TO 746
      DO 747 I=2,NLM1
      IF(B0(I).EQ.0.) GO TO 747
      IF(SMALB.EQ.0.)SMALB=B0(I)
      IF(B0(I).LT.SMALB) SMALB=B0(I)
      IF(B0(I).GT.BIGB) BIGB=B0(I)
747 CONTINUE
746 CONTINUE
      TEM5=SMALB/BIGB
      SIZZEE=SIZE
      IF(TEM5.LT.1.E-5) SIZZEE=ALOG(1000./TEM5)
      IF(SIZZEE.GT.SIZE) SIZE=SIZZEE
      IF(.NOT.SPLG) GO TO 1052
      SPLG=.FALSE.
      DO 4 I=1,NS
      IF(IUSE(I).LT.1000) GO TO 4
      EN(1,I)=0.
      ENLN(I)=0.
      IUSE(I)=-IUSE(I)
      4 CONTINUE
      WRITE(6,15)
15 FORMAT(16H REMOVE SOLUTION )
      IQ1=IQ1-1
      ENLS=0.
      ENNS=0.
1052 CALL EQLBRM(.TRUE.)
      CALL CONDOC(PFLAG)
1334 TP = .FALSE.
      HP=.FALSE.
      SP=.TRUE.
      S0 = SSUM(1)
334 TMELT=0.
      TROT = 3
      TAI = .FALSE.
C**** KKKK=1
C**** WRITE(1,9876) KKKK
      GAM=GAMMAS(1)
      IF(GAM.EQ.0.) GAM=1.05
      APP(2)/=((GAM+1.)/2.)*(GAM/(GAM-1.))
      PP = PPP(1)/APP(2)
      TT=2.*TT/(GAM+1.)

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ROCK6260
ROCK6270
ROCK6280
ROCK6290
ROCK6300
ROCK6310
ROCK6320
ROCK6330
ROCK6340
ROCK6350
ROCK6360
ROCK6370
ROCK6380
ROCK6390
ROCK6400
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ROCK6480
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ROCK6630
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ROCK6670
ROCK6680
ROCK6690
ROCK6700
ROCK6710
ROCK6720
ROCK6730
ROCK6740
ROCK6750
ROCK6760
ROCK6770
ROCK6780
ROCK6790
ROCK6800
ROCK6810

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      ISV = 1
      GO TO 878
195 IF(NPT.NE.2) CALL CONDUCT(PFLAG)
      IF(IPP.GE.4) GO TO 38
      USQ = 2.*(HSUM(1)-HSUM(NPT)) * RR
C**** KKKK=2
C**** WRITE(1,9876) KKKK
      IF (IPP.GT.2) GO TO 988
C
C   THROAT
C**** KKKK=3
C**** WRITE(1,9876) KKKK
C
198 IF(.NOT.THI) GO TO 191
      GAMMAS(2) = 8.
      GO TO 899
38 DX=DXI
C**** KKKK=18
C**** WRITE(1,9876) KKKK
      UMHD=UE
      USQ=UMHD*UMHD
      IF(NMPATH.EQ.3.AND.IPP.NE.3)GO TO 31
      AEAT(NPT)=(ENN+EMM)*TTT(NPT)/(PP*UMHD*AWT)
31 CONTINUE
      TSAV1=8314.3*GAMMAS(NPT)*TTT(NPT)/WM(NPT)
      IF(TSAV1.LE.8.8D8)GO TO 988
      PMTEST=PP*USQ/TSAV1
      IF(PMTEST.GT.PCRIT)GO TO 988
      ISV=8
      GO TO 868
191 ASQ=GAMMAS(2)*TT*ENN*RR
C**** KKKK=4
C**** WRITE(1,9876) KKKK
      IF(EOL)WRITE(6,194)APP(2),TT
194 FORMAT(7H PC/PT= , F9.6, 6H T= , F9.2)
      IF(IDEBUG.EQ.1.OR.IDEBUG.EQ.2) WRITE(6,923)USQ,ASQ
923 FORMAT(5H8USQ=,E15.8,5X,4HASQ=,E15.8)
      DH = (USQ-ASQ)/ASQ
      IF(DH.LT.8.) DH=-DH
      IF(DH.LE.8.4E-4.OR.ITROT.EQ.8) GO TO 899
      IF(JSOL.NE.8) GO TO 925
      IF(TMELT.EQ.8.) GO TO 192
      DLT = ALOG(TMELT/TT)
      DD = DLT*CPR(2)/(ENN*DLVTP(2))
C**** KKKK=11
C**** WRITE(1,9876) KKKK
      PP = PP*EXP(DD)
      APP(2) = P(IP)/PP
      THI = .TRUE.
      GO TO 331
295 TMELT = TT
192 APP(2) = APP(2)/(1.+(USQ-ASQ)/(ENN*TT*RR*(GAMMAS(2)+1.)))
193 PP = P(IP)/APP(2)
      ITROT = ITROT-1
C**** KKKK=5
C**** WRITE(1,9876) KKKK

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ROCK6828
ROCK6838
ROCK6848
ROCK6858
ROCK6868
ROCK6878
ROCK6888
ROCK6898
ROCK6908
ROCK6918
ROCK6928
ROCK6938
ROCK6948
ROCK6958
ROCK6968
ROCK6978
ROCK6988
ROCK6998
ROCK7008
ROCK7018
ROCK7028
ROCK7038
ROCK7048
ROCK7058
ROCK7068
ROCK7078
ROCK7088
ROCK7098
ROCK7108
ROCK7118
ROCK7128
ROCK7138
ROCK7148
ROCK7158
ROCK7168
ROCK7178
ROCK7188
ROCK7198
ROCK7208
ROCK7218
ROCK7228
ROCK7238
ROCK7248
ROCK7258
ROCK7268
ROCK7278
ROCK7288
ROCK7298
ROCK7308
ROCK7318
ROCK7328
ROCK7338
ROCK7348
ROCK7358
ROCK7368
ROCK7378

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      GO TO 331
899  CONTINUE
      UMHD=DSORT(USQ)
      AWT =ELN*TT/(PP*UMHD)
C**** KKKK=6
C**** WRITE(1,9876) 'KKKK
      PCPLT = ALOG(APP(2))
      IF(NFZ.EQ.2) EQL = SEQL
      CALL CONDOC(PFLAG)
C
C
      900 ISV =0
C**** KKKK=7
C**** WRITE(1,9876) 'KKKK
      IF(NMPATH.EQ.3.AND.IPP.NE.3)GO TO 787
      IF(IPP.EQ.3)UMHD=DSORT(USQ)
      AEAT(NPT) = (ELN+EMM)*TTT(NPT)/(PP*UMHD*AWT)
      787 CONTINUE
      IF(TT.EQ.0.) GC TO 860
      IF(PCP(1).EQ.0.0.AND.IPP.GT.2)AREA=.TRUE.
      IF(AREA) GO TO 800
      IF(IPP.LT.NPP) GO TO 859
      788 IF(NSUB.EQ.0.AND.NSUP.EQ.0) GO TO 860
      AREA = .TRUE.
C
C      PCP ESTIMATES FOR AREA RATIOS
C
      800 IF(ITNUM.NE.0) GO TO 810
      DLNP = 1.
C**** KKKK=12
C**** WRITE(1,9876) 'KKKK
      ITNUM = 1
      ARATIO = SUBAR(ISUB)
      IF(NSUB.LE.0) ARATIO=SUPAR(ISUP)
      IF(EQL.OR.NFZ.LT.3) GO TO 798
      IF(ARATIO.GT.AEAT(NFZ)) GO TO 798
      WRITE(6,884)
      GO TO 834
      798 ELN = ALOG(ARATIO)
      IF(NSUB.LE.0) GO TO 799
      APPL = PCPLT/(SUBAR(ISUB)+(10.587*ELN*ELN+9.454)*ELN)
      IF(ARATIO.LT.1.09) APPL=.9*APPL
      IF(ARATIO.GT.10.) APPL=APPL/ARATIO
      GO TO 859
      799 IF(NFZ.EQ.IPP) ISUPSV = ISUP
      IF (SUPAR(ISUP).LT.2.) GO TO 805
      IF(ISUP.GT.1.AND.SUPAR(ISUP-1).GE.2.) GO TO 802
      APPL = GAUSS(2)+ELN*1.4
      GO TO 859
      805 APPL = SQRT(ELN*(1.535+3.294*ELN))+PCPLT
      GO TO 859
C
C      TEST FOR CONVERGENCE ON APEA RATIO.
C
      810 CONTINUE
C**** KKKK=15
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ROCK7380
ROCK7390
ROCK7400
ROCK7410
ROCK7420
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ROCK7920
ROCK7930
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C**** WRITE(1,9376) KKKK                                ROCK7940
IF(IDEBUG.LE.0.OR.NPT.LT.1) GO TO 809                    ROCK7950
WRITE(6,1811)ITNUM,ARATIO,AEAT(NPT),APP(NPT),DLNP        ROCK7960
1811 FORMAT (6HWRITE=,I2,5X,15HASSIGNED AE/AT=,F15.8,5X,6HAE/AT=,F15.8, ROCK7970
15X,5HPC/P=,F15.8,5X,13HDELTA LN PCP=,F15.8)              ROCK7980
809 TSAV4 = (AEAT(NPT)-ARATIO)/ARATIO                    ROCK7990
IF(ABS(TSAV4).LE.CHECK)GO TO 330                          ROCK8000
DELTAE=TSAV4                                              ROCK8010
IF(ABS(DLNP).LT.CHECK) GO TO 830                          ROCK8020
AEATL= ALOG(AEAT(NPT))                                    ROCK8030
ITNUM = ITNUM+1                                           ROCK8040
IF(ITNUM.GT.10) GO TO 840                                  ROCK8050
C                                                         ROCK8060
C IMPROVED PCP ESTIMATES.                                ROCK8070
C                                                         ROCK8080
ASQ = GAMMAS(NPT)*ENN*RR*TT                              ROCK8090
DLNPE = GAMMAS(NPT)*USQ/(USQ-ASQ)                         ROCK8100
802 DLNP = DLNPE*(ELN-AEATL)                              ROCK8110
APPL = APPL+DLNP                                           ROCK8120
IF(ITNUM.EQ.1) GO TO 859                                   ROCK8130
IF(APPL.LT.0.) APPL=.000001                               ROCK8140
APP(NPT) = EXP(APPL)                                       ROCK8150
PP = P(IP)/APP(NPT)                                       ROCK8160
GO TO 331                                                  ROCK8170
C                                                         ROCK8180
830 ITNUM = 0                                              ROCK8190
AEAT(NPT) = ARATIO                                         ROCK8200
C.....ONLY 1 AREA RATIO ALLOWED.....                   ROCK8210
IF(ITNUM.EQ.0)GO TO 859                                    ROCK8220
IF(NSUB.LE.0) GO TO 834                                    ROCK8230
ISUB = ISUB+1                                              ROCK8240
IF(ISUB.LE.NSUB) GO TO 800                                ROCK8250
ISUB = 1                                                   ROCK8260
NSUB = -NSUB                                               ROCK8270
IF(ISUP.LE.NSUP) GO TO 800                                ROCK8280
GO TO 835                                                  ROCK8290
834 ISUP = ISUP+1                                          ROCK8300
ITNUM=0                                                    ROCK8310
IF(ISUP.LE.NSUP) GO TO 800                                ROCK8320
ISUP = ISUPSV                                             ROCK8330
835 AREA = .FALSE.                                         ROCK8340
ISUB=1                                                     ROCK8350
NSUB=0                                                     ROCK8360
GO TO 860                                                  ROCK8370
840 WRITE(6,841) ARATIO                                    ROCK8380
841 FORMAT(34H0DID NOT CONVERGE FOR AREA RATIO =,F10.5)  ROCK8390
GO TO 830                                                  ROCK8400
C                                                         ROCK8410
C TEST FOR OUTPUT -- END OF PCP,SUBAR,AND SUPAR SCHEDULES OR NPT=13. ROCK8420
C                                                         ROCK8430
859 ISV = NPT                                              ROCK8440
C**** KKKK=8                                              ROCK8450
C**** WRITE(1,9876) KKKK                                  ROCK8460
IF(NPT.NE.13) GO TO 870                                    ROCK8470
860 IF(EQL) GO TO 861                                      ROCK8480
IF(NFZ.GT.1) GO TO 861                                    ROCK8490

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      CPR(NFZ) = CPRF
      GAMMAS(NFZ) = CPRF/(CPRF-1./WM(NFZ))
      861 CONTINUE
C**** KKKK=13
C**** WRITE(1,9876) KKKK
      842 IF(JJPATH.GE.0)GO TO 843
      NPT=NPT-1
      IPP=IPP-1
      IF(NPT.EQ.2.AND.IPP.GT.2)GO TO 3001
      843 CALL RKTOUT
      3001 CONTINUE
      IF(JJPATH.GE.0)GO TO 305
      WRITE(6,3008)
      3008 FORMAT(5X,29HSTOP 5 IS NORMAL CHANNEL STOP,/,7X,
      *54HIT OCCURS WHEN XPOSITION EXCEEDS INPUTTED XXSTOP VALUE)
      STOP 5
      305 CONTINUE
      IF(IPP.GE.NPP)WRITE(6,4095) IPP,NPP
      4095 FORMAT(/,1X,10(1H*),23HPROGRAM STOPS WHEN IPP=,I6,
      *2X,12IS .GE. NPP=,I6/,10X,26HNPP IS SET TWICE IN ROCKET)
      DLNP=1.
C**** KKKK=14
C**** WRITE(1,9876) KKKK
      IF(TT.EQ.0.) AREA=.FALSE.
      IF(.NOT.EOL.AND.TT.EQ.0.) WRITE(6,862)
      862 FORMAT(105H0CALCULATIONS WERE STOPPED BECAUSE NEXT POINT IS MORE
      1HAN 50 DEG BELOW TEMP RANGE OF A CONDENSED SPECIES)
      IF (ISV.EQ.0) GO TO 990
      IDEBUG = IDEBUG-13
      IF(EQL) WRITE(6,865)
      865 FORMAT(1H1)
      NPT=2
C
C      SET INDICES AND ESTIMATES FOR NEXT POINT.
C
      870 NPT = NPT + 1
C**** KKKK=9
C**** WRITE(1,9876) KKKK
      IF(.NOT.AREA) GO TO 57
      IF(IPP.LE.2)GO TO 57
      NSUP=0
      NPP=500
      NSUB=0
      AREA=.FALSE.
      PCP(1)=PPP(1)/PPP(3)
      57 CONTINUE
      IF(.NOT.EQL.AND.(ISV.NE.1.OR.SEQL)) GO TO 380
      IF(ISV.EQ.1) ISV = -1
      IF(NS.GT.1)CALL SAVE
      880 IPP = IPP+1
      881 IF(IPP.LT.3)GO TO 107
      17 CONTINUE
      40 CALL MHD(JJPATH)
      882 CONTINUE
      IF(JJPATH)842,10,883
      883 APP(NPT)=PPP(1)/PPP(NPT)

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ROCK8500
 ROCK8510
 ROCK8520
 ROCK8530
 ROCK8540
 ROCK8550
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 ROCK8570
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 ROCK8590
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 ROCK8610
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 ROCK8640
 ROCK8650
 ROCK8660
 ROCK8670
 ROCK8680
 ROCK8690
 ROCK8700
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 ROCK8970
 ROCK8980
 ROCK8990
 ROCK9000
 ROCK9010
 ROCK9020
 ROCK9030
 ROCK9040
 ROCK9050

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      GO TO 300                                ROCK9060
100 CONTINUE                                ROCK9070
C**** KKKK=16                                ROCK9080
C**** WRITE(1,9876) KKKK                    ROCK9090
      IF (NPT.EQ.2) GO TO 331                ROCK9100
C**** KKKK=17                                ROCK9110
C**** WRITE(1,9876) KKKK                    ROCK9120
      IF (AREA) GO TO 885                    ROCK9130
      APP(NPT) = PCP(IPP-2)                  ROCK9140
      IF (APP(NPT).EQ.0.0) GO TO 885          ROCK9150
      IF (EQL) GO TO 886                     ROCK9160
      IF (APP(NPT).GE.APP(NFZ)) GO TO 886     ROCK9170
      WRITE(6,884)                           ROCK9180
884 FORMAT(//,1X,114HSUPERSONIC PRESSURE RATIOS MUST BE IN ASCENDING ORDER
1000 POINTS OUT OF ORDER WERE OMITTED FROM FROZEN CALCULATIONS)
      GO TO 880                                ROCK9210
885 APP(NPT) = EXP(APPL)                      ROCK9220
886 PP = P(IP)/APP(NPT)                      ROCK9230
      GO TO 331                                ROCK9240
C                                              ROCK9250
C      END OF PCP, SUBAR, AND SUPAR SCHEDULES.  ROCK9260
C                                              ROCK9270
990 IF (IDEBUG.LT.0) IDEBUG=IDEBUG+13        ROCK9280
C**** KKKK=18                                ROCK9290
C**** WRITE(1,9876) KKKK                    ROCK9300
      IF (NSUB.LT.0) NSUB=-NSUB              ROCK9310
      IF (.NOT.FROZ) GO TO 997               ROCK9320
C                                              ROCK9330
C      SET UP FOR FROZEN.                    ROCK9340
C                                              ROCK9350
      IF (EQL) GO TO 991                     ROCK9360
      IF (NFZ.EQ.1) GO TO 997               ROCK9370
      NFZ=1                                  ROCK9380
991 EQL = .FALSE.                            ROCK9390
      IF (NS.GT.1) CALL SAVE                 ROCK9400
      TT = TTT(NFZ)                         ROCK9410
      IPP = NFZ                              ROCK9420
      IF (NFZ.EQ.NPT) GO TO 860              ROCK9430
      NPT = NFZ                              ROCK9440
      ENN = 1./WM(NFZ)                      ROCK9450
C**** KKKK=19                                ROCK9460
C**** WRITE(1,9876) KKKK                    ROCK9470
      IF (NFZ.EQ.1) GO TO 334                ROCK9480
      NSUB = -NSUB                          ROCK9490
      IF (APP(NFZ).GE.APP(2)) GO TO 994      ROCK9500
      WRITE(6,993)                          ROCK9510
993 FORMAT(//,28X,77HFREEZING IS NOT ALLOWED AT A SUBSONIC POINT, FROZEN
1000 CALCULATIONS WERE OMITTED)
      GO TO 997                                ROCK9530
994 IF (NFZ.LT.NPP) GO TO 870                ROCK9540
      GO TO 788                                ROCK9550
997 NPT = 1                                  ROCK9560
C                                              ROCK9570
C      ARE THERE MORE ASSIGNED,              ROCK9580
C      1) CHAMBER PRESSURES(IP = NP)        ROCK9590
C      2) CHAMBER TEMPERATURES(IT = NT)     ROCK9600
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C      3) O/F VALUES (IOF = NOF)
C
C**** KKKK=21
C**** WRITE(1,9876) KKKK
      IF(IP.EQ.NP.AND.IT.EQ.NT.AND.IOF.EQ.NOF) GO TO 1000
      WRITE(6,865)
      IF(NS.GT.1)CALL SAVE
      TT = TTT(1)
      IF(NPPP.EQ.1.OR.RKTO) GO TO 998
      NSUB = 1
998  CONTINUE
      IF(IT.GE.NT) GO TO 999
      IT = IT+1
      TT = T(IT)
      GO TO 322
999  IF (IOF.GE.NO) GO TO 1000
      GO TO 321
1000 RETURN
      END
      SUBROUTINE MHD(JJPATH)
C
C
C
C      THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED
C      FOR NON-CDC MACHINES
C
      DOUBLE PRECISION TTT,TM,PP,SIGMA,SIG,VLMI,VLM,ENINIT
      DOUBLE PRECISION ENN,EMM,SUMN,AWT
      DOUBLE PRECISION HSUM,SSUM,CPR,DLVPT,DLVPT,GAMMAS,COEF,EN,S0
      DOUBLE PRECISION S,ENLN,H0,SV,XMAX,ERROR,NE,X0,XH,XN
      DOUBLE PRECISION XL,XHM,DEX,DACC,XS,TSAV1,AANS,ATERM,AMULT
      DOUBLE PRECISION X0CRIT,ACCRT,ACCRT2,XLSTP,XCLOSE,DDXSAV
      DOUBLE PRECISION TSAV2,TSAB3,TSAB4,TSTORE,DXOUTP,XXSTOP
      DOUBLE PRECISION XHNOPT,XHOLD,RHOUE,UEDP
      DOUBLE PRECISION XHINC,XHINCC,XHMIN,XFIX,XMINC,XMIND
C
      LOGICAL SHOCK,MMHG,UV,DET,SIUNIT,NSQM,CALCH
      LOGICAL HP,SP,TP,NEW,IONS,MOLES,FROZ,EOL,PSIA,RKT,VOL,TV
      LOGICAL FA,ERATIO,FPCT,OTTO
      LOGICAL CONVG,LOGV,SFLG,AREA,HPTH,SPATH
      LOGICAL NEQL,FIRST,ONCE,PRINTX,TWOSTG
      REAL INTERP
      DIMENSION IFL(4),IFL1(4)
      DIMENSION OUTP(4,3),OUTR(4,3)
      COMMON/SPNOPT/KBEGR(35),KKIJJ,XHINC,XFIX,XHNOPT,XHMIN
      COMMON/XPRINT/PRINTX
      COMMON/SETUPS/ITYPE,CHLOSS,CHHEAT,RHOUE,UEDP
      COMMON/TOSTAR/XHSTRT
      COMMON/START/FIRST
      COMMON/MISC/S0,ENN,SUMN,TT,ATOM(3,101),LLMT(30),B0(30),B0P(30,2)
1  ,TM,TLOW,TMID,THIGH,CPSUM,PP,OF,EQRAT,FPCT,R,RR,HSUB0,CA(2),AM(2)
2  ,HPP(2),FH(2),VMIN(2),VPLS(2),WP(2),DATX(30),NAME(30,5)
3  ,ANUM(30,5),PECWT(30),ENTH(30),FAZ(30),RTEMP(30),FOX(30),DENS(30)
4  ,RHOP,RMW(30),TLN,CR,OXF(30),ENNL,ENSAVE,ENLSAV,TRACE,SIZE
      COMMON/MHDD/SSUMV,DX,DXI,XJY(26),AI(26),UE,NITER,NSTOP,SIG(26),YPPM
X  ,BZ,XK,PIPP
      COMMON/INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM

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      ROCK9620
      ROCK9630
      ROCK9640
      ROCK9650
      ROCK9660
      ROCK9670
      ROCK9680
      ROCK9690
      ROCK9700
      ROCK9710
      ROCK9720
      ROCK9730
      ROCK9740
      ROCK9750
      ROCK9760
      ROCK9770
      ROCK9780
      ROCK9790
      ROCK9800
      MHD 5
      MHD 10
      MHD 15
      MHD 20
      MHD 25
      MHD 30
      MHD 35
      MHD 40
      MHD 45
      MHD 50
      MHD 55
      MHD 60
      MHD 65
      MHD 70
      MHD 75
      MHD 80
      MHD 85
      MHD 90
      MHD 95
      MHD 100
      MHD 105
      MHD 110
      MHD 115
      MHD 120
      MHD 125
      MHD 130
      MHD 135
      MHD 140
      MHD 145
      MHD 150
      MHD 155
      MHD 160
      MHD 165
      MHD 170
      MHD 175
      MHD 180
      MHD 185

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1      ,NS,KMAT,IMAT,IO1,NOF,MOMIT,IP,NEW,NSUB,NSUP,ITM,CPCVFR,CPCVEQMHD 190
2      ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCHMHD 195
3      ,IOSAVE,LSAVE,ISUP,ISUB,ITNUM MHD 200
COMMON/PERF/PCP(22),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)MHD 205
1      ,APP(13),AEAT(13),CSTR,EQL,FROZ,SS0,AREA,AWT MHD 210
COMMON/POINTS/ HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13) MHD 215
1      ,GATEAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13) MHD 220
2      ,VLM(13),TOTEN(13) MHD 225
COMMON/CSIG/SIGMA(13) MHD 230
COMMON/EQ/NEQL,ACCURC,HMIN MHD 235
COMMON/NEQ/B0N(30),EMM,SNEQ,NQ1,NSK,NEQPT MHD 240
DIMENSION SPECNM( 30,3),DATA(30),AC(40),DAT(4,3) MHD 245
COMMON/DIFEQ/ AKF1(30),AKF2(30), MHD 250
* AKF3(30),NJR(30,4),NJP(30,4),MAR(30,4),MAP(30,4), MHD 255
* AP(30,4),AR(30,4),NJ1,NOMIT,VLMI MHD 260
COMMON/MIKE0/ITE1,ITE2,ITE3,IMPRNT,NMPATH,NUMIV,XINDP(1) MHD 265
COMMON/MIKE1/ATERM,AMULT,VELIN(1) MHD 270
COMMON/MIKE2/HPATH,SPATH,PRESIN(1) MHD 275
COMMON/MIKE3/AREAIN(1) MHD 280
COMMON/MIKE5/NNNNN,X0CRIT,DUMMIN(1) MHD 285
COMMON/MIKE6/SPECNM MHD 290
COMMON/MIKE7/CHCALC,CHNLEN,IPRRKT,TMPSTP,TDIFUN,TEOLBM MHD 295
C... NMPATH DESCRIBES THE VECTOR TO BE INPUTTED MHD 300
C      1=INPUT VELOCITY MHD 305
C      2=INPUT PRESSURE MHD 310
C      3=INPUT AREA MHD 315
C... NUMIV IS THE NO. OF POINTS INPUTTED(MAX. =NUMIVM=90) MHD 320
C... ITE1 IS STARTING LOCATION OF P OR UE CALCULATIONS MHD 325
C... ITE2 IS POSITION OF S (OR H) CALCULATION MHD 330
C... ITE3 IS NO. OF EQUATIONS TO SOLVE(OTHER THAN NOMIT ONES) MHD 335
COMMON/SPECE1/NSPCMX,NCMAX,NELMX,TEMP(175,2),SUB(600,3),S(1) MHD 340
COMMON/SPECE2/ENLN(1) MHD 345
COMMON/SPECE3/H0(1) MHD 350
COMMON/SPECE5/IUSE(1) MHD 355
COMMON/SPECE7/SCONMX(1) MHD 360
COMMON/TSTG/TWOSTG,ALPH,NLM1,XELMC(30),XMWC(1) MHD 365
COMMON/DBGVEC/DXOUTP(1) MHD 370
COMMON/KGM/EN(13,1) MHD 375
COMMON/THMF/COEF(2,7,1) MHD 380
COMMON/STOIC/A(30,1) MHD 385
C... NSPCMX REFERS TO THE MAXIMUM NO. OF SPECIES ALLOWED MHD 390
C... NCMAX REFERS TO THE MAXIMUM NO. OF CONDENSED SPECIES ALLOWED MHD 395
C      THIS IS FIXED AND REFERS TO THE SIZE OF TEMP(N,2) IN COMMON MHD 400
C      SPECE1.....MUST CHANGE THIS COMMON EVERYWHERE IF A LARGER SMHD 405
C      IS NEEDED MHD 410
C... NELMX REFERS TO THE MAXIMUM NO. OF ELEMENTS ALLOWED MHD 415
C      THIS IS FIXED AND REFERS TO THE SIZE OF XELMC(N) AND A(N,NSMHD 420
C      .....MUST CHANGE COMMON TSTG AND STOIC EVERYWHERE IF MHD 425
C      A LARGER SIZE IS NEEDED MHD 430
C MHD 435
C MHD 440
C MHD 445
DIMENSION B3(3),NE(8,32) MHD 445
DIMENSION SV(12,32),XMAX(32),ERROR(32),PW(32,32),IPS(32),PC(32) MHD 450
DIMENSION AANS(32),IICLK(32) MHD 455
C MHD 460
EQUIVALENCE (OTTO,CPCVFR),(CPCVEQ,LOGV) MHD 465

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C	DATA B3/4HTRH,4HD BO,4HDY /	MHD	470
	DATA XXMAX/.0/,NCONMX/1,SSSSUM/1.0/	MHD	475
	DATA REACT,PRODT/4HPEAC,4HPROD/	MHD	480
	DATA BLANK/1H/,ACCCRT/1.0D-12/,ACCCRT2/-1.0D-12/,ENINIT/1.0D-12/	MHD	485
	DATA NUMIVM/.0/,DXIMAX/.03/,DXCALC/1.0/,TTMAX/.0/	MHD	490
	DATA XCLOSE/1.0D-4/,IICHXS/5/,IHALFS/20/	MHD	495
	DATA IFL/1H,3*1H+/,IFL1/1H=,3*1H+/	MHD	500
	DATA XMIND/5.0D-12/,XMINC/1.0D-10/	MHD	505
C+	NAMLIST COMMENTED OUT FOR PRIME	MHD	510
C+	UNCOMMENT READ AND COMMENT OUT CALL NMLST	MHD	515
	NAMLIST/CHNLIN/NMPATH,IMPRNT,XXSTOP,UEINP,ITYPE	MHD	520
C	NPTM1=NPT-1	MHD	525
	IF(IPP.GT.13.AND.NPTM1.EQ.2)NPTM1=13	MHD	530
	IF(JJPATH.EQ.-10)GO TO 27	MHD	535
	IF(JJPATH.EQ.0)GO TO 29	MHD	540
	IF(.NOT.FIRST)GO TO 29	MHD	545
	ICASEC=0	MHD	550
	KAREA=0	MHD	555
	IMREAD=0	MHD	560
	JVELFL=0	MHD	565
	XHSTRT=1.0E-5	MHD	570
	DO 26 I=1,35	MHD	575
26	KBEGN(I)=0	MHD	580
	XCLOSE=0.001*DXI	MHD	585
	IF(XVSTRT.GT.XCLOSE)XHSTRT=XCLOSE	MHD	590
	XCLOSE=DXI	MHD	595
	IF(DXI.GT.DXIMAX)XCLOSE=DXIMAX	MHD	600
	XCLOSE=0.01*(XCLOSE+XHSTRT)	MHD	605
	WRITE(1,4047) XCLOSE,DXI,DXIMAX,XHSTRT	MHD	610
4047	FORMAT(1X,5(1H.),4(1X,G13.5))	MHD	615
	XFIX=1.0	MHD	620
	XHNQPT=50.0*XHSTRT	MHD	625
	XHINC=0.5*XHNQPT	MHD	630
	XHINC=XHINC-XHSTRT/5.0	MHD	635
	XHNM1N=10.0*XFSTRT	MHD	640
	KKILCJ=0	MHD	645
	XINDP(1)=0.0	MHD	650
	DUMMIN(1)=0.0	MHD	655
	NORD=3	MHD	660
	IHALF=0	MHD	665
	IF(IPRRKT.LT.0)GO TO 28	MHD	670
	WRITE(1,3002) NPT,PPP(NPT),SSUM(NPT),UE	MHD	675
	WRITE(1,9016) 1PP,NQOPT	MHD	680
28	CONTINUE	MHD	685
	IF(NUMIVM.NE.0)NUMIV=NUMIVM	MHD	690
	KSPEC=0	MHD	695
	ITE1=0	MHD	700
	ITE2=0	MHD	705
	ITE3=0	MHD	710
	AMULT=8314.3D0	MHD	715
	IF(NEQPT.LT.3)GO TO 29	MHD	720
	NOIT=0	MHD	725
	NJ1=0	MHD	730
29	CONTINUE	MHD	735
		MHD	740
		MHD	745

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      IF(IMPRNT.GE.2)WRITE(1,9876) IPP,NEOPT
9876  FORMAT(1X,25(1H*),4HIPP=,I4,3X,6HNEOPT=,I6)
      IF(IPP.EQ.NEOPT)GO TO 27
      IF(JUPATH.EQ.0)GO TO 3017
      IF(NEOPT.EQ.1)GO TO 403
      IF(FIRST)GO TO 4
      GO TO 120
27  CONTINUE
      IF(NPTM1.LT.1)NPTM1=1
      IF(IPRRKT.GE.0)WRITE(1,3002)NPTM1,PPP(NPTM1),SSUM(NPTM1),UE
      NQ1=0
      NSK=NS
      NOMIT=0
      NJ1=0
C  **** NON-EQL STATES FOLLOW
      1  READ(5,2)(DATA(I),I=1,15)
      2  FORMAT(5(3A4,3X))
      IF(DATA(1).EQ.BLANK)GO TO 130
C  **** PRINT CONTENTS OF DLIT CARD
      WRITE(6,3)(DATA(I),I=1,15)
      3  FORMAT(1X,5(3A4,3X))
      DO 140 I=4,15,3
      IF (DATA(I).EQ.BLANK)GO TO 1
      NOMIT=NOMIT+1
      SPECNM(NOMIT,1)=DATA(I)
      SPECNM(NOMIT,2)=DATA(I+1)
      SPECNM(NOMIT,3)=DATA(I+2)
140  CONTINUE
      GO TO 1
C  **** BEGIN LOOP FOR READING SPECES
130  CONTINUE
      NNNNN=NOMIT+NSK
      IF(NNNNN.LE.NSPCMX)GO TO 133
      NC2=NC
132  IF(NNNNN.EQ.NOMIT)NNNNN=NSK
      WRITE(6,9001) NSPCMX,NCMAX,NNNNN,NC2
9001  FORMAT(1X,44HNOT ENOUGH STORAGE FOR FINITE RATE EQUATIONS/,5X,
      *7HNSPCMX=,I4,2X,6HNCMAX=,I4,2X,15HWE NEED NSPCMX=,I5,
      *10H OR NCMAX=,I5,2X,25H...DLIT REACTIONS IGNORED/,10X,
      *29HSEE ERROR MESSAGES FOR SRCHCC)
      NEOPT=100000
      NOMIT=0
      NSK=NS
      NNNNN=0
      IF(JJPATH.EQ.-10)STOP 10
      IF(JJPATH.EQ.0)GO TO 3017
      IF(FIRST)GO TO 4
      IF(KKSPEC.EQ.0)GO TO 120
      GO TO 128
133  CONTINUE
      HCNON=0
      NC2=NC-1
      NNNNN=NOMIT
      DO 101 K=1,NOMIT
      KN=0
      NC1=0

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MHD 750
MHD 755
MHD 760
MHD 765
MHD 770
MHD 775
MHD 780
MHD 785
MHD 790
MHD 795
MHD 800
MHD 805
MHD 810
MHD 815
MHD 820
MHD 825
MHD 830
MHD 835
MHD 840
MHD 845
MHD 850
MHD 855
MHD 860
MHD 865
MHD 870
MHD 875
MHD 880
MHD 885
MHD 890
MHD 895
MHD 900
MHD 905
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MHD 945
MHD 950
MHD 955
MHD 960
MHD 965
MHD 970
MHD 975
MHD 980
MHD 985
MHD 990
MHD 995
MHD 1000
MHD 1005
MHD 1010
MHD 1015
MHD 1020
MHD 1025

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DO 20 I=1,NS
  IF(IUSE(I).NE.0) NC1=NC1+1
  DO 30 J=1,3
    IF(SPECNM(K,J).NE.SUB(I,J))GO TO 25
  30 CONTINUE
C **** WE HAVE A MATCH---GENERATE X ARRAYS
  IF(IABS(IUSE(I)).LT.1000) GO TO 800
  WRITE(6,700)
700 FORMAT(38H1ERROR - SOLUTION SPECIES ON DLIT CARD )
  STOP
800 IN=NSK+K
  DO 801 J=1,3
    SUB(IN,J)=SUB(I,J)
  801 CONTINUE
  DO 802 INL=1,NLM
    A(INL,IN)=A(INL,I)
  802 CONTINUE
  DO 803 I1=1,NPTM1
    EN(I1,IN)=EN(I1,I)
    IUSE(IN)=IUSE(I)
    IF(IUSE(I).GT.0)NQ1=NQ1+1
    IF(IUSE(I).LT.0)IUSE(IN)=-IUSE(IN)
  85 DO 90 K1=1,7
    DO 102 J1=1,2
      COEF(J1,K1,IN)=COEF(J1,K1,I)
  102 CONTINUE
  90 CONTINUE
C...RESHUFFLE MOLECULAR WEIGHTS
  XMWC(IN)=XMWC(I)
C...FIX TEMP ARRAY IF CONDENSED SPECIES...ALSO COUNT NO. OF THEM REM.
  IF(IUSE(I).EQ.0)GO TO 20
  NCNON=NCNON+1
  TSAV2=TEMP(NC1,1)
  TSAV3=TEMP(NC1,2)
  IF(NC1.GT.NC2)GO TO 1117
  DO 1119 KK=NC1,KC2
    JJ=KK+1
    DO 1118 J=1,2
      1118 TEMP(KK,J)=TEMP(JJ,J)
  1119 CONTINUE
  1117 CONTINUE
  TEMP(NC,1)=TSAV2
  TEMP(NC,2)=TSAV3
  GO TO 20
  25 KN=KN+1
980 DO 150 J4=1,3
  150 SUB(KN,J4)=SUB(I,J4)
  IUSE(KN)=IUSE(I)
C...RE HUFFLE MOLECULAR WEIGHTS
  XMWC(KN)=XMWC(I)
  DO 805 INL=1,NLM
    A(INL,KN)=A(INL,I)
  806 CONTINUE
  DO 804 I1=1,NPTM1
    EN(I1,KN)=EN(I1,I)
  804 ENLN(KN)=ENLN(I)

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MHD 1030
MHD 1035
MHD 1040
MHD 1045
MHD 1050
MHD 1055
MHD 1060
MHD 1065
MHD 1070
MHD 1075
MHD 1080
MHD 1085
MHD 1090
MHD 1095
MHD 1100
MHD 1105
MHD 1110
MHD 1115
MHD 1120
MHD 1125
MHD 1130
MHD 1135
MHD 1140
MHD 1145
MHD 1150
MHD 1155
MHD 1160
MHD 1165
MHD 1170
MHD 1175
MHD 1180
MHD 1185
MHD 1190
MHD 1195
MHD 1200
MHD 1205
MHD 1210
MHD 1215
MHD 1220
MHD 1225
MHD 1230
MHD 1235
MHD 1240
MHD 1245
MHD 1250
MHD 1255
MHD 1260
MHD 1265
MHD 1270
MHD 1275
MHD 1280
MHD 1285
MHD 1290
MHD 1295
MHD 1300
MHD 1305

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      DO 161 K2=1,7
      DO 80 J3=1,2
      COEF(J3,K2,KN)=COEF(J3,K2,I)
800 CONTINUE
161 CONTINUE
200 CONTINUE
   NS=NS-1
101 CONTINUE
      DO 810 I=1,NOMIT
      NSI=NS+I
      NSKI=NSK+I
      DO 820 J=1,3
      SUB(NSI,J)=SUB(NSKI,J)
820 CONTINUE
      DO 805 I1=1,NPTM1
      EN(I1,NSI)=EN(I1,NSKI)
805 CONTINUE
      DO 830 K1=1,7
      DO 840 J1=1,2
      COEF(J1,K1,NSI)=COEF(J1,K1,NSKI)
840 CONTINUE
830 CONTINUE
      IUSE(NSI)=IUSE(NSKI)
C...RESHUFFLE MOLECULAR WEIGHTS
      XMWC(NSI)=XMWC(NSKI)
      DO 850 INL=1,NLM
      A(INL,NSI)=A(INL,NSKI)
850 CONTINUE
810 CONTINUE
C      ISV=3
      IF(NC2.GT.NCMAX)GO TO 132
      NC=NC-NCNON
      IF(NEOPT.NE.1)CALL SAVE
      NSK1=NSK+1
      DO 244 J=1,3
      SUB(NSK1,J)=B3(J)
      IQ1=IQ1-NQ1
      IF(JJPATH.EQ.-10)RETURN
403 CONTINUE
      IF(NEOPT.EQ.1)NEOPT=2
      NSK1=NSK+1
      DO 404 I=1,30
      DO 404 J=1,4
      MAR(I,J)=0
      MAP(I,J)=0
      NJR(I,J)=0
404 NJP(I,J)=0
      NJ2=0
      200 READ(5,2001) (DATA(I),I=1,3),(AC(J),(DAT(J,I),I=1,3),
      * J=1,4)
2001 FORMAT(3A4,4(F3.0,3A4))
      DO 600 J=1,4
      DO 600 I=1,3
      IIX=J*3+I
600 DATA(IIX)=DAT(J,I)
      NREACT=0

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MHD 1310
MHD 1315
MHD 1320
MHD 1325
MHD 1330
MHD 1335
MHD 1340
MHD 1345
MHD 1350
MHD 1355
MHD 1360
MHD 1365
MHD 1370
MHD 1375
MHD 1380
MHD 1385
MHD 1390
MHD 1395
MHD 1400
MHD 1405
MHD 1410
MHD 1415
MHD 1420
MHD 1425
MHD 1430
MHD 1435
MHD 1440
MHD 1445
MHD 1450
MHD 1455
MHD 1460
MHD 1465
MHD 1470
MHD 1475
MHD 1480
MHD 1485
MHD 1490
MHD 1495
MHD 1500
MHD 1505
MHD 1510
MHD 1515
MHD 1520
MHD 1525
MHD 1530
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MHD 1545
MHD 1550
MHD 1555
MHD 1560
MHD 1565
MHD 1570
MHD 1575
MHD 1580
MHD 1585

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      IF(DATA(1) .EQ. BLANK) GO TO 218
      IF(DATA(1) .EQ. REACT) GO TO 228
      IF(DATA(1) .EQ. PRODT) GO TO 238
      GO TO 288
228 NJ1=NJ1+1
      GO TO 231
238 NJ2=NJ2+1
231 DO 248 I=4,15,3
      IF(DATA(I) .NE. BLANK) GO TO 282
      IF(DATA(I) .EQ. REACT) GO TO 288
      IF(DATA(I) .EQ. PRODT) GO TO 283
      GO TO 288
282 NREACT=NREACT+1
      IF(DATA(1) .EQ. REACT) AR(NJ1,NREACT)=AC(NREACT)
      IF(DATA(1) .EQ. PRODT) AP(NJ2,NREACT)=AC(NREACT)
      DO 241 II=1,NSK1
      DO 242 J=1,3
      IJ1=I+J-1
      IF(DATA(IJ1) .NE. SIB(II,J)) GO TO 241
242 CONTINUE
      IF(DATA(1) .EQ. REACT) NJR(NJ1,NREACT)=II
      IF(DATA(1) .EQ. PRODT) NJP(NJ2,NREACT)=II
      IF(II .LE. NS .OR. II .EQ. NSK1) GO TO 241
      IF(DATA(1) .EQ. REACT) MAR(NJ1,NREACT)=II
      IF(DATA(1) .EQ. PRODT) MAP(NJ2,NREACT)=II
241 CONTINUE
248 CONTINUE
      IF(DATA(1) .EQ. PRODT) GO TO 288
      GO TO 288
283 READ(5,2888) (DATA(I),I=1,6)
2888 FORMAT(3A4,3E10.4)
      AKF1(NJ1)=DATA(4)
      AKF2(NJ1)=DATA(5)
      AKF3(NJ1)=DATA(6)
      GO TO 288
C*** REARRANGE DIFFERENTIAL EQUATIONS,INSERTING AND INITIALIZING NOMIT EQMHD
218 CONTINUE
      IF(NJ1 .EQ. 0) GO TO 9889
C.....THIS SECTION WILL OUTPUT TO (FORTRAN LOGICAL UNIT 6) THE SET
C      OF FINITE RATE REACTIONS AS WELL AS THEIR RATE EQUATION
      WRITE(6,9884)
9884 FORMAT(1H1,54X,25HNON-EQUILIBRIUM REACTIONS)
      DO 9888 II=1,NJ1
      DO 9887 JJ=1,4
      IX=MAR(II,JJ)-NS
      IX=MAP(II,JJ)-NS
      IF(NJR(II,JJ) .NE. 0) IX1=JJ
      IF(NJP(II,JJ) .NE. 0) IX2=JJ
9887 CONTINUE
      IF(IX1.LE.0.OR.IX2.LE.0)GO TO 9888
      IF(IX1.GT.4)IX1=4
      IF(IX2.GT.4)IX2=4
      DO 9814 IX=1,IX1
      IXX=IJR(II,IX)
      DO 9818 JJ=1,3
9818 OUTR(IX,JJ)=SUB(IXX,JJ)

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MHD 1598
MHD 1595
MHD 1608
MHD 1605
MHD 1618
MHD 1615
MHD 1628
MHD 1625
MHD 1638
MHD 1635
MHD 1648
MHD 1645
MHD 1658
MHD 1655
MHD 1668
MHD 1665
MHD 1678
MHD 1675
MHD 1688
MHD 1685
MHD 1698
MHD 1695
MHD 1708
MHD 1705
MHD 1718
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MHD 1725
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MHD 1748
MHD 1745
MHD 1758
MHD 1755
MHD 1768
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MHD 1798
MHD 1795
MHD 1808
MHD 1805
MHD 1818
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MHD 1825
MHD 1838
MHD 1835
MHD 1848
MHD 1845
MHD 1858
MHD 1855
MHD 1868
MHD 1865

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9014 CONTINUE
      DO 9015 IX=1,IX2
        IXX=NJP(II,IX)
        DO 9011 JJ=1,3
9011 OUTP(IX,JJ)=SUB(IXX,JJ)
9015 CONTINUE
      WRITE(6,9006) II,(IFL(IX),AR(II,IX),(OUTP(IX,JJ),JJ=1,3),
        * IX=1,IX1),(IFL1(IX),AP(II,IX),(OUTP(IX,JJ),
        * JJ=1,3),IX=1,IX2)
9006 FORMAT(///IX,I2,4X,A1,F4.1,2X,3A4,5(1X,A1,F4.1,2X,3A4))
      WRITE(6,9005) AKF1(II),AKF2(II),AKF3(II)
9005 FORMAT(/17H CHEMICAL RATE - ,1PE12.4,4H*T**,0PF10.4,
        * 6H*EXP(-,1PE13.4,3H/T))
9008 CONTINUE
      WRITE(6,9012)
9012 FORMAT(//)
C.....ALL RATE EQUATIONS PRINTED
9009 CONTINUE
      IF(FIRST)GO TO 9013
      TSAV1=NE(1,ITE1)
      TSAV2=NE(1,ITE1+1)
      TSAV3=NE(1,ITE2)
      TSAV4=NE(1,ITE3)
9013 CONTINUE
      DO 212 J=1,NOMIT
        NSPJ=NS+J
        IF(EN(NPTM1,NSPJ).LE.0.000)EN(NPTM1,NSPJ)=ENINIT
        IF(NJ1.EQ.0.AND).EN(NPTM1,NSPJ).LE.ACCCRT)KBEGN(J)=-1
212  NE(1,J)=EN(NPTM1,NSPJ)
        IF(FIRST)GO TO 4
        ITE1=ITE1+NOMIT
        ITE2=ITE2+NOMIT
        ITE3=ITE3+NOMIT
        IF(ITE3.GT.32)STOP 7
        IF(JJPATH.EQ.0)GO TO 3017
        TE(1,ITE1)=TSAV1
        NE(1,ITE1+1)=TSAV2
        NE(1,ITE2)=TSAV3
        NE(1,ITE3)=TSAV4
        IF(KKSPEC.EQ.0)GO TO 120
        DO 213 K=1,ITE2
          ICHX(K)=0
          XMAX(K)=DABS(NE(1,K))
          IF(XMAX(K).LE.ACCCRT)XMAX(K)=ACCCRT
213  CONTINUE
          JSTART=0
          NOMNJ1=NOMIT*NJ1
          GO TO 128
C
4  JSTART=0
   FIRST=.FALSE.
   ITE1=NOMIT+1
   ITE2=ITE1+1
   ITE3=ITE2+1
   IF(ITE3.GT.32)STOP 7
C... INPUT PATH CONTROL AND NO. OF INPUTS IN APPROPRIATE VECTORS

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MHD 1870
MHD 1875
MHD 1880
MHD 1885
MHD 1890
MHD 1895
MHD 1900
MHD 1905
MHD 1910
MHD 1915
MHD 1920
MHD 1925
MHD 1930
MHD 1935
MHD 1940
MHD 1945
MHD 1950
MHD 1955
MHD 1960
MHD 1965
MHD 1970
MHD 1975
MHD 1980
MHD 1985
MHD 1990
MHD 1995
MHD 2000
MHD 2005
MHD 2010
MHD 2015
MHD 2020
MHD 2025
MHD 2030
MHD 2035
MHD 2040
MHD 2045
MHD 2050
MHD 2055
MHD 2060
MHD 2065
MHD 2070
MHD 2075
MHD 2080
MHD 2085
MHD 2090
MHD 2095
MHD 2100
MHD 2105
MHD 2110
MHD 2115
MHD 2120
MHD 2125
MHD 2130
MHD 2135
MHD 2140
MHD 2145

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      IF(IMREAD.NE.0)GO TO 3014                      MHD 2150
      IF(NEOPT.LT.3)GO TO 3011                      MHD 2155
      UE=0.0                                          MHD 2160
      IF(PCP(1).EQ.1.0)GO TO 3011                  MHD 2165
      UE=DSORT(2.D0*3314.3D0*(HSUM(1)-HSUM(NPTM1))) MHD 2170
3011 CONTINUE                                         MHD 2175
C**** INPUT THE FOLLOWING VARIABLES IN NAMELIST 'CHNLIN' MHD 2180
C      NMPATH=PATH DESCRIBING INPUTS WHERE 1 MEANS INPUT VELOCITY MHD 2185
C                                          2 MEANS INPUT PRESSURE MHD 2190
C                                          3 MEANS INPUT AREA MHD 2195
C                                          -1 MEANS CONSTANT VEL. USED MHD 2200
C                                          AT CHANNEL ENTRANCE MHD 2205
C                                          -2 MEANS CONSTANT PRESSURE USED MHD 2210
C                                          AT CHANNEL ENTRANCE MHD 2215
C                                          -3 MEANS CONSTANT AREA USED MHD 2220
C                                          AT CHANNEL ENTRANCE MHD 2225
C                                          0 IS DEFAULT VALUE (TO -1) MHD 2230
C      IMPRNT IS DEBUG LEVEL OF OUTPUT MHD 2235
C      THE GREATER IN MAG. THE MORE OUTPUT MHD 2240
C      DEFAULT VALUE IS 0 MHD 2245
C      XXSTOP IS POSITION IN CHANNEL TO CEASE CALCULATIONS MHD 2250
C      0.0 DEFAULTS TO 10.001*DXI OR 10 POINTS WILL BE CALULATED MHD 2255
C      UEINP REFERS TO THE REQUESTED INITIAL VELOCITY AT THE CHANNEL ENTRMHD 2260
C      (0 DEFAULTS TO CALCULATING THE MHD 2265
C      STARTING VALUE BASED ON HSUM(1)-HSUM(NPTM1)) MHD 2270
C      ITYPE REFERS TO SET OF EQUATIONS TO BE SOLVED MHD 2275
C      ITYPE=1 FOR MHD FORMULATION MHD 2280
C      ITYPE=2 TO ADD FRICTION TERMS TO MHD FORMULATION MHD 2285
C      ITYPE=999 OR NEGATIVE NO. TO SET DERIVATIVES TO 0 MHD 2290
C      ITYPE =0 DEFAULTS TO ITYPE=1 MHD 2295
C.....THE FORMAT FOR XXSTOP AND UEINP IS 2F10.0 MHD 2300
      XXSTOP=0.0 MHD 2305
      UEINP=0.0 MHD 2310
      ITYPE=0 MHD 2315
CCCCC READ(11,3000) NMPATH,IMPRNT,XXSTOP,UEINP,ITYPE MHD 2320
      READ(11,CHNLIN) MHD 2325
C**** CALL NMLST('CHNLIN',0,11,NMPATH,IMPRNT,XXSTOP,UEINP,ITYPE) MHD 2330
      IF(ITYPE.EQ.0)ITYPE=1 MHD 2335
      IF(ITYPE.LT.0)ITYPE=999 MHD 2340
      IF(UEINP.NE.0.0)UE=UEINP MHD 2345
      IF(XXSTOP.EQ.0.0D0)XXSTOP=10.001*DX MHD 2350
      IF(IMPRNT.GE.1)WRITE(1,7000)NMPATH,IMPRNT,XXSTOP,UEINP,ITYPE MHD 2355
7000 FORMAT(1X,10(1H*),14HCHANNEL INPUTS,10(1H*)/,7X,7HNMPATH=,I3/, MHD 2360
      *7X,7HIMPRNT=,I3/,7X,7HXXSTOP=,G13.5/,7X, MHD 2365
      *6HUEINP=,G13.5/,7X,6HITYPE=,I3) MHD 2370
7001 FORMAT(1X,10(1H*),14HCHANNEL INPUTS,10(1H*)/,7X,7HNMPATH=,I3/, MHD 2375
      *7X,7HIMPRNT=,I3/,7X,7HXXSTOP=,G13.5/,7X, MHD 2380
      *6HUEINP=,G13.5/,7X,6HITYPE=,I3/,10X,20HINDEPENDENT VARIABLE,10X, MHD 2385
      *13HDEPENDENT VARIABLE) MHD 2390
7002 FORMAT(14X,F12.5,17X,F12.5) MHD 2395
      IF(NMPATH)3020,3016,3030 MHD 2400
3020 CONTINUE MHD 2405
      READ(11,3001,END=3025) XTNDP(1),DUMMIN(1) MHD 2410
      IF(XTNDP(1).GE.0.0)GO TO 3025 MHD 2415
      NMPATH=-NMPATH MHD 2420
      NUMIV=1 MHD 2425

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      GO TO 4005                                MHD 2430
3025 CONTINUE                                MHD 2435
      IF(NMPATH.GE.-3)GO TO 3014                MHD 2440
3016 NMPATH=-1                                MHD 2445
      GO TO 3014                                MHD 2450
3030 IF(NMPATH.GT.3)GO TO 3016                MHD 2455
C... INPUT INDEPENDENT AND DEPENDENT VARIABLE(IN PAIRS...ONE SET PER LINMHD 2460
      KOUNT=0                                MHD 2465
      5 KOUNT=KOUNT+1                          MHD 2470
      IF(KOUNT.GT.NUMIV)GO TO 3010             MHD 2475
      READ(11,3001,END=3010) XINDP(KOUNT),DUMMIN(KOUNT) MHD 2480
      IF(XINDP(KOUNT).NE.0.0)GO TO 5           MHD 2485
      IF(DUMMIN(KOUNT).NE.0.0)GO TO 5          MHD 2490
      KOUNT=KOUNT-1                            MHD 2495
      GO TO 5                                  MHD 2500
3010 NUMIV=NUMIV                              MHD 2505
      NUMIV=KOUNT-1                            MHD 2510
      IF(NUMIV.LE.0)NUMIV=1                    MHD 2515
C*****WISH TO INTEGRATE FROM THROAT TO 0.0 IF XINDP(1) .LT. 0.0 MHD 2520
      IF(XINDP(1).GE.0.0)GO TO 4009           MHD 2525
C...XINDP(1) IS NEGATIVE(ACTUAL DISTANCE OF THROAT RELATIVE TO 0.0) MHD 2530
C...DUMMIN(1) CONTAINS THE PRESSURE AT CHAN. ENTRANCE(0.0 POINT) MHD 2535
      PRESSURE IS ASSUMED LINEAR FROM THROAT TO 0.0 MHD 2540
C      CALCULATE: PSLOPE=(DUMMIN(1)-PPP(THROAT))/(-XINDP(1)) MHD 2545
      WHERE PPP(THROAT)=PPP(NPTM1)            MHD 2550
C...SET THE FOLLOWING VARIABLES TO CONTROL INTEGRATING FROM THROAT MHD 2555
C      KKSPEC=-NMPATH,BZ=0.0,NMPATH=2,NUMIV=2,NORD=1, MHD 2560
C      PRESIN(1)=PPP(THROAT)=PPP(NPTM1), MHD 2565
C      PRESIN(2)=PPP(CHAN. ENTRANCE)=DUMMIN(1), MHD 2570
C      NE(1,ITE1)=UE, MHD 2575
C      NE(1,ITE3)=PPP(THROAT)*101325.0 MHD 2580
C...NOTE,THE REMAINING SETS OF (XINDP,DUMMIN) DATA POINTS WILL MHD 2585
C      REFLECT THE ACTUAL VELOCITY,PRESSURE,OR AREA PROFILE DATA MHD 2590
C      IN THE CHANNEL (DEPENDING ON THE INPUT VALUE OF NMPATH) MHD 2595
C.....IF ACTUAL AREA PROFILE WILL RESULT SET UP DUMMY INTEGRATION VAR. MHD 2600
      IF(NUMIV.LT.3)GO TO 4003                MHD 2605
      WRITE(6,7001) NMPATH,IMPRNT,XXSTOP,UEINP,ITYPE MHD 2610
      WRITE(6,7002) XINDP(K),DUMMIN(K),K=1,NUMIV MHD 2615
4005 CONTINUE                                MHD 2620
      IF(NMPATH.NE.3)GO TO 4002                MHD 2625
C...AREA PROFILE WILL DEFINE CHANNEL CALCULATIONS MHD 2630
      ITE2=ITE2+1                              MHD 2635
      ITE3=ITE2+1                              MHD 2640
      IF(ITE3.GT.32)STOP 7                     MHD 2645
      NE(1,ITE1+1)=140.0                      MHD 2650
4002 NUMIVS=NUMIV-1                          MHD 2655
      BZSAV=BZ                                MHD 2660
      KKSPEC=-NMPATH                          MHD 2665
      BZ=0.0                                  MHD 2670
      NUMIV=2                                  MHD 2675
      NORD=1                                  MHD 2680
      PRESIN(1)=PPP(NPTM1)                     MHD 2685
      PRESIN(2)=DUMMIN(1)                     MHD 2690
      NE(1,ITE3)=PPP(NPTM1)*101325.0          MHD 2695
      NE(1,ITE1)=UE                            MHD 2700
      PSLOPE=(DUMMIN(1)-PPP(NPTM1))/XINDP(1) MHD 2705

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      IF (IMPRNT.GE.0) WRITE(1,4001) NMPATH, XINDP(1), DUMMIN(1), PSLOPE
4001  FORMAT(1X,10(IH*),I3,3(5X,F10.4))
      GO TO 3014
4009  CONTINUE
      GO TO(4010,4020,4030), NMPATH
C... INPUT VELOCITY VECTOR
4010  DO 4012 K=1, NUMIV
4012  VELIN(K)=DUMMIN(K)
      UECALC=0.0
      NE(1,ITE3)=UE
      NE(1,ITE1)=PPP(NPTM1)*101325.
      IF (NUMIV.GE.2) GO TO 3014
      NUMIV=2
      VELIN(2)=VELIN(1)
      XINDP(2)=XINDP(1)+1.0
      GO TO 3014
C... INPUT PRESSURE VECTOR
4020  DO 4022 K=1, NUMIV
4022  PRESIN(K)=DUMMIN(K)
      IF (NUMIV.GE.2) GO TO 4023
      NUMIV=2
      PRESIN(2)=PRESIN(1)
      XINDP(2)=XINDP(1)+1.0
4023  NE(1,ITE1)=UE
      NE(1,ITE3)=PPP(NPTM1)*101325.0
      GO TO 3014
C... INPUT AREA VECTOR
4030  ITE2=ITE2+1
      IF (ITE2.GT.32) STOP 7
      DO 4032 K=1, NUMIV
4032  AREAIN(K)=DUMMIN(K)
      NE(1,ITE1)=PPP(NPTM1)*101325.
      NE(1,ITE1+1)=UE
      IF (NUMIV.GE.2) GO TO 3014
      NUMIV=2
      AREAIN(2)=AREAIN(1)
      XINDP(2)=XINDP(1)+1.0
3014  CONTINUE
      IF (NMPATH.LT.0) GO TO 3037
      IF (XINDP(1).LT.0.0) GO TO 3037
      WRITE(6,7001) NMPATH, IMPRNT, XXSTOP, UEINP, ITYPE
      WRITE(6,7002) (XINDP(K), DUMMIN(K), K=1, NUMIV)
3037  CONTINUE
      IF (KKSPEC.LT.0) NMPATH=2
      IMREAD=1
      IF (XXSTOP.LT.0.0D0) GO TO 129
      JJPATH=KKSPEC
      IF (NPT.EQ.3 .AND. JJPATH.EQ.0) RETURN
      JJPATH=1
3017  CONTINUE
      IF (NMPATH.GT.0) GO TO 3036
      NUMIV=2
      XINDP(1)=0.0
      XINDP(2)=1.0
      NMPATH=-NMPATH
      WRITE(6,7001) NMPATH, IMPRNT, XXSTOP, UEINP, ITYPE

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MHD 2710
MHD 2715
MHD 2720
MHD 2725
MHD 2730
MHD 2735
MHD 2740
MHD 2745
MHD 2750
MHD 2755
MHD 2760
MHD 2765
MHD 2770
MHD 2775
MHD 2780
MHD 2785
MHD 2790
MHD 2795
MHD 2800
MHD 2805
MHD 2810
MHD 2815
MHD 2820
MHD 2825
MHD 2830
MHD 2835
MHD 2840
MHD 2845
MHD 2850
MHD 2855
MHD 2860
MHD 2865
MHD 2870
MHD 2875
MHD 2880
MHD 2885
MHD 2890
MHD 2895
MHD 2900
MHD 2905
MHD 2910
MHD 2915
MHD 2920
MHD 2925
MHD 2930
MHD 2935
MHD 2940
MHD 2945
MHD 2950
MHD 2955
MHD 2960
MHD 2965
MHD 2970
MHD 2975
MHD 2980
MHD 2985

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      GO TO (3015,3028,3029),NMPATH
C....CONSTANT VELOCITY AT CHANNEL ENTRANCE
3015 CONTINUE
      JVELFL=1
      GO TO 3036
C....CONSTANT PRESSURE VALUE AT CHANNEL ENTRANCE USED
3028 CONTINUE
      PRESIN(1)=PPP(3)
      PRESIN(2)=PPP(3)
      WRITE(6,7002) (XINDP(K),PRESIN(K),K=1,2)
      GO TO 3036
C....CONSTANT AREA VALUE AT CHANNEL ENTRANCE USED
3029 CONTINUE
      IF(KAREA.EQ.1)GO TO 3038
      KAREA=1
      ITE2=ITE2+1
      IF(ITE2.GT.32)STOP 7
3038 CONTINUE
      AREAIN(1)=AEAT(3)
      AREAIN(2)=AEAT(3)
      WRITE(6,7002) (XINDP(K),AREAIN(K),K=1,2)
3036 CONTINUE
3000 FORMAT(2I3,3F10.0,I4)
3001 FORMAT(2F10.0)
CXXX NE(1,ITE2)=SSUM(NPTM1)*AMULT
3002 FORMAT(1X,6HIN MHD,2X,I3,2X,3(F15.7,2X))
      XHM=HMIN
      DACC=ACCURC
      IF(JJPATH.NE.0)GO TO 3024
      JJPATH=1
      IF(NEOPT.LT.3)GO TO 3027
      UE=UEINP
      IF(PCP(1).EQ.1.0)GO TO 3027
      IF(UE.EQ.0.0)UE=DSQRT(16528.6*(HSUM(1)-HSUM(NPTM1)))
3027 CONTINUE
      VMOC(NPTM1)=UE
      GO TO (3023,3021,3022),NMPATH
C... PLACE VELOCITY IN FIRST POS.(INPUT PRESSURE)
3021 NE(1,ITE1)=UE
      NE(1,ITE3)=PPP(NPTM1)*101325.
C.... INITIAL PRESSURE MUST BE COMPAT. WITH PREVIOUS CALCULATION(NPTM1)
      KKOLD=0
      IF(PRESIN(1).NE.PRESIN(2))KKOLD=1
      PRESIN(1)=PPP(NPTM1)
      IF(KKOLD.EQ.0)PRESIN(2)=PRESIN(1)
      GO TO 3024
C... SET UP VECTORS FOR CASE OF AREA INPUTTED
3022 CONTINUE
      NE(1,ITE1)=PPP(NPTM1)*101325.
      NE(1,ITE1+1)=UE
C.... INITIAL AREA MUST BE COMPAT. WITH PREVIOUS CALCULATION(NPTM1)
      KKOLD=0
      IF(AREAIN(1).NE.AREAIN(2))KKOLD=1
      AREAIN(1)=AEAT(NPTM1)
      IF(KKOLD.EQ.0)AREAIN(2)=AREAIN(1)
      GO TO 3024

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MHD 2990
MHD 2995
MHD 3000
MHD 3005
MHD 3010
MHD 3015
MHD 3020
MHD 3025
MHD 3030
MHD 3035
MHD 3040
MHD 3045
MHD 3050
MHD 3055
MHD 3060
MHD 3065
MHD 3070
MHD 3075
MHD 3080
MHD 3085
MHD 3090
MHD 3095
MHD 3100
MHD 3105
MHD 3110
MHD 3115
MHD 3120
MHD 3125
MHD 3130
MHD 3135
MHD 3140
MHD 3145
MHD 3150
MHD 3155
MHD 3160
MHD 3165
MHD 3170
MHD 3175
MHD 3180
MHD 3185
MHD 3190
MHD 3195
MHD 3200
MHD 3205
MHD 3210
MHD 3215
MHD 3220
MHD 3225
MHD 3230
MHD 3235
MHD 3240
MHD 3245
MHD 3250
MHD 3255
MHD 3260
MHD 3265

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C...SET UP VECTORS FOR CASE OF VELOCITY INPUTTED          MHD 3270
3023 CONTINUE                                             MHD 3275
C.... INITIAL VELOCITY MUST BE COMPAT. WITH PREVIOUS CALCULATION(NPTM1) MHD 3280
      IF(VELIN(1).EQ.VELIN(2))JVELFL=1                    MHD 3285
      VELIN(1)=UE                                          MHD 3290
      IF(JVELFL.EQ.0)GO TO 3026                            MHD 3295
      VELIN(2)=UE                                          MHD 3300
      WRITE(6,7002) (XINDP(K),VELIN(K),K=1,2)             MHD 3305
      JVELFL=0                                             MHD 3310
3026 NE(1,ITE1)=PPP(NPTM1)*101325.                        MHD 3315
      NE(1,ITE3)=UE                                        MHD 3320
3024 CONTINUE                                             MHD 3325
      X0=XINDP(1)                                          MHD 3330
      IF(DX)3031,3032,3033                                MHD 3335
3031 DX=-DX                                               MHD 3340
      DXIMAX=DX                                           MHD 3345
      GO TO 3033                                           MHD 3350
3032 DX=DXIMAX                                           MHD 3355
3033 CONTINUE                                             MHD 3360
      DXSAV=DX                                             MHD 3365
      XL=0.                                                MHD 3370
      FIRST=.FALSE.                                       MHD 3375
      ONCE=.FALSE.                                        MHD 3380
120 CONTINUE                                             MHD 3385
      IF(IPP.GE.NEQPT)*FIX=0.75                           MHD 3390
      IF(IMPRNT.GE.0)WRITE(1,3002) NPTM1,PPP(NPTM1),SSUM(NPTM1),UE MHD 3395
      PRINTX=.TRUE.                                       MHD 3400
      XL=XL+DX                                             MHD 3405
      IF(KKSPEC)121,122,124                               MHD 3410
C... SET SPECIAL CONTROLS TO INTERPOLATE FROM THROAT TO 0.0 MHD 3415
121 XL=0.0                                                MHD 3420
      ITE=ITE2                                             MHD 3425
      NOMNJ1=NOMIT                                         MHD 3430
C...INTEGRATE FROM THROAT TO 0.0 IF THERE ARE RATE EQUATIONS OR MHD 3435
C CHANNEL HEAT LOSS OR NON-MHD FORMULATION              MHD 3440
      IF(NJ1.NE.0)GO TO 123                               MHD 3445
      IF(NOMIT.NE.0)GO TO 123                             MHD 3450
      IF(CHCALC.NE.0.0)GO TO 123                          MHD 3455
      IF(ITYPE.EQ.999)GO TO 5000                          MHD 3460
      IF(ITYPE.EQ.1)GO TO 5000                            MHD 3465
      GO TO 123                                           MHD 3470
C... SET VARIABLES FOR FIRST PASS THROUGH                MHD 3475
122 DX=DXSAV                                              MHD 3480
      NOMNJ1=NOMIT                                         MHD 3485
      IF(IPP.GE.NEQPT)NOMNJ1=NOMIT*NJ1                   MHD 3490
      X0=0.0                                               MHD 3495
      XL=X0+DX                                             MHD 3500
      KKSP=C=1                                             MHD 3505
123 CONTINUE                                             MHD 3510
      XH=X15TRT                                           MHD 3515
      DXCALC=DXIMAX*ACCURC                                 MHD 3520
      IF(XH.GT.DXCALC)XH=DXCALC                           MHD 3525
      ITE=ITE2                                             MHD 3530
      DDX=DX                                               MHD 3535
      IF (DX.GT.DXIMAX)DDX=DXIMAX                         MHD 3540
      DDXXSAV=DDX                                          MHD 3545

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      HP=H*PATH
      SP=SPATH
      ATERM=SSUM(NPTM1)
      AMULT=8314.3D0
      NE(1,ITE2)=ATERM*AMULT
      IF(.NOT.HP)GO TO 126
      ATERM=HSUM(NPTM1)
      AMULT=8314.3D0
      NE(1,ITE2)=ATERM*AMULT+.5*UE*UE
126  CONTINUE
      IF(KKSPEC.LT.0)GO TO 5060
      ICASEC=0
C***** PROBLEM WITH CASE OF ELIMINATING EQUATIONS WITH 0 DERIVATIVES
C***** IN DIFFUN AND....(SPECIFICALLY CAN NOT ELIMINATE H OR S CALC)
C***** TURNED OFF FOLLOWING CODE BY IF(ICASEC.EQ.0)GO TO 5060
C***** UNTIL SEE ***** LINE
C      IF(ICASEC.EQ.0)GO TO 5063
      IF(NOMIT.EQ.0)GO TO 5052
128  IF(NJ1.NE.0)GO TO 5052
C*** DO NOT INTEGRATE NOMIT EQUATIONS
      DO 5050 K=1,NOMIT
      DUMPHIN(K)=NE(1,K)
5050  CONTINUE
      DO 5051 K=ITE1,ITE3
      KMNOM=K-NOMIT
      KBEGN(KMNOM)=0
5051  NE(1,KMNOM)=NE(1,K)
      ITE1=1
      ITE2=ITE2-NOMIT
      ITE3=ITE3-NOMIT
      ITE=ITE2
      GO TO 5060
5052  ITE=ITE2
      ICASEC=0
C***** PROBLEM WITH CASE OF ELIMINATING EQUATIONS WITH 0 DERIVATIVES
C***** IN DIFFUN AND....(SPECIFICALLY CAN NOT ELIMINATE H OR S CALC)
C***** TURNED OFF FOLLOWING CODE BY IF(ICASEC.EQ.0)GO TO 5060
C***** UNTIL SEE ***** LINE
      IF(ICASEC.EQ.0)GO TO 5060
      IF(BZ.NE.0.0)GO TO 5060
      IF(SPATH)GO TO 5053
      ITE=ITE-1
      ICASEC=1
      AANS(ITE2)=NE(1,ITE2)
      GO TO 5054
5053  IF(NJ1.NE.0)GO TO 5054
      ITE=ITE-1
      ICASEC=1
      AANS(ITE2)=NE(1,ITE2)
5054  XREG0=100.0
      IF(ICASEC.EQ.0)GO TO 5060
      IF(NJ1.LE.1)GO TO 5060
      IEOSLV=1
      GO TO(5055,5056,5057),NM*PATH
5055  ATEST=INTERP(XREG0,XINDP,VELIN,1,NUMIV,DINT,IER)
      VARC=VELIN(1)

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MHD 3550
MHD 3555
MHD 3560
MHD 3565
MHD 3570
MHD 3575
MHD 3580
MHD 3585
MHD 3590
MHD 3595
MHD 3600
MHD 3605
MHD 3610
MHD 3615
MHD 3620
MHD 3625
MHD 3630
MHD 3635
MHD 3640
MHD 3645
MHD 3650
MHD 3655
MHD 3660
MHD 3665
MHD 3670
MHD 3675
MHD 3680
MHD 3685
MHD 3690
MHD 3695
MHD 3700
MHD 3705
MHD 3710
MHD 3715
MHD 3720
MHD 3725
MHD 3730
MHD 3735
MHD 3740
MHD 3745
MHD 3750
MHD 3755
MHD 3760
MHD 3765
MHD 3770
MHD 3775
MHD 3780
MHD 3785
MHD 3790
MHD 3795
MHD 3800
MHD 3805
MHD 3810
MHD 3815
MHD 3820
MHD 3825

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      GO TO 5058                                MHD 3830
5056 ATEST=INTERP(XREG0,XINDP,PRESIN,1,NUMIV,DINT,IER) MHD 3835
      VARC=PRESIN(1)                            MHD 3840
      GO TO 5058                                MHD 3845
5057 ATEST=INTERP(XREG0,XINDP,AREAIN,1,NUMIV,DINT,IER) MHD 3850
      VARC=AREAIN(1)                            MHD 3855
      IEQSLV=2                                  MHD 3860
5058 IF(ATEST.NE.VARC)GO TO 5060                MHD 3865
      ITE=ITE-IEQSLV                            MHD 3870
      AANS(ITE1)=NE(1,ITE1)                     MHD 3875
      IF(NMPATH.EQ.3)AANS(ITE1+1)=NE(1,ITE1+1) MHD 3880
C**** IF(ICASEC.EQ.1)GO TO 5060                MHD 3885
C**** TSTORE=NE(1,ITE1)                       MHD 3890
C**** NE(1,ITE1)=NE(1,ITE2)                   MHD 3895
C**** ICASEC=2                                 MHD 3900
C***** ABOVE CODE TO BE TURNED ON.           MHD 3905
5060 CONTINUE                                  MHD 3910
      IF(IMPRNT.LE.2)GO TO 5062                 MHD 3915
      DXOUTP(1)=NOMIT                           MHD 3920
      JJJJ=NOMIT                                MHD 3925
      IF(JJJJ.LE.0)JJJJ=1                      MHD 3930
      DXOUTP(2)=NE(1,JJJJ)                     MHD 3935
      DXOUTP(3)=DUMMIN(1)                      MHD 3940
      DXOUTP(4)=ITE1                           MHD 3945
      DXOUTP(5)=NE(1,ITE1)                     MHD 3950
      DXOUTP(6)=ITE2                           MHD 3955
      DXOUTP(7)=NE(1,ITE2)                     MHD 3960
      DXOUTP(8)=ITE                            MHD 3965
      DXOUTP(9)=ATEST                          MHD 3970
      DXOUTP(10)=VARC                          MHD 3975
      DXOUTP(11)=NJ1                           MHD 3980
      DXOUTP(12)=ICASEC                       MHD 3985
      N7MOJT=12                                MHD 3990
      NUMDBG=15                                MHD 3995
      CALL DBGOUT(NUMOUT,HP,SP,DXOUTP,NUMDBG) MHD 4000
5062 CONTINUE                                  MHD 4005
      IHALF=0                                   MHD 4010
      DO 127 K=1,ITE                           MHD 4015
      ICHK(K)=0                                 MHD 4020
      XMAX(K)=DABS(NE(1,K))                     MHD 4025
      IF(XMAX(K).LE.ACCCRT)XMAX(K)=ACCCRT       MHD 4030
127 CONTINUE                                  MHD 4035
124 CONTINUE                                  MHD 4040
      IF(X0.GE.XL)GO TO 2022                    MHD 4045
2020 XN=X0+XH                                  MHD 4050
      XLSTP=XL+XCLOSE                           MHD 4055
      IF(XN.LE.XLSTP)GO TO 2022                MHD 4060
      XH=XL-X0+XCLOSE                           MHD 4065
      XN=X0+XH                                  MHD 4070
      DDX=XH                                    MHD 4075
      IF(DDX.LE.0.001D0)DDX=0.001D0          MHD 4080
2023 CONTINUE                                  MHD 4085
      IF(NOMIT.EQ.0)GO TO 5061                 MHD 4090
      IF(NJ1.NE.0)GO TO 5061                  MHD 4095
      DO 5059 K=1,NOMIT                        MHD 4100
      XNS=K+NS                                  MHD 4105

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EN(NPT,KNS)=DUMMIN(K)	MHD 4110
5059 CONTINUE	MHD 4115
5061 CONTINUE	MHD 4120
XHOLD=XH	MHD 4125
IF(I PRNT.LT.2)GO TO 3009	MHD 4130
WRITE(1,3006) X0,XL,XN,XH	MHD 4135
3007 FORMAT(1X,3(F15.5,X))	MHD 4140
3006 FORMAT(1X,2(1H*),11HX0,XL,XN,XH,2X,F10.7,2X,F8.5,2X,F10.7,	MHD 4145
*2X,F15.12)	MHD 4150
3009 CONTINUE	MHD 4155
IF(XN.LE.XXSTOP)GO TO 125	MHD 4160
3035 IF(NEOPT.GE.3)GO TO 129	MHD 4165
WRITE(6,3132)	MHD 4170
3132 FORMAT(1X/,1X,10(1H*),30HOUTPUTS AT MAXIMUM TEMPERATURE,10(1H*))	MHD 4175
WRITE(6,3131) TTMAX,XXMAX,VVMAX,SSSSUM	MHD 4180
IF(IMPRNT.GT.0)WRITE(1,3131) TTMAX,XXMAX,VVMAX,SSSSUM	MHD 4185
WRITE(6,3133)	MHD 4190
3133 FORMAT(5X,7HSPECIES,15X,13HMOLE FRACTION)	MHD 4195
DO 325 KKSET=1,NCONMX	MHD 4200
SSSOUT=SCONMX(KKSET)/SSSSUM	MHD 4205
WRITE(6,3134) (SUB(KKSET,NNSET),NNSET=1,3),SSSOUT	MHD 4210
325 CONTINUE	MHD 4215
3134 FORMAT(5X,3A4,7X,G13.5)	MHD 4220
3131 FORMAT(1X,10(1H*),6HTMAX=,G13.4,2X,6HAT X=,G13.5,2X,	MHD 4225
*5HVEL=,G13.5,2X,10HMOLES/KG=,G13.5)	MHD 4230
129 CONTINUE	MHD 4235
DXOUTP(1)=XN	MHD 4240
DXOUTP(2)=XXSTOP	MHD 4245
DXOUTP(3)=NEOPT	MHD 4250
DXOUTP(4)=TTT(NPT)	MHD 4255
DXOUTP(5)=TTPSTP	MHD 4260
DXOUTP(6)=KSAV	MHD 4265
NUMOUT=6	MHD 4270
NUMDBG=16	MHD 4275
IF(IMPRNT.GT.0)CALL DBGOUT(NUMOUT,HP,SP,DXOUTP,NUMDBG,	MHD 4280
JJPATH=-1	MHD 4285
RETURN	MHD 4290
125 CONTINUE	MHD 4295
KKIIJJ=KKIIJJ-1	MHD 4300
IF(KKIIJJ.LT.0)KKIIJJ=0	MHD 4305
KKOLD=KKIIJJ	MHD 4310
CALL DIFSUB(ITE,X0,NE,SV,XH,XHM,DDX,DACC,2,XMAX,ERROR,	MHD 4315
* KFLAG,JSTART,6,PW,IPS,PC,32)	MHD 4320
IF(IMPRNT.GE.2)WRITE(1,3006)X0,XL,XN,XH	MHD 4325
IF(KBEGN(35).LT.0)GO TO 3332	MHD 4330
IF(DDX.NE.DDXSAV)DDX=DDXSAV	MHD 4335
C.....REMOVE FINITE RATE TERMS THAT HAVE APPROACHED ZERO	MHD 4340
IF(NOMIT.LE.0)GO TO 4041	MHD 4345
DO 4040 KK=1,NOMIT	MHD 4350
IF(KBEGN(KK).LT.0)GO TO 4040	MHD 4355
IF(NE(1,KK).GE.XMINC)GO TO 4039	MHD 4360
IF(NE(1,KK).GE.XMIND)GO TO 4040	MHD 4365
IF(KBEGN(KK).EQ.0)GO TO 4040	MHD 4370
KBEGN(KK)=-1	MHD 4375
CADDED NEXT LINE AS A TEST	MHD 4380
C KBEGN(KK)=0	MHD 4385

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      IF(CHCALC.EQ.0.0)KBEGN(KK)=0
C... ZERO OUT SAVED ARRAYS FOR DIFSUB
      DO 4044 LL=1,ITE
C... RESET XMAX ARRAY FOR RESTART
      XMAX(LL)=DABS(NE(1,LL))
      IF(XMAX(LL).LE.ACCCRT)XMAX(LL)=ACCCRT
4044 CONTINUE
      SV(1,KK)=0.0
      DO 4045 JJ=2,12
      SV(JJ,KK)=0.0
      IF(JJ.GT.8)GO TO 4045
      NE(JJ,KK)=0.0
4045 CONTINUE
      IF(IMPRT.GE.0)WRITE(1,4046) KK,NE(1,KK)
4046 FORMAT(2X,6HREMOVE,I3,4H EQU,5X,6HVALUE=,G13.5)
      JSTART=0
      GO TO 4040
4039 KBEGN(KK)=1
4040 CONTINUE
      IF(JSTART.EQ.0)GO TO 2020
4041 CONTINUE
      IF(KKIIJJ.LE.0)GO TO 2038
CCCC IF(IMPRT.GT.0)WRITE(1,2037) KKIIJJ,KKOLD,X0,NE(1,7)
2037 FORMAT(1X,1H.,7HKKIIJJ=,I5,1X,6HKKOLD=,I5,1X,3HX0=,G13.5,3X,
      *3HV7=,G13.5)
      IF(KKIIJJ.EQ.KKOLD)KKIIJJ=KKIIJJ-1
      IF(XH.LT.XHINCC)GO TO 2039
      XH=XHINC
      GO TO 2039
2038 CONTINUE
2039 CONTINUE
      IF(KFLAG.LT.0) GO TO 2040
      ONCE=.FALSE.
      DO 308 K=1,ITE2
      IF(KBEGN(K).LT.0)GO TO 308
      IF(NE(1,K).LE.ACCRT2) GO TO 302
308 CONTINUE
315 CONTINUE
      IF(NEOPT.GE.3)GO TO 318
      IF(TT.LE.TTMAX)GO TO 318
      TTMAX=TT
      XXMAX=X0
      IF(NMPATH.EQ.1)GO TO 316
      IVPOS=ITE1-2+NMPATH
      VVMA=NE(1,IVPOS)
      GO TO 317
316 VVMA/=INTERP(XXMAX,XINDP,VELIN,NORD,NUMIV,DINT,IER)
317 IF(NCONMX.LE.1)NCONMX=NS+NOMIT
      SSSUM=0.0
314 DO 319 KKSET=1,NS
      SCONMX(KKSET)=EN(NPT,KKSET)
      IF(SCONMX(KKSET).LT.0.0)SCONMX(KKSET)=0.0
      SSSUM=SSSUM+SCONMX(KKSET)
319 CONTINUE
      IF(NOMIT.EQ.0)GO TO 318
      KKSET=NS

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MHD 4390
MHD 4395
MHD 4400
MHD 4405
MHD 4410
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MHD 4455
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MHD 4470
MHD 4475
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MHD 4485
MHD 4490
MHD 4495
MHD 4500
MHD 4505
MHD 4510
MHD 4515
MHD 4520
MHD 4525
MHD 4530
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MHD 4555
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MHD 4570
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MHD 4595
MHD 4600
MHD 4605
MHD 4610
MHD 4615
MHD 4620
MHD 4625
MHD 4630
MHD 4635
MHD 4640
MHD 4645
MHD 4650
MHD 4655
MHD 4660
MHD 4665

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DO 320 NNSET=1,NOMIT
KKSET=KKSET+1
SCONMX(KKSET)=NE(1,NNSET)
IF(SCONMX(KKSET).LT.0.0)SCONMX(KKSET)=0.0
SSSSUM=SSSSUM+SCONMX(KKSET)
320 CONTINUE
318 CONTINUE
XN=X0
DO 311 K=1,ITE2
IF(K/EGN(K).LT.0)GO TO 311
TSAV1=DABS(NE(1,K))
IF(TSAV1.GT.ACCCRT)GO TO 3331
CCCCC IF(IMPRNT.GE.1)WRITE(1,3334) K,NE(1,K),XMAX(K),ERROR(K)
3334 FORMAT(1X,2(1H+),3H K=,I3,4H NE=,G13.5,6H XMAX=,G13.5,
*5H ERR=,G13.5)
GO TO 311
3331 CONTINUE
KSAV=K
IF(TSAV1.LT.XMAX(K)*DACC ) GO TO 312
311 CONTINUE
IF(XN.LT.XL) GO TO 2022
2022 XS=(XL-X0)/XH
J1=JSTART+1
IF(XS.NE.0.D0) GO TO 2030
J1=1
XS=1.
2030 IF(NOMNJ1.EQ.0) GO TO 2031
DO 601 II=1,NOMIT
IINS=II+NS
EN(NPT,IINS)=0.
DO 602 J=1,J1
602 EN(NPT,IINS)=EN(NPT,IINS)+NE(J,II)*XS**(J-1)
601 CONTINUE
2031 CONTINUE
DO 620 J=1,ITE
620 AANS(J)=0.0D0
DO 603 J=1,J1
TSAV1=XS**(J-1)
DO 604 K=1,ITE
AANS(K)=AANS(K)+NE(J,K)*TSAV1
604 CONTINUE
603 CONTINUE
605 CONTINUE
C**** IF(1/ASEC.NE.2)GO TO 618
C**** AANS(ITE2)=AANS(ITE1)
C**** AANS(ITE1)=TSTORE
618 CONTINUE
IF(KKSPEC.LT.0)GO TO 619
TSAV2=XINDP(NUMIV-1)
IF(XN.GE.TSAV2)NORD=1
619 CONTINUE
GO TO(622,621,623),NMPAT4
C...INTERPOLATE PRESSURE,SET VEL. AND ENTROPY
621 XREG0=XL
PPINT=INTERP(XREG0,XINDP,PRESIN,NORD,NUMIV,DINT,IER)
PP=PPINT

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MHD 4670
MHD 4675
MHD 4680
MHD 4685
MHD 4690
MHD 4695
MHD 4700
MHD 4705
MHD 4710
MHD 4715
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MHD 4730
MHD 4735
MHD 4740
MHD 4745
MHD 4750
MHD 4755
MHD 4760
MHD 4765
MHD 4770
MHD 4775
MHD 4780
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MHD 4790
MHD 4795
MHD 4800
MHD 4805
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MHD 4875
MHD 4880
MHD 4885
MHD 4890
MHD 4895
MHD 4900
MHD 4905
MHD 4910
MHD 4915
MHD 4920
MHD 4925
MHD 4930
MHD 4935
MHD 4940
MHD 4945

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      UE=AANS(ITE1)
      GO TO 624
C...INTERPOLATE VELOCITY,SET PRESSURE AND ENTROPY
622 XREG0=XL
      UE=INTERP(XREG0,XINDP,VELIN,NORD,NUMIV,DINT,IER)
      PP=AANS(ITE1)/101325.
      GO TO 624
C...INTERPOLATE AREA,SET VEL. ,PRESSURE ,AND ENTROPY
623 XREG1=XL
      ARINT=INTERP(XREG0,XINDP,AREAIN,NORD,NUMIV,DINT,IER)
      PP=AANS(ITE1)/101325.
      UE=AANS(ITE1+1)
      AEAT(NPT)=ARINT
624 CONTINUE
      IF(SP)S0=AANS(ITE2)/AMULT
      IF(HP)H0= (AANS(ITE2)-0.5*UE*UE)/AMULT
      KBEGN(35)=0
625 VMOC(NPT)=UE
626 CONTINUE
      IF(IMPRNT.GE.0)WRITE(1,3003) PP,S0,UE,ARINT,H0
3003 FORMAT(1X,12HMD FROM DIF,2X,F12.7,2X,F9.5,2X,F15.7,2(2X,F10.5))
      IF(KKSPEC.GE.0)GO TO 5040
C.....CONDITIONS AT CHANNEL ENTRANCE DETERMINED
C      RESET VARIABLES FOR CHANNEL CALCULATIONS
5000 PPP(NPT)=PRESIN(2)
      UE=NE(1,ITE1)
      XL=0.0
      JSTART=0
      JJPATH=0
      NMPATH=-KKSPEC
      KKSPEC=0
      BZ=BZSAV
      IF(NUMIVS.GE.2)GO TO 5005
C.....SET CHANNEL PROFILE AS CONSTANT VEL. OR PRESSURE OR AREA
      IF(NMPATH.NE.3)GO TO 5002
C... FLAG CONSTANT CHANNEL AREA
      KAREA=1
      NMPATH=-3
      RETURN
C... SET CONSTANT VELOCITY OR PRESSURE
5002 NUMIV=2
      XINDP(1)=0.0
      XINDP(2)=1.0
      WRITE(6,7001) NMPATH,IMPRNT,XXSTOP,UEINP,ITYPE
      GO TO (5003,5004),NMPATH
C...CONSTANT VELOCITY
5003 JVELFL=1
      RETURN
C...CONSTANT PRESSURE
5004 PRESIN(1)=PPP(NPT)
      WRITE(6,7002) (XINDP(K),PRESIN(K),K=1,2)
      RETURN
C... RESE" APPROPRIATE PROFILE
5005 CONTINUE
      NUMIV=NUMIVS
      GO TO (5010,5020,5030),NMPATH

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MHD 4950
MHD 4955
MHD 4960
MHD 4965
MHD 4970
MHD 4975
MHD 4980
MHD 4985
MHD 4990
MHD 4995
MHD 5000
MHD 5005
MHD 5010
MHD 5015
MHD 5020
MHD 5025
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MHD 5185
MHD 5190
MHD 5195
MHD 5200
MHD 5205
MHD 5210
MHD 5215
MHD 5220
MHD 5225

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C...RESET VELOCITIES
5010 DO 5015 K=1,NUMIVS
      KP1=K+1
      XINDP(K)=XINDP(KP1)
5015 VELIN(K)=DUMMIN(KP1)
      XINDP(1)=0.0
      RETURN
C...RESET PRESSURES
5020 DO 5025 K=1,NUMIVS
      KP1=K+1
      XINDP(K)=XINDP(KP1)
5025 PRESIN(K)=DUMMIN(KP1)
      XINDP(1)=0.0
      RETURN
C...RESET AREAS
5030 DO 5035 K=1,NUMIVS
      KP1=K+1
      XINDP(K)=XINDP(KP1)
5035 AREAIN(K)=DUMMIN(KP1)
      XINDP(1)=0.0
      RETURN
5040 CONTINUE
      CALL EQLBRM(.TRUE.)
      CALL CONDOC(.TRUE.)
      TT=TTT(NPT)
      IF(I2P.LE.4)RETURN
      TTSAV=TTT(NPTM1)
      IF(NPT.EQ.3)TTSAV=TTT(13)
      IF(TT.GE.TTSAV)RETURN
      TDIFUN=TMPSTP
      IF(TT.LE.TMPSTP)GO TO 3035
      RETURN
312 IF(X0.GE.XL) GO TO 2022
      IF(IMPRNT.LT.0)GO TO 3330
      WRITE(1,3335) KSAV
      WRITE(1,3336) (K,NE(1,K),XMAX(K),ERROR(K),K=1,ITE)
3335 FORMAT(1X,5(1H+),37HNE,XMAX,ERROR ARRAY FROM GEARS METHOD,3X,I2)
3336 FORMAT(1X,I2,2X,G13.5,2X,G13.5,2X,G13.5)
3330 CONTINUE
C-----
CCC IF(XH.GT.XHSTRT)XH=XHSTRT
CCC JSTART=0
CCC XMAX(KSAV)=DABS(NE(1,KSAV))
CCC ICHK(KSAV)=ICHK(KSAV)+1
CCC IF(ICHK(KSAV).GT.ICHKKS)GO TO 3338
CCC IF(KSAV.NE.0)GO TO 2020
C-----
      DO 313 K=1,ITE
      XMAX(K)=DABS(NE(1,K))
      IF(XMAX(K).LE.ACCCRT) XMAX(K)=ACCCRT
313 CONTINUE
      IF(KSAV.LE.0)GO TO 3337
      ICHK(KSAV)=ICHK(KSAV)+1
      IF(ICHK(KSAV).EQ.ICHKKS)GO TO 3338
CCCC IF(ICHK(KSAV).GT.1)GO TO 2020
3337 CONTINUE

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MHD 5230
MHD 5235
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MHD 5495
MHD 5500
MHD 5505

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	JSTART=0	MHD 5510
	IF(XH.LT.XHSTRT)GO TO 2020	MHD 5515
	XH=XHSTRT	MHD 5520
	IF(XH.GT.DXCALC)XH=DXCALC	MHD 5525
	GO TO 2020	MHD 5530
302	CONTINUE	MHD 5535
	IF(K.EQ.ITE2 .AND. HP)GO TO 315	MHD 5540
	IIHALF=IIHALF+1	MHD 5545
	IF(IIHALF.LE.IHALFS)GO TO 3339	MHD 5550
3338	CONTINUE	MHD 5555
	IPP=IPP-1	MHD 5560
	NPT=NPT-1	MHD 5565
	GO TO 129	MHD 5570
3332	CONTINUE	MHD 5575
	KBEGN(35)=-KBEGN(35)	MHD 5580
3339	CONTINUE	MHD 5585
	JSTART=-1	MHD 5590
	XH=XH/2.	MHD 5595
	IF(IMPRNT.LT.0)GO TO 2020	MHD 5600
	WRITE(1,3335) JSTART	MHD 5605
	WRITE(1,3336) (K,NE(1,K),XMAX(K),ERROR(K),K=1,ITE)	MHD 5610
	GO TO 2020	MHD 5615
2040	CONTINUE	MHD 5620
	KSAV=0	MHD 5625
	WRITE(1,3005) KFLAG	MHD 5630
	WRITE(6,3005) KFLAG	MHD 5635
3005	FORMAT(1X,10(1H*),7H KFLAG=,I5)	MHD 5640
	IF(KFLAG.NE.-4 .OR. ONCE) GO TO 2041	MHD 5645
	ONCE=.TRUE.	MHD 5650
	GO TO 312	MHD 5655
2041	WRITE(6,3004) KFLAG	MHD 5660
	ISV=0	MHD 5665
	IPP=IPP-1	MHD 5670
	NPT=NPT-1	MHD 5675
	CALL RKTOUT	MHD 5680
3004	FORMAT(23H ERROR - KFLAG =,I3)	MHD 5685
	STOP	MHD 5690
	END	MHD 5695
	SUBROUTINE SRCHCC	SRCC 10
C		SRCC 20
C	SEARCH FILE 7 FOR THERMO DATA FOR SPECIES TO BE CONSIDERED	SRCC 30
C		SRCC 40
C	THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR	SRCC 50
C	NON-CDC MACHINES	SRCC 60
C		SRCC 70
	DOUBLE PRECISION TTT,TM,PP,SIGMA,SIG,VLM1,VLM	SRCC 80
	DOUBLE PRECISION ENN,SUMN	SRCC 90
	DOUBLE PRECISION COLF,S,EN,S0	SRCC 100
C		SRCC 110
	INTEGER SUB,OMIT,FND,TOOBIG,ARRAY(80)	SRCC 120
C		SRCC 130
	LOGICAL SHOCK,MMHG,UV,DETN,SIGNIT,NSOM,CALCH	SRCC 140
	LOGICAL HP,SP,IP,NEWR,IONS,MOLES,FROZ,EQL,PSYA,RKT,VOL,TV,SV	SRCC 150
	LOGICAL FA,ERATIO,FPCT,OTTO,SFLG	SRCC 160
	LOGICAL NEOL,CONVG,LOGV,SFLG,AREA,TWOSTG	SRCC 170

C	PROGRAM NEQMDH(INPUT,OUTPUT,TAPE7,TAPE5=INPUT,TAPE6=OUTPUT)	MAIN 10	PAGE 0048
C		SRCC 180	
C	DIMENSION MT(4),B(4),NAM(3),TOOBIG(3,50)	SRCC 190	
C		SRCC 200	
	COMMON/MISC/S0,ENN,SUMN,TT,ATOM(3,101),LLMT(30),B0(30),B0P(30,2)	SRCC 210	
	1 ,TM,'LOW,TMID,THIGH,CPSUM,PP,OF,EORAT,FPCT,R,RR,HSUB0,AC(2),AM(2)	SRCC 220	
	2 ,HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(30),NAME(30,5)	SRCC 230	
	3 ,ANUM(30,5),PECWT(30),ENTH(30),FAZ(30),RTEMP(30),FOX(30),DEMS(30)	SRCC 240	
	4 ,RHOP,RMW(30),TLN,CR,OXF(30),ENNL,ENSAVE,ENLSAV ,TRACE	SRCC 250	
	COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,ISV, N2P, MOLES,NP,NT,NPT,NLM	SRCC 260	
	1 ,NS,KMAT,IMAT,IQ1,NOF,VOMIT,IP,NEWR,NSUB,NSUP,ITM,CPCVFR,CPCVEQ	SRCC 270	
	2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NF2,CALCHS	SRCC 280	
	3 ,IQSAVE,LSAVE,ISUP,ISUB,ITNUM	SRCC 290	
	COMMON/SPECE1/NSPCMX,NCMAX,NELMX,TEMP(175,2),SUB(600,3),S(1)	SRCC 300	
	COMMON/SPECE5/IUSE(1)	SRCC 310	
	COMMON/SPECE8/OMIT(3,1)	SRCC 320	
	COMMON/SPECE9/DATE(2,1)	SRCC 330	
	COMMON/KGM/EN(13,1)	SRCC 340	
	COMMON/THMF/COEF(2,7,1)	SRCC 350	
	COMMON/STOIC/A(30,1)	SRCC 360	
	COMMON/TSTG/TWOSTG,ALPH,NLM1,XELMC(30),XMC(1)	SRCC 370	
C...	NSPCMX REFERS TO THE MAXIMUM NO. OF SPECIES ALLOWED	SRCC 380	
C...	NCMAX REFERS TO THE MAXIMUM NO. OF CONDENSED SPECIES ALLOWED	SRCC 390	
C	THIS IS FIXED AND REFERS TO THE SIZE OF TEMP(N,2) IN COMMON	SRCC 400	
C	SPECE1.....MUST CHANGE THIS COMMON EVERYWHERE IF A LARGER	SRCC 410	
C	IS NEEDED	SRCC 420	
C...	NELMX REFERS TO THE MAXIMUM NO. OF ELEMENTS ALLOWED	SRCC 430	
C	THIS IS FIXED AND REFERS TO THE SIZE OF XELMC(N) AND A(N,NSS	SRCC 440	
C	MUST CHANGE COMMON TSTG AND STOIC EVERYWHERE IF	SRCC 450	
C	A LARGER SIZE IS NEEDED	SRCC 460	
C		SRCC 470	
C		SRCC 480	
C	EQUIVALENCE (ENDD,END)	SRCC 490	
	EQUIVALENCE (OTTO,CPCVFR),(CPCVEQ,LOGV)	SRCC 500	
	EQUIVALENCE (XT,IXT)	SRCC 510	
C		SRCC 520	
	DATA GAS/1HG/,END/3HEND/,IIFLG/0/	SRCC 530	
C.....		SRCC 540	
C		SRCC 550	
C..	WRITE(1,8888) NOMIT,(OMIT(I,1),I=1,3)	SRCC 560	
	871 FORMAT(35H0INSUFFICIENT STORAGE FOR FOLLOWING,13,8H SPECIES)	SRCC 570	
	880 FORMAT(8(3X,3A4))	SRCC 580	
	872 FORMAT(1X,25(1H*),38HFATAL ERROR NOT ENOUGH SPECIES STORAGE/,	SRCC 590	
	*10X,50HCHANGE VALUE OF NSPCMX AND APPROPRIATE VECTORS IN ,	SRCC 600	
	*22HCOMMON IN THE MAIN PGM)	SRCC 610	
	873 FORMAT(1X,20HNEW SIZE GREATER 600,5X,	SRCC 620	
	*47HCHANGE SIZE OF SUB(600,3) ARRAY IN ALL ROUTINES)	SRCC 630	
	8888 FORMAT(1X,6HNOMIT=,13,2X,6HOMIT= ,3A4)	SRCC 640	
	8999 FORMAT(/,1X,40HOUTPUT MOLECULAR WEIGHTS OF THE ELEMENTS/,1X,	SRCC 650	
	*3HNO.,2X,4HNAME,2X,13HMOLECULAR WT.)	SRCC 660	
	8998 FORMAT(1X,12,3X,A4,5X,F10.3)	SRCC 670	
C.....		SRCC 680	
C***	INITIALIZE MOLECULAR WTS. OF ELEMENTS AND SPECIES	SRCC 690	
C	AS WELL AS A(I,J)	SRCC 700	
	NCKOUN=0	SRCC 710	
	DO 300 I=1,NLM	SRCC 720	
	300 XELMC(I)=0.0	SRCC 730	


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      DO 301 J=1,NSPCMX
      XMWC(J)=0.0
      DO 301 I=1,NLM
      A(I,J)=0.0
301 CONTINUE
C... DETERMINE AND STORE MOLECULAR WTS. OF THE ELEMENTS
C**** WRITE(1,8999)
      DO 320 I=1,NLM
      IXT=LLMT(I)
      DO 315 K=1,101
      IF(XT.NE.ATOM(1,K))GO TO 315
      XELMC(I)=ATOM(2,K)
C**** WRITE(1,8998) I,XT,XELMC(I)
      GO TO 320
315 CONTINUE
320 CONTINUE
C**** WRITE(1,8997)
8997 FORMAT(/,1X,39HOUTPUT MOLECULAR WEIGHTS OF THE SPECIES/,1X,
*3HNO.,2X,12HSPECIES NAME,2X,13HMOLECULAR WT.)
8996 FORMAT(1X,13,2X,3A4,5X,F10.3)
      I2B = 0
      NC= 0
      IX= 0
      NCOUNT=0
      MAXNS=6000
      IF(MAXNS.LT.NSPCMX)MAXNS=NSPCMX
C CHECK DIMENSION FOR NUMBER OF SPECIES
C
      SUB(1,1) = END
C
C READ TEMPERATURE RANGES FOR COEFFICIENTS OF GASEOUS SPECIES.
C
      READ(7,5) TLOW,TMID,THIGH
5 FORMAT (3F10.3)
      NS = 1
      IBLK=0
C
C BEGIN LOOP FOR READING SPECIES DATA FROM TAPE.
C
      7 READ(7,10,ERR=999)ARRAY,(NAM(I),I=1,3),DATE(1,NS),DATE(2,NS),
      1 (MT(J),B(J),J=1,4),PHAZ,T1,T2
10 FORMAT(80A1,T1,3A4,6X,2A3,4(A2,F3.0),A1,2F10.3)
      IBLK=IBLK+1
      DO 9930 J=1,4
      IF(B(J).EQ.-0.)B(J)=0.
9930 CONTINUE
      IF(T1.EQ.-0.)T1=0.
      IF(T2.EQ.-0.)T2=0.
      NCOUNT=NCOUNT+1
      IF(NAM(1).EQ.END) GO TO 171
      READ(7,20,ERR=999)((COEF(I,J,NS),J=1,7),I=1,2)
20 FORMAT (5E15.8)
      IF(NOMIT.EQ.0) GO TO 810
      DO 805 I=',NOMIT
      DO 804 J=1,3
      IF(OMIT(J,I).NE.NAM(J)) GO TO 805
      SRCC 740
      SRCC 750
      SRCC 760
      SRCC 770
      SRCC 780
      SRCC 790
      SRCC 800
      SRCC 810
      SRCC 820
      SRCC 830
      SRCC 840
      SRCC 850
      SRCC 860
      SRCC 870
      SRCC 880
      SRCC 890
      SRCC 900
      SRCC 910
      SRCC 920
      SRCC 930
      SRCC 940
      SRCC 950
      SRCC 960
      SRCC 970
      SRCC 980
      SRCC 990
      SRCC1000
      SRCC1010
      SRCC1020
      SRCC1030
      SRCC1040
      SRCC1050
      SRCC1060
      SRCC1070
      SRCC1080
      SRCC1090
      SRCC1100
      SRCC1110
      SRCC1120
      SRCC1130
      SRCC1140
      SRCC1150
      SRCC1160
      SRCC1170
      SRCC1180
      SRCC1190
      SRCC1200
      SRCC1210
      SRCC1220
      SRCC1230
      SRCC1240
      SRCC1250
      SRCC1260
      SRCC1270
      SRCC1280
      SRCC1290

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804 CONTINUE
GO TO 7
805 CONTINUE
810 CONTINUE
XMWSUM=0.0
DO 820 K=1,4
IF(B(K).EQ.0.) GO TO 825
DO 168 I=1,NLM
IF(LLMT(I).EQ.MT(K)) GO TO 818
168 CONTINUE
IF(NS.GT.NSPCMX) GO TO 7
DO 819 J=1,NLM
819 A(J,NS) = 0.
GO TO 7
C... DETERMINE MOLECULAR WT. OF THIS SPECIES AND SET COEF.
818 CONTINUE
XMWSUM=XMWSUM+B(K)*XELMC(I)
IF(NS.LE.NSPCMX)A(I,NS)=B(K)
820 CONTINUE
825 CONTINUE
XMWC(NS)=XMWSUM
C++++ WRITE(1,8996) NS,(NAM(I),I=1,3),XMWSUM
828 DO 829 I=1,3
829 SUB(NS,I) = NAM(I)
IF(NS.LE.NSPCMX)GO TO 835
IF(NS.LE.MAXNS)GO TO 170
I2B = I2B+1
DO 826 I=1,3
826 TOOBIG(I,I2B) = NAM(I)
GO TO 7
835 CONTINUE
IUSE(NS) = 0
IF(PHAZ.EQ.GAS) GO TO 170
C
C CONDENSED SPECIES
C
IF(NC.LT.NCMAX)GO TO 900
NCKOUN=NCKOUN+1
GO TO 7
900 CONTINUE
NC= NC+1
200 TEMP(NC,1)=T1
TEMP(NC,2)= T2
IX= IX+1
IF(NS.EQ.1.OR.IUSE(NS-1).EQ.0) GO TO 145
DO 830 I=1,NLM
IF(A(I,NS).NE.A(I,NS-1)) GO TO 145
830 CONTINUE
IX= IX-1
145 IUSE(NS)= -IX
170 NS= NS+1
GO TO 7
C
C END CARD HAS BEEN READ.
C
171 NS= NS-1

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SRCC1300
SRCC1310
SRCC1320
SRCC1330
SRCC1340
SRCC1350
SRCC1360
SRCC1370
SRCC1380
SRCC1390
SRCC1400
SRCC1410
SRCC1420
SRCC1430
SRCC1440
SRCC1450
SRCC1460
SRCC1470
SRCC1480
SRCC1490
SRCC1500
SRCC1510
SRCC1520
SRCC1530
SRCC1540
SRCC1550
SRCC1560
SRCC1570
SRCC1580
SRCC1590
SRCC1600
SRCC1610
SRCC1620
SRCC1630
SRCC1640
SRCC1650
SRCC1660
SRCC1670
SRCC1680
SRCC1690
SRCC1700
SRCC1710
SRCC1720
SRCC1730
SRCC1740
SRCC1750
SRCC1760
SRCC1770
SRCC1780
SRCC1790
SRCC1800
SRCC1810
SRCC1820
SRCC1830
SRCC1840
SRCC1850

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231 NEWR=.FALSE.                                SRCC1860
    WRITE(6,172)                                SRCC1870
172 FORMAT(42H0SPECIES BEING CONSIDERED IN THIS SYSTEM ) SRCC1880
    DO 174 I=1,NS,5                             SRCC1890
      I5= I+4                                    SRCC1900
      IF(NS.LT.I5) I5=NS                        SRCC1910
174 WRITE (6,176)(LATE(1,J),DATE(2,J),SUB(J,1),SUB(J,2),SUB(J,3),J=I, SRCC1920
      1 I5)                                     SRCC1930
      WRITE(6,995) NS,NLM,NC,IX,I2B,NREAC,NCOUNT SRCC1940
995 FORMAT(7I10)                                SRCC1950
      WRITE(6,996)(LLMT(I), I=1,NLM)           SRCC1960
996 FORMAT(10X,A4)                             SRCC1970
176 FORMAT(5(5X,2A3,2X,3A4))                   SRCC1980
      IF(NCKOUN.NE.0)WRITE(6,8094) NCMAX,NCKOUN SRCC1990
8994 FORMAT(1X,50(1H*),/,10X,26HTOO MANY CONDENSED SPECIES,/,10X, SRCC2000
      *14HPROGRAM ALLOWS,I4,2X,5HLAST,I3,      SRCC2010
      *61HIGNORED UPDATE TEMP(NC,2) VECTOR IN COMMON/SPECE1/ EVERYWHERE) SRCC2020
      IF(NS.LE.NSPCMX)RETURN                   SRCC2030
      KOUNT=NS-NSPCMX                           SRCC2040
      JOUT=NSPCMX+1                             SRCC2050
      WRITE(6,872)                              SRCC2060
      WRITE(6,871) KOUNT                        SRCC2070
      WRITE(6,880)((SUB(J,K),K=1,3),J=JOUT,NS) SRCC2080
      NS=0                                       SRCC2090
      IF(I2B.GT.0) GO TO 870                    SRCC2100
      RETURN                                    SRCC2110
870 WRITE(6,871) I2B                            SRCC2120
      WRITE(6,880)(TOOBIG(1,J),TOOBIG(2,J),TOOBIG(3,J),J=1,I2B) SRCC2130
      WRITE(6,873)                              SRCC2140
      RETURN                                    SRCC2150
999 WRITE(6,9999) IBLK,ARRAY                   SRCC2160
9999 FORMAT(29H0 JAVAF TABLE ERROR AT BLOCK ,I4/1H0,80A1) SRCC2170
      STOP                                     SRCC2180
      END                                     SRCC2190
      SUBROUTINE RKTOUT                          RKTO 10
C                                             RKTO 20
C ROCKET PERFORMANCE PARAMETERS              RKTO 30
C                                             RKTO 40
C THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR RKTO 50
C NON-CDC MACHINES                          RKTO 60
C                                             RKTO 70
C      DOUBLE PRECISION TTT,TM,PP,SIGMA,SIG,VLMI,VLM,DXOUTP    RKTO 80
C      DOUBLE PRECISION ENN,EMM,SUMN,AWT                      RKTO 90
C      DOUBLE PRECISION HSUM,SS,WM,CPR,DLVTP,DLVPT,GAMMAS,S0   RKTO 100
C      DOUBLE PRECISION S,EN,TSV1,TSV2,TSV4                   RKTO 110
C                                             RKTO 120
C      LOGICAL SHOCK,MHMG,UV,DETN,SIUNIT,NSQM,CALCH           RKTO 130
C      LOGICAL HP,SP,TP,NEWR,IONS,MOLES,FROZ,EQL,PSIA,RKT,VOL,TV,SV RKTO 140
C      LOGICAL ERATIO,FPCT,OTTO,SFLG                         RKTO 150
C      LOGICAL NEQL,CONVG,LOGV,SFLG,AREA                     RKTO 160
C                                             RKTO 170
C      DIMENSION NV(13),Z(10,4)                              RKTO 180
C                                             RKTO 190
C      COMMON/POINTS/HSUM(13),SUM(13),CPR(13),DLVTP(13),DLVPT(13) RKTO 200
C      1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13) RKTO 210
C      2 ,VL(13),TOTN(13)                                     RKTO 220

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COMMON/MISC/SS,ENN,SUMN,TT,ATOM(3,101),LLMT(30),B0(30),B0P(30,2) RKTO 230
1 ,EM,1LOW,TMID,THIGH,CPSJM,PP,OF,EORAT,FPCT,R,RR,HSUB0,AC(2),AM(2)RKTO 240
2 ,HPP(2),RH(2),VMIN(2),VELS(2),WP(2),DATA(30),NAME(30,5) RKTO 250
3 ,ANIM(30,5),PECWT(30),ENTH(30),FAZ(30),RTEMP(30),FOX(30),DENS(30)RKTO 260
4 ,HOP,RMW(30),TLN,CR,OXF(30),ENNL,ENSAVE,ENLSAV,TRACE RKTO 270
COMMON/IN0X/ IDEBUG,CONVS,TP,HP,SP,ISV, NPP, MOLES,NP,NT,NPT,NLM RKTO 280
1 ,NS,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWNR,NSUB,NSUP,ITM,CPCVFR,CPCVEQ RKTO 290
2 ,IONS,NC,NSLRT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCHRKTO 300
3 ,IOSAVE,LSAVE,ISUP,ISUB,ITNUM RKTO 310
COMMON/PERF/PCP(22),VMOC(13),SPIM(13),VAC(13),SUBAR(13),SUPAR(13)RKTO 320
1 ,APP(13),AEAT(13),CSTR,EQL,FROZ,SS0,AREA,AWT RKTO 330
COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4) RKTO 340
1 ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2 RKTO 350
2 ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0 RKTO 360
COMMON/MHDD/SSUMW,DX,DXI,XJY(26),AI(26),UE,NITER,NSTOP,SIG(26),IPPRKTO 370
X ,BZ,XK,PIPP RKTO 380
COMMON/NEQ/B0N(30),EMM,SNEQ,NO1,NSK,NEOPT RKTO 390
COMMON/SPEC1/NSPCMX,NCMAX,NELMX,TEMP(175,2),SUB(600,3),S(1) RKTO 400
COMMON/DBGVEC/DXOUTP(1) RKTO 410
COMMON/KGM/EN(13,1) RKTO 420
C... NSPCMX REFERS TO THE MAXIMUM NO. OF SPECIES ALLOWED RKTO 430
C... NCMAX REFERS TO THE MAXIMUM NO. OF CONDENSED SPECIES ALLOWED RKTO 440
C THIS IS FIXED AND REFERS TO THE SIZE OF TEMP(N,2) IN COMMON RKTO 450
C SPEC1.....MUST CHANGE THIS COMMON EVERYWHERE IF A LARGER SRKTO 460
C IS NEEDED RKTO 470
C... NELMX REFERS TO THE MAXIMUM NO. OF ELEMENTS ALLOWED RKTO 480
C THIS IS FIXED AND REFERS TO THE SIZE OF XELMC(N) AND A(N,NSRKTO 490
C .....MUST CHANGE COMMON TSTG AND STOIC EVERYWHERE IF RKTO 500
C A LARGER SIZE IS NEEDED RKTO 510
C RKTO 520
C RKTO 530
C DIMENSION XDMIKE(13) RKTO 540
C RKTO 550
C EQUIVALENCE (V(1),NV(1)) RKTO 560
C EQUIVALENCE (OTTO,CPCVFR),(CPCVEQ,LOGV) RKTO 570
C RKTO 580
C DATA EXIT/4HEXIT/ RKTO 590
C RKTO 600
5000 FORMAT(1X,14HTOTAL MOL WT ,1X,12(F8.3,1X),F8.3) RKTO 610
5001 FORMAT(1X,44HALL OUTPUTS FOR TOTAL MIXTURE(GAS+CONDENSED),1X, RKTO 620
*28HUNLESS SPECIFIED DIFFERENTLY) RKTO 630
5004 FORMAT(1X,4A4,16X,11I9) RKTO 640
5005 FORMAT(1X,4A4,16X,11(1X,F8.1)) RKTO 650
C RKTO 660
IF(.NOT.EQL) GO TO 636 RKTO 670
WRITE(6,37) RKTO 680
37 FORMAT(1H1/50X,32HTHEORETICAL MHD CORE PERFORMANCE /) RKTO 690
GO TO 39 RKTO 700
366 WRITE(6,38) RKTO 710
38 FORMAT(1H1,26X,78HTHEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN CRKTO 720
10MPOSITION DURING EXPANSION /) RKTO 730
IF(NFZ.GT.1) WRITE(6,63')NFZ RKTO 740
637 FORMAT(58X,11HAFTER POINT',I2) RKTO 750
39 IF(TTT(1).EQ.T(IT)) WRITE(6,737) RKTO 760
737 FORMAT (52X,28HAT AN ASSIGNED TEMPERATURE ) RKTO 770
TEM = PPP(1)*14.696006 RKTO 780

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      WRITE (6,40) TEM
40  FORMAT(5H0PC = ,F8.1,5H PSIA)
      CALL OUT1
      IF(NDIPT.LT.0)WRITE(6,5001)
      NEX = NPT - 2
      DO 862 I = 1,NEX
862  V(I) = DX*FLOAT(IPP - NPT - 1 + I)
      WRITE(6,48) (V(I),I=1,NEX)
48  FORMAT(1H0,55X,18HAXIAL STATION (M) /
      * 1H0,16X,16HCHAMBER THROAT ,11F9.3)

C
C  PRESSURE RATIOS
C
      FMT(4) = FMT(6)
      CALL VARFMT (APP,NPT)
      WRITE (6,FMT) FR1,FB,FB,FB,(APP(J),J=1,NPT)
      CALL OUT2

C
      AGV = 1.
      GC = 1.
      IF (R.GT.2.) GO TO 198
      GC = 32.174
      AGV = 9.80665
198  CONTINUE
      TSAV1=2.0*RR
      TSAV3=RR/(AGV*AGV)
      IF(NEOPT.LT.3)TSAV2=UE
      DO 202 K = 2,NPT
      IF(NEOPT.GE.3)GO TO 197
      IF(K.GE.4)GO TO 197
      IF(IPP.LE.13)GO TO 199
197  CONTINUE
      TSAV4=HSUM(1)-HSUM(K)
      IF(TSAV4.LE.0.0D0)GO TO 199
      TSAV2=DSQRT(TSAV1*TSAV4)
199  CONTINUE
      SPIM(K)=TSAV2/AGV

C
C  AW (A/W) IN UNITS OF SEC/ATM
C
      AW = TSAV3*TTT(K)/(PPP(K)*
      WM(K)*SPIM(K))
      IF(K.NE.2)GO TO 200
      CSTR = GC*PPP(1)*AW
      IF(NEOPT.LT.3)GO TO 200
      VMOC(2)=SPIM(2)*AGV
      AEAT(2) = 1.
200  VACI(K)=SPIM(K)+PPP(K)*AW
      IF (SONVEL(K).NE.0.) VMOC(K)=VMOC(K)/SONVEL(K)
      NV(K)= CSTR + .5
202  CONTINUE

C
C  MACH NUMBER
C
      VMOC(1)=0.
      DELT=ABS(VMOC(2)-1.0)
      IF(DELT.LT.1.0E-2)VMOC(2)=1.0

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RKTO 790
RKTO 800
RKTO 810
RKTO 820
RKTO 830
RKTO 840
RKTO 850
RKTO 860
RKTO 870
RKTO 880
RKTO 890
RKTO 900
RKTO 910
RKTO 920
RKTO 930
RKTO 940
RKTO 950
RKTO 960
RKTO 970
RKTO 980
RKTO 990
RKTO1000
RKTO1010
RKTO1020
RKTO1030
RKTO1040
RKTO1050
RKTO1060
RKTO1070
RKTO1080
RKTO1090
RKTO1100
RKTO1110
RKTO1120
RKTO1130
RKTO1140
RKTO1150
RKTO1160
RKTO1170
RKTO1180
RKTO1190
RKTO1200
RKTO1210
RKTO1220
RKTO1230
RKTO1240
RKTO1250
RKTO1260
RKTO1270
RKTO1280
RKTO1290
RKTO1300
RKTO1310
RKTO1320
RKTO1330
RKTO1340

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      IF(GAMMAS(2).EQ.0.) VMOC(2)=0.
      FMT(1) = F4
      WRITE(6,FMT)(FN(I),I=1,4),(VMOC(J),J=1,NPT)
      WRITE(6,208)
208  FORMAT(1H)
C
C  AREA RATIO
C
      FMT(4) = FMT9X
      CALL VARFMT(AEAT,NPT)
      FMT(5) = FB
      WRITE(6,FMT)(FA1,FA2,FB,FB,(AEAT(J),J=2,NPT)
C
C  C*
C
C*****
C  OUTPUT TOTN(I) INVERSE OR TOTAL MOLES/KG(USED IN CALCULATING MOLE FRR
      DO 5099 I=1,NPT
5099  XDMIKE(I)=1.0/TOTN(I)
      WRITE(6,5080)(XDMIKE(I),I=1,NPT)
C.....NEXT 4 OUTPUTS ARE NOT WANTED...THUS,SKIP
C          BY ADDING NEXT 2 LINES AND APPROPRIATE 4 LINES LATER
      ISKIP=10
      IF(ISKIP.EQ.10)GO TO 5096
C*****
      FMT(5) = FMT13
      FMT(6) = FMTI9
      FMT(7) = FB
      WRITE(6,FMT)(FR(I),I=1,4),(NV(J),J=2,NPT)
C
C  CF - THRUST COEFFICIENT
C
      FMT(6) = FMT(8)
      FMT(7) = F3
      DO 212 I=2,NPT
212  V(I)=GC*SPIM(I)/CSTR
      WRITE(6,FMT)(FC1,FB,FB,FB,(V(J),J=2,NPT)
C
C  VACUUM IMPULSE
C
      FMT(5) = FMT13
      FMT(7) = F1
      WRITE(6,FMT)(FA(I),I=1,4),(VACI(J),J=2,NPT)
C
C  SPECIFIC IMPULSE
C
      WRITE(6,FMT)(FI(I),I=1,4),(SPIM(J),J=2,NPT)
C.....ADDED NEXT 4 LINES TO DELETE OUTPUTTING OF C*,CF,IVAC,ISP
      GO TO 5095
5096  CONTINUE
      FMT(6)=FMT(8)
5095  CONTINUE
      WRITE(6,208)
      FMT(4) = FB
      FMT(5) = FMT13
      FMT(7) = F5

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RKTO1350
RKTO1360
RKTO1370
RKTO1380
RKTO1390
RKTO1400
RKTO1410
RKTO1420
RKTO1430
RKTO1440
RKTO1450
RKTO1460
RKTO1470
RKTO1480
RKTO1490
RKTO1500
RKTO1510
RKTO1520
RKTO1530
RKTO1540
RKTO1550
RKTO1560
RKTO1570
RKTO1580
RKTO1590
RKTO1600
RKTO1610
RKTO1620
RKTO1630
RKTO1640
RKTO1650
RKTO1660
RKTO1670
RKTO1680
RKTO1690
RKTO1700
RKTO1710
RKTO1720
RKTO1730
RKTO1740
RKTO1750
RKTO1760
RKTO1770
RKTO1780
RKTO1790
RKTO1800
RKTO1810
RKTO1820
RKTO1830
RKTO1840
RKTO1850
RKTO1860
RKTO1870
RKTO1880
RKTO1890
RKTO1900

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      IF(EQL) GO TO 312
      WRITE(6,310)
310  FORMAT(15HMOLE FRACTIONS //)
C
C   MOLE FRACTIONS - FROZEN
C
      TRA = 5.E-6
      IF(TRACE.NE.0.) TRA=TRACE
      LINE = 0
      DO 430 K = 1, NS
      V(LINE+1) = EN(NFZ,K)/TOTN(NFZ)
      IF(V(LINE+1).LT.TRA) GO TO 424
      LINE = LINE+1
      Z(LINE,1) = SUB(K,1)
      Z(LINE,2) = SUB(K,2)
      Z(LINE,3) = SUB(K,3)
      Z(LINE,4) = V(LINE)
424  IF (LINE.NE.4.AND.K.NE.NS) GO TO 430
      IF (LINE.EQ.0) GO TO 312
      WRITE (6,426) (Z(LN,1),Z(LN,2),Z(LN,3),Z(LN,4),LN=1,LINE)
426  FORMAT (1H,4(3A4,F9.5,7X))
      LINE = 0
430  CONTINUE
312  CALL OUT3
1000  CONTINUE
      RETURN
      END
      SUBROUTINE CPHS
C   CALCULATES THERMODYNAMIC PROPERTIES FOR INDIVIDUAL SPECIES
C
C   THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR
C   NON-CDC MACHINES
C
      DOUBLE PRECISION TTT,TM,PP,SIGMA,SIG,VLMI,VLM
      DOUBLE PRECISION ENN,EMM,SUMN
      DOUBLE PRECISION COEF,S,EN,H0,S0
C
      LOGICAL SHOCK,MMHG,UV,DEPN,SIUNIT,NSOM,CALCH
      LOGICAL HP,SP,IP,NEW,IONS,MOLES,FROZ,SOL,PSIA,RKT,VOL,TV,SV
      LOGICAL FA,ERATIO,FPCT,OTTO,SFLG
      LOGICAL NEQL,CONVG,LOGV,SFLG,AREA
C
      COMMON/MISC/S0,ENN,SUMN,TT,ATOM(3,101),LLMT(30),B0(30),B0P(30,2)
1   ,TM,TLOW,TMID,THIGH,CPSUM,PP,OF,EQPAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
2   ,HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(30),NAME(30,5)
3   ,ANUM(30,5),PECWT(30),ENTH(30),FAZ(30),RTEMP(30),FOX(30),DENS(30)
4   ,RHOP,RMV(30),TLN,CR,OXF(30),ENNL,ENSAVE,ENLSAV,TRACE,SIZE
      COMMON/INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM
1   ,NS,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEW,NSUB,NSUP,ITM,CPCVFR,CPCVEQ
2   ,IONS,IC,NSERT,JSOL,JLIT,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH
3   ,IOSAVE,LSAVE,ISUP,ISUB,ITRUM
      COMMON/NEQ/EN(30),MM,SLEQ,NQ1,NSK,NEQPT
      COMMON/SPACE1/NSPCMX,NCMX,NELMX,TEMP(1/5,2),SUB(500,3),S(1)
      COMMON/SPACE3/NO(1)
      COMMON/SPACE5/USE(1)
      COMMON/KGM/EN(13,1)

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RKTO1910
RKTO1920
RKTO1930
RKTO1940
RKTO1950
RKTO1960
RKTO1970
RKTO1980
RKTO1990
RKTO2000
RKTO2010
RKTO2020
RKTO2030
RKTO2040
RKTO2050
RKTO2060
RKTO2070
RKTO2080
RKTO2090
RKTO2100
RKTO2110
RKTO2120
RKTO2130
RKTO2140
RKTO2150
RKTO2160
RKTO2170
CPHS 10
CPHS 20
CPHS 30
CPHS 40
CPHS 50
CPHS 60
CPHS 70
CPHS 80
CPHS 90
CPHS 100
CPHS 110
CPHS 120
CPHS 130
CPHS 140
CPHS 150
CPHS 160
CPHS 170
CPHS 180
CPHS 190
CPHS 200
CPHS 210
CPHS 220
CPHS 230
CPHS 240
CPHS 250
CPHS 260
CPHS 270
CPHS 280
CPHS 290

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COMMON/THMP/COEF(2,7,1) CPHS 300
C... N5PCMX REFERS TO THE MAXIMUM NO. OF SPECIES ALLOWED CPHS 310
C... NCMAX REFERS TO THE MAXIMUM NO. OF CONDENSED SPECIES ALLOWED CPHS 320
C THIS IS FIXED AND REFERS TO THE SIZE OF TEMP(N,2) IN COMMON CPHS 330
C SPECE1.....MUST CHANGE THIS COMMON EVERYWHERE IF A LARGER SCPHS 340
C IS NEEDED CPHS 350
C... NELMX REFERS TO THE MAXIMUM NO. OF ELEMENTS ALLOWED CPHS 360
C THIS IS FIXED AND REFERS TO THE SIZE OF XELMC(N) AND A(N,NSCPHS 370
C .....MUST CHANGE COMMON TSTG AND STOIC EVERYWHERE IF CPHS 380
C A LARGER SIZE IS NEEDED CPHS 390
C CPHS 400
C CPHS 410
EQUIVALENCE (J,JS1) CPHS 420
EQUIVALENCE (OTTO,CPCVFR),(CPCVEQ,LOGV) CPHS 430
C CPHS 440
K = 1 CPHS 450
IF(TT.LE.TMID)K = 2 CPHS 460
KK = 0 CPHS 470
CPSUM=0. CPHS 480
90 CONTINUE CPHS 490
DO 92 IIK=1,7 CPHS 500
IF(COEF(K,IIK,J).NE.0.000)GO TO 97 CPHS 510
92 CONTINUE CPHS 520
IF (IUSE(J).LT.0) GO TO 150 CPHS 530
C CPHS 540
C IF COEFFICIENTS ARE ZERO, USE OTHER TEMPERATURE INTERVAL CPHS 550
C CPHS 560
KK = K CPHS 570
K = 1 CPHS 580
IF (KK.EQ.1) K = 2 CPHS 590
97 CONTINUE CPHS 600
S(J) = (((COEF(K,5,J)/4.)*TT+ COEF(K,4,J)/3.)*TT+ COEF(K,3,J)/2. CPHS 610
1)* TT+COEF(K,2,J))*TT+ COEF(K,1,J)*TLN + COEF(K,7,J) CPHS 620
H0(J) = (((COEF(K,5,J)/5.)*TT+ COEF(K,4,J)/4.)*TT+ COEF(K,3,J)/3. CPHS 630
1)* TT+ COEF(K,2,J)/2.)*TT+ COEF(K,1,J) + COEF(K,6,J)/TT CPHS 640
CPXXX= (((COEF(K,5,J)*TT+ COEF(K,4,J))*TT+ COEF(K,3,J))*TT CPHS 650
1 + COEF(K,2,J))*TT+ COEF(K,1,J) CPHS 660
CPSUM=CPSUM+CP:XX*EN(NPT,J) CPHS 670
IF (YK.EQ.0) GO TO 150 CPHS 680
K = KK CPHS 690
KK = 0 CPHS 700
150 CONTINUE CPHS 710
IF(J.EQ.NSK) RETURN CPHS 720
J=J+1 CPHS 730
GO TO 90 CPHS 740
200 RETURN CPHS 750
END CPHS 760
SUBROUTINE OUT1 OUT1 10
C OUT1 20
C OUT1 30
C THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR OUT1 40
C NON-CDC MACHINES OUT1 50
C OUT1 60
DOUBLE PRECISION TTT,TM,PP,SIGMA,SIG,VLM1,VLM OUT1 70
DOUBLE PRECISION ENN,SUMN OUT1 80
DOUBLE PRECISION HSUM,SSUM,CPR,DIUVD,DIUVD, GAMMAS,SG OUT1 90

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DOUBLE PRECISION G,X,S                                OUT1 100
C                                                       OUT1 110
LOGICAL SHOCK,MMHG,UV,DETN,SIUNIT,NSQM,CALCH          OUT1 120
LOGICAL HP,SP,TP,NEWIR,IONS,MOLES,PSIA,RKT,VOL,TV,SV  OUT1 130
LOGICAL ERATIO,FPCT,OTTO                              OUT1 140
LOGICAL NEOL,CONVG,LOGV                               OUT1 150
C                                                       OUT1 160
DIMENSION NV(13),Z(10,3),HEAD(15),YX(5),YN(5),FSB(3) OUT1 170
C                                                       OUT1 180
COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13) OUT1 190
1 ,GA IMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13) OUT1 200
2 ,VLM(13),TOTN(13)                                    OUT1 210
COMMON/MISC/S0,ENN,SUMN,TT,ATOM(3,101),LLMT(30),B0(30),B0P(30,2) OUT1 220
1 ,TM,TLOW,TMID,THIGH,CPSUM,PP,OF,EORAT,FPCT,R,RR,HSUB0,AC(2),AM(2) OUT1 230
2 ,HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(30),NAME(30,5) OUT1 240
3 ,ANUM(30,5),PECWT(30),ENTH(30),FAZ(30),RTEMP(30),FOX(30),DENS(30) OUT1 250
4 ,RHOP,RMW(30),TLN,CR,OXF(30),ENNL,ENSAVE,ENLSAV ,TRACE OUT1 260
COMMON /DOUBLE/ G(60,61), X(60)                       OUT1 270
COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,ISV, NPP, MOLES,NP,NT,NPT,NLM OUT1 280
1 ,NS,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWIR,NSUB,NSUP,ITM,CPCVFR,CPCVEQ OUT1 290
2 ,IONS,NC,NSERT,JSOL,JLID,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NF2,CALCHOUT1 OUT1 300
3 ,IQSAVE,LSAVE,ISUP,ISUB,ITNUM                        OUT1 310
COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4) OUT1 320
1 ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2 OUT1 330
2 ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0,FRHO(4) OUT1 340
C                                                       OUT1 350
COMMON/CSIG/SIGMA(13)                                  OUT1 360
COMMON/SIGOUT/FNEL(3),ANE(15),FIONS(3),AIONS(15),FSIGWO(4), OUT1 370
XFSIG(4),SIGM(15),PFREQ(3),TOTAL(15)                 OUT1 380
COMMON/SPECE1/NSPCMX,NCMAX,NELMX,TEMP(175,2),SUB(600,3),S(1) OUT1 390
C... NSPCMX REFERS TO THE MAXIMUM NO. OF SPECIES ALLOWED OUT1 400
C... NCMAX REFERS TO THE MAXIMUM NO. OF CONDENSED SPECIES ALLOWED OUT1 410
C THIS IS FIXED AND REFERS TO THE SIZE OF TEMP(N,2) IN COMMON OUT1 420
C SPECE1.....MUST CHANGE THIS COMMON EVERYWHERE IF A LARGER SOUT1 430
C IS NEEDED                                             OUT1 440
C... NELMX REFERS TO THE MAXIMUM NO. OF ELEMENTS ALLOWED OUT1 450
C THIS IS FIXED AND REFERS TO THE SIZE OF XELMC(N) AND A(N,NSOUT1 460
C .....MUST CHANGE COMMON TSTG AND STOIC EVERYWHERE IF OUT1 470
C A LARGER SIZE IS NEEDED                             OUT1 480
EQUIVALENCE (V(1),NV(1)),(IB,FB)                     OUT1 490
EQUIVALENCE (OTTO,CPCVFR),(CPCVEQ,LOGV)              OUT1 500
C                                                       OUT1 510
HEAD=(1H ,2A4,5 (A2,F8.5,3X),5 X,F7.5,F13.3,4X,A1,F10.2,F9.4) OUT1 520
C                                                       OUT1 530
DATA HEAD/4H(1H ,4H,2A4,2H,5,4H(A2,,4HF8.5 ,4H,3X),2H,5 ,2HX, OUT1 540
1 ,4HF7.5 ,4H,F13 ,4H,3,4 ,4HX,A1 ,4H,F10 ,4H,2,F ,4H9.4)/ OUT1 550
DATA FUEL/4HFUEL/,OXID/4HOXID/,ANT/3HANT/,OX/1HO/,I2/2H00/ OUT1 560
1 ,YN/2H,1, 2H,2, 2H,3, 2H,4, 2H,5 /,F75/4HF7.5/ OUT1 570
2 ,YX/3H,57,3H,44,3H,31,3H,18,2H,5 /,F73/4HF7.3/ OUT1 580
C                                                       OUT1 590
IF(KASE.NE.0) WRITE (6,3) KASE                        OUT1 600
3 FORMAT (9H CASE NO. ,I8)                            OUT1 610
IF (MOLES) GO TO 18                                    OUT1 620
WRITE (6,5)                                             OUT1 630
IF(ABS(R-RR/4184.)) .LT. 0.01) WRITE(6,4)            OUT1 640
IF(ABS(R-RR/4184.)) .GE. 0.01) WRITE(6,7)            OUT1 650

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5 FORMAT (77X,46HWT FRACTION    ENERGY    STATE    TEMP    DENSITY)    OUT1 660
4 FORMAT (10X,16HCHEMICAL FORMULA,51X,21H(SEE NOTE)    CAL/MOL,10X,    OUT1 670
1    5HDEG K,4X,4HG/CC )    OUT1 680
7 FORMAT (10X,16HCHEMICAL FORMULA,51X,22H(SEE NOTE)    KJ/KG-MOL,9X,    OUT1 690
1    5HDEG K,4X,4HG/CC )    OUT1 700
GO TO 19    OUT1 710
18 WRITE (6,6)    OUT1 720
IF(ABS(R-RR/4184.) .LT. 0.01) WRITE(6,8)    OUT1 730
IF(ABS(R-RR/4184.) .GE. 0.01) WRITE(6,9)    OUT1 740
6 FORMAT (79X,5HMOLES,7X,    33H ENERGY    STATE    TEMP    DENSITY)    OUT1 750
8 FORMAT (10X,16HCHEMICAL FORMULA,66X,7HCAL/MOL    ,10X,    OUT1 760
1    13HDEG K    G/CC )    OUT1 770
9 FORMAT (10X,16HCHEMICAL FORMULA,65X,9HKJ/KG-MOL,10X,    OUT1 780
1    13HDEG K    G/CC )    OUT1 790
19 DO 15 N=1,NREAC    OUT1 800
IF(FOX(N).NE.OX)GO TO 10    OUT1 810
HD1 = OXID    OUT1 820
HD2 = ANT    OUT1 830
GO TO 11    OUT1 840
10 HD1 = FUEL    OUT1 850
HD2 = FB    OUT1 860
11 DO 13 J=1,5    OUT1 870
IF(NAME(N,J).EQ.IZ.OR.NAME(N,J).EQ.IB) GO TO 14    OUT1 880
13 CONTINUE    OUT1 890
J=6    OUT1 900
14 J=J-1    OUT1 910
HEAD(3)=YN(J)    OUT1 920
HEAD(7)=YX(J)    OUT1 930
HEAD(9) = F75    OUT1 940
IF(PECWT(N).GE.10.) HEAD(9)=F73    OUT1 950
ETH = ENTH(N)    OUT1 960
IF(ABS(R-RR/4184.) .GE. 0.01) ETH=ETH*4.184    OUT1 970
WRITE(6,HEAD)HD1,HD2,(NAME(N,J),ANUM(N,J),JJ=1,J),PECWT(N),ETH    OUT1 980
1 ,FAZ(N),RTEMP(N),DENS(N)    OUT1 990
15 CONTINUE    OUT11000
FPC = 100./(1.+OF)    OUT11010
WRITE(6,20) OF ,FPC,EQRAT,RHOP    OUT11020
20 FORMAT (10X,15X, 4HO/F=, F8.4,4X,13HPERCENT FUEL=,F8.4,4X,    OUT11030
1    19HEQUIVALENCE RATIO= ,F7.4,4X,17HREACTANT DENSITY=,F8.4//)    OUT11040
C    OUT11050
AGV = 9.80665    OUT11060
RETURN    OUT11070
END    OUT11080
SUBROUTINE OUT2    OUT2 10
C    OUT2 20
C    OUT2 30
C    THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR    OUT2 40
C    NON-CDC MACHINES    OUT2 50
C    OUT2 60
DOUBLE PRECISION TTT,TM,PP,SIGMA,SIG,VLMI,VLM    OUT2 70
DOUBLE PRECISION ENN,SUMN,AWT    OUT2 80
DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS,S0    OUT2 90
DOUBLE PRECISION G,X,S,T0AV1    OUT2 100
C    OUT2 110
LOGICAL SHOCK,MMHG,UV,DETN,SIUNIT,NSQM,CALCH    OUT2 120
LOGICAL HP,SP,TP,NEW,IONS,MOLES,FROZ,EQL,PSIA,RKT,VOL,TV,SV    OUT2 130

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C      PROGRAM NSQNHDI INPUT,OUTPUT,TAPE7 TAPE5=INPUT,TAPE6=OUTPUT)      MAIN 10      PAGE 0059

      LOGICAL ERATIO,FPCT,OTTO      OUT2 140
      LOGICAL NEQL,CONVG,LOGV,AREA      OUT2 150
C      DIMENSION NV(13),Z(10,3),HEAD(15),YX(5),YN(5),FSB(3)      OUT2 160
      DIMENSION VNAME(4),BZNAM(4),BETNAM(4),HNAME(4)      OUT2 170
C      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)      OUT2 180
      1 ,CAMVAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)      OUT2 190
      2 ,VLM(13),TOTN(13)      OUT2 200
      COMMON/MISC/S0,ENN,SUMN,TT,ATOM(3,101),LLMT(30),B0(30),B0P(30,2)      OUT2 210
      1 ,TM,TLOW,TMID,THIGH,CPSUM,PP,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)      OUT2 220
      2 ,HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(30),NAME(30,5)      OUT2 230
      3 ,ANUM(30,5),PECWT(30),ENTH(30),FAZ(30),RTEMP(30),FOX(30),DENS(30)      OUT2 240
      4 ,RHOP,RMW(30),TLN,CR,OX(30),ENNL,ENSAVE,ENLSAV,TRACE      OUT2 250
      COMMON /DOUBLE/ G(60,61), X(60)      OUT2 260
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,ISV, NPP, MOLES,NP,NT,NPT,NLM      OUT2 270
      1 ,NS,KMAT,IMAT,IQ1,NOF,NCMIT,IP,NEW,NSUB,NSUP,ITM,CPCVFR,CPCVEQ      OUT2 280
      2 ,IONS,NC,NSERT,JSOL,JLI,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCHOUT      OUT2 290
      3 ,IQAVE,LSAVE,ISUP,ISUB,ITNUM      OUT2 300
      COMMON/PERF/PCP(22),%MOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)      OUT2 310
      1 ,APP(13),AEAT(13),CSTR,EQL,FROZ,SS0,AREA,AWT      OUT2 320
      COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)      OUT2 330
      1 ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2      OUT2 340
      2 ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0,FRHO(4)      OUT2 350
C      COMMON/CSIG/SIGMA(13)      OUT2 360
      COMMON/MIKE8/EXIN,BZOUT(13),BETOUT(13)      OUT2 370
      * COMMON/SIGOUT/FNEL(3),ANE(15),FIONS(3),AIONS(15),FSIGWO(4),      OUT2 380
      XFSIG(4),SIGM(15),FFREQ(3),TOTAL(15)      OUT2 390
      COMMON/SPECE1/HSPCMX,NCMAX,NELMX,TEMP(175,2),SUB(600,3),S(1)      OUT2 400
C... NSPCMX REFERS TO THE MAXIMUM NO. OF SPECIES ALLOWED      OUT2 410
C... NCMAX REFERS TO THE MAXIMUM NO. OF CONDENSED SPECIES ALLOWED      OUT2 420
C      THIS IS FIXED AND REFERS TO THE SIZE OF TEMP(N,2) IN COMMON      OUT2 430
C      SPECE1.....MUST CHANGE THIS COMMON EVERYWHERE IF A LARGER      OUT2 440
C      IS NEEDED      OUT2 450
C... NELMX REFERS TO THE MAXIMUM NO. OF ELEMENTS ALLOWED      OUT2 460
C      THIS IS FIXED AND REFERS TO THE SIZE OF XELMC(N) AND A(N,NSOUT      OUT2 470
C      .....MUST CHANGE COMMON TSTG AND STOIC EVERYWHERE IF      OUT2 480
C      A LARGER SIZE IS NEEDED      OUT2 490
C      EQUIVALENCE (V(1),NV(1)),(IB,FB)      OUT2 500
      EQUIVALENCE (OTTO,CPCVFR),(CPCVEQ,LOGV)      OUT2 510
C      HEAD=(1H,2A4,5 (A2,F8.5,3X),5 X,F7.5,F13.3,4X,A1,F10.2,F9.4)      OUT2 520
C      DATA HEAD/4H(1H,4H,2A4,2H,5,4H(A2,4HF3.5,1H,3X),2H,5,2HX,      OUT2 530
      1 ,4HF7.5,4I,F13,4H,3,4,4HX,A1,4H,F10,1H,2,F,4H9.4)/      OUT2 540
      DATA FUEL/4HFUEL/,OX1D/4HOXID/,ANT/3HANT/,OX/1HO/,IZ/2H00/      OUT2 550
      1 ,YN/2H,1,2H,2,2H,3,2H,4,2H,5/,F75/4HF7.5/      OUT2 560
      2 ,YX/3H,5,3H,14,3H,31,3H,18,2H,5/,F73/4HF7.3/      OUT2 570
      DATA VNAME/4HVVO,4HCITY,4H,M/S,2H,C/      OUT2 580
      DATA HNAME/4HTOTA,4HLH(,4H,2H,4)/      OUT2 590
      DATA BZNAME/3HMMVG,4HFELD(,4H,2H,4)/      OUT2 600
      DATA FEIN/4H,1H,1H,1H/      OUT2 610
C      OUT2 620
C      OUT2 630
C      OUT2 640
C      OUT2 650
C      OUT2 660
C      OUT2 670
C      OUT2 680
C      OUT2 690

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      FMT(4) = FMT(6)
C
C PRESSURE
C
      JSLOT=0
50 IF(ABS(R-RR/4184.) .LT. 0.01) GO TO 60
      DO 55 I =1,NPT
55 V(I) = PPP(I)*101325.
      CALL EFMT(NPT,FP,V)
      GO TO 64
60 CALL VARFMT (PPP,NPT)
      WRITE (6,FMT)(FP(I),I=1,4),(PPP(J),J=1,NPT)
      JSLOT=1
C
C TEMPERATURE
C
64 DO 65 I=1,NPT
      NV(I)= TTT(I)+.5
65 CONTINUE
      FMT(4)= FMT13
      FMT(5)= FMTI9
      WRITE (6,FMT)(FT(I),I=1,4),(NV(J),J=1,NPT)
C
C DENSITY
C
      *
      VNUM = 10000.
      IF (R.LT.2.) VNUM=1.
      DO 70 I=1,NPT
      IF (VLM(I).NE.0.) V(I)=VNUM/VLM(I)
70 CONTINUE
      CALL EFMT(NPT,FRHO,V)
C
C ENTHALPY
C
      DO 75 I=1,NPT
      V(I) = HSUM(I) * R
75 CONTINUE
      FMT(5)= FB
      FMT(7) = F1
      WRITE (6,FMT)(FH(I),I=1,4),(V(J),J=1,NPT)
C
C ENTROPY
C
      FMT(7)=F4
77 DO 78 I=1,NPT
      V(I) = SSUM(I) * R
78 CONTINUE
      WRITE (6,FMT)(FS(I),I=1,4),(V(J),J=1,NPT)
      WRITE (6,80)
80 FORMAT ( 1H )
C
C MOLECULAR WEIGHT
C
      FMT(7)= F3
      WRITE (6,FMT)(FM(I),I=1,4),(WM(J),J=1,NPT)
C

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OUT2 700
OUT2 710
OUT2 720
OUT2 730
OUT2 740
OUT2 750
OUT2 760
OUT2 770
OUT2 780
OUT2 790
OUT2 800
OUT2 810
OUT2 820
OUT2 830
OUT2 840
OUT2 850
OUT2 860
OUT2 870
OUT2 880
OUT2 890
OUT2 900
OUT2 910
OUT2 920
OUT2 930
OUT2 940
OUT2 950
OUT2 960
OUT2 970
OUT2 980
OUT2 990
OUT21000
OUT21010
OUT21020
OUT21030
OUT21040
OUT21050
OUT21060
OUT21070
OUT21080
OUT21090
OUT21100
OUT21110
OUT21120
OUT21130
OUT21140
OUT21150
OUT21160
OUT21170
OUT21180
OUT21190
OUT21200
OUT21210
OUT21220
OUT21230
OUT21240
OUT21250

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C (DLV/DLP)T OUT21260
C OUT21270
  FMT(7)=F5 OUT21280
  IF(EQL) WRITE(6,FMT)(FV(I),I=1,4),(DLVPT(J),J=1,NPT) OUT21290
C OUT21300
C (DIV/DLT)P OUT21310
C OUT21320
  FMT(7)= F4 OUT21330
  IF(EQL) WRITE(6,FMT)(FD(I),I=1,4),(DLVTP(J),J=1,NPT) OUT21340
C OUT21350
C HEAT CAPACITY OUT21360
C OUT21370
  DO 85 I=1,NPT OUT21380
  V(I) = CPR(I) * R OUT21390
85 CONTINUE OUT21400
  WRITE(6,FMT)(FC(I),I=1,4),(V(J),J=1,NPT) OUT21410
C OUT21420
C GAMMA(S) OUT21430
C OUT21440
  FMT(7) = F4 OUT21450
  WRITE(6,FMT)(FG(I),I=1,4),(GAMMAS(J),J=1,NPT) OUT21460
C OUT21470
  IF(NPT.LE.2)GO TO 7071 OUT21480
C...VELOCITY OUT21490
  WRITE(6,1050) (VNAME(I),I=1,4),(VMOC(J),J=3,NPT) OUT21500
C... TOTAL H OUT21510
  ACON=R/RR OUT21520
  DO 7070 I=3,NPT OUT21530
  V(I)=(HSUM(I)*RR+.5*VMOC(I)*VMOC(I))*ACON OUT21540
7070 CONTINUE OUT21550
  WRITE(6,1050) (HNAME(I),I=1,4),(V(J),J=3,NPT) OUT21560
C... MAGNETIC FIELD OUT21570
  WRITE(6,1050) (BZNAME(I),I=1,4),(BZOUT(J),J=3,NPT) OUT21580
C... BETA OUT21590
  WRITE(6,1050) (BETNAME(I),I=1,4),(BETOUT(J),J=3,NPT) OUT21600
7071 CONTINUE OUT21610
1050 FORMAT(1X,4A4,16X,13(1X,F8.2)) OUT21620
C OUT21630
C SONIC VELOCITY OUT21640
C OUT21650
  FMT(7)= F1 OUT21660
  ADIV=1.0/RR OUT21670
  DO 95 I = 1,NPT OUT21680
  TSAV1 = (GAMMAS(I)*TTT(I))/(WM(I)*ADIV) OUT21690
  IF(TSAV1.LE.0.0000)TSAV1=1.0000 OUT21700
  TSAV1=DSQRT(TSAV1) OUT21710
  SONVEL(I)=TSAV1 OUT21720
95 CONTINUE OUT21730
  WRITE(6,FMT)(FL(I),I=1,4),(SONVEL(J),J=1,NPT) OUT21740
C OUT21750
C CONDUCTIVITY OUT21760
C WR TE(6,96)(SIGMA(I),I=1,NPT) OUT21770
96 FORMAT(11H ***** 13F7.4) OUT21780
  CALL EFMT(NPT,FNEL,ANE) OUT21790
  CALL EFMT(NPT,FIONS,AIONS) OUT21800
  FMT(7)=F4 OUT21810

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C	PROGRAM NEOMHD(INPUT,OUTPUT,TAPE7,TAPE5=INPUT,TAPE6=OUTPUT)	MAIN 10	PAGE 0062
	WRITE(6,FMT)FSIG,(SIGMA(I),I=1,NPT)	OUT21820	
	WRITE(6,FMT)FSIGWO,(SIGMA(I),I=1,NPT)	OUT21830	
	CALL EFMT(NPT,FFREQ,TOTAL)	OUT21840	
	RETURN	OUT21850	
	END	OUT21860	
	SUBROUTINE OUT3	OUT3 10	
C		OUT3 20	
C		OUT3 30	
C	THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR	OUT3 40	
C	NON-CDC MACHINES	OUT3 50	
C		OUT3 60	
	DOUBLE PRECISION TTT,TM,PP,SIGMA,SIG,VLMI,VLM	OUT3 70	
	DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS,S0	OUT3 80	
	DOUBLE PRECISION ENN,EMM,SUMN,AWT	OUT3 90	
	DOUBLE PRECISION G,X,S,EN,ENLS	OUT3 100	
C		OUT3 110	
	LOGICAL SHOCK,MMHG,UV,DETN,SIUNIT,NSOM,CALCH	OUT3 120	
	LOGICAL HP,SP,"P,NEVR,IONS,MOLES,FROZ,EQL,PSIA,RKT,VOL,TV,SV	OUT3 130	
	LOGICAL ERATIO,FPCT,OTTO,SFLG	OUT3 140	
	LOGICAL NEQL,CONVG,LOGV,SFLG,AREA	OUT3 150	
C		OUT3 160	
	DIMENSION NV(13),Z(10,3),HEAD(15),YX(5),YN(5),FSB(3)	OUT3 170	
C		OUT3 180	
	COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)	OUT3 190	
	1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)	OUT3 200	
	2 ,VLM(13),TOTN(13)	OUT3 210	
	COMMON/SOLUT/NSOL,ISOLN(3,16),SFLG,SUMSN,ENNS,ENLS	OUT3 220	
	COMMON/MISC/S0,ENN,SUMN,TT,ATOM(3,101),LLMT(30),B0(30),B0P(30,2)	OUT3 230	
	1 ,TM,TLOW,TMID,THIGH,CPSUM,PP,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)	OUT3 240	
	2 ,HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(30),NAME(30,5)	OUT3 250	
	3 ,ANUM(30,5),PECWT(30),ENTH(30),FAZ(30),RTEMP(30),FOX(30),DENS(30)	OUT3 260	
	4 ,RHOP,RMW(30),TLN,CR,OXF(30),ENNL,ENSAVE,ENLSAV,TRACE	OUT3 270	
	COMMON /DOUBLE/ G(60,61), X(60)	OUT3 280	
	COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,ISV, NPP, MOLES,NP,NT,NPT,NLM	OUT3 290	
	1 ,NS,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEW,NSUB,NSUP,ITM,CPCVFR,CPCVEQ	OUT3 300	
	2 ,IONS,NC,NSERT,JSOL,JLIM,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCHOUT	OUT3 310	
	3 ,IQSAVE,LSAVE,ISUP,ISUB,ITNUM	OUT3 320	
	COMMON/PERF/PCP(22),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)	OUT3 330	
	1 ,APP(13),AEAT(13),CSTR,EQL,FROZ,SS0,AREA,AWT	OUT3 340	
	COMMON/OUTP/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)	OUT3 350	
	1 ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2	OUT3 360	
	2 ,FH1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0,FRHO(4)	OUT3 370	
C		OUT3 380	
	COMMON/CSIG/SIGMA(13)	OUT3 390	
	COMMON/SIGOUT/FNEL(3),ANE(15),FIONS(3),AIONS(15),FSIGWO(4),	OUT3 400	
	XFSIG(4),SIGM(15),FFREQ(3),TOTAL(15)	OUT3 410	
	COMMON/NEQ/B0N(30),EMM,SFEQ,NQ1,NSK,NEQPT	OUT3 420	
	COMMON/SPECE1/NSPCIX,NCMAX,NELMX,TEMP(175,2),SUB(600,3),S(1)	OUT3 430	
	COMMON/SPECE5/IUSE(1)	OUT3 440	
	COMMON/KGM/EN(13,1)	OUT3 450	
C..	NSPCMX REFERS TO THE MAXIMUM NO. OF SPECIES ALLOWED	OUT3 460	
C...	NCMAX REFERS TO THE MAXIMUM NO. OF CONDENSED SPECIES ALLOWED	OUT3 470	
C	THIS IS FIXED AND REFERS TO THE SIZE OF TEMP(N,2) IN COMMON	OUT3 480	
C	SPECE1.....MUST CHANGE THIS COMMON EVERYWHERE IF A LARGER	OUT3 490	
C	IS NEEDED	OUT3 500	
C...	NELMX REFERS TO THE MAXIMUM NO. OF ELEMENTS ALLOWED	OUT3 510	

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C          THIS IS FIXED AND REFERS TO THE SIZE OF XELMC(N) AND A(N,NSOUT3 520
C          .....MUST CHANGE COMMON TSTG AND STOIC EVERYWHERE IF OUT3 530
C          A LARGER SIZE IS NEEDED OUT3 540
C          EQUIVALENCE (V(1),NV(1)),(IB,FB) OUT3 550
C          EQUIVALENCE (OTTO,CPCVFR),(CPCVEQ,LOGV) OUT3 560
C          HEAD=(1H,2A4,5 (A2,F8.5,3X),5 X,F7.5,F13.3,4X,A1,F10.2,F9.4) OUT3 570
C          OUT3 580
C          OUT3 590
C          DATA HEAD/4H(1H,4H,2A4,2H,5,4H(A2,,4HF8.5,4H,3X),2H,5,2HX, OUT3 600
1          ,4HF7.5,4H,F13,4H,3,4,4HX,A1,4H,F10,4H,2,F,4H9.4)/ OUT3 610
C          DATA FUEL/4HFUEL/,OXID/4HOXID/,ANT/3HANT/,OX/1HO/,IZ/2H00/ OUT3 620
1          ,YN/2H,1,2H,2,2H,3,2H,4,2H,5/,F75/4HF7.5/ OUT3 630
2          ,YX/3H,57,3H,44,3H,31,3H,18,2H,5/,F73/4HF7.3/ OUT3 640
C          OUT3 650
C          OUT3 660
C          OUT3 670
C          TRA = 5.E-6 OUT3 680
C          IF(TRACE.NE.0.) TRA= TRACE OUT3 690
C          IF(.NOT.EQL) GO TO 331 OUT3 700
C          OUT3 710
C          MOLE FRACTIONS - EQUILIBRIUM OUT3 720
C          OUT3 730
C          WRITE (6,80) OUT3 740
80      FORMAT(1H ) OUT3 750
C          FMT(7)= F5 OUT3 760
C          WRITE(6,310) OUT3 770
310     FORMAT(/1X,14HMOLE FRACTIONS //) OUT3 780
C          NSP1=NS+1 OUT3 790
C          NNSTOP=NSK OUT3 800
C          DO 330 K=1,NNSTOP OUT3 810
C          IF(K.EQ.NSP1)WRITE(6,400) OUT3 820
400     FORMAT(/1X,31HMOLE FRACTIONS OF NEOL SPECIES //) OUT3 830
C          DO 315 I=1,NPT OUT3 840
C          V(I) = EN(I,K)/TOTN(I) OUT3 850
C          IF(V(I).LT.0.0)V(I)=0.0 OUT3 860
315     CONTINUE OUT3 870
C          DO 316 I=1,NPT OUT3 880
C          IF(TRACE.EQ.0.) GO TO 317 OUT3 890
C          IF(V(I).GE.TRACE) GO TO 325 OUT3 900
317     IF(V(I).GE.(5.E-6)) GO TO 320 OUT3 910
316     CONTINUE OUT3 920
C          GO TO 330 OUT3 930
320     WRITE (6,FMT) SUB(K,1),SUB(K,2),SUB(K,3),FB,(V(I),I=1,NPT) OUT3 940
C          GO TO 330 OUT3 950
325     FSB(1) = SUB(K,1) OUT3 960
C          FSB(2) = SUB(K,2) OUT3 970
C          FSB(3) = SUB(K,3) OUT3 980
C          CALL EFMT(NPT,FSB,V) OUT3 990
330     CONTINUE OUT31000
C          IF(.NOT.SFLG) GO TO 331 OUT31010
C          WRITE(6,6000) OUT31020
6000    FORMAT(36H00SPECIES IN SOLUTION AT LAST STATION ) OUT31030
C          II=1 OUT31040
601     IZI=2 OUT31050
C          DO 600 I=II,NS OUT31060
C          IF(IUSE(I).LT.1000) GO TO 600 OUT31070

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      IZI=IZI+1                                OUT31080
      DO 602 J=1,3                             OUT31090
602  Z(IZI,J)=SUB(I,J)                         OUT31100
      IF(IZI.GE. 10) GO TO 603                  OUT31110
600  CONTINUE                                  OUT31120
      I=NS                                       OUT31130
      IF(IZI.EQ. 0) GO TO 331                   OUT31140
603  WRITE(6,345) ((Z(JJ,LN),LN=1,3),JJ=1,IZI) OUT31150
      IF(I.EQ. NS) GO TO 331                   OUT31160
      II=I                                       OUT31170
      GO TO 601                                 OUT31180
331  WRITE(6,335) TRA                           OUT31190
335  FORMAT(83H0ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE OUT31200
      IE FRACTIONS WERE LESS THAN ,E12.5,28H FOR ALL ASSIGNED CONDITIONS/ OUT31210
      2/)                                       OUT31220
      LINE= 0                                  OUT31230
      NN = 1                                    OUT31240
      IF(EQL) NN=NPT                            OUT31250
      DO 350 K=1,NNSTOP                        OUT31260
      DO 340 I=1,NN                            OUT31270
      IF((EN(I,K)/TOTN(I)).GE.TRA) GO TO 343    OUT31280
340  CONTINUE                                  OUT31290
      LINE= LINE+1                             OUT31300
      Z(LINE,1)= SUB(K,1)                      OUT31310
      Z(LINE,2)= SUB(K,2)                      OUT31320
      Z(LINE,3)= SUB(K,3)                      OUT31330
343  IF ((LINE.NE.10) .AND. K.NE.NNSTOP) GO TO 350 OUT31340
      IF (LINE.EQ.0) GO TO 1000                OUT31350
      WRITE(6,345) (Z(LN,1),Z(LN,2),Z(LN,3),LN=1,LINE) OUT31360
345  FORMAT (10(1X,3A4))                      OUT31370
      LINE= 0                                  OUT31380
350  CONTINUE                                  OUT31390
      IF(.NOT.MOLES) WRITE(6,360)              OUT31400
360  FORMAT(78H0NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXI OUT31410
      2DANT IN TOTAL OXIDANTS )               OUT31420
1000  RETURN                                  OUT31430
      END                                       OUT31440
      SUBROUTINE EQLBRM(FLAG)                  EQLB 5
C  ROUTINE TO CALCULATE EQUILIBRIUM COMPOSITION AND PROPERTIES EQLB 10
C  EQLB 15
C  EQLB 20
C  THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR EQLB 25
C  NON-CDC MACHINES EQLB 30
C  EQLB 35
      DOUBLE PRECISION TTT,TM,PP,SIGMA,SIG,VLMI,VLM EQLB 40
      DOUBLE PRECISION ENN,EMM,SUMN,AWT EQLB 45
      INTEGER SJF EQLB 50
      DOUBLE PRECISION HSUM,SS,TM,CPR,DLVTP,DLVPT,GAMMAS,SUMM,SS,SS EQLB 55
      DOUBLE PRECISION X,G,SUM,SUM2,E,S,EN,ENLN,H0,DELN,CONSSS EQLB 60
      DOUBLE PRECISION ENL,PISAVE,DLNT,AA,ENLS,ENNEIM,CRCRIT EQLB 65
      DOUBLE PRECISION X0CRIT,ENSPEC EQLB 70
      DOUBLE PRECISION ENNSSS,ENMAX,XXXSUM EQLB 75
      DOUBLE PRECISION DP1TP,DP1PT,DLNTP,DLNPT EQLB 80
      DOUBLE PRECISION DXOUTP,SOLMAX,ENTOT,ENLNT,SUMS EQLB 85
      DOUBLE PRECISION CPOLD EQLB 90
      DOUBLE PRECISION SUM1,AAON,CONTST,AMBDA,AMBDA1,AACHK,AAMAX CSUM 91

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C
LOGICAL SHOCK,MMHG,WV,DETN,SIUNIT,NSOM,CALCH          EQLB 95
LOGICAL HP,SP,TP,NEWNR,IONS,MOLES,FROZ,EQL,PSIA,RKT,VOL,TV,SV EQLB 100
LOGICAL FA,ERATIO,FPCT,OTTO                          EQLB 105
LOGICAL N2L,CONVG,LOGV,STG,AREA,I35,RITE,FLAG        EQLB 110
DIMENSION JJDUM(16),KKDUM(48),XXXSUM(16),NNDUM(10)    EQLB 115
DIMENSION PISAVE(30)                                  EQLB 120
C
COMMON/SPACE1/NSPCMX,NCMAX,NELMX,TEMP(175,2),SUB(600,3),S(1) EQLB 125
COMMON/SPECE2/ENLN(1)                                 EQLB 130
COMMON/SPECE3/ENLN(1)                                 EQLB 135
COMMON/SPECE4/ENLN(1)                                 EQLB 140
COMMON/SPECE5/IUSE(1)                                  EQLB 145
COMMON/SPECE6/SLN(1)                                  EQLB 150
COMMON/KGM/EN(13,1)                                   EQLB 155
COMMON/STOIC/A(30,1)                                  EQLB 160
C... NSPCMX REFERS TO THE MAXIMUM NO. OF SPECIES ALLOWED EQLB 165
C... NCMAX REFERS TO THE MAXIMUM NO. OF CONDENSED SPECIES ALLOWED EQLB 170
C      THIS IS FIXED AND REFERS TO THE SIZE OF TEMP(N,2) IN COMMON EQLB 175
C      SPECE1.....MUST CHANGE THIS COMMON EVERYWHERE IF A LARGER EQLB 180
C      IS NEEDED                                         EQLB 185
C... NELMX REFERS TO THE MAXIMUM NO. OF ELEMENTS ALLOWED EQLB 190
C      THIS IS FIXED AND REFERS TO THE SIZE OF XELMC(N) AND A(N,NSEQLB 195
C      .....MUST CHANGE COMMON TSTG AND STOIC EVERYWHERE IF EQLB 200
C      A LARGER SIZE IS NEEDED                         EQLB 205
C
COMMON/SOLUT/NSOL,ISOLN(3,16),SFLG,SUMSN,ENNS,ENLS    EQLB 210
COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVPT(13),DLVPT(13) EQLB 215
1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13) EQLB 220
2 ,VLH(13),TOTN(13)                                    EQLB 225
COMMON/MISC/S0,ENN,SUMN,TT,ATOM(3,101),LLMT(30),B0(30),B0P(30,2) EQLB 230
1 ,TM,TLOW,TMID,THIGH,CPSUM,PP,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2) EQLB 235
2 ,HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(30),NAME(30,5) EQLB 240
3 ,ANUM(30,5),PECWT(30),ENTH(30),FAZ(30),RTEMP(30),FOX(30),DENS(30) EQLB 245
4 ,RHOP,RMW(30),TLN,CR,OXF(30),ENNL,ENSAVE,ENLSAV,TRACE,SIZE EQLB 250
COMMON/DOUBLE/ G(60,61), X(60) EQLB 255
COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,ISV, NPP, MOLES,NP,NT,NPT,NLM EQLB 260
1 ,NS,KMAT,IMAT,IQ1,NOF,ROMIT,IP,NEWNR,NSUB,NSUP,ITM,CPCVFR,CPCVEQ EQLB 265
2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCHEQLB 270
3 ,IQSAVE,LSAVE,ISUP,ISUB,ITNUM EQLB 275
COMMON/NEQ/B0N(30),EMM,SIEQ,NQ1,NSK,NEQPT EQLB 280
COMMON/MHDD/SSUMW,DX,DXI,XJY(26),AI(26),UE,NITER,NSTOP,SIG(26),IPPEQLB 285
X ,BZ,XK,PPPP EQLB 290
COMMON/NUM/NUMB1 EQLB 295
COMMON/MIKE0/IIDUM(3),IMPRNT,NMPATH,NUMIV,XINDP(1) EQLB 300
COMMON/MIKE5/MOMIT,X0CRIT,DUMMIN(1) EQLB 305
COMMON/MIKE7/CHICALC,CHNLEN,IPRRKT,TMPSTP,TDIFUN,TEQLBM EQLB 310
COMMON/NS1SPC/IRSPEC,ENSPEC,RKT EQLB 315
COMMON/AREASV/PPITP(30),DLNTP,DPIPT(30),DLNPT EQLB 320
COMMON/DBGVNC/DXOUTP(1) EQLB 325
EQUIVALENCE (NERT,ISINGV) EQLB 330
EQUIVALENCE (OTTO,CPCVFR),(CPCVEQ,LOGV) EQLB 335
C
DATA IE/IHE/,SMALNO/1.E-6/,SMNOL/-13.815511/,E/2.718281828459/ EQLB 340
DATA IEQLFL/0/,KSUB0M/5/,PISAVE/30*0./,TEMP0/0./,TEMP1/0./,LP1/1/ EQLB 345
DATA CRCRIT/1.0D-12/,TTCPT/150.0/,TMELTM/150./,TMELTP/150./ EQLB 350

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	DATA TMELTS/150./,TTBOT/1000./,TPMLTS/50.000/	EQLB 375
	DATA CONST/1.0D-5/,AACON/1.0D-4/,CONSSS/5.0D-5/	EQLB 380
	DATA NRMOVS/0/,ITN/35/,SLIMAX/1.0D-4/	EQLB 385
	DATA NSOLSV/0/,TRAMIN/1.0E-7/	EQLB 390
	DATA JPHCHN/0/,CPOLE/0.009/,JREM/0/,NPTOLD/0/,TMLTMN/1.00/	EQLB 395
C	ENNEMM=0.	EQLB 400
	IF(NS.EQ.1)GO TO 532	EQLB 405
	IAFLG=0	EQLB 410
	IF(NPT.EQ.NPTOLD)GO TO 396	EQLB 415
	NPTOLD=NPT	EQLB 420
	JREM=0	EQLB 425
396	CONTINUE	EQLB 430
	IF(IPP.LT.NEOPT)GO TO 397	EQLB 435
	TMELTM=TMLTMN	EQLB 440
	TMELTP=TMLTMN	EQLB 445
	TTCRIT=TMLTMN	EQLB 450
397	CONTINUE	EQLB 455
	IADDSL=0	EQLB 460
	SSZEG=0.	EQLB 465
	KSUB=0	EQLB 470
	KKKK=0	EQLB 475
	KKTEM=0	EQLB 480
	IF(NRMOVS.NE.NPT)NRMOVS=0	EQLB 485
	NUMB1=0	EQLB 490
	IF(TRACE.NE.0.) ITN=50	EQLB 495
	IF(NPT.LE.2)ITN=70	EQLB 500
	CONSAV=CONST	EQLB 505
	AACONS=AACON	EQLB 510
405	CONTINUE	EQLB 515
	JCONS=0	EQLB 520
	IKWRIT=ITN-2	EQLB 525
	PIE = 0.	EQLB 530
	I35 = .FALSE.	EQLB 535
	ENL = ENNL	EQLB 540
	RITE = .FALSE.	EQLB 545
	IF(IDEBUG.GT.0.AND.NPT.GE.IDEBUG) RITE=.TRUE.	EQLB 550
	LOGV = .FALSE.	EQLB 555
	TLN = ALOG(TT)	EQLB 560
	CONVG = .FALSE.	EQLB 565
	NUMB=0	EQLB 570
	IF(.NOT.TP)GO TO 309	EQLB 575
	ITN=100	EQLB 580
	TMELTS=TPMLTS	EQLB 585
	IF(.NOT.SF.G)GO TO 309	EQLB 590
C	INITIAL ESTIMATES	EQLB 595
	JPHCHN=0	EQLB 600
	ENN = .1	EQLB 605
	ENNL = -2.3025851	EQLB 610
	ENL=ENNL	EQLB 615
	SUMN = ENN	EQLB 620
	XI = NS - NC	EQLB 625
	IF(XI.EQ.0.)XI=1.	EQLB 630
	XI = ENN/XI	EQLB 635
	XLN = ALOG(XI)	EQLB 640
	IQ1=0	EQLB 645
		EQLB 650

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      INC=0
      JJSOLD=0
      DO 303 J=1,NS
      IF(IUSE(J).EQ.0)GO TO 302
      INC=INC+1
      IF(IUSE(J).LE.1000)GO TO 300
      IUSE(J)=-IUSE(J)
C... SHOULD THIS SPECIES BE FROZEN OUT OF SOLUTION
      JJDUM(1)=J
      TMELT=TEMP(TNC,1)-TMELTS
      IF(TT.GT.TMULT)GO TO 301
C...YES,REMOVE IT,SET SOLID FLAG
      JJSOLD=JJSOLD+1
      NSOL=NSOL-1
      KKDUM(JJSOLD)=IUSE(J)-1000
      IUSE(J)=IUSE(J)+1000
CCCCC IF(KASE.EQ.7777)WRITE(1,4021)J,IUSE(J),KKDUM(JJSOLD)
      WRITE(6,4029) (SUB(J,KK),KK=1,3),TMELTS
300 IF(IUSE(J).GT.0)IUSE(J)=-IUSE(J)
301 EN(NPT,J)=0.0
      ENLN(J)=0.0
      DELN(J)=0.0
      GO TO 303
302 DELN(J)=0.0
      EN(NPT,J) = XI
      ENLN(J) = XLN
303 CONTINUE
      SFLG=.FALSE.
      ENNS=0.0
      ENLS=0.0
      IF(NSOL.NE.1)GO TO 304
      NSOL=0
      M=JJDUM(1)
      JJSOLD=JJSOLD+1
      KKDUM(JJSOLD)=IUSE(M)-1000
      IUSE(M)=IUSE(M)+1000
CCCCC IQ1=IQ1+1
CCCCC IF(KASE.EQ.7777)WRITE(1,4021)M,IUSE(M),KKDUM(JJSOLD)
304 CONTINUE
      IF(NSOL.EQ.0)WRITE(6,8002)
      IF(JJSOLD.EQ.0)GO TO 308
C...RESET IUSE OF SOLID SPECIES THAT FROZE OUT OF SOLUTION
      DO 307 KK=1,NS
      IF(IUSE(KK).GE.-2000)GO TO 307
      DO 306 JJ=1,JJSOLD
      IF(IUSE(KK).NE.KKDUM(JJ))GO TO 306
C...FOUND THE CORRESPONDING SOLID( ADD 2000 )
      IUSE(KK)=IUSE(KK)+2000
CCCCC IF(IUSE(KK).GT.0)IQ1=IQ1+1
CCCCC IF(KASE.EQ.7777)WRITE(1,4021)KK,IUSE(KK),KKDUM(JJ)
306 CONTINUE
307 CONTINUE
308 IQ1 = NLH+1+IQ1
309 CONTINUE
      JS1 = 1
      CALL CPHS

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EQLB 655
EQLB 660
EQLB 665
EQLB 670
EQLB 675
EQLB 680
EQLB 685
EQLB 690
EQLB 695
EQLB 700
EQLB 705
EQLB 710
EQLB 715
EQLB 720
EQLB 725
EQLB 730
EQLB 735
EQLB 740
EQLB 745
EQLB 750
EQLB 755
EQLB 760
EQLB 765
EQLB 770
EQLB 775
EQLB 780
EQLB 785
EQLB 790
EQLB 795
EQLB 800
EQLB 805
EQLB 810
EQLB 815
EQLB 820
EQLB 825
EQLB 830
EQLB 835
EQLB 840
EQLB 845
EQLB 850
EQLB 855
EQLB 860
EQLB 865
EQLB 870
EQLB 875
EQLB 880
EQLB 885
EQLB 890
EQLB 895
EQLB 900
EQLB 905
EQLB 910
EQLB 915
EQLB 920
EQLB 925
EQLB 930

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      JKSOL=NSOL
      ENNEMM=ENN+EMM
      TM=PP/ENNEMM
C+.  GROK0
CCCCC DXOUTP(1)=PP
CCCCC DXOUTP(2)=ENNEMM
CCCCC DXOUTP(3)=ENN
CCCCC DXOUTP(4)=EMM
CCCCC DXOUTP(5)=0.0
CCCCC NUMOUT=5
CCCCC NUMDBG=301
CCCCC IF(TM.LE.0.0D0)CALL DBGO'UT(NUMOUT,HP,SP,DXOUTP,NUMDBG)
C+.
CCCCC TM = DLOG(PP/(ENN+EMM))
      TM=DLOG(TM)
      IF(MOMIT.EQ.0)GO TO 403
      BIGB=B0(1)-B0N(1)
      SMALB=BIGB
      IF(BIGB.GT.0.0)GO TO 404
      I=1
      WRITE(1,9898) I,B0(I),B0N(I),BIGB
      STOP 4
404  CONTINUE
      IF(IMPRNT.GE.3)WRITE(1,9875) MOMIT,BIGB
9875  FORMAT(1X,6HMO'IT=,I3,1X,7HDELTAB=,G12.3)
      NNLOOP=NLM
      IF(IONS)NNLOOP=NLM-1
      IF(NNLOOP.LE.1)GO TO 403
      DO 402 I=2,NNLOOP
      TSAV1=B0(I)-B0N(I)
      IF(TSAV1.GT.0.0)GO TO 401
      WRITE(1,9898) I,B0(I),B0N(I),TSAV1
9898  FORMAT(1X,12HERROR STOP 4,2X,25HI B0(I) B0N(I) DIFFERENCE,/,
      *1X,I4,3(1X,G11.3))
      STOP 4
401  CONTINUE
      IF(TSAV1.LT.SMALB)SMALB=TSAV1
      IF(TSAV1.GT.BIGB)BIGB=TSAV1
402  CONTINUE
      TSAV1=SMALB/BIGB
      TSAV3=SIZE
      TSAV2=SIZE
      IF(TSAV1.LT.1.E-5)TSAV3=ALOG(1000./TSAV1)
      IF(TSAV3.GT.SIZE)SIZE=TSAV3
      IF(IMPRNT.GE.3)WRITE(1,9877) SMALB,BIGB,TSAV2,TSAV3,SIZE
9877  FORMAT(1X,26HSMALB BIGB SIZE TSAV3 SIZE,/,1X,5(G11.3,1X))
403  CONTINUE
      IF(I.P.NE.NEOPT)GO TO 2001
      IF(I.Q.LF.L.NE.0)GO TO 2001
      IF(NJK.EQ.NS)GO TO 2001
      TM=PP/ENN
C+.  GROK1
CCCCC DXOUTP(1)=PP
CCCCC DXOUTP(2)=ENN
CCCCC DXOUTP(3)=1.0
CCCCC NUMOUT=3

```

```

EQLB 935
EQLB 940
EQLB 945
EQLB 950
EQLB 955
EQLB 960
EQLB 965
EQLB 970
EQLB 975
EQLB 980
EQLB 985
EQLB 990
EQLB 995
EQLB1000
EQLB1005
EQLB1010
EQLB1015
EQLB1020
EQLB1025
EQLB1030
EQLB1035
EQLB1040
EQLB1045
EQLB1050
EQLB1055
EQLB1060
EQLB1065
EQLB1070
EQLB1075
EQLB1080
EQLB1085
EQLB1090
EQLB1095
EQLB1100
EQLB1105
EQLB1110
EQLB1115
EQLB1120
EQLB1125
EQLB1130
EQLB1135
EQLB1140
EQLB1145
EQLB1150
EQLB1155
EQLB1160
EQLB1165
EQLB1170
EQLB1175
EQLB1180
EQLB1185
EQLB1190
EQLB1195
EQLB1200
EQLB1205
EQLB1210

```

```

CCCCC NUMDBG=302
CCCCC IF(TM.LE.0.000)CALL DBGOUT(NUMOUT,HP,SP,DXOUTP,NUMDBG)
C+.
CCCCC TM=DLOG(PP/ENN)
      TM=DLOG(TM)
2001 CONTINUE
      LE=NLM
      LI=0
      IF(LSAVE.EQ.0.OR.NLM.EQ.LSAVE) GO TO 32
      LI=LSAVE+1
      DO 499 I=LI,NLM
      DO 499 J = 1,NS
      IF(A(I,J).EQ.0.) GO TO 499
      IF(IUSE(J).NE.0) GO TO 499
      EN(NPT,J) = 1.E-8
      ENLN(J) = -SIZE
499 CONTINUE
32 LS=NLM
   LZ=LS
   IF(IONS)LZ=LS-1
   IF(NPT.GT.1 .AND. LI.EQ.0) GO TO 43
33 IF(.NOT.SHOCK) WRITE(6,244)(LLMT(I),I=1,NLM)
244 FORMAT (4H0PT ,14(5X,A4))
C
C      BEGIN ITERATION
C
43 IF(NUMB.GE.ITN)GO TO 14
C**** IF(NUMB.GE.IKWRT.AND.AA.EQ.1.0)RITE=.TRUE.
      IF(RITE)WRITE(6,6666) NUMB
6666 FORMAT(1X,25(1H*),9HDEBUG AT ,I3)
      NUMB1=NUMB+1
      NUMB=NUMB+1
      AA=1.0
      IF(.NOT.CONVG) GO TO 62
C...WARNING MUST IABS(NMPATH) IF CAN ITERATE FROM THROAT TO 0.0
      IF(NMPATH.EQ.3)GO TO 61
      IF(.NOT.FLAG) GO TO 186
61 SUMN = ENN
      IF(JSOL.EQ.0) GO TO 62
      ENSOL = EN(NPT,JSOL)
      EN(NPT,JSOL) = EN(NPT,JSOL)+EN(NPT,JLIQ)
      IUSE(JLIQ) = -IUSE(JLIQ)
      IQ1 = IQ1-1
      DLVTP(NPT) = 0.
      CPR(NPT) = 0.
      GAMMAS(NPT) = 0.
      LOGV = .TRUE.
62 CALL MATRIX(FLAG)
      IQ2 = IQ1 + 1
      IF(CONVG) IMAT=IMAT-1
      IF(.NOT.RITE) GO TO 72
      IF(.NOT.CONVG) GO TO 88
      IF(.NOT.LOGV) WRITE(6,81)
81 FORMAT(15H0T DERIV MATRIX)
      IF(LOGV) WRITE(6,82)
82 FORMAT(15H0P DERIV MATRIX)

```

EOLB1215
EOLB1220
EOLB1225
EOLB1230
EOLB1235
EOLB1240
EOLB1245
EOLB1250
EOLB1255
EOLB1260
EOLB1265
EOLB1270
EOLB1275
EOLB1280
EOLB1285
EOLB1290
EOLB1295
EOLB1300
EOLB1305
EOLB1310
EOLB1315
EOLB1320
EOLB1325
EOLB1330
EOLB1335
EOLB1340
EOLB1345
EOLB1350
EOLB1355
EOLB1360
EOLB1365
EOLB1370
EOLB1375
EOLB1380
EOLB1385
EOLB1390
EOLB1395
EOLB1400
EOLB1405
EOLB1410
EOLB1415
EOLB1420
EOLB1425
EOLB1430
EOLB1435
EOLB1440
EOLB1445
EOLB1450
EOLB1455
EOLB1460
EOLB1465
EOLB1470
EOLB1475
EOLB1480
EOLB1485
EOLB1490

```

      GO TO 89
88 WRITE(6,772) NUMB
772 FORMAT (11H0ITERATION ,I3,6X,7HMATRIX //)
89 DO 911 I=1,IMAT
911 WRITE (6,73) (G(I,K),K=1,KMAT)
72 ISINGV=0
CALL GAUSS
IF(ISINGV.NE.0) GO TO 774
IF(.NOT.RITE) GO TO 773
WRITE (6,73)(LLMT(I),I=1,NLM)
373 FORMAT (7H0PI ,9(A4,10X))
WRITE (6,73)(X(I),I=1,IMAT)
73 FORMAT (9E14.6)
773 IF(.NOT.CONVG) GO TO 85
IF(.NOT.LOGV) GO TO 174
IF(NMPATH.NE.3)GO TO 171
C... STORE PRESSURE DERIVITIVES...DPIPT AND DLNPT
DO 8140 KK=1,NLM
DPIPT(KK)=X(KK)
8140 CONTINUE
DLNPT=X(IQ1)
GO TO 171
C
C TEMPERATURE DERIVATIVES--CONVG=T, LOGV=F
C
174 DLVTP(NPT) = 1.-X(IQ1)*(ENN/(ENN+EMM))
IF(DLVTP(NPT).LT.25.) GO TO 175
DLVTP(NPT) = 0.
DLVPT(NPT) = 0.
CPR(NPT) = 0.
GAMMAS(NPT) = 0.
GO TO 186
175 CPR(NPT) = G(IQ2,IQ2)
DO 176 J=1,IQ1
CPR(NPT) = CPR(NPT)-G(IQ2,J)*X(J)
176 CONTINUE
C
C PRESSURE DERIVATIVE--CONVG=T, LOGV=T
C
LOGV = .TRUE.
IF(NMPATH.NE.3)GO TO 62
C... STORE PRESSURE DERIVITIVES...DPITP AND DLNTP
DO 8145 KK=1,NLM
DPITP(KK)=X(KK)
8145 CONTINUE
DLNTP=X(IQ1)
GO TO 62
C
C SINGULAR MATRIX
C
774 IF(.NOT.CONVG) GO TO 775
WRITE(6,172) ISINGV
172 FORMAT(28H0DERIVATIVE MATRIX SINGULAR ,5X,7HISINGV=,I5)
GO TO 1171
775 IF(.NOT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.TT.GT.100.) GO TO 871
WRITE(6,874)

```

EQLB1495
 EQLB1500
 EQLB1505
 EQLB1510
 EQLB1515
 EQLB1520
 EQLB1525
 EQLB1530
 EQLB1535
 EQLB1540
 EQLB1545
 EQLB1550
 EQLB1555
 EQLB1560
 EQLB1565
 EQLB1570
 EQLB1575
 EQLB1580
 EQLB1585
 EQLB1590
 EQLB1595
 EQLB1600
 EQLB1605
 EQLB1610
 EQLB1615
 EQLB1620
 EQLB1625
 EQLB1630
 EQLB1635
 EQLB1640
 EQLB1645
 EQLB1650
 EQLB1655
 EQLB1660
 EQLB1665
 EQLB1670
 EQLB1675
 EQLB1680
 EQLB1685
 EQLB1690
 EQLB1695
 EQLB1700
 EQLB1705
 EQLB1710
 EQLB1715
 EQLB1720
 EQLB1725
 EQLB1730
 EQLB1735
 EQLB1740
 EQLB1745
 EQLB1750
 EQLB1755
 EQLB1760
 EQLB1765
 EQLB1770

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874 FORMAT(96H0LOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE EQLB1775
      1BEEN INCLUDED ON AN INSERT CARD, RESTART ) EQLB1780
      GO TO 873 EQLB1785
871 WRITE (6,74) NJMB,ISINGV EQLB1790
      74 FORMAT(27H0SINGULAR MATRIX, ITERATION ,I3,10H VARIABLE,I3) EQLB1795
      IF(ISINGV.LT.IQ1) GO TO 390 EQLB1800
960 DO 970 JJ = 1, NS EQLB1805
      IF(.NOT.IONS) GO TO 965 EQLB1810
      IF(LMT(NLM).EQ.1E) GO TO 965 EQLB1815
      IF(A(LS,JJ).NE.0.) GO TO 970 EQLB1820
965 IF(IUSE(JJ).NE.0) GO TO 970 EQLB1825
      IF(EN(NPT,JJ).NE.0.) GO TO 970 EQLB1830
      EN(NPT,JJ) = SMALNO EQLB1835
      ENLN(JJ) = SMNOL EQLB1840
970 CONTINUE EQLB1845
      GO TO 873 EQLB1850
C EQLB1855
C OBTAIN CORRECTIONS TO THE ESTIMATES EQLB1860
85 KK=NLM+1 EQLB1865
      IF(TP) X(IQ2)=0. EQLB1870
      DLNT= X(IQ2) EQLB1875
      SUM = X(IQ1) EQLB1880
      SUMS=0.0 EQLB1885
      IF(SFLG) SUMS=X(IQ1-1) EQLB1890
      DO 100 J=1,NS EQLB1895
      IF(IUSE(J).GT.1000) GO TO 102 EQLB1900
      IF (IUSE(J)) 171,98,100 EQLB1905
98 IF(NLM.GE.L2) GO TO 95 EQLB1910
      DELN(J)=0. EQLB1915
      DO 96 I=LP1,LS EQLB1920
      IF(A(I,J).NE.0.) GO TO 101 EQLB1925
96 CONTINUE EQLB1930
95 DELN(J) = H0(J)*DLNT-H0(J)+S(J)-ENLN(J)-TM+SUM EQLB1935
      X *ENN/(ENN+EMM) EQLB1940
103 DO 99 K=1,NLM EQLB1945
      DELN(J)= DELN(J)+A(K,J)*X(K) EQLB1950
99 CONTINUE EQLB1955
      IF(PIE.NE.0.) DELN(J)=DELN(J)+A(LS,J)*PIE EQLB1960
      GO TO 101 EQLB1965
102 DELN(J)=H0(J)*DLNT-H0(J)+S(J)+ENLS-ENLN(J)+SUMS EQLB1970
      GO TO 103 EQLB1975
100 DELN(J) = X(KK) EQLB1980
      KK = KK + 1 EQLB1985
101 CONTINUE EQLB1990
C EQLB1995
C CALCULATE CONTROL FACTOR,AMBDA EQLB2000
C EQLB2005
      ENN1=E**ENL-EMM1 EQLB2010
C**** IF(IPP.EQ.1)GO TO 2002 EQLB2015
      IF(IPP.NE.NEQP)GO TO 2002 EQLB2020
      IF(IFOLFL.NE.0)GO TO 2002 EQLB2025
      IF(NK.EQ.NS)GO TO 2002 EQLB2030
      ENL=ALOG(LNN1) EQLB2035
      IFOL=L=1 EQLB2040
2002 CONTINUE EQLB2045
      AMBDA= 1. EQLB2050

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      AMBDA1= 1.
      SUM X(IQ1)
      IF (SUM.LT.0.) SUM=-SUM
      IF (DLNT.GT.SUM) SUM=DLNT
      IF (-DLNT.GT.SUM) SUM=-DLNT
      IF (SUMS.GT.SUM) SUM=SUMS
      IF (-SUMS.GT.SUM) SUM=-SUMS
      ENTOT=ENN+EMM+LNN
      ENLNT=DLOG(ENTOT)
      DO 917 J=1,NS
      IF (IUSE(J).EQ.0) GO TO 916
      IF (IUSE(J).LE.1000) GO TO 917
      IF (IUSE(J).GE.2000) GO TO 917
916 CONTINUE
      IF ((EN(NPT,J).GT.0.) .AND. DELN(J).GT.SUM) SUM = DELN(J)
      IF ((EN(NPT,J).NE.0.) .OR. DELN(J).LE.0.) GO TO 917
      SUM1=(ENN*X(IQ1)+ENNS*X(IQ1-1))/ENTOT
      SUM1=(-9.212-ENLN(J)+ENLNT)/(DELN(J)-SUM1)
      IF (SUM1.LT.0.) SUM1=-SUM1
      IF (SUM1.LT.AMBDA1) AMBDA1 = SUM1
917 CONTINUE
      IF (SUM.GT.2.) AMBDA=2./SUM
      IF (AMBDA1.LT.AMBDA) AMBDA = AMBDA1
      IF (.NOT.RITE) GO TO 111

C
C INTERMEDIATE OUTPUT
C
      WRITE(6,923) TT,ENN, ENL,PP,TM,AMBDA
923 FORMAT (3H0T=,E15.8,6H ENN=,E15.8,7H ENNL=E15.8,5H PP=,E15.8,
1 9H LN P/N=E15.8,8H AMBDA=E15.8 )
      WRITE (6,924)
924 FORMAT(1H0,18X,2HNJ,12X,5HLN NJ,8X,9HDEL LN NJ,9X,6HH0J/RT,9X,5H0J/RT,
1J/R,10X,7H-G0J/RT,8X,6H-GJ/RT )
      DO 926 J=1,NS
      GNEG1 = S(J)-H0(J)
      GNEG2 = GNEG1
      IF (IUSE(J).EQ.0) GNEG2=GNEG2-ENLN(J)-TM
      IF (IUSE(J).GT.1000) GNEG2=GNEG2-ENLN(J)+ENLS
      WRITE (6,925) SUB(J,1),SUB(J,2),
1SUB(J,3),EN(NPT,J),ENLN(J),DELN(J),H0(J),S(J),GNEG1,GNEG2
925 FORMAT (1X,3A4,7E15.6)
926 CONTINUE
      WRITE (6,110)
110 FORMAT('E0')

C
C APPLY CORRECTIONS TO ESTIMATES
C
      111 SUM = 0.
C+
CCCC IF (KASE.EQ.7777) WRITE(1,8888) NUMB,TT,ENN,ENL,PP,S0,SSUM(NPT)
8888 FORMAT(1X,3H AT,I3,4H TT=,G13.5,
*21H ENN ENL PP S0 SSUM =,5(1X,G13.5))
C....IS VALUE OF ENN GOING TO 1.0
      IF (ENN.GE.CPCRT) GO TO 8330
C....YES,DO NOT CALCULATE THAT TEMPERATURE
      WRITE(6,8838) NUMB,TT,ENN,ENL,PP,S0,SSUM(NPT)

```

EQLB2055
 EQLB2060
 EQLB2065
 EQLB2075
 EQLB2080
 CSUM2081
 CSUM2082
 CSUM2083
 CSUM2084
 EQLB2085
 CSUM2090
 CSUM2091
 CSUM2092
 CSUM2093
 EQLB2095
 EQLB2100
 CSUM2106
 CSUM2107
 EQLB2110
 EQLB2115
 EQLB2120
 EQLB2125
 EQLB2130
 EQLB2135
 EQLB2140
 EQLB2145
 EQLB2150
 EQLB2155
 EQLB2160
 EQLB2165
 EQLB2170
 EQLB2175
 EQLB2180
 EQLB2185
 EQLB2190
 EQLB2195
 EQLB2200
 EQLB2205
 EQLB2210
 EQLB2215
 EQLB2220
 EQLB2225
 EQLB2230
 EQLB2235
 EQLB2240
 EQLB2245
 EQLB2250
 EQLB2255
 EQLB2260
 EQLB2265
 EQLB2270
 EQLB2275
 EQLB2280
 EQLB2285
 EQLB2290
 EQLB2295


```

      IF(KASE.NE.7777)WRITE(1,8888)NUMB,TT,ENN,ENL,PP,SS,SSUM(NPT)
      KKTEM=10
      GO TO 14
8888 CONTINUE
      BIGN = 0.
      DO 113 J=1,NS
      IF(IUSE(J).GT.1000) GO TO 117
      IF (IUSE(J)) 113,112,114
112 ENLN(J)=ENLN(J)+AMBDA*DELN(J)
      EN(NPT,J) = 0.
      IF(NLM.GE.LZ) GO TO 212
      DO 215 I=LP1,LS
      IF(A(I,J).NE.0.)GO TO 113
215 CONTINUE
212 IF((ENLN(J)- ENL+SIZE).LE.0.) GO TO 113
      EN(NPT,J) = E*ENLN(J)
414 SUM = SUM+EN(NPT,J)
      GO TO 113
117 ENLN(J)=ENLN(J)+AMBDA*DELN(J)
      IF((ENLN(J)- ENL+SIZE).LE.0.) GO TO 113
      EN(NPT,J)=E*ENLN(J)
      GO TO 113
114 EN(NPT,J) = EN(NPT,J) + AMBDA * DELN(J)
113 CONTINUE
      SUMN = SUM
      IF (TP) GO TO 115
      TLN= TLN+AMBDA*DLNT
      TT = EXP(TLN)
      JS1 = 1
      CALL CPHS
115 ENL = ENL+AMBDA*X(IQ1)
      ENN = E*ENL
      IF(.NOT.SFLG)GO TO 4020
CCCCC IF(KASE.NE.7777)GO TO 4022
CCCCC WRITE(1,4023) ENLS,ENNS,AMBDA,X(IQ1-1),X(IQ1)
4023 FORMAT(1X,12HL.N.A.X-1.X=,5(1X,G12.4))
4022 CONTINUE
      ENLS=ENLS+AMBDA*X(IQ1-1)
      ENNS=E*ENLS
      IF(IMPRT.GE.3)WRITE(1,9988) ENL,ENN,ENLS,ENNS,SIZE
9988 FORMAT(1X,20(1H*),22HENL ENN ENLS ENNS SIZE,/1X,5(G11.3,1X))
      IF((ENLS-ENL+SIZE).GT.0.)GO TO 4020
      SFLG=.FALSE.
      NRMOVS=NPT
      IQ1=IQ1-1
      DO 4000 J=1,NS
      IF(IUSE(J).LE.1000)GO TO 4000
      EN(NPT,J)=0.
      DELN(J)=0.
      IUSE(J)=-IUSE(J)
4000 CONTINUE
      ENNS=0.
      WRITE(6,4010)
4010 FORMAT(1X,10(1H*),16HSOLUTION REMOVED)
      WRITE(6,9088)ENL,ENN,ENLS,ENNS,SIZE
      IF(TP)GO TO 43

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```

EQLB2300
EQLB2305
EQLB2310
EQLB2315
EQLB2320
EQLB2325
EQLB2330
EQLB2335
EQLB2340
EQLB2345
EQLB2350
EQLB2355
EQLB2360
EQLB2365
EQLB2370
EQLB2375
EQLB2380
EQLB2385
EQLB2390
EQLB2395
EQLB2400
EQLB2405
EQLB2410
EQLB2415
EQLB2420
EQLB2425
EQLB2430
EQLB2435
EQLB2440
EQLB2445
EQLB2450
EQLB2455
EQLB2460
EQLB2465
EQLB2470
EQLB2475
EQLB2480
EQLB2485
EQLB2490
EQLB2495
EQLB2500
EQLB2505
EQLB2510
EQLB2515
EQLB2520
EQLB2525
EQLB2530
EQLB2535
EQLB2540
EQLB2545
EQLB2550
EQLB2555
EQLB2560
EQLB2565
EQLB2570
EQLB2575

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```

      JS1=1
      CALL CPHS
      GO TO 43
4020 CONTINUE
      ENNEMM=ENN+EMM
      TM=PP/ENNEMM
      IF(TM.GT.0.0)GO TO 8881
C+.  GROK2
CCCCC DXOUTP(1)=PP
CCCCC DXOUTP(2)=ENNEMM
CCCCC DXOUTP(3)=ENN
CCCCC DXOUTP(4)=EMM
CCCCC DXOUTP(5)=2.0
CCCCC NUMOUT=5
CCCCC NUMDBG=303
CCCCC CALL DBGOUT(NUMOUT,HP,SP,DXOUTP,NUMDBG)
      GO TO 873
C+.  8881 CONTINUE
      TM=DLOG(TM)
      IF (LLMT(NLM).NE.IE) GO TO 116
C
C    CHECK ON REMOVING IONS
C
      DO 1116 J = 1,NS
      IF (A(NLM,J).EQ.0.) GO TO 1116
      IF (EN(NPT,J).GT.0.) GO TO 116
1116 CONTINUE
      PIE = X(NLM)
      NLM = NLM-1
      IQ1 = IQ1-1
      WRITE(6,4027)
4027 FORMAT(3X,12HIONS REMOVED)
      GO TO 43
C
C    TEST FOR CONVERGENCE
C
116 CONTINUE
      DXOUTP(NUMB)=X(IQ1)
      NUMOUT=ITN+NUMB
      DXOUTP(NUMOUT)=AMBDA
      IF (AMBDA.LT.1.) GO TO 43
      SUM = X(IQ1)
      IF (SUM.LT.0.) SUM = -SUM
      IF(ENTOT.EQ.0.0)ENTOT=ENN+EMM+ENNS
      SUM=ENN*SUM/ENTOT
      IF (SUM.GT.CONST) GO TO 43
      IF(.NOT.S.FLG)GO TO 118
      SUM=DABS(X(IQ1-1))
      SUM=ENNS*SUM/ENTOT
      IF(SUM.GT.CONST)GO TO 43
118 CONTINUE
      AAMAX=0.0
      AACHK=SUMN+EMM+ENCONV+ENNS
      DO 130 J=1,NS
      IF (IUSE(J).LT.0) GO TO 130

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```

EQLB2580
EQLB2585
EQLB2590
EQLB2595
EQLB2600
EQLB2605
EQLB2610
EQLB2615
EQLB2620
EQLB2625
EQLB2630
EQLB2635
EQLB2640
EQLB2645
EQLB2650
EQLB2655
EQLB2660
EQLB2665
EQLB2670
EQLB2675
EQLB2680
EQLB2685
EQLB2690
EQLB2695
EQLB2700
EQLB2705
EQLB2710
EQLB2715
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EQLB2740
EQLB2745
EQLB2750
EQLB2755
EQLB2760
EQLB2765
EQLB2770
EQLB2775
EQLB2780
EQLB2785
EQLB2790
EQLB2795
CSUM2796
EQLB2797
EQLB2805
CSUM2806
CSUM2807
CSUM2808
CSUM2809
CSUM2809
EQLB2810
EQLB2816
EQLB2820
EQLB2825

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      IF(AACHK.EQ.0.0)GO TO 7777
      AA= DELN(J)/AACHK
      IF(AA.LT.0.) AA= AA
      IF (IUSE(J).EQ.0 .OR. IUSE(J).GT.1000) AA = AA*EN(NPT,J)
      IF(AA.GT.AAMAX)AAMAX=AA
CCCCC IF(KASE.NE.7777)GO TO 130
CCCCC IF(AA.LE.CONST)GO TO 130
CCCCC WRITE(1,4024) J,AA,AACHK,DELN(J),EN(NPT,J),IUSE(J)
4024 FORMAT(1X,3(1H*),17HJ.A.AA.D.EN.IUSE=,I3,1X,4(G13.5,1X),I4)
130 CONTINUE
7777 CONTINUE
      AA=AAMAX
      IF(AA.GT.CONST)GO TO 43
      LE=NLM
      IF(TRACE.EQ.0.) GO TO 275
      IF(TRACE.GE.TRAMIN)GO TO 275
C ***** CHECK FOLLOWING FIF B0(I), ETC., ARE REVISED
C WHEN TRACE NOT 0. *****
      TEM=1.
      KKTEM=1
      IF(NUMB.EQ.1)GO TO 128
225 DO 126 I =1,NLM
      TEM = 0.
      IF(X(I).EQ.0.) GO TO 126
      TEM=(PISAVE(I)-X(I))/X(I)
      IF(TEM.LT.0.) TEM=-TEM
      IF(TEM.GT..001) GO TO 128
226 CONTINUE
228 DO 129 I=1,NLM
229 PISAVE(I)=X(I)
      IF(TEM.GT..001) GO TO 43
222 DO 225 I=1,NLM
      IF(B0(I).LE.1.0E-8) GO TO 227
      SUM = 0.
      DO 223 J=1,NS
223 SUM = SUM+EN(NPT,J)*A(I,J)
      TSUM=B0(I)-SUM-B0N(I)
      IF(ABS(TSUM)/B0(I).GT..0001) GO TO 43
225 CONTINUE
      IF(TEM=0)
227 IF(.NOT.IONS) GO TO 275
C
C CHECK ON ELECTRON BALANCE
C
      ITER=1
      IF(PIE.EQ.0.) GO TO 229
      LE=NLM+1
      X(LE)=PIE
229 SUM2 = 0.
      SUM = 0.
      PIE = X(LE)
      DO 230 J=1,NSK
      IF(IUSE(J).LT.0.OR.A(LS,J).EQ.0.) GO TO 230
      EN(NPT,J)=0.
      ENE=0.
      IF(ENLN(J).GT.-87.) ENE=E*ENLN(J)

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EQLB2830
EQLB2835
EQLB2840
EQLB2845
EQLB2850
EQLB2855
EQLB2860
EQLB2865
EQLB2870
EQLB2875
EQLB2880
EQLB2885
EQLB2890
EQLB2895
EQLB2900
EQLB2905
EQLB2910
EQLB2915
EQLB2920
EQLB2925
EQLB2930
EQLB2935
EQLB2940
EQLB2945
EQLB2950
EQLB2955
EQLB2960
EQLB2965
EQLB2970
EQLB2975
EQLB2980
EQLB2985
EQLB2990
EQLB2995
EQLB3000
EQLB3005
EQLB3010
EQLB3015
EQLB3020
EQLB3025
EQLB3030
EQLB3035
EQLB3040
EQLB3045
EQLB3050
EQLB3055
EQLB3060
EQLB3065
EQLB3070
EQLB3075
EQLB3080
EQLB3085
EQLB3090
EQLB3095
EQLB3100
EQLB3105

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	IF((SMLN(J)-ENL+SIZE).LE.0.) GO TO 231	EQLB3110
	IF(.NOT.J)=ENE	EQLB3115
	IF(L.MT(NLM).EQ.IE) PIE=0.	EQLB3120
231	AN = A(LS,J)*ENE	EQLB3125
	SUM = SUM+AN	EQLB3130
	SUM2 = SUM2+AN*A(LS,J)	EQLB3135
230	CONTINUE	EQLB3140
	IF(SUM2.EQ.0.) GO TO 275	EQLB3145
	DPIE = -SUM/SUM2	EQLB3150
	DO 250 J=1,NS	EQLB3155
	IF(A(LS,J).EQ.0.) GO TO 250	EQLB3160
	ENLN(J) = ENLN(J)+A(LS,J)*DPIE	EQLB3165
250	CONTINUE	EQLB3170
	IF(ABS(DPIE).LE.0001) GO TO 270	EQLB3175
	X(LE)=X(LE)+DPIE	EQLB3180
255	ITER=ITER+1	EQLB3185
	IF(ITER.LE.80) GO TO 229	EQLB3190
	WRITE(6,260)	EQLB3195
260	FORMAT(37H0DID NOT CONVERGE ON ELECTRON BALANCE)	EQLB3200
	GO TO 873	EQLB3205
270	IF(LLMT(NLM).NE.IE.OR.PIE.EQ.0.) GO TO 275	EQLB3210
	NLM=ULM-1	EQLB3215
	IQ1=IQ1-1	EQLB3220
275	CONTINUE	EQLB3225
	IF(IPRRKT.GE.3)WRITE(1,9182) NPT,ITN,NUMB	EQLB3230
C		EQLB3235
C	CALCULATE ENTROPY, CHECK ON DELTA S FOR SP PROBLEMS	EQLB3240
C		EQLB3245
	TOTN(NPT) = 0.	EQLB3250
	SSUM(NPT) = 0.	EQLB3255
	DO 183 J=1,NS	EQLB3260
	IF(IUSE(J).LT.0) GO TO 183	EQLB3265
	TOTN(NPT) = TOTN(NPT) + EN(NPT,J)	EQLB3270
	SS = S(J)	EQLB3275
	IF(IUSE(J).EQ.0) SS=SS-ENLN(J)-TM	EQLB3280
	IF(IUSE(J).GT.1000) SS=SS-ENLN(J)+ENLS	EQLB3285
	SSUM(NPT) = SSUM(NPT)+SS*CN(NPT,J)	EQLB3290
183	CONTINUE	EQLB3295
C		EQLB3300
C	**** ADD NON-EQ CONTRIBUTION	EQLB3305
C		EQLB3310
	IF(IPP.LT.NEOPT)GO TO 184	EQLB3315
	IF(NSK.EQ.NS)GO TO 184	EQLB3320
	NSP1=NS+1	EQLB3325
	DO 185 J=NSP1,NSK	EQLB3330
	IF(IUSE(J).LT.0)GO TO 185	EQLB3335
	TOTN(NPT)=TOTN(NPT)+EN(NPT,J)	EQLB3340
	SS=S(J)	EQLB3345
	IF(IUSE(J).EQ.0)SS=SS-ENLN(J)-TM	EQLB3350
	SSUM(NPT)=SSUM(NPT)+SS*CN(NPT,J)	EQLB3355
185	CONTINUE	EQLB3360
184	CONTINUE	EQLB3365
	IF(.NOT.SP)GO TO 13	EQLB3370
C+.	IF(AA.LE.AACON)GO TO 13	EQLB3375
	SS = SSUM(NPT) -S0	EQLB3380
	IF(DABS(SJ).LE.CON33S)GO TO 1180	EQLB3385

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      IF(NUMB.GE.ITN)GO TO 276      EQLB3390
      GO TO 43                      EQLB3395
1180 CONTINUE                      EQLB3400
      IF(RITE) WRITE(6,1183) SS     EQLB3405
1183 FORMAT(12H0DELTA S/P =,E15.8) EQLB3410
C                                  EQLB3415
      13 CONVG= .TRUE.             EQLB3420
C.ADD                              EQLB3425
      IAFLG=0                       EQLB3430
      GO TO 160                     EQLB3435
      14 CONTINUE                   EQLB3440
      IF(KKTEM.NE.0)GO TO 276       EQLB3445
      IF(A1.LE.AACON)GO TO 275      EQLB3450
      IF(IAFLG.EQ.0)GO TO 276       EQLB3455
      IF(AA.GE.1.0)GO TO 276        EQLB3460
      IF(CHNLEN.LT.0.0)GO TO 276    EQLB3465
      KSUB0=KSUB0+1                 EQLB3470
      IF(KSUB0.GT.KSUB0M)GO TO 276  EQLB3475
      HSUB0=1.001*HSUB0             EQLB3480
      GO TO 386                     EQLB3485
276 CONTINUE                       EQLB3490
      IF(ITN.EQ.0)ITN=30             EQLB3495
      WRITE(6,973) ITN,NPT           EQLB3500
973 FORMAT(1HL,I3,69H ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREME EQLB3505
      INTS FOR THE POINT I5)         EQLB3510
      IF(LIPNT.LT.0)GO TO 4444      EQLB3515
      NUMDEG=2                      EQLB3520
      IF(N1.NE.1)CALL DBGOUT(NUMOUT,HP,SP,DXOUTP,NUMQBG) EQLB3525
      NUMCBG=3                      EQLB3530
      DXOUTP(1)=J                   EQLB3535
      DXOUTP(2)=NPT                 EQLB3540
      DXOUTP(3)=EN(NPT,J)           EQLB3545
      DXOUTP(4)=TRACE               EQLB3550
      IF(SP)DXOUTP(4)=SS            EQLB3555
      DXOUTP(5)=AMBDA               EQLB3560
      DXOUTP(5)=AMPDA1              EQLB3565
      DXOUTP(7)=SUM                  EQLB3570
      DXOUTP(8)=SUM1                EQLB3575
      DXOUTP(9)=AA                  EQLB3580
      DXOUTP(10)=TEM                 EQLB3585
C...DXOUTP(11)=TMELT FOR CONDENSED SPECIES FOR WHICH IAFLG=1 EQLB3590
      DXOUTP(12)=VE                  EQLB3595
      DXOUTP(13)=NLM                 EQLB3600
      DXOUTP(14)=TSUM                EQLB3605
      DXOUTP(15)=EN(NPT,1)           EQLB3610
      DXOUTP(16)=EMM                 EQLB3615
      DXOUTP(17)=ENN                 EQLB3620
      DXOUTP(18)=IQ1                 EQLB3625
      DXOUTP(19)=X(IQ1)              EQLB3630
      DXOUTP(20)=DLN                 EQLB3635
      DXOUTP(21)=ENL                 EQLB3640
      DXOUTP(22)=TT                  EQLB3645
      DXOUTP(23)=TEMP0               EQLB3650
      DXOUTP(24)=TEMP1               EQLB3655
      DXOUTP(25)=NS                  EQLB3660
      DO 4445 I=1,NLM                EQLB3665

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4445 DXOUTP(I+25)=B0(I)                                EQLB3670
      NUMOUT=25+NLM                                     EQLB3675
      CALL DBGOUT(NUMOUT,HP,SP,DXOUTP,NUMDBG)           EQLB3680
4444 CONTINUE                                           EQLB3685
      IF(KKTEM.EQ.10)GO TO 873                          EQLB3690
      IF(NS.LE.1)GO TO 873                              EQLB3695
      IF(NC.EQ.0.OR.I35) GO TO 873                     EQLB3700
      I35 = .TRUE.                                       EQLB3705
      IF (.NOT.HP.OR.NPT.NE.1.OR.TT.GT.100.) GO TO 261 EQLB3710
      WRITE(6,874)                                       EQLB3715
      GO TO 873                                          EQLB3720
261 NCOND = IQ1-NLM-2                                    EQLB3725
      IF(TP) NCOND=NCOND+1                              EQLB3730
      IF(NCOND.NE.1.OR.ENN.GT.1.E-4) GO TO 873          EQLB3735
C HIGH TEMPERATURE, INCLUDED CONDENSED CONDITION       EQLB3740
      WRITE(6,265)                                       EQLB3745
265 FORMAT(31H0TRY REMOVING CONDENSED SPECIES)         EQLB3750
      ENN = .1                                           EQLB3755
      ENL = -2.3025851                                   EQLB3760
      SUMN = ENN                                        EQLB3765
      XI = NS - NC                                       EQLB3770
      XI = ENN/XI                                        EQLB3775
      XLN = ALOG(XI)                                    EQLB3780
      DO 432 J=1,NS                                     EQLB3785
      IF(IUSE(J).GT.0 .AND. IUSE(J).LT.1000) IUSE(J)=-IUSE(J) EQLB3790
      EN(NPT,J) = 0.                                     EQLB3795
      ENLN(J) = 0.                                       EQLB3800
      IF (IUSE(J).NE.0) GO TO 432                       EQLB3805
      EN(NPT,J) = XI                                     EQLB3810
      ENLN(J) = XLN                                     EQLB3815
432 CONTINUE                                           EQLB3820
      IQ1 = NLM+1                                       EQLB3825
      GO TO 40                                          EQLB3830
C                                                       EQLB3835
C CONVERGENCE TESTS ARE SATISFIED, TEST CONDENSED SPECIES AND/OR SOLE EQLB3840
C                                                       EQLB3845
160 TN=NUMB                                             EQLB3850
      IF(.NOT.SHOCK .AND. FLAG)WRITE(6,771) NPT,(X(IL),IL=1,LE),TN EQLB3855
      IF(IPRRKT.GE.2)WRITE(1,771) NPT,(X(IL),IL=1,LE),TN EQLB3860
771 FORMAT (I3,(2X,14F9.3))                           EQLB3865
      IF(.NOT.SFLG) GO TO 180                           EQLB3870
      INC=0                                              EQLB3875
      DO 910 J=1,NS                                     EQLB3880
      IF(IUSE(J).EQ.0) GO TO 910                        EQLB3885
      INC=INC+1                                          EQLB3890
      IF(IUSE(J) .LT. 1000) GO TO 910                  EQLB3895
      TMELT=TEMP(INC,1) - TMELTS                       EQLB3900
      IF(TT .GT. TMELT) GO TO 910                      EQLB3905
      IUX=-IUSE(J) - 1000                              EQLB3910
      IUSE(J)=IUSE(J)-1000                             EQLB3915
      JJSOLD=1                                           EQLB3920
      DO 901 KK=1,NSOLOC                                EQLB3925
      JJ=JJDUM(KK)                                       EQLB3930
      IF(JJ.LT.0)JJ=-JJ                                  EQLB3935
      IF(JJ.NE.J)GO TO 901                              EQLB3940
      JJDUM(KK)=0                                        EQLB3945

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      GO TO 902
901 CONTINUE
      JJSOLD=0
902 IADDSL=0
      DO 913 JJ=1,NS
      IF(IUSE(JJ).EQ.IUX) IUSE(JJ)=IUSE(JJ)+2000
      IF(IUSE(JJ).LE.1000)GO TO 913
      SUMM=0.0
      DO 903 L2=1,NLM
903 SUMM=SUMM+A(L2,JJ)*X(L2)
      SUM2=SUMM-H0(JJ)+S(JJ)
      DO 904 KK=1,NSOLC
      MM=JJDUM(KK)
      IF(M1.LT.0)MM=-MM
      KKSAY=KK
      IF(MM.EQ.JJ)GO TO 905
904 CONTINUE
C... NO MATCH.....RESET IUSE AND CONTINUE
      IUSE(JJ)=IUSE(JJ)-1000
      GO TO 913
905 JJSOLD=JJSOLD+1
      JJDUM(KKSAY)=-JJ
      XXXSUM(KKSAY)=SUM2
      IF(SUM2.GT.0.000)GO TO 907
      JJDUM(KKSAY)=JJ
907 CONTINUE
      IF(JJSOLD.EQ.NSOLC)GO TO 909
913 CONTINUE
909 CONTINUE
      NSOL = NSOL -1
      IQ1 = IQ1 + 1
      JREM=0
      WRITE(6,8001) (SUB(J,JJ),JJ=1,3)
8001 FORMAT(1X,3A4,23H FROZEN OUT OF SOLUTION )
      IF(NSOL.GT.1)GO TO 8109
      DO 912 KK=1,NS
      IF(IUSE(KK).LT.-2000) IUSE(KK)=IUSE(KK)+2000
      IF(IUSE(KK).LT.1000)GO TO 912
      IUX=KK
      IUSE(KK)=IUSE(KK) - 1000
912 CONTINUE
      WRITE(6,8002)
8002 FORMAT(/1X,7(1H*),25HSOLUTION NO LONGER EXISTS,7(1H*))
      NSOL =0
      ENNS=0
      SFLG=.FALSE.
      GO TO 908
910 CONTINUE
910 CONTINUE
      IF(NSOL.LE.0.OR.SFLG)GO TO 908
      IF(NCMOVS.NE.0)GO TO 908
981 TEST=0.
      IF(IMPRNT.GE.3)WRITE(1,8003) NSOL
8003 FORM,T(1X,/,1X,J3,17H SOLUTION SPECIES/,2X,3HNO.,4X,4HSUM2,8X,
      *4HSUMM,8X,5H0(J),7X,4HS(J),8X,4HTEST)
8004 FORMAT(1X,I3,2X,5(G11.3,2X))

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EQLB3950
EQLB3955
EQLB3960
EQLB3965
EQLB3970
EQLB3975
EQLB3980
EQLB3985
EQLB3990
EQLB3995
EQLB4000
EQLB4005
EQLB4010
EQLB4015
EQLB4020
EQLB4025
EQLB4030
EQLB4035
EQLB4040
EQLB4045
EQLB4050
EQLB4055
EQLB4060
EQLB4065
EQLB4070
EQLB4075
EQLB4080
EQLB4085
EQLB4090
EQLB4095
EQLB4100
EQLB4105
EQLB4110
EQLB4115
EQLB4120
EQLB4125
EQLB4130
EQLB4135
EQLB4140
EQLB4145
EQLB4150
EQLB4155
EQLB4160
EQLB4165
EQLB4170
EQLB4175
EQLB4180
EQLB4185
EQLB4190
EQLB4195
EQLB4200
EQLB4205
EQLB4210
EQLB4215
EQLB4220
EQLB4225

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8005 FORMAT(57X,G13.5)
      SSZEG=0.0
      INC=0
      NSOL=0
      JJSOLD=0
      DO 8104 J=1,NS
      IF(IUSE(J).EQ.0)GO TO 8104
      INC=INC+1
      IF(IUSE(J).GE.-1000)GO TO 8104
      IF(IUSE(J).LE.-2000)GO TO 8104
C... SHOULD ANY SPECIES BE IMMEDIATELY FROZEN OUT OF SOLUTION
      TMELT=TEMP(INC,1)-TMELTS
      IF(TT.GT.TMELT)GO TO 8103
C... YES, REMOVE IF AND FLAG ITS IUSE TO FIX CORRESPONDING SOLID
      JJSOLD=JJSOLD+1
      KKDUM(JJSOLD)=IUSE(J)-1000
      IUSE(J)=IUSE(J)+1000
      NSOL=NSOL+1
      EN(NPT,J)=0.0
      DELN(J)=0.0
CCCC IF(KASE.EQ.7777)WRITE(1,4021)J,IUSE(J),KKDUM(JJSOLD)
4021 FORMAT(10X,5(1H*),8HSPECIES=,I4,7H IUSE=,I5,8H KKDUM=,I5)
      WRITE(6,4029) (SUB(J,KK),KK=1,3),TMELTS
4029 FORMAT(1X,3A4,31H REMOVED FROM SOLUTION AS TT IS,F8.2,
      *23H DEG K BELOW MELTING PT)
      GO TO 8104
C... DOES THIS SPECIES CONTRIBUTE ENOUGH TO ADD SOLUTION
8100 SUMM=0.
C... STORE ITS POSITION IN JJDUM
      NSOL=NSOL+1
      JJDUM(NSOL)=J
      DO 8101 L2=1,NLM
8101 SUMM=SUMM+A(L2,J)*X(L2)
      SUM2=SUMM-H0(J)+S(J)
C... SAVE ITS SUM2 VALUE IN XXXSUM
      XXXSUM(NSOL)=SUM2
      IF(SUM2.GT.0.000)GO TO 8102
C... SUM2 .LT. 0.0 MEANS THIS SPECIES IS NOT AS PROMINENT
      JJDUM(NSOL)=J
      GO TO 8103
8102 SSZEG=SSZEG+SUM2
      IF(SUM2.GE.40.000)SUM2=1.0
8103 IF(IMPRNT.GE.3)WRITE(1,8004)J,SUM2,SUMM,H0(J),S(J),TEST
      TEST=TEST+DEXP(SUM2)
8104 CONTINUE
      NSOL=NSOL
C... RESET IUSE OF SOLID SPECIES THAT FROZE OUT OF SOLUTION
      IF(J.SOLD.EQ.0)GO TO 8107
      DO 8106 KK=1,NS
      IF(IUSE(KK).GE.-2000)GO TO 8106
      DO 8105 JJ=1,JJSOLD
      IF(IUSE(KK).NE.KKDUM(JJ))GO TO 8105
C... FOUND THE CORRESPONDING SOLID( ADD 2000 )
      EN(NPT,KK)=0.0
      DELN(KK)=0.0
      IUSE(KK)=IUSE(KK)+2000

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EOLB4230
EOLB4235
EOLB4240
EOLB4245
EOLB4250
EOLB4255
EOLB4260
EOLB4265
EOLB4270
EOLB4275
EOLB4280
EOLB4285
EOLB4290
EOLB4295
EOLB4300
EOLB4305
EOLB4310
EOLB4315
EOLB4320
EOLB4325
EOLB4330
EOLB4335
EOLB4340
EOLB4345
EOLB4350
EOLB4355
EOLB4360
EOLB4365
EOLB4370
EOLB4375
EOLB4380
EOLB4385
EOLB4390
EOLB4395
EOLB4400
EOLB4405
EOLB4410
EOLB4415
EOLB4420
EOLB4425
EOLB4430
EOLB4435
EOLB4440
EOLB4445
EOLB4450
EOLB4455
EOLB4460
EOLB4465
EOLB4470
EOLB4475
EOLB4480
EOLB4485
EOLB4490
EOLB4495
EOLB4500
EOLB4505


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CCCC IF(KASE.EQ.7777)WRITE(1,4021)KK,IUSE(KK),KKDUM(JJ)
8105 CONTINUE
8106 CONTINUE
C... MAKE SURE THERE ARE SOME SPECIES IN SOLUTION
8107 IF(NSOL-1)8112,8113,8115
C....ONLY 1 SPECIES IN SOLUTION REMOVE IT
8113 CONTINUE
      MM=JJDUM(1)
      IF(MM.LT.0)MM=-MM
      NSOL=0
      ENNS=0.0
      IUX=IUSE(MM)-1000
      IUSE(MM)=IUSE(MM)+1000
      DO 8114 KK=1,MM
      IF(IUSE(KK).EQ.IUX)IUSE(KK)=IUSE(KK)+2000
8114 CONTINUE
      SSZEG=0.0
8112 WRITE(6,8002)
CCCC IF(KASE.EQ.7777)WRITE(1,8002)
      GO TO 908
C.... MORE THAN 1 SPECIES IN SOLUTION...SHOULD SOLUTION BE ADDED....
8115 CONTINUE
      IF(IMPRINT.GE.3)WRITE(1,8005)TEST
      IF(TEST.GE.1.)GO TO 8108
      SSZEG=0.0
      GO TO 908
8108 IF(SSZEG.EQ.0.0)SSZEG=-.00001
      IF(SSZEG.GT.0.0)SSZEG=-SSZEG
      GO TO 908
C
C ADD SOLUTION TO PROBLEM
34 CONTINUE
      JREM=0
      JPHCHN=0
      IADDSL=1
8109 CONTINUE
      ENNS=SOLMAX
      ENLS=ALOG(ENNS)
      NSOLNG=0
      NSOL=0
      ENNS55=0.0
      ENMAX=SOLMAX/NSOL
      DO 8117 KK=1,NSOL
      IF(JJDUM(KK))8116,8117,8110
      C... THIS PATH MEANS (H0(J)-S(J)-SUMM).GT.0.0
8110 CONTINUE
      J=JJDUM(KK)
      IF(IUSE(J).LT.-1000)IUSE(J)=-IUSE(J)
      EN(NPT,J)=CRCRIT
      SUM2=XXSUM(KK)
      IF(SUM2.LE.-19.000)GO TO 8111
      EN(NPT,J)=SOLMAX*DEXP(SUM2)
      IF(EN(NPT,J).LT.CRCRIT)EN(NPT,J)=CRCRIT
      IF(EN(NPT,J).GT.ENMAX)EN(NPT,J)=ENMAX
CCCC IF(KASE.EQ.7777)WRITE(1,4025)J,EN(NPT,J)
4025 FORMAT(1X,4(1H*),2HJ=,I4,1X,3HEN=,G13.5)

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EQLB4510
EQLB4515
EQLB4520
EQLB4525
EQLB4530
EQLB4535
EQLB4540
EQLB4545
EQLB4550
EQLB4555
EQLB4560
EQLB4565
EQLB4570
EQLB4575
EQLB4580
EQLB4585
EQLB4590
EQLB4595
EQLB4600
EQLB4605
EQLB4610
EQLB4615
EQLB4620
EQLB4625
EQLB4630
EQLB4635
EQLB4640
EQLB4645
EQLB4650
EQLB4655
EQLB4660
EQLB4665
EQLB4670
EQLB4675
EQLB4680
EQLB4685
EQLB4690
EQLB4695
EQLB4700
EQLB4705
EQLB4710
EQLB4715
EQLB4720
EQLB4725
EQLB4730
EQLB4735
EQLB4740
EQLB4745
EQLB4750
EQLB4755
EQLB4760
EQLB4765
EQLB4770
EQLB4775
EQLB4780
EQLB4785

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8111 NSOL (=NSOL1+1
      ENNSSS=ENNSSS+TN(NPT,J)
      ENLN(J)=DLOG(EN(NPT,J))
      GO TO 8117
C... THIS PATH MEANS (H0(J)-S(J)+SUMM) .LE. 0.0
8116 NSOLNG=NSOLNG+1
8117 CONTINUE
      IF(NSOLNG.EQ.0 GO TO 8119
      AADIV=NSOL-NSOL1
      ENMAX=(SOLMAX-ENNSSS)/AADIV
CCCCC IF(KASE.EQ.7777)WRITE(1,4026) NSOLNG,ENMAX,ENNSSS,AADIV
4026 FORMAT(1X,3(1H*),7HNSOLNG=,I3,1X,19HENMAX.ENNSSS.AADIV=,
      *3(1X,G13.5))
      ENNSSS=DLOG(ENMAX)
      DO 8118 KK=1,NSOLC
      IF(JJDUM(KK).GE.0)GO TO 8118
      J=-JJDUM(KK)
      IF(IUSE(J).LT.-1000)IUSE(J)=-IUSE(J)
      EN(NPT,J)=ENMAX
CCCCC IF(KASE.EQ.7777)WRITE(1,4025) J,EN(NPT,J)
      ENLN(J)=ENNSSS
8118 CONTINUE
8119 IF(IADDSL.EQ.0)GO TO 908
      SFLG=.TRUE.
      IQ1=IQ1+1
      WRITE(6,9006)
9006 FORMAT(13H ADD SOLUTION )
C***GROK
      KKKK=1
      GO TO 40
908 IF(NC.EQ.0) GO TO 143
C***GROK
      KKKK=2
      DO 146 J=1,NS
      IF(EN(NPT,J).GE.0.) GO TO 146
      IF(IUSE(J).LE.0 .OR. IARS(IUSE(J)) .GT. 1000) GO TO 146
      IF(J.NE.JSOL .AND. J.NE.JLIQ) GO TO 147
      JSOL = 0
      JLIQ = 0
147 IQ1 = IQ1 - 1
      EN(NPT,J) = 0.
      DELN(J)=0.
      JREM=J
      JKEE=J
      WRITE(6,391) SUB(J,1),SUB(J,2),SUB(J,3)
      GO TO 166
146 CONTINUE
      SIZEG = 0.
      IF(NPMOVS.NE.0)SSZEG=0.0
      IF(.NOT.SFLG)SIZEG=SSZEG
C***GROK
      KKKK=3
      INC = 0
CCCCC IF(KASE.EQ.7777)WRITE(1,8007)
8007 FORMAT(2X,1HJ,5X,4HDELG,3X,5HHE0(J),7X,4HS(J),9X,3HSUM,8X,
      *5HSIZEG,7X,5HSSZEG)

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EQLB4790
EQLB4795
EQLB4800
EQLB4805
EQLB4810
EQLB4815
EQLB4820
EQLB4825
EQLB4830
EQLB4835
EQLB4840
EQLB4845
EQLB4850
EQLB4855
EQLB4860
EQLB4865
EQLB4870
EQLB4875
EQLB4880
EQLB4885
EQLB4890
EQLB4895
EQLB4900
EQLB4905
EQLB4910
EQLB4915
EQLB4920
EQLB4925
EQLB4930
EQLB4935
EQLB4940
EQLB4945
EQLB4950
EQLB4955
EQLB4960
EQLB4965
EQLB4970
EQLB4975
EQLB4980
EQLB4985
EQLB4990
EQLB4995
EQLB5000
EQLB5005
EQLB5010
EQLB5015
EQLB5020
EQLB5025
EQLB5030
EQLB5035
EQLB5040
EQLB5045
EQLB5050
EQLB5055
EQLB5060
EQLB5065

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DO 170 J = 1, NS
JKEEP=J
IF (IUSE(J).EQ.0) GO TO 170
INC=INC+1
IF (IABS(IUSE(J)).GE.1000) GO TO 170
CSOL IUX=ABS(IUSE(J))
CSOL IF(IUX.GE.3000)GO TO 170
CSOL IF(IUX.GT.2000)GO TO 8160
CSOL IF(IUX.GE.1000)GO TO 170
8160 CONTINUE
IF(NUM.GE.LZ) GO TO 164
DO 162 I=LP1,LS
IF (A(I,J).NE.0.) GO TO 170
162 CONTINUE
164 IF(RITE) WRITE(6,144)(SUB(J,I),I=1,3),TEMP(INC,1),TEMP(INC,2),IUSE(J),EN(NPT,J)
144 FORMAT (1H0,3A4,2F10.3,3X,5HIUSE=,I4,E15.7)
IF(EN(NPT,J).GT.0.) GO TO 169
KG = 1
IF(IUSE(J).EQ.-IUSE(J+1)) GO TO 154
IF(J.EQ.1.OR.IUSE(J).NE.-IUSE(J-1)) GO TO 153
KG = -1
154 JKG = J + KG
TMELT = TEMP(INC,1)
IMP = INC + KG
IF(TMELT.EQ.TEMP(IMP,2)) GO TO 158
TMELT = TEMP(INC,2)
IF (TMELT.EQ.TEMP(IMP,1)) GO TO 157
WRITE (6,156) (SUB(J,I),I=1,3)
156 FORMAT (51H03 PHASES OF A CONDENSED SPECIES ARE OUT OF ORDER -,1X,
1 3A4)
GO TO 873
C
C JTH SPECIES A SOLID (EN=0), (J+KG)TH SPECIES A LIQUID (EN IS +)
C
157 CONTINUE
TTCOLP=ABS(TT-TMELT)
IF(TCOLP.GT.TCRIT)GO TO 152
IAFLG=1
DXOUTP(11)=TMELT
152 CONTINUE
IF(TT.GT.TMELT) GO TO 169
IF (TP.AND.TT.EQ.TMELT) GO TO 169
IF ('P) GO TO 1165
IF(I2P.GE.NEOPT)GO TO 1165
IF (TT.LE (TMELT-TMELTM)) GO TO 1165
CPSV IF(TT.LE.TEQLPM)GO TO 2003
CPSV IF(TT.LE.TTBO1)GO TO 116,
2003 CONTINUE
J3OL = J
JL1Q = JKG
GO TO 159
C
C JTH SPECIES A LIQUID(EN=0), (J+KG)TH SPECIES A SOLID (EN IS +)
C
158 CONTINUE

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      TTCOMP=ABS(TT-TMELT)
      IF(TTCOMP.GT.TTCRIT)GO TO 151
      TAFL=1
      DEOUTP(11)=TMELT
151  CONTINUE
      IF (TT.LT.TMELT) GO TO 169
      IF (TP.AND.TT.EQ.TMELT) GO TO 169
      IF (TP) GO TO 1165
      IF(IPP.GE.NEQPT)GO TO 1165
      IF (TT.GE.(TMELT+TMELTP)) GO TO 1165
CPSV IF(TT.LE.1EQLEBM)GO TO 2884
CPSV IF(TT.LE.TTHOT)GO TO 1165
2884  CONTINUE
      JSOL = JKG
      JLIQ = J
159  CONTINUE
      EN(NPT,JKG) = .5 * EN(NPT,JKG)
      EN(NPT,J) = EN(NPT,JKG)
CPSV TLN = ALOG (TMELT)
CPSV TT = TMELT
CPSV GO TO 165
      KSUBM=1
      WRITE(6,8889) (SUB(J,KK),KK=1,3),(SUB(JKG,KK),KK=1,3),TT,TMELT
      WRITE(1,8289) (SUB(J,KK),KK=1,3),(SUB(JKG,KK),KK=1,3),TT,TMELT
8889  FORMAT(1X,10(1H*),30HWARNING TRIPLE PT. OF SPECIES ,6A4,
      *11H APPROACHED/,5X,3HTT=,F10.2,2X,6HTMELT=,F10.2,/,1X,50(1H*))
      GO TO 165
C
C  WRONG PHASE INCLUDED FOR T INTERVAL, SWITCH EN
1165 CONTINUE
      IF(J.EQ.JPHCHN)GO TO 169
      JPHCHN=JKG
      EN(NPT,J) = EN(NPT,JKG)
      IUSE(J) = -IUSE(J)
      IUSE (JKG) = -IUSE(JKG)
      EN(NPT,JKG)= 0.
      WRITE(6,161) (SUB(JKG,I),I=1,3),(SUB(J,K),K=1,3)
161  FORMAT(23H PHASE CHANGE, REPLACE ,3A4,5HWITH ,3A4)
CCCCC IF(KASE.EQ.7777)WRITE(1,8122) JKG,J,TT,TMELT
8122  FORMAT(5X,I4,12H REPLACED BY,I5,18H FOR TT AND TMELT=,
      *2(1X,F11.3),1X,25(1H.))
      GO TO 48
153  IF (TT.LT.TEMP(INC,1) .AND.TEMP(INC,1).NE.TLOW) GO TO 169
      IF (TT.GT.TEMP(INC,2)) GO TO 169
C
C
      SUM = 0.
      DO 167 I = 1,NLM
      SUM=SUM+A(I,J)*X(I)
167  CONTINUE
      DELG = H0(J)-S(J)-SUM
      IF(RITE) WRITE(6,163)DELG,SIZEG
      IF(DELG.GE.0.0)GO TO 169
CCCCC IF(KASE.EQ.7777)WRITE(1,8886)J,DELG,H0(J),S(J),SUM,SIZEG,SSZEG
8886  FORMAT(1X,I3,6(1X,G11.3))
168  FORMAT (18H G0-SUM(AIJ*PII) =E15.7,10X,17HMAX NEG DELTA G =,E15.7)

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EQLB5350
EQLB5355
EQLB5360
EQLB5365
EQLB5370
EQLB5375
EQLB5380
EQLB5385
EQLB5390
EQLB5395
EQLB5400
EQLB5405
EQLB5410
EQLB5415
EQLB5420
EQLB5425
EQLB5430
EQLB5435
EQLB5440
EQLB5445
EQLB5450
EQLB5455
EQLB5460
EQLB5465
EQLB5470
EQLB5475
EQLB5480
EQLB5485
EQLB5490
EQLB5495
EQLB5500
EQLB5505
EQLB5510
EQLB5515
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EQLB5555
EQLB5560
EQLB5565
EQLB5570
EQLB5575
EQLB5580
EQLB5585
EQLB5590
EQLB5595
EQLB5600
EQLB5605
EQLB5610
EQLB5615
EQLB5620
EQLB5625

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      IF(DELG.GE.SIZEG) GO TO 169
      SIZEG = DELG
      JDELG = J
169  IF(INC.EQ.NC) GO TO 1160
170  CONTINUE
1160 IF (SIZEG.EQ.0.) GO TO 143
      IF(NRMOVS.NE.0)GO TO 1162
      IF(SIZEG.EQ.SSIZEG)GO TO 34
1162 CONTINUE
      IF(JKEEP.EQ.JREM)GO TO 143
      JKEEP= JDELG
165  IF(JKEEP.EQ.JREM)GO TO 143
      IQ1 = IQ1 + 1
      WRITE (6,136) SUB(JKEEP,1),SUB(JKEEP,2),SUB(JKEEP,3)
136  FORMAT (5H ADD ,3A4)
166  IUSE(JKEEP) = - IUSE(JKEEP)
CSOL IF(IUSE(JKEEP).GT.2000)IUSE(JKEEP)=IUSE(JKEEP)-2000
C***GROK...LIST NEXT 15 LINES
      KKKK=KKKK-1F
      40 CONVG = .FALSE.
      KKKK=KKKK+100
      GO TO 385
143  CONTINUE
      KKKK=KKKK+1000
      IF(.NOT.TP) GO TO 386
385  JS1=1
      CALL CPHS
386  CONTINUE
      IF(IPRRKT.GE.3)WRITE(1,9182) NPT,KKKK,NUMB
9182 FORMAT(1X,10(1H*),3(2X,15))
      NUMB=0
      AA=1.0
      GO TO 43
390 IF(ISINGV.LE.NLM) GO TO 194
C
C REMOVE CONDENSED SPECIES TO CORRECT SINGULARITY
C
      JC=ISINGV-NLM
      INC=0
      DO 392 J=1,NS
      IF(IUSE(J).LE.0 .OR. IABS(IUSE(J)).GT.1000) GO TO 392
      INC=INC+1
      IF(INC.NE.JC) GO TO 392
      IF(J.EQ.JCONS) GO TO 960
      IQ1=I/1-1
      JCONJ=J
      EN(NPT,J)=0.
      JREM=J
      IUSE(J)=-IUSE(J)
      WRITE(6,391) SUB(J,1),SUB(J,2),SUB(J,3)
391  FORMAT (8H REMOVE ,3A4)
      GO TO 40
392 CONTINUE
C
C FIND NEW COMPONENT
C

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EQLB5630
EQLB5635
EQLB5640
EQLB5645
EQLB5650
EQLB5655
EQLB5660
EQLB5665
EQLB5670
EQLB5675
EQLB5680
EQLB5685
EQLB5690
EQLB5695
EQLB5700
EQLB5705
EQLB5710
EQLB5715
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EQLB5745
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EQLB5755
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EQLB5770
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EQLB5800
EQLB5805
EQLB5810
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EQLB5845
EQLB5850
EQLB5855
EQLB5860
EQLB5865
EQLB5870
EQLB5875
EQLB5880
EQLB5885
EQLB5890
EQLB5895
EQLB5900
EQLB5905

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394 IF(. . T.IONS) TO TO 400                                EQLB5910
      IF(LLMT(NLM).NE.0) GO TO 400                          EQLB5915
      DO 395 J=1, NS                                         EQLB5920
      IF(A(NLM,J).NE.0.) EN(NPT,J)=0.                      EQLB5925
395 CONTINUE                                                  EQLB5930
      PIE=(NLM)                                              EQLB5935
      NLM=NLM-1                                              EQLB5940
      IQ1=IQ1-1                                              EQLB5945
      IF(ISINGV.GT.NLM) GO TO 43                            EQLB5950
400 DO 430 LC=1, NLM                                         EQLB5955
      IF(LC.EQ.ISINGV) GO TO 430                             EQLB5960
      DO 420 J=1, NS                                         EQLB5965
      IF(A(LC,J).EQ.0.) GO TO 420                            EQLB5970
      IF(EN(NPT,J).EQ.0.) GO TO 420                          EQLB5975
      IF(A(ISINGV,J).EQ.0.) GO TO 420                        EQLB5980
      JB=J                                                    EQLB5985
      GO TO 431                                              EQLB5990
420 CONTINUE                                                  EQLB5995
430 CONTINUE                                                  EQLB6000
      IF(IC.EQ.0 .AND. NLM.GT.1) GO TO 530                  EQLB6005
      GO TO 960                                              EQLB6010
431 WRITE(6,435) SUB(JB,1), SUB(JB,2), SUB(JB,3)           EQLB6015
435 FORMAT (18H0NEW COMPONENT IS ,3A4)                     EQLB6020
      WRITE(6,436) SUB(JB,1)                                EQLB6025
436 FORMAT (27H0PI AND B0 WILL BE LABELED ,A4)             EQLB6030
      LLMT(LC)=SUB(JB,1)                                     EQLB6035
      IC=0                                                    EQLB6040
C                                                            EQLB6045
C CALCULATE NEW COEFFICIENTS                                EQLB6050
C                                                            EQLB6055
      ACJ=A(LC,JB)                                           EQLB6060
      IF (A(LC,JB).EQ.1.) GO TO 460                         EQLB6065
      B0(LC)=B0(LC)/ACJ                                       EQLB6070
      B0P(LC,1)=B0P(LC,1)/ACJ                                EQLB6075
      B0P(LC,2)=B0P(LC,2)/ACJ                                EQLB6080
      DO 455 J=1, NS                                         EQLB6085
      A(LC,J)=A(LC,J)/ACJ                                    EQLB6090
455 CONTINUE                                                  EQLB6095
460 DO 470 I=1, LS                                           EQLB6100
      IF (A(I,JB).EQ.0. .OR. I.EQ.LC) GO TO 470            EQLB6105
      TEM = A(I,JB)                                           EQLB6110
      DO 465 J=1, NS                                         EQLB6115
      A(I,J)=A(I,J)-A(LC,J)*TEM                             EQLB6120
      II (ABS(A(I,J)).LT.1.E-5) A(I,J)=0.                   EQLB6125
465 CONTINUE                                                  EQLB6130
      B0(I)=B0(I) - B0(LC)*TEM                               EQLB6135
      B0P(I,1)=B0P(I,1) - B0P(LC,1)*TEM                     EQLB6140
      B0P(I,2)=B0P(I,2) - B0P(LC,2)*TEM                     EQLB6145
470 CONTINUE                                                  EQLB6150
      IF(.NOT.RITE) GO TO 490                                EQLB6155
      DO 430 J=1, NS                                         EQLB6160
      WRITE (6,475) SUB(J,1), (A(I,J),I=1,LS)              EQLB6165
475 FORMAT (1H ,A4,4X,5F10.3)                               EQLB6170
480 CONTINUE                                                  EQLB6175
490 IF(ISINGV.EQ.NLM) GO TO 530                             EQLB6180
C SWITCH ORDER OF ISINGV AND NLM COMPONENTS, REDUCE MATRIX EQLB6185

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500 DO 510 J=1,NS
    AA=A(ISINGV,J)
    A(ISINGV,J)=A(NLM,J)
510 A(NLM,J)=AA
    IA=LLMT(ISINGV)
    LLMT(ISINGV)=LLMT(NLM)
    LLMT(NLM)=IA
    B0(ISINGV)=B0(NLM)
    B0(NLM)=0.
    DO 520 I = 1,2
    B0P(ISINGV,I)=B0P(NLM,I)
    B0P(NLM,I)=0.
520 CONTINUE
530 IQ1=IQ1-1
    IF(TRACE.NE.0.) WRITE (6,525)
525 FORMAT(29H0TRACE SPECIES NOT CALCULATED )
    LP1=NLM
    NLM=NLM-1
531 IF(.NOT.IONS) GO TO 33
    WRITE(6,244) (LLMT(I),I=1,NLM),IE
    GO TO 43
C*** SPECIAL EQUIL CALCULATIONS FOR CASE WHERE NS .LE. 1
532 KOUNT=0
    KKTEM=1
    EN(NPT,1)=B0(1)/A(1,1)
    IF(IRSPEC.NE.0) EN(NPT,1)=ENSPEC
    TOTN NPT)=0.
    DO 4011 I=1,NSK
    TOTN(NPT)=TOTN(NPT)+EN(NPT,I)
    IF(IUSE(I).EQ.0) ENNEMM=FNNEMM+EN(NPT,I)
4011 CONTINUE
C*** IF(ENNEMM.GT.X0CRIT)GO TO 1001
    IF(IMPRT.LE.3)GO TO 533
    DXOUTP(1)=NLM
    DXOUTP(2)=ENN
    DXOUTP(3)=EMM
    DXOUTP(4)=B0(1)
    DXOUTP(5)=A(1,1)
    NUMOUT=5
    NUMDBG=4
    CALL DBGOUT(NUMOUT,4P,SP,DXOUTP,NUMDBG)
533 KOUNT=KOUNT+1
    IF(KOUNT.GT.30)GO TO 14
    JS1=1
    TLN=ALOG(TT)
    ALL CPHS
    HSUM(NPT)=0.0
    SSUM(NPT)=0.0
    ELPEMM=PP/ENNEMM
C+ GROF4
CCCCC DXOUTP(1)=PP
CCCCC DXOUTP(2)=ENNEMM
CCCCC DXOUTP(3)=ENN
CCCCC DXOUTP(4)=EMM
CCCCC DXOUTP(5)=4.0
CCCCC NUMOUT=5

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EQLB6190
EQLB6195
EQLB6200
EQLB6205
EQLB6210
EQLB6215
EQLB6220
EQLB6225
EQLB6230
EQLB6235
EQLB6240
EQLB6245
EQLB6250
EQLB6255
EQLB6260
EQLB6265
EQLB6270
EQLB6275
EQLB6280
EQLB6285
EQLB6290
EQLB6295
EQLB6300
EQLB6305
EQLB6310
EQLB6315
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EQLB6335
EQLB6340
EQLB6345
EQLB6350
EQLB6355
EQLB6360
EQLB6365
EQLB6370
EQLB6375
EQLB6380
EQLB6385
EQLB6390
EQLB6395
EQLB6400
EQLB6405
EQLB6410
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EQLB6435
EQLB6440
EQLB6445
EQLB6450
EQLB6455
EQLB6460
EQLB6465

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CCCCC NUMDBG=304
CCCCC 17(ELPENM.LE.0.0D0)CALL DBGOUT(NUMOUT,HP,SP,DXOUTP,NUMDBG)
C+.
    ELPENM=DLOG(ELPENM)
    DO 534 J=1,NSK
    HSUM(NPT)=HSUM(NPT)+H0(J)*EN(NPT,J)
    ENLNJ=0.
    IF(EN(NPT,J).GT.0.)ENLNJ=DLOG(EN(NPT,J))
    ENJELP=ENLNJ+ELPENM
    SSSS=S(J)
    IF(IUSE(J).EQ.0)SSSS=S(J)-ENJELP
    SSUM(NPT)=SSUM(NPT)+SSSS*EN(NPT,J)
534 CONTINUE
    DELT=0.0-SSUM(NPT)
    IF(HP)DELT=HSUB0/TT-HSUM(NPT)
    DELT=DELT/CPSUM
    TEMP0=ABS(DELT)
    AMBDA=2./TEMP0
    IF(AMBDA.GT.1.)AMBDA=1
    TEMP1=ALOG(TT)+AMBDA*DELT
    TT=EXP(TEMP1)
    IF(TEMP0.LE..5E-4)GO TO 1171
    GO TO 533
C CALCULATE EQUILIBRIUM PROPERTIES
1171 IF(ENNEMM.LE.0.0D0)ENNEMM=ENN+EMM
    DLVPT(NPT) = -1.
    DLVTP(NPT) = 1.
    CPR(NPT) = CPSUM
    GAMMAS(NPT)=CPSUM/(CPSUM-ENNEMM)
C...GROK1
    IF(GAMMAS(NPT).GT.1.0D0)GO TO 186
    IF(IPRRKT.LE.0)GO TO 5001
    DXOUTP(1)=1.
    DXOUTP(2)=CPSUM
    DXOUTP(3)=ENNEMM
    DXOUTP(4)=GAMMAS(NPT)
    NUMOUT=4
    NUMDBG=6
    CALL DBGOUT(NUMOUT,HP,SP,DXOUTP,NUMDBG)
5001 CONTINUE
    IF(CHNLEN.LT.0.0)GO TO 5010
    KSUB0=KSUB0+1
    IF(KSUB0.GT.KSUB0M)GO TO 5010
    HSUB=1.001*HSUB0
    CONVG=.FALSE.
    GO TO 386
    171 DLVPT(NPT) = -1. + X(IQ1)*(ENN/(ENN+EMM))
C...GROX0
    IF(DLVPT(NPT).IT.0.0D0)GO TO 177
5011 IF(IPRRKT.LE.0)GO TO 5001
    DXOUTP(1)=0.0
    DXOUTP(2)=IQ1
    DXOUTP(3)=NPT
    DXOUTP(4)=X(IQ1)
    DXOUTP(5)=ENN
    DXOUTP(6)=EMM

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EQLB6470
 EQLB6475
 EQLB6480
 EQLB6485
 EQLB6490
 EQLB6495
 EQLB6500
 EQLB6505
 EQLB6510
 EQLB6515
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 EQLB6670
 EQLB6675
 EQLB6680
 EQLB6685
 EQLB6690
 EQLB6695
 EQLB6700
 EQLB6705
 EQLB6710
 EQLB6715
 EQLB6720
 EQLB6725
 EQLB6730
 EQLB6735
 EQLB6740
 EQLB6745


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      DXOUTP(7)=DLVPT(NPT)
      NUMOUT=7
      NUMDLG=7
      CALL DBGOUT(NUMOUT,HP,SP,DXOUTP,NUMDBG)
5882 CONTINUE
      IF(CHNLEN.LT.8.8)GO TO 5818
      KSUB8=KSUB8+1
      IF(KSUB8.GT.KSUB8M)GO TO 5818
      HSUB8=1.881*HSUB8
      CONVG=.FALSE.
      GO TO 386
177 CONTINUE
      IF(JLIQ.EQ.8) GO TO 199
      IF(TT.LE.TEOLBM)GO TO 196
      IF(TT.LE.TTBOT)GO TO 198
196 EN(NPT,JSOL) = ENSOL
      IUSE(JLIQ) = -IUSE(JLIQ)
      HSUM(NPT) = HSUM(NPT)+EN(NPT,JLIQ)*(H8(JLIQ)-H8(JSOL))
      IQ1 = IQ1+1
      GAMMAS(NPT) = -1./DLVPT(NPT)
C...GROK2
      IF(GAMMAS(NPT).GT.1.8D8)GO TO 186
      IF(IPRRKT.LE.8)GO TO 5883
      DXOUTP(1)=2.
      DXOUTP(2)=DLVPT(NPT)
      DXOUTP(3)=GAMMAS(NPT)
      NUMOJT=3
      NUMDBG=8
      CALL DBGOUT(NUMOUT,HP,SP,DXOUTP,NUMDBG)
5883 CONTINUE
      IF(CHNLEN.LT.8.8)GO TO 5818
      KSUB8=KSUB8+1
      IF(KSUB8.GT.KSUB8M)GO TO 5818
      HSUB8=1.881*HSUB8
      CONVG=.FALSE.
      GO TO 386
198 CONTINUE
      WRITE(6,197) JLIQ,TT,TTBOT
197 FORMAT(1X,18(1H*),14HWARNING..JLIQ=,I4,13HTT AND TTBOT=,
      *2(1X,G12.4))
      IF(IPRRKT.GE.2)WRITE(1,177) JLIQ,TT,TTBOT
199 GAMMAS(NPT) = -1./((DLVPT(NPT)+(DLVTP(NPT)**2)*(ENN+EMM)/CPR(NPT))
C...GROK3
      IF(GAMMAS(NPT).GT.1.8D8)GO TO 186
      IF(IPRRKT.LE.8)GO TO 5881
      DXOUTP(1)=3.
      DXOUTP(2)=DLVPT(NPT)
      DXOUTP(3)=DLVTP(NPT)
      DXOUTP(4)=ENN
      DXOUTP(5)=EMM
      DXOUTP(6)=CPR(NPT)
      DXOUTP(7)=GAMMAS(NPT)
      NUMOUT=7
      NUMDLG=9
      CALL DBGOUT(NUMOUT,HP,SP,DXOUTP,NUMDBG)
5884 CONTINUE

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EQLB6758
EQLB6755
EQLB6768
EQLB6765
EQLB6778
EQLB6775
EQLB6788
EQLB6785
EQLB6798
EQLB6795
EQLB6808
EQLB6805
EQLB6818
EQLB6815
EQLB6828
EQLB6825
EQLB6838
EQLB6835
EQLB6848
EQLB6845
EQL36858
EQLB6855
EQLB6868
EQLB6865
EQLB6878
EQLB6875
EQLB6888
EQLB6885
EQLB6898
EQLB6895
EQLB6908
EQLB6905
EQLB6918
EQLB6915
EQLB6928
EQLB6925
EQLB6938
EQLB6935
EQLB6948
EQLB6945
EQLB6958
EQLB6955
EQLB6968
EQLB6965
EQLB6978
EQLB6975
EQLB6988
EQLB6985
EQLB6998
EQLB6995
EQLB7008
EQLB7005
EQLB7018
EQLB7015
EQLB7028
EQLB7025

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      IF(CHNLEN.LT.0.0)GO TO 5010
      KSUB0=KSUB0+1
      IF(KSUB0.GT.KSUB0M)GO TO 5010
      HSUB0=1.001*HSUB0
      CONVG=.FALSE.
      GO TO 386
5010 GAMMAS(NPT)=1.0001
186 TTT(NPT) = TT
187 CONTINUE
      IF(CPR(NPT).NE.0.0D0)CPOLD=CPR(NPT)
      IF(CPR(NPT) EQ.0.0D0)CPR(NPT)=CPOLD
      IF(ENNEMM.LE.0.0D0)ENNEMM=ENN+EMM
      ENNL=ENL
      PPP(NPT)=PP
      VLM(NPT) = RR*ENNEMM*TT/(101.325*PP)
      IF(IMPRNT.LT.100)GO TO 1111
      DXOUTP(1)=TLN
      DXOUTP(2)=AMBDA
      DXOUTP(3)=DLNT
      DXOUTP(4)=TT
      DXOUTP(5)=TMELT
      DXOUTP(6)=VLM(NPT)
      DXOUTP(7)=PP
      DXOUTP(8)=NPT
      DXOUTP(9)=ENN
      DXOUTP(10)=EMM
      DXOUTP(11)=SUMN
      NUMOUT=11
      NUMDBG=5
      CALL DBGOUT(NUMOUT,HP,SP,DXOUTP,NUMDBG)
1111 CONTINUE
      HSUM(NPT) = HSUM(NPT)*TT
      WM(NPT) = 1./ENNEMM
      IF(NS.LE.1)GO TO 1001
      IF(.NOT.FLAG)GO TO 1001
188 IF(TRACE.EQ.0.)GO TO 200
      IF(NS.EQ.0)GO TO 200
      DO 1200 J=1,NS
      IF(IUSE(J).NE.0) GO TO 1200
      IF(NLM.GE.L2) GO TO 287
      DO 280 I=LP1,L3
      IF(A(I,J).NE.0.) GO TO 1200
280 CONTINUE
287 IF(ENLN(J).GT.-87.) EN(NPT,J)=E**ENLN(J)
1200 CONTINUE
200 IF(.NOT.RITE) GO TO 863
      WRITE(6,201) NPT, PP,TT,HSUM(NPT),SSUM(NPT),WM(NPT),CPR(NPT)
      IT,DLVPT(NPT),DLVTP(NPT),GAMMAS(NPT),VLM(NPT)
201 FORMAT (7H POINT=I3,3X,2HT=E13.6,3X,2HT=E13.6,3X,4HH/R=E13.6,3X,4HE
      1./R=E13.6//3X, 5HWM=E13.6,3X,5HCP/R=E13.6,3X,6HDLVPT=E13.6,3X,6HDLVE
      2TP=E13.6,3X,9TGAMMA(S)=E13.6,3X,2HV=E13.6)
863 IF(TT.GE.TLOW.AND.TT.LE.THIGH.OR.SHOCK) GO TO 1000
      WRITE(6,329) TT,NPT
329 FORMAT(17H THE TEMPERATURE=E12.4,26H IS OUT OF RANGE FOR POINT,I5)
      IF(TT.GE.TLOW/1.5.AND.TT.LE.THIGH*1.25) GO TO 1000
      NPT = NPT+1

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EQLB7030
 EQLB7035
 EQLB7040
 EQLB7045
 EQLB7050
 EQLB7055
 EQLB7060
 EQLB7065
 EQLB7070
 EQLB7075
 EQLB7080
 EQLB7085
 EQLB7090
 EQLB7095
 EQLB7100
 EQLB7105
 EQLB7110
 EQLB7115
 EQLB7120
 EQLB7125
 EQLB7130
 EQLB7135
 EQLB7140
 EQLB7145
 EQLB7150
 EQLB7155
 EQLB7160
 EQLB7165
 EQLB7170
 EQLB7175
 EQLB7180
 EQLB7185
 EQLB7190
 EQLB7195
 EQLB7200
 EQLB7205
 EQLB7210
 EQLB7215
 EQLB7220
 EQLB7225
 EQLB7230
 EQLB7235
 EQLB7240
 EQLB7245
 EQLB7250
 EQLB7255
 EQLB7260
 EQLB7265
 EQLB7270
 EQLB7275
 EQLB7280
 EQLB7285
 EQLB7290
 EQLB7295
 EQLB7300
 EQLB7305

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C
C      ERROR, SET TT=0
C
C      873 TT=0.
C      NPT = NPT-1
C      1000 LSAVE=NLM
C      IQ1=IQ1+LS-NLM
C      NLF=LS
C      1001 CONTINUE
C      1002 CONTINUE
C      RETURN
C      END
C      SUBROUTINE SAVE
C
C      SAVES OR USES COMPOSITIONS FROM PREVIOUS POINT AS INITIAL ESTIMATES
C
C      THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR
C      NON-CDC MACHINES
C
C      DOUBLE PRECISION TM,PP,SIGMA,SIG,VLMI,VLM
C      DOUBLE PRECISION ENN,SUMN
C      DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS,TTT,VLM
C      DOUBLE PRECISION S,EN,ENLN,H0,DELN,S0,DXOUTP
C
C      LOGICAL SHOCK,MMHG,UV,DETN,SIUNIT,NSOM,CALCH
C      LOGICAL HP,SP,TP,NEW,IONS,MOLES,FROZ,EQL,PSIA,RKT,VOL,TV,SV
C      LOGICAL FA,ERATIO,FPCT,OTTO,SFLG
C      LOGICAL NEQL,CONVG,LOGV,AREA
C
C      COMMON/MISC/S0,ENN,SUMN,TT,ATOM(3,101),LLMT(30),B0(30),B0P(30,2)
C      1 ,TM,TLOW,TMID,THIGH,CPSUM,PP,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
C      2 ,HPP(2),PH(2),VMIN(2),VPLS(2),WP(2),DATA(30),NAME(30,5)
C      3 ,ANUM(30,5),PECWT(30),ENTH(30),FAZ(30),RTEMP(30),FOX(30),DENS(30)
C      4 ,RHOP,RMA(30),TLN,CR,OXF(30),ENNL,ENSAVE,ENLSAV,TRACE,SIZE
C      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM
C      1 ,NS,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEW,NSUB,NSUP,ITM,CPCVFR,CPCVEQ
C      2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH
C      3 ,IOJAVE,LSAVE,ISUP,ISUB,ITNUM
C      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),
C      *GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13),
C      *VLM(13),TOTN(13)
C
C      COMMON/SPEC1/NSPCMX,NCMAX,NELMX,TEMP(175,2),SUB(600,3),S(1)
C      COMMON/SPEC2/ENLN(1)
C      COMMON/SPEC5/USE(1)
C      COMMON/SPEC6/TLN(1)
C      COMMON/KG1/EM(13,1)
C... NSPCMX REFERS TO THE MAXIMUM NO. OF SPECIES ALLOWED
C... NCMAX REFERS TO THE MAXIMUM NO. OF CONDENSED SPECIES ALLOWED
C      THIS IS FIXED AND REFERS TO THE SIZE OF TEMP(N,2) IN COMMON
C      SPEC1.....MUST CHANGE THIS COMMON EVERYWHERE IF A LARGER
C      IS NEEDED
C... NELMX REFERS TO THE MAXIMUM NO. OF ELEMENTS ALLOWED
C      THIS IS FIXED AND REFERS TO THE SIZE OF XELMC(N) AND A(N,NSAVE
C      .....MUST CHANGE COMMON TSTG AND STOIC EVERYWHERE IF

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EQLB7310
EQLB7315
EQLB7320
EQLB7325
EQLB7330
EQLB7335
EQLB7340
EQLB7345
EQLB7350
EQLB7355
EQLB7360
EQLB7365
SAVE 10
SAVE 20
SAVE 30
SAVE 40
SAVE 50
SAVE 60
SAVE 70
SAVE 80
SAVE 90
SAVE 100
SAVE 110
SAVE 120
SAVE 130
SAVE 140
SAVE 150
SAVE 160
SAVE 170
SAVE 180
SAVE 190
SAVE 200
SAVE 210
SAVE 220
SAVE 230
SAVE 240
SAVE 250
SAVE 260
SAVE 270
SAVE 280
SAVE 290
SAVE 300
SAVE 310
SAVE 320
SAVE 330
SAVE 340
SAVE 350
SAVE 360
SAVE 370
SAVE 380
SAVE 390
SAVE 400
SAVE 410
SAVE 420
SAVE 430
SAVE 440

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C	PROGRAM NEQMDH(INPUT,OUTPUT,TAPE7,TAPE5=INPUT,TAPE6=OUTPUT)	MAIN 10	PAGE 0092
C			
C	A LARGER SIZE IS NEEDED	SAVE 450	
C	COMMON/DBGVEC/DXOUTP(1)	SAVE 460	
C		SAVE 470	
C	EQUIVALENCE (AC(1),JSOLS),(AC(2),JLIQS)	SAVE 480	
C	EQUIVALENCE (OTTO,CPCVFR),(CPCVEQ,LOGV)	SAVE 490	
C		SAVE 500	
C		SAVE 510	
C	IF(ISV)100,10,200	SAVE 520	
C		SAVE 530	
C	NEXT POINT FIRST T IN SCHEDULE, USE PREVIOUS COMPOSITIONS FOR THIS T	SAVE 540	
C		SAVE 550	
C	10 IQ1 = IQSAVE	SAVE 560	
C	JSOL = JSOLS	SAVE 570	
C	JLIQ = JLIQS	SAVE 580	
C	ENN = ENSAVE	SAVE 590	
C	ENNL = ENLSAV	SAVE 600	
C	NLM = LSAVE	SAVE 610	
C	DO 50 J = 1,NS	SAVE 620	
C	IF (IUSE(J).EQ.0) GO TO 20	SAVE 630	
C	EN(NPT,J) = SLN(J)	SAVE 640	
C	IF(IUSE(J).GT.0) IUSE(J) = - IUSE(J)	SAVE 650	
C	IF (EN(NPT,J).NE.0.)IUSE(J) = -IUSE(J)	SAVE 660	
C	GO TO 50	SAVE 670	
C	20 EN(NPT,J) = 0.	SAVE 680	
C	ENLN(J) = SLN(J)	SAVE 690	
C	IF(SLN(J).EQ.0.) GO TO 50	SAVE 700	
C	IF ((ENLN(J)-ENNL + 18.5).LE.0.) GO TO 50	SAVE 710	
C	EN(NPT,J) = 2.718281828459**ENLN(J)	SAVE 720	
C	50 CONTINUE	SAVE 730	
C	GO TO 1000	SAVE 740	
C		SAVE 750	
C	FIRST T--SAVE COMPOSITIONS FOR FUTURE POINTS WITH THIS T	SAVE 760	
C		SAVE 770	
C	100 ISV = -ISV	SAVE 780	
C	JSOLS = JSOL	SAVE 790	
C	JLIQS = JLIQ	SAVE 800	
C	IQSAVE = IQ1	SAVE 810	
C	ENSAVE = ENN	SAVE 820	
C	ENLSAV = ENNL	SAVE 830	
C	LSAVE = NLM	SAVE 840	
C	DO 150 J = 1,NS	SAVE 850	
C	SLN(J) = ENLN(J)	SAVE 860	
C	IF(IUSE(J).NE.0) SLN(J)=EN(ISV,J)	SAVE 870	
C	150 CONTINUE	SAVE 880	
C		SAVE 890	
C	USE COMPOSITIONS FROM PREVIOUS POINT	SAVE 900	
C		SAVE 910	
C	200 CONTINUE	SAVE 920	
C	DO 300 J = 1,NS	SAVE 930	
C	EN(NPT,J) = EN(ISV,J)	SAVE 940	
C	300 CONTINUE	SAVE 950	
C	1000 RETURN	SAVE 960	
C	END	SAVE 970	
C	SUBROUTINE DIFFUN(X,N,EEN)	DIFF 10	
C		DIFF 20	
C		DIFF 30	

C	THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED	DIFF 40
C	FOR NON-CDC MACHINES	DIFF 50
C		DIFF 60
	DOUBLE PRECISION TTT, TM, PP, SIGMA, SIG, VLMI, VLM, ATERM, AMULT	DIFF 70
	DOUBLE PRECISION ENN, EMM, SUMN, AWT	DIFF 80
	DOUBLE PRECISION HSUM, SSUM, CPR, DLVTP, DLVPT, GAMMAS, AVN, SUM, GSUM	DIFF 90
	DOUBLE PRECISION X0CRIT, CRCRIT, FFF, OQQ	DIFF 100
	DOUBLE PRECISION RHOVE, UEDP	DIFF 110
	DOUBLE PRECISION EN, S, ENLN, H0, X, N, EEN, ENM, F, S0	DIFF 120
	DOUBLE PRECISION ENP, ENR, AKB, AKF, TSAV1, TSAV2	DIFF 130
	DOUBLE PRECISION DXOUTP, ENR1, ENR2, TSAV5, BNEW, SAVED, SAVEH	DIFF 140
	DOUBLE PRECISION A11, A22, SVEL, WWW, TSAV3, B11, B22, SAVELL	DIFF 150
	DOUBLE PRECISION DPITP, DPIPT, DLNTP, DLNPT, DELN, DFSUDM	DIFF 160
C		DIFF 170
	LOGICAL SHOCK, MMHG, UV, DETN, SIUNIT, NSQM, CALCH	DIFF 180
	LOGICAL HP, SP, TP, NEWR, IONS, MOLES, FROZ, EQL, PSIA, RKT, VOL, TV, SV	DIFF 190
	LOGICAL FA, ERATIO, FPCT, OTTO	DIFF 200
	LOGICAL NEQL, CONVG, LOGV, FELG, AREA, PRINTX, HPATH, SPATH	DIFF 210
	REAL INTERP	DIFF 220
C		DIFF 230
	COMMON/SPNOPT/KBEGN(35), XKIIJJ, DFSUDM(4)	DIFF 240
	COMMON/TOSTAR/XHSTRT	DIFF 250
	COMMON/MHDD/SSUMW, DX, DXI, XJY(26), AI(26), UE, NITER, NSTOP, SIG(26), IPPDIFF	DIFF 260
	* ,EZ, XK, PIPP	DIFF 270
	COMMON/INDX/IDEBUG, CONVG, TP, HP, SP, ISV, NPP, MOLES, NP, NT, NPT, NLM	DIFF 280
	* ,NS, KMAT, IMAT, IQ1, NOF, MOMIT, IP, NEWR, NSUB, NSUP, ITM, CPCVFR, CPCVEQ	DIFF 290
	* ,IONS, NC, NSERT, JSOL, JLI2, KASE, NREAC, IC, JS1, VOL, SHOCK, IT, NFZ, CALCHDIFF	DIFF 300
	* ,IQCAVE, LSAVE, ISUP, ISUB, ITNUM	DIFF 310
	COMMON/POINTS/HSUM(13), SSUM(13), CPR(13), DLVTP(13), DLVPT(13)	DIFF 320
	* ,GAMMAS(13), P(26), T(26), V(13), PPP(13), WM(13), SONVEL(13), TTT(13)	DIFF 330
	* ,VLM(13), TOTEN(13)	DIFF 340
	COMMON/PERF/PCP(22), VMOC(13), SPIM(13), VACI(13), SUBAR(13), SUPAR(13)	DIFF 350
	1 ,APP(13), AFAT(13), CSTR, EQL, FROZ, S00, AREA, AWT	DIFF 360
	DIMENSION N(8, 32), EEN(32)	DIFF 370
	COMMON/XPRINT/ PRINTX	DIFF 380
	COMMON/CSIG/SIGMA(13)	DIFF 390
	COMMON/DIFEQ/ AKF1(30), AKF2(30),	DIFF 400
	* AKF3(30), NJR(30, 4), NJP(30, 4), MAR(30, 4), MAP(30, 4),	DIFF 410
	* AP(30, 4), AR(30, 4), NJ1, NMIT, VLMI	DIFF 420
	COMMON/NEQ/B0N(30), EMM, SNEQ, NQ1, NSK, NEOPT	DIFF 430
	COMMON/MISC/S0, ENN, SUMN, TT, ATOM(3, 101), LLMT(30), B0(30), B0P(30, 2)	DIFF 440
	1 ,TM, TLOW, TMID, THIGH, CPSUM, PP, OF, EQRAT, FPCT, R, RR, HSUB0, AC(2), AM(2)	DIFF 450
	2 ,HPP(2), KH(2), VMIN(2), VELS(2), WP(2), DATA(30), NAME(30, 5)	DIFF 460
	3 ,ANUM(30, 5), PECWT(30), ENTH(30), FAZ(30), RTEMP(30), FOX(30), DENS(30)	DIFF 470
	4 ,RHAP, RMT(30), TLN, CR, OXF(30), ENNL, ENSAVE, ENLSAV, TRACE, SIZE	DIFF 480
	COMMON/MIKE0/ITE1, ITE2, ITE3, IMPRNT, NMPATH, NUMIV, XINDP(1)	DIFF 490
	COMMON/MIKE1/ATERM, AMULT, VELIN(1)	DIFF 500
	COMMON/MIKE2/HPATH, SPATH, PRESIN(1)	DIFF 510
	COMMON/MIKE3/ARFAIN(1)	DIFF 520
	COMMON/MIKE5/NNNNN, X0CRIT, DUMMIN(1)	DIFF 530
	COMMON/MIKE7/CALC, CHNLN, LPRRKT, TMPSTP, TDIFUN, TEOLBM	DIFF 540
	COMMON/MIKE8/EN, BZOUT(3), BETOUT(13)	DIFF 550
	COMMON/SIGOUT/INEL(3), ANE(15), FIONS(3), AIONS(15), FSIGWO(4),	DIFF 560
	FSIG(4), SFEM(15), FFREQ(3), TOTAL(15)	DIFF 570
	COMMON/SPECE1/NPCMA, NCMA, NELMX, TEMP(175, 2), SUB(600, 3), S(1)	DIFF 580
	COMMON/SPECE2/ENLN(1)	DIFF 590

CZZZ CALL DBGOUT(NUMOUT,HP,SP,DXOUTP,NUMDBG)
CZZZZZ

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      ENM=0.
      DO 961 I=NS1,NSK
      ENLN(I)=0.
      IF(EN(NPT,I).GT.0.) ENLN(I)=DLOG(EN(NPT,I))
962  IF(IUSE(I).NE.0) GO TO 961
C***  IF(EN(NPT,I).LE.0.0D0)GO TO 961
      ENM=ENM+EN(NPT,I)
961  CONTINUE
901  CONTINUE
      CALL EQLBRM(.FALSE.)
      IF(TT.GT.TDIFUN)GO TO 904
      IF(TT.NE.0.0)GO TO 905
      IF(NS.NE.1)GO TO 905
      KBEGN(35)=KBEGN(35)+1
      IF(KBEGN(35).GT.2)STOP 20
      KBEGN(35)=-KBEGN(35)
      IF(KBEGN(35).EQ.-2)RETURN
      IPP=IPP-1
      IF(TT.NE.0.0)NPT=NPT-1
      CALL RKTOUT
      IPP=IPP+1
      IF(TT.NE.0.0)NPT=NPT+1
      RETURN
905  ISV=0
      IPP=IPP-1
      IF(TT.NE.0.0)NPT=NPT-1
      CALL RKTOUT
      IF(ISTPFL.EQ.1)STOP 6
      STOP 20
904  CONTINUE
      CALL CONDOC(.FALSE.)
      VLMI=VLM(NPT)*1.E-3
      AVN=6.02252D26/VLMI
      IF(PRINTX.AND.IMPRNT.GE.2) WRITE(1,9997) X,AVN
9997  FORMAT(/14H DIFFUN - X=,1PE13.4,13H AVN/VLMI=,1PE13.4)
      XJY(NPT)=SIGMA(NPT)*UE*(XK-1.D0)*BZ
      SUM=0.
      SAVEI=0.0D0
      SAVEH=0.0D0
      SAVELL=0.0D0
      I=NPT
      IF(NOMIT.EQ.0) GO TO 902
      JSI=1
      TLN=ALOG(TT)
      CALL CPHS
      ENM=0.
      DO 910 J=1,NSK
      IF(IUSE(J).LT.0)GO TO 910
      IF(J.LE.NS)GO TO 903
      IF(EN(I,J).GT.0.0D0)GO TO 903
      IF(X.GT.XHSTRT)GO TO 903
      EN(I,J)=CRCRIT
903  CONTINUE
      IF(IUSE(J).EQ.0) ENM=ENM+EN(I,J)

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DIFF1600
DIFF1610
DIFF1620
DIFF1630
DIFF1640
DIFF1650
DIFF1660
DIFF1670
DIFF1680
DIFF1690
DIFF1700
DIFF1710
DIFF1720
DIFF1730
DIFF1740
DIFF1750
DIFF1760
DIFF1770
DIFF1780
DIFF1790
DIFF1800
DIFF1810
DIFF1820
DIFF1830
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DIFF1880
DIFF1890
DIFF1900
DIFF1910
DIFF1920
DIFF1930
DIFF1940
DIFF1950
DIFF1960
DIFF1970
DIFF1980
DIFF1990
DIFF2000
DIFF2010
DIFF2020
DIFF2030
DIFF2040
DIFF2050
DIFF2060
DIFF2070
CDIF2071
DIFF2080
DIFF2090
DIFF2100
DIFF2110
DIFF2120

910	CONTINUE	DIFF2130
	IF(ENM.LE.0.000)ENM=CRCRIT	DIFF2140
	EN(I,NSK1)=ENM	DIFF2150
902	IF(NJ1 .LE. 0) GO TO 204	DIFF2160
	IF(NMPATH.NE.3)GO TO 4001	DIFF2170
C...	INITIALIZE DELN ARRAY TO 0.0(TO BE USED FOR FINITE RATE DERIV.)	DIFF2180
	DO 4000 KK=1,NSK1	DIFF2190
	DELN(KK)=0.0	DIFF2200
4000	CONTINUE	DIFF2210
4001	CONTINUE	DIFF2220
	IF(IMPRNT.GE.3)WRITE(1,2054) 1,ENM,TTT(I),UE	DIFF2230
2054	FORMAT(1X,2HI=,I2,1X,4HEM=,G13.5,5H TTT=,G13.5,4H UE=,G13.5)	DIFF2240
	KOUNT=29	DIFF2250
	DO 101 K=1,NJ1	DIFF2260
	ENR=1.	DIFF2270
	ENP=1.	DIFF2280
	RPOW=0.	DIFF2290
	POW=0.	DIFF2300
	GSUM=0.	DIFF2310
	DO 302 M=1,4	DIFF2320
	NX=NCP(K,M)	DIFF2330
	IF(NX .EQ. 0) GO TO 1	DIFF2340
	NX1=NX	DIFF2350
	IF(NX .EQ. NSK1) NX1=0	DIFF2360
	AX=AP(K,M)	DIFF2370
	IF(NX1.EQ.0)GO TO 812	DIFF2380
	GSUM=GSUM+AX*(H0(NX)-S(NX))	DIFF2390
	IF(IMPRNT.LT.100)GO TO 812	DIFF2400
	DXOUTP(1)=K	DIFF2410
	DXOUTP(2)=AX	DIFF2420
	DXOUTP(3)=NX	DIFF2430
	DXOUTP(4)=H0(NX)	DIFF2440
	DXOUTP(5)=S(NX)	DIFF2450
	DXOUTP(6)=GSUM	DIFF2460
	DXOUTP(7)=TT	DIFF2470
	NUMOUT=7	DIFF2480
	NUMDBG=18	DIFF2490
	CALL DBGOUT(NUMOUT,HP,SP,DXOUTP,NUMDBG)	DIFF2500
812	CONTINUE	DIFF2510
	POW=POW+AX	DIFF2520
	IF(NX1.GT.NS)GO TO 814	DIFF2530
C***	IF(EN(I,NX).LE.CRCRIT)GO TO 1	DIFF2540
	ENP=ENP*EN(I,NX)**AX	DIFF2550
	GO TO 1	DIFF2560
814	CONTINUE	DIFF2570
	NXNS=NX-NS	DIFF2580
C***	IF(NX1.LE.NS)GO TO 1	DIFF2590
	IF(KBEGN(WYNS).EQ.-1)GO TO 101	DIFF2600
	TSBV3=N(1,NXNS)	DIFF2610
	IF(TSAV3.GT.0.000)GO TO 7005	DIFF2620
	IF(X.GT.XLSTRT)GO TO 7001	DIFF2630
	TSBV3=CRCRIT	DIFF2640
	GO TO 7005	DIFF2650
7001	CONTINUE	DIFF2660
	ENP=0.0	DIFF2670
	GO TO 1	DIFF2680

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7005 CONTINUE
ENP=ENP*TSV3**AX
1 NX=NJR(K,M)
IF(NX.EQ.0) GO TO 302
NX1=NX
IF(NX1.EQ.NSK1) NX1=0
AX=AR(K,M)
IF(NX1.EQ.0) GO TO 813
GSUM=GSUM1-AX*(H0(NX)-S(NX))
IF(IMFRNT.LT.100) GO TO 813
DXOUTP(1)=-K
DXOUTP(2)=AX
DXOUTP(3)=NX
DXOUTP(4)=H0(NX)
DXOUTP(5)=S(NX)
DXOUTP(6)=GSUM
DXOUTP(7)=TT
NUMDBG=19
CALL DBGOUT(NUMOUT,HP,SP,DXOUTP,NUMDBG)
813 CONTINUE
POW=POW-AX
RPOW=RPOW+AX
IF(NX1.GT.NS) GO TO 815
C*** IF(EN(I,NX).LE.CRCRIT) GO TO 302
ENR=ENR*EN(I,NX)**AX
GO TO 302
815 CONTINUE
NXNS=NX-NS
C*** IF(NX1.LE.NS) GO TO 302
IF(KBEGN(NXNS).EQ.-1) GO TO 101
TSV3=N(1,NXNS)
IF(TSV3.GT.0.0D0) GO TO 7008
IF(X.GT.XHSTRT) GO TO 7006
TSV3=CRCRIT
GO TO 7008
7006 CONTINUE
ENR=0.0
GO TO 302
7008 CONTINUE
ENR=ENR*TSV3**AX
302 CONTINUE
C
AKB=(PP/ENM)**POW/DEXP(-GSUM)
AKF=AKF1(K)*TTT(I)**AKF2(K)*DEXP(-DBLE(AKF3(K))/TTT(I))
C
C
TSV1=ENP*AKB
TSV2=ENR
ENR=J.0
IF(TSV1.EQ.TSV2) GO TO 810
TSV3=DAES(TSV1)
TSV5=DAES(TSV2)
IF(TSV3.LT.TSV5) TSV3=TSV5
TSV5=DAES(TSV1-TSV2)/TSV3
IF(TSV5.LE.1.0D-6) GO TO 810
ENR=(TSV2-TSV1)*AKF*((1.0D-6*AVN)**(RPOW-1.))

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DIFF3240

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810 CONTINUE
  IF(IMPRNT.LE.1)GO TO 816
  IF(PRINTX) WRITE(1,9998) K,AKF,AKB,ENP,TSAV2,POW,RPOW,ENR
9998 FORMAT(1X,8HREACTION,13,2X,4HAKF=,G13.5,2X,4HAKB=,G13.5,
  *2X,4HENP=,G13.5,2X,4HENR=,G13.5,2X,4HPOW=,F9.5,2X,5HRPOW=,F9.5/,
  *7X,5HREACTION RATE=(ENR-ENP*AKB)*AKF*((1.D-6*AVN)**(RPOW-1.))=,
  *G13.5)
816 CONTINUE
  IF(IMPRNT.LT.9)GO TO 811
  DXOUTP(1)=K
  DXOUTP(2)=GSUM
  DXOUTP(3)=ENP
  DXOUTP(4)=TSAV2
  DXOUTP(5)=TSAV1
  DXOUTP(6)=TSAV3
  DXOUTP(7)=TSAV5
  C*** DXOUTP(8)=ENM
  C*** DXOUTP(9)=PP
  C*** DXOUTP(10)=POW
  C*** DXOUTP(11)=(PP/ENM)**POW
  C*** DXOUTP(12)=DEXP(-GSUM)
  C*** NUMOUT=12
  NUMOUT=7
  NUMDBG=20
  CALL DBGOUT(NUMOUT,HP,SP,DXOUTP,NUMDBG)
811 CONTINUE
C
  KOUNT=KOUNT+1
  DXOUTP(KOUNT)=ENR
C
  DO 103 M=1,4
  NX=MAP(K,M)
  IF(NX.EQ.0)GO TO 426
  IF(NX.EQ.NSK1)GO TO 426
  NXNS=NX-NS
  EEN(NXNS)=EEN(NXNS)+ENR*AP(K,M)/UE
426 NX=MAR(K,M)
  IF(NX.EQ.0)GO TO 103
  IF(NX.EQ.NSK1)GO TO 103
  NXNS=NX-NS
  EEN(NXNS)=EEN(NXNS)-ENR*AR(K,M)/UE
103 CONTINUE
  IF(HP.AND.NMPA*H.NE.3)GO TO 101
  SAVED=0.0D0
  SAVED3=0.0
  DO 3002 M=1,4
  NX=NJR(K,M)
  IF(NX.EQ.0)GO TO 3003
  IF(IUSE(NX).LT.0)GO TO 3003
  SAVE=-AR(K,M)*ENR
  DELN(NX)=DELN(NX)+SAVE
  F=H0(NX)-S(NX)
  IF(IUSE(NX).EQ.0)F=F+ENLN(NX)+DLOG(DBLE(PPP(I))/ENM)
  SUM=SUM+F*SAVE*AMULT/UE
  NX=MAR(K,M)
  IF(NX.EQ.0)GO TO 3003

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DIFF3800

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      IF(IUSE(NX).GT.0)GO TO 4014
C... SUM GAS CONTRIBUTIONS IN NON-EQL. POOL
      SAAVEE3=SAVEE3-AR(K,M)
      SAAVEL=SAVEL+SAVE
C... SUM CONDENSED CONTRIBUTION*H0 IN NON-EQL. POOL
4014 SAAVEH=SAVEH+SAVE*H0(NX)
3003 NX=NJP(K,M)
      IF(NX.EQ.0)GO TO 3002
      IF(IUSE(NX).LT.0)GO TO 3002
      SAAVE=AP(K,M)*ENR
      DELN(NX)=DELN(NX)+SAAVE
      F=H0(NX)-S(NX)
      IF(IUSE(NX).EQ.0)F=F+ENL1(NX)+DLOG(DBLE(PPP(I))/ENM)
      SUM=SUM+F*SAAVE*AMULT/UE
      NX=MAP(K,M)
      IF(NX.EQ.0)GO TO 3002
      IF(IUSE(NX).GT.0)GO TO 4024
C... SUM GAS CONTRIBUTIONS IN NON-EQL. POOL
      SAAVEE3=SAVEE3+AP(K,M)
      SAAVEL=SAVEL+SAVE
C... SUM CONDENSED CONTRIBUTION*H0 IN NON-EQL. POOL
4024 SAAVEH=SAVEH+SAVE*H0(NX)
3002 CONTINUE
      IF(ABS(SAAVEE3).LT.1.0E-8)SAVEL=0.0
      SAAVEL=SAVEL+SAVEL
101 CONTINUE
      SAAVEL=SAVELL
      IF(IMPRNT.LT.100)GO TO 204
      DXOUTP(1)=N(1,1)
      DXOUTP(2)=SAVEL
      DXOUTP(3)=SAAVEH
      DXOUTP(4)=ENM
      DXOUTP(5)=AKF
      DXOUTP(6)=AKB
      DXOUTP(7)=ENP
      DXOUTP(8)=SUM
      DXOUTP(9)=UE
      DXOUTP(10)=ENR
      DXOUTP(11)=ENM
      DXOUTP(12)=POW
      DXOUTP(13)=RPOW
      DXOUTP(14)=GSUM
      DXOUTP(15)=AVN
      DXOUTP(16)=XJY(I)
      DXOUTP(17)=TTT(I)
      DXOUTP(18)=EEN(1)
      DXOUTP(19)=EEN(2)
      DXOUTP(20)=EEN(3)
      DXOUTP(21)=EEN(4)
      DXOUTP(22)=EEN(5)
      DXOUTP(23)=EEN(6)
      DXOUTP(24)=EEN(7)
      DXOUTP(25)=EEN(8)
      DXOUTP(26)=EEN(9)
      DXOUTP(27)=EEN(10)
      DXOUTP(28)=EEN(11)

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DXOUTP(29)=EEN(12)
DXOUTP(38)=NOMIT
DXOUTP(39)=NS
DXOUTP(40)=NSK1
DXOUTP(41)=EN(I,NSK1)
DXOUTP(42)=VLMI
DXOUTP(43)=I
DXOUTP(44)=ENN
DXOUTP(45)=RR
DXOUTP(46)=R
DXOUTP(47)=TLN
DXOUTP(48)=CPSUM
DXOUTP(49)=S0
DXOUTP(50)=HSU30
DXOUTP(51)=PP
NUMDBG=21
DO 401 J=NS1,NSK
  KKKK=J-NS+NUMOUT
  DXOUTP(KKKK)=EN(I,J)
401 DXOUTP(KKKK+NSK)=B0N(J-NS)
  NUMOUT=2*(NSK-NS1+1)+NUMOUT
  CALL DBGOUT(NUMOUT,HP,SP,DXOUTP,NUMDBG)
  IMPRNT=IMPRNT-100
  NUMOUT=25
  NUMDBG=22
  DO 403 L=1,NJ1
    DXOUTP(1)=L
    DO 402 J=1,4
      K=(J-1)*6+2
      DXOUTP(K)=AR(L,J)
      DXOUTP(K+1)=AP(L,J)
      DXOUTP(K+2)=NJR(L,J)
      DXOUTP(K+3)=NJP(L,J)
      DXOUTP(K+4)=MAR(L,J)
      DXOUTP(K+5)=MAP(L,J)
    402 CONTINUE
    CALL DBGOUT(NUMOUT,HP,SP,DXOUTP,NUMDBG)
  403 CONTINUE
204 SIG(I)=SIGMA(I)
C*****DETERMINE FFF AND QQQ TERMS FOR SOLVING
C      THE FOLLOWING DIFFERENTIAL EQUATIONS
C      (1) DP/DX=-RHO*UE*DUE/DX+FFF
C          WHERE UE=VELOCITY
C          AND D MEANS DERIVATIVE OF
C      (2) DH/DX=-UE*DUE/DX+QQQ/(RHO*UE)
C          WHERE QQQ CONTAINS A HEAT LOSS TERM(IF APPLICABLE)
C          AND DH/DX=D(H0+0.5*UE*UE)/DX
C          OR DH/DX=QQQ/(RHO*UE)
C          WHERE H=TOTAL ENTHALPY
C OR (2) DS/DX=(QQQ-FFF*UE)/(RHO*UE*TEMPERATURE)-(FINITE RATE TERM)
C.....FOR ANY PROBLEM THE USER MUST GENERATE A GENERAL FORCE(FFF)
C      AND HEAT(QQQ) BY CALLING SUBROUTINE SETEQ
C.....SUBROUTINE(NPT,FFF,QQQ,TSAV3,XREG0)
C          WHERE NPT=CURRENT CHANNEL POINT
C          FFF=FORCE TERM(DOUBLE PRECISION)
C          QQQ=HEAT TERM(DOUBLE PRECISION)

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C          TSAV3=(QQQ-VELOCITY*FFF) AND IS DOUBLE PRECISION      DIFF4930
C          XREG0 IS THE CURRENT X POSITION IN THE CHANNEL           DIFF4940
C                                                                    DIFF4950
C*****FOLLOWING RETRIEVAL OF HEAT VALUE TO BE DELETED          DIFF4960
C....RETRIEVE THE HEAT VALUE                                     DIFF4970
C          IF(NMPATH.EQ.1)UE=INTERP(XREG0,XINDP,VELIN,NORD,NUMIV,DINT,IER) DIFF4980
CCCCC UEDP=UE                                                    DIFF4990
CCCCC CHHEAT=N(1,ITE2)                                           DIFF5000
CCCCC IF(ITYPE.NE.1)GO TO 280                                     DIFF5010
          CHHEAT=N(1,ITE2)-0.5*UE*UE                             DIFF5020
          280 CONTINUE                                           DIFF5030
C                                                                    DIFF5040
C... SET VALUE OF RHO*UE IN RHOUE                                DIFF5050
          RHOUE=UE/VLMI                                           DIFF5060
          CALL SETEQ(NPT,FFF,QQQ,TSAV3,XREG0)                     DIFF5070
C                                                                    DIFF5080
          IF(IPRNT0.GT.0)WRITE(1,2050) NMPATH                     DIFF5090
          GO TO (291,292,293),NMPATH                             DIFF5100
C... VELOCITY GIVEN,CALC. DP/DX AND DS/DX OR DH/DX              DIFF5110
          291 CONTINUE                                           DIFF5120
          IF(IPRNT0.GT.0)WRITE(1,2051) (XINDP(KK),VELIN(KK),KK=1,NUMIV) DIFF5130
C... GET VELOCITY DERIVATIVE AND CALC. DP/DX                    DIFF5140
          EEN(ITE1)=FFF-RHOUE*DINT                                DIFF5150
          N(1,ITE3)=UE                                           DIFF5160
          GO TO 294                                               DIFF5170
C... PRESSURE GIVEN,CALC. DUE/DX AND DS/DX OR DH/DX             DIFF5180
          292 CONTINUE                                           DIFF5190
          IF(IPRNT0.GT.0)WRITE(1,2051) (XINDP(KK),PRESIN(KK),KK=1,NUMIV) DIFF5200
C... GET PRESSURE DERIVATIVE AND CALC. DUE/DX                   DIFF5210
          PPINT=INTERP(XREG0,XINDP,PRESIN,NORD,NUMIV,DINT,IER)   DIFF5220
          PP=PPINT*101325.                                         DIFF5230
          DINT=DINT*101325.                                         DIFF5240
          EEN(ITE1)=(FFF-DINT)/RHOUE                               DIFF5250
          N(1,ITE3)=PP                                             DIFF5260
          GO TO 294                                               DIFF5270
C... AREA GIVEN,CALCULATE DP/DX,DUE/DX,DS/DX OR DH/DX          DIFF5280
          293 CONTINUE                                           DIFF5290
          2060 FORMAT(1X,3(1H*),4(1X,F10.2),14)                   DIFF5300
          IF(IPRNT0.GT.0)WRITE(1,2051) (XINDP(KK),AREAIN(KK),KK=1,NUMIV) DIFF5310
C...SET TSAV5=1.0/AMULT=1.0/GAS CONSTANT=1.0/8314.3           DIFF5320
          TSAV5=1.0/AMULT                                         DIFF5330
          IF(IPRRKT.LT.4)GO TO 297                                 DIFF5340
          DXOUTP(1)=GAMMAS(I)                                     DIFF5350
          DXOUTP(2)=TTT(I)                                         DIFF5360
          DXOUTP(3)=WM(I)                                          DIFF5370
          NUMOUT=3                                                 DIFF5380
          NUMDBG=306                                               DIFF5390
          CALL DBGOUT(NUMOUT,HP,SP,DXOUTP,NUMDBG)                 DIFF5400
C          REPLACE BY ADD2DIFFUN                                  DIFF5410
          297 CONTINUE                                           DIFF5420
          IF(GAMMAS(I).EQ.0.0D0.OR.CPR(I).EQ.0.0D0)GO TO 905     DIFF5430
          WRITE(1,2060) 3VEL,UE,VLMI,CPR(I),I                   DIFF5440
C...SET TSAV4=(TOTAL MOL. WT.)/(8314.3*GAMMA*TEMPERATURE)     DIFF5450
          TSAV4=(TSAV5*WM(I))/(GAMMAS(I)*TTT(I))                DIFF5460
C...DERTMA IS THE VALUE OF THE DP/DX,DUE/DX DETERMINANT        DIFF5470
          DERTMA=UE*UE*TSAV4-1.0                                  DIFF5480

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      IF (ABS(DERTMA).GE.0.0001) GO TO 4041
      TSAV4=SQRT(1.0/TSAV4)
      WRITE(6,2053) XREG0,DERTMA,UE,TSAV4
2053  FORMAT(/,1X,10(1H*),14HPROGRAM STOP 6,10(1H*)/,10X,2HX=,7X,
      *G13.5/,10X,9HM*M-1.0= ,G13.5/,10X,9HVELOCITY=G13.5/,10X,
      *9HSON VEL= ,G13.5/)
      ISTOP=1
      GO TO 905
4041  CONTINUE
      DERTMA=UE*TSAV4-1.0/UE
      ARINT=INTERP(XREG0,XINDP,AREAIN,NORD,NUMIV,DINT,IER)
      ACPR=CPR(I)*AMULT
      TSAV5=DLVTP(I)/(TTT(I)*ACPR)
C.....SOLVE FOR B11 TERM DEFINED AS FOLLOWS
C      B11=-7/10UE*(DA/DX)/A+(QQQ-F*UE)*TSAV5-FFF/UE-BNEW
C      WHERE A STANDS FOR APEL AND DA/DX IS THE DERIVATIVE
C      TSAV5=(D(LOG(VOLUME),/DT)/(TEMPERATURE*CP*8314.3)
C      BNEW=CONTRIBUTION DUE TO FINITE RATE CHEMISTRY=UE*PHI
C      AS PHI=(R/UE)-(CON1*SAVEL+CON2*SAVEH+EQL. CONTRIB)
C      WITH SAVEH AND SAVED THE NON-EQL TERMS
C      SAVEH=SUM(WI*HJ/RHO)
C      SAVED=SUM(WI/RHO)
C.....DETERMINE CONTRIBUTION DUE TO SAVED AND SAVEDH AND SET
C      CONSTANTS TSAV1,TSAV2,AND SAVEDL
C      TSAV1=-TTT(I)/(PP*VLMI*VLMI)
C      TSAV2=1.0/(VLMI*ACPR)
C      SAVEDL=ENN/(ENN+EMM)
C      IF(NOMSAV.LE.0)GO TO 4050
      TSAV1=-TTT(I)/(N(1,I*E1)*VLMI*VLMI)
      TSAV2=DLVTP(I)/(VLMI*ACPR)
      SAVEDL=ENN/(ENN+EMM)
      A11=TSAV1*(1.0-SAVEDL*DLNPT)+TSAV2*SAVELL*DLNTP
      SAVEDL=A11*SAVEL
      SAVEDH=TSAV2*SAVEH
      SAVEDL=SAVEL+SAVEH
      IF(IMPRT.LE.3)GO TO 4044
      TSAV1=SAVELL*VLMI*AMULT
      WRITE(1,2055) TSAV4,SAVEL,SAVEH,TTT(I)
2055  FORMAT(1X,7H TSAV4=G11.3,7H SAVEDL=G11.3,7H SAVEDH=G11.3,
      *5H TTT=G11.3)
4044  CONTINUE
C... DETERMINE CONTRIBUTION DUE TO EQUIL. POOL
      A11=0.0
      B11=0.0
      IF(IMPRT.EQ.0)GO TO 4055
      IIPAL=0
      DO 4050 KK=1,N3
      IF(IUSE(KK).LT.0)GO TO 4049
      IF(DELN(KK).EQ.0.0D0)GO TO 4050
      SAVEDL=0.0
      SAVEDH=0.0
      DO 4045 JJ=1,NLM
      SAVEDL=SAVEL+A(JJ,KK)*DPIPT(JJ)
      SAVEDH=SAVEH+A(JJ,KK)*DPITP(JJ)
4045  CONTINUE

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      A11=A11+DELN(KK)*SAVEL
      B11=B11+DELN(KK)*SAVEH
4049 IIPAJ=1
4050 CONTINUE
C... GET TOTAL FINITE RATE CONTRIBUTION
      A11=TSAV1*A11
      B11=TSAV2*B11
4055 BNEW=AMULT*(SAVELL+A11+B11)
      IF(IMPRNT.GE.3)WRITE(1,2056)BNEW,A11,B11,SAVELL
2056 FORMAT(1X,5HBNEW=,G13.5,5H A11=,G13.5,5H B11=,G13.5,
      *8H SAVELL=,G13.5)
4058 CONTINUE
C... DETERMINE B11
      B11=-RHOUE*DINT/ARINT+TSAV3*TSAV5-FFF/UE-BNEW
C... SET UP DP/DX AND DUE/DX
      EEN(ITE1)=B11/DEPTMA
      EEN(ITE1+1)=(FFF-EEN(ITE1))/RHOUE
      AEAT(I)=ARINT
C... CALCULATE DS/DX OR DH/DX
294 CONTINUE
      IF(IMPRNT.LE.0)GO TO 295
      IF(NMPATH.NE.2)PPINT=PP
      NUMDBG=17
      WRITE(1,2052) NMPATH,XREG0,PPINT,UE,ARINT,DINT,NUMDBG
2050 FORMAT(1X,20HINPUTS ARE FOR PATH ,I3)
2051 FORMAT(1X,3(F10.3,2X,F10.3))
2052 FORMAT(1X,I3,1X,F10.7,1X,F10.3,1X,F13.5,1X,F10.4,1X,F10.2,
      *2X,11HDBG OUT NO.,I2)
295 CONTINUE
      IPRNT0=0
      IF(SP)EEN(ITE2)=TSAV3/(RHOUE*TTT(I))-SUM
      IF(HP)EEN(ITE2)=QQQ/RHOUE
      IF(IMPRNT.LT.0)GO TO 890
      IF(PRINTX)WRITE(1,9999) (II,N(1,II),EEN(II),II=1,ITE3)
9999 FORMAT(2(3X,I3,2G13.4))
890 PRINTX=.FALSE.
      RETURN
      END
      SUBROUTINE SETEQV(NPT,FFF,QQQ,TSAV3,XREG0)
C..... THIS SUBROUTINE DEFINES THE GENERAL FORCE TERM AND QQQ TERM
C TO SOLVE CHANNEL EQUATIONS
      DOUBLE PRECISION FFF,QQQ,TSAV2,TSAV3,TSAV4,SIG,TSAV1,FFFS,QQQS
      DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS,TTT,VLM
      DOUBLE PRECISION RHOUE,UEDP,TSAV5,TSAV6
      DOUBLE PRECISION CON1,CON2,CON3,CON4,CON5,CON6
      LOGICAL HPATH,SPATH
      COMMON/SETUPS/ITYPE,CHLOSS,CHHEAT,RHOUE,UEDP
      COMMON/MIKE0/ITE1,ITE2,ITE3,IMPRNT,NMPATH,NUMIV,XINDP(1)
      COMMON/MIKE3/AREAIN(1)
      COMMON/MHDD/SSUMW,DX,DXI,XJY(26),AI(26),UE,NITER,NSTOP,SIG(26),IPPS
      * ,BZ,XK,PIPP
      COMMON/MIKE2/HPATH,SPATH,PRESIN(1)
      COMMON/MIKE7/CHCALC,CHNLIN,IPRKT,TMPSTP,TDIFUN,TEQLBM
      COMMON/MIKE8/EXIN,BZOUT(13),BETOUT(13)
      COMMON/SIGOUT/FNEL(3),ANE(15),FIONS(3),AIONS(15),PSIGWO(4),
      *FSIG(4),SIGM(15),FFREQ(3),TOTAL(15)

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DIFF6050
DIFF6060
DIFF6070
DIFF6080
DIFF6090
DIFF6100
DIFF6110
DIFF6120
DIFF6130
DIFF6140
DIFF6150
DIFF6160
DIFF6170
DIFF6180
DIFF6190
DIFF6200
DIFF6210
DIFF6220
DIFF6230
DIFF6240
DIFF6250
DIFF6260
DIFF6270
DIFF6280
DIFF6290
DIFF6300
DIFF6310
DIFF6320
DIFF6330
DIFF6340
DIFF6350
DIFF6360
DIFF6370
DIFF6380
DIFF6390
DIFF6400
DIFF6410
DIFF6420
SETE 10
SETE 20
SETE 30
SETE 40
SETE 50
SETE 60
SETE 70
SETE 80
SETE 90
SETE 100
SETE 110
SETE 120
SETE 130
SETE 140
SETE 150
SETE 160
SETE 170
SETE 180

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COMMON/POINTS/ HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13) SETE 190
1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13) SETE 200
2 ,VLM(13),TOTEN(13) SETE 210
C SETE 220
DATA IENTER/0/ SETE 230
C SETE 240
C SETE 250
C SETE 260
C.....WHICH SET OF EQUATIONS TO BE USED SETE 270
C...ITYPE DEFINES HOW MANY TERMS WILL BE USED TO DEFINE FFF AND QQQ SETE 280
C NOTE CONTRIBUTIONS ARE ADDITIVE...IF ITYPE=2 THEN FFF AND QQQ SETE 290
C WILL BE FORMED BY THE ITYPE=1 AND ITYPE=2 CONTRIBUTIONS SETE 300
C ETC. FOR ITYPE=3 ..... SETE 310
C ITYPE IS PROGRAMMED TO BE 1 OR 2 OR 999(WHERE ALL TERMS ARE SET=0.0) SETE 320
C IF(ITYPE.EQ.999)GO TO 9999 SETE 330
C*****MHD CHANNEL EQUATIONS ITYPE=1 OR GREATER SETE 340
100 CONTINUE SETE 350
C SETE 360
C.....FOR THIS MHD CHANNEL PROBLEM SETE 370
C FFF=SIGMA*UE*BZ*BZ*(K-1) SETE 380
C QQQ=FFF*UE*K SETE 390
C..... SETE 400
C TSAV1=XK-1.D0 SETE 410
C... DETERMINE IF CURRENT VALUE OF BZ CAUSES YOU TO EXCEED THE SETE 420
C INPUTTED VALUE OF EXIN WHERE SETE 430
C... EXNEW=1.7583E11*BZ*BZ*(XK-1.0)/TOTAL(NPT) SETE 440
C TSAV2=BZ*BZ SETE 450
C BETOUT(NPT)=BETOUT(3) SETE 460
C AAAA=EXIN*BZ*TOTAL(NPT) SETE 470
C IF(AAAA.EQ.0.0)GO TO 110 SETE 480
C TSAV3=1.7583D11/TOTAL(NPT) SETE 490
C TSAV4=TSAV3*UE*TSAV1 SETE 500
C EXNEW=TSAV4*TSAV2 SETE 510
C EXCOMP=ABS(EXNEW) SETE 520
C... DID WE EXCEED VALUE INPUTTED SETE 530
C IF(EXCOMP.LE.EXIN)GO TO 105 SETE 540
C... YES,RECALCULATE BZ SO THAT EXNEW=EXIN SETE 550
C TSAV2=EXIN/TSAV4 SETE 560
C TSAV2=DABS(TSAV2) SETE 570
C TSAV4=DSORT(TSAV2) SETE 580
C BZ=TSAV4 SETE 590
105 BETOUT(NPT)=BZ*TSAV3 SETE 600
C IF(IMPRTN.GE.4)WRITE(1,9989) XREG0,EXNEW,BZ,BETOUT(NPT) SETE 610
9989 FORMAT(1X,2HX=,F10.7,2X,5HEXNEW=,G13.5,2X,3HBZ=,G13.5, SETE 620
*2X,5HBETA=,G13.5) SETE 630
110 CONTINUE SETE 640
C BETOUT(NPT)=BZ SETE 650
C.....DEFINE VARIABLES MAKING UP FFF AND QQQ SETE 660
C TSAV2=BZ*BZ SETE 670
C TSAV1=(K-1) SETE 680
C SIG IS SIG MA AND UE IS VELOCITY SETE 690
C SETE 700
C FFF=SIG(NPT)*TSAV2*TSAV1*UE SETE 710
C TSAV4=UE*FFF SETE 720
C QQQ=AK*TSAV4 SETE 730
C SETE 740

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C.....ANY HEAT LOSS TERM...STORED IN CHLOSS          SETE 750
  IF(CHCALC.EQ.0.0)GO TO 125                            SETE 760
CCCCC IF(ITYPE.NE.1)GO TO 125                          SETE 770
C      NO HEAT LOSS ALLOWED FOR SPATH PROBLEMS          SETE 780
  IF(SPATH)GO TO 125                                    SETE 790
C...CALCULATE HEAT LOSS USING AN INPUT CHCALC AND CURRENT VALUE(CHHEAT) SETE 800
C... CHLOSS=-(CHHEAT-CHCALC)/CHNLEN                     SETE 810
  CHLOSS=(CHCALC-CHHEAT)/CHNLEN                         SETE 820
  QQQ=QQQ+CHLOSS*RHOUE                                  SETE 830
  IENTER=IENTER+1
  IF(IENTER.LT.100)GO TO 125
CCCCC IF(NITER.EQ.1)WRITE(8,9887) XREG0,CHLOSS,CHCALC,CHHEAT
9887 FORMAT(1X,2HX=,G13.5,8H CHLOSS=,G13.5,8H CHCALC=,G13.5,
  *8H CHHEAT=,G13.5)
  IENTER=0
  IF(IPRRKT.GE.4)WRITE(1,9898) CHLOSS,CHCALC,CHNLEN,CHHEAT SETE 840
9898 FORMAT(1X,24HCHAN. LOSS,2ASS,LEN,HEAT/,1X,4(G12.4,1X)) SETE 850
  125 CONTINUE                                          SETE 860
  IF(ITYPE.NE.1)GO TO 200                              SETE 870
C.....DEFINE TSAV3 AS (QQQ-FFF*UE)                     SETE 880
  TSAV3=QQQ-TSAV4                                       SETE 890
  RETURN                                                SETE 900
C.....ITYPE=2 OR GREATER                                SETE 910
200 CONTINUE                                           SETE 920
C...SAVE FFF AND QQQ TERMS JUST CALCULATED FOR ITYPE=1 SETE 930
  FFFS=FFF                                              SETE 940
  QQQS=QQQ                                              SETE 950
C... CALCULATE NEW FFF AND QQQ AND ADD TO SAVED RESULTS. SETE 960
  FFF=0.0                                              SETE 970
  QQQ=0.0                                              SETE 980
  FFF=FFF+FFFS                                         SETE 990
  QQQ=QQQ+QQQS                                         SETE1000
  IF(ITYPE.NE.2)GO TO 300                              SETE1010
C.....RETURN QQQ-UE*FFF IN TSAV3                       SETE1020
  TSAV3=QQQ-UE*FFF                                     SETE1030
  RETURN                                                SETE1040
C.....ITYPE=3 OR GREATER                                SETE1050
300 CONTINUE                                           SETE1060
C... SAVE FFF AND QQQ PREVIOUSLY CALCULATED           SETE1070
  FFFS=FFF                                              SETE1080
  QQQS=QQQ                                              SETE1090
C... CALCULATE NEW FFF AND QQQ AND ADD TO SAVED RESULTS SETE1100
  FFF=0.0                                              SETE1110
  QQQ=0.0                                              SETE1120
  FFF=FFF+FFFS                                         SETE1130
  QQQ=QQQ+QQQS                                         SETE1140
  IF(ITYPE.NE.3)GO TO 400                              SETE1150
C.....RETURN QQQ-UE*FFF IN TSAV3                       SETE1160
  TSAV3=QQQ-UE*FFF                                     SETE1170
  RETURN                                                SETE1180
C.....ITYPE=4 OR GREATER                                SETE1190
400 CONTINUE                                           SETE1200
C... SAVE FFF AND QQQ PREVIOUSLY CALCULATED           SETE1210
  FFFS=FFF                                              SETE1220
  QQQS=QQQ                                              SETE1230
C... CALCULATE NEW FFF AND QQQ AND ADD TO SAVED RESULTS SETE1240

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      FFF=0.0
      QQQ=0.0
      FFF=FFF+FFFS
      QQQ=QQQ+Q QS
C.....RETURN QQQ-UE*FFF IN TSAV3
      TSAV3=QQQ-UE*FFF
      RETURN
C*****DEFAULT FFF,QQQ,TSAV3 VALUES TO 0.0
9999 CONTINUE
      FFF=0.0
      QQQ=J.0
      TSAV3=0.0
      RETURN
      END
C.....THIS PACKAGE CONTAINS THE FOLLOWING SUBROUTINES
C      (1) REACT
C      (2) HCALC
C      (3) MATRIX
C      (4) CONDUCT
C      (5) NEWOF
C.....
      SUBROUTINE REACT
C
      DOUBLE PRECISION S0,ENN,SUMN
      DOUBLE PRECISION TTT,TM,PP,SIGMA,SIG,VLMI,VLM
C
      LOGICAL SHOCK,MMHG,JV,DETN,SIUNIT,NSQM,CALCH
      LOGICAL HP,SP,TP,NEWNR,IONS,MOLES,FROZ,EQL,PSIA,RKT,VOL,TV,SV
      LOGICAL FA,EFATIO,FPCT,OTTO
      LOGICAL NEOL,CONVG,LOGV,AREA,TWOSTG
C
      DIMENSION ANAME(30,5),V(30),LLMTS(30),SB0P(30,2),B0PT(30,2)
C
      COMMON/MISC/S0,ENN,SUMN,TT,ATOM(3,101),LLMT(30),B0(30),B0P(30,2)
1  ,TM,TLOW,TMID,THIGH,CPSJM,PP,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
2  ,HP2(2),PH(2),VMIN(2),VPLS(2),WP(2),DATA(30),NAME(30,5)
3  ,ANUM(30,5),PECWT(30),ENTH(30),FAZ(30),RTEMP(30),FOX(30),DENS(30)
4  ,RHOP,RMT(30),TLN,CR,OXF(30),ENNL,ENSAVE,ENLSAV,TRACE
      COMMON/INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM
1  ,NG,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWNR,NSUB,NSUP,ITM,CPCVFR,CPCVEQ
2  ,IONS,NC,FSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCHREAC
3  ,IQSAVE,LSAVE,ISUP,ISUB,ITNUM
      COMMON/TSTG/TWOSTG,ALPH,NLM1,XELMC(30),XMMC(1)
      COMMON/MJKE4/PCWFT(2),HPP2(2),PCWSD(2),B0P2(30,2)
C
      EQUIVALENCE (NAME(1,1),ANAME(1,1)),(NLM,L),(BLANK,LANK)
      EQUIVALENCE (OTTO,CPCVFR),(CPCVEQ,LOGV)
C
      DATA MOL/1HM/,CX/1HO/,LAWK/1H/,IZERO/2H00/,NLS/0/,ZERO/1H0/
      DATA DAJ/1HJ/
C
      DO 17 K=1,2
      WP(K)=0.
      HPP(K)=0.
      RH(K)=0.
      VPLS(K)=0.

```

```

      SETE1250
      SETE1260
      SETE1270
      SETE1280
      SETE1290
      SETE1300
      SETE1310
      SETE1320
      SETE1330
      SETE1340
      SETE1350
      SETE1360
      SETE1370
      SETE1380
      REAC 10
      REAC 20
      REAC 30
      REAC 40
      REAC 50
      REAC 60
      REAC 70
      REAC 80
      REAC 90
      REAC 100
      REAC 110
      REAC 120
      REAC 130
      REAC 140
      REAC 150
      REAC 160
      REAC 170
      REAC 180
      REAC 190
      REAC 200
      REAC 210
      REAC 220
      REAC 230
      REAC 240
      REAC 250
      REAC 260
      REAC 270
      REAC 280
      REAC 290
      REAC 300
      REAC 310
      REAC 320
      REAC 330
      REAC 340
      REAC 350
      REAC 360
      REAC 370
      REAC 380
      REAC 390
      REAC 400
      REAC 410
      REAC 420

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      VMIN(K)=0.
      AM(K)=0.
      PCWFT(K)=0.0
      PCWSD(K)=0.0
      HPP2(K)=0.0
      DO 8 J=1,30
      LLMT(J)=0
      EOP(J,K)=0.
      BOP2(J,K)=0.0
      BOP1(J,K)=0.0
8 CONTINUE
10 CONTINUE
      TOUT2=0.0
      IF(TWOSTG)TOUT2=1.0
      NFUEL = 0
      N=1
      L=1
C
C      READ AND WRITE REACTANT CARDS
C
20 READ(5,21)(NAME(N,I),ANUM(N,I),I=1,5),PECWT(N),MOLE,ENTH(N),FAZ(N)
1 ,RTEMP(N),CORJ,FOX(N),DENS(N)
21 FORMAT(5(A2,F7.5),F7.5,A1,F9.5,A1,F7.0,2A1,F8.5)
DO 9801 IOP=1,5
9801 IF(ANUM(N,IOP).EQ.-0.)ANTM(N,IOP)=0.
      IF(PECWT(N).EQ.-0.)PECWT(N)=0.
      IF(ENTH(N).EQ.-0.)ENTH(N)=0.
      IF(RTEMP(N).EQ.-0.)RTEMP(N)=0.
      IF(DENS(N).EQ.-0.)DENS(N)=0.
      IF(NAME(N,1).EQ.LANK) GO TO 200
C*****PECWT INPUT FIELD IS RESTRICTED TO F7.5 *****
C      IF THE ABOVE INPUT VALUE WAS 0.0 THEN
C      IMMEDIATELY READ THE CORRECT VALUE IN
C      FORMAT (10X,E13.5) PLACING THE E IN COLUMN 20 OF THIS CARD
C      THE INPUT CARD WILL BE..(4X,PECWT=,E13.5)
C.....NOTE,IF THIS INPUT CARD IS LEFT OUT,THE REMAINING
C      REACTANTS WILL BE INPUTTED AS GARBAGE.....
      IF(PECWT(N).EQ.0.0)READ(5,22) PECWT(N)
22 FORMAT(10X,E13.5)
C
      IF(L.EQ.0)GO TO 20
      WRITE (6,31)(NAME(N,I),ANUM(N,I),I=1,5),PECWT(N),MOLE,ENTH(N),FAZ
1 (N),RTEMP(N),CORJ,FOX(N),DENS(N)
31 FORMAT(1X,5(A2,1X,F7.4,2X),G13.5,2X,A1,F11.2,2X,A1,2X,F9.3,2(2X,
1 A1),3X,F3.5)
35 IF(MOLE.EQ.MOL) MOLES=.TRUE.
      IF (CORJ.EQ.DAJ) ENTH(N)=ENTH(N)/4.184
C
C      IF OXIDANT, K=1
C      IF FUEL, K=2
C
      IF(FOX(N).EQ.ZERO) FOX('=)OX
      IF (PECWT(N).EQ.0.) PECWT(N)=1.
      K = 1
      IF(FOX(N).EQ.OX) GO TO 37
      K = 2

```

```

REAC 430
REAC 440
REAC 450
REAC 460
REAC 470
REAC 480
REAC 490
REAC 500
REAC 510
REAC 520
REAC 530
REAC 540
REAC 550
REAC 560
REAC 570
REAC 580
REAC 590
REAC 600
REAC 610
REAC 620
REAC 630
REAC 640
REAC 650
REAC 660
REAC 670
REAC 680
REAC 690
REAC 700
REAC 710
REAC 720
REAC 730
REAC 740
REAC 750
REAC 760
REAC 770
REAC 780
REAC 790
REAC 800
REAC 810
REAC 820
REAC 830
REAC 840
REAC 850
REAC 860
REAC 870
REAC 880
REAC 890
REAC 900
REAC 910
REAC 920
REAC 930
REAC 940
REAC 950
REAC 960
REAC 970
REAC 980

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```

      NFUEL = NFUEL+1
37 DO 38 J=1,30
      DATA(J) = 0.
38 CONTINUE
      RM=0.
C
C      STORE ATOMIC SYMBOLS IN LLMT ARRAY.
C      CALCULATE MOLECULAR WEIGHT.
C      TEMPORARILY STORE ATOMIC VALENCE IN V.
C
      DO 100 JJ=1,5
      IF(ANUM(N,JJ).EQ.0.)GO TO 101
      IF(ANAME(N,JJ).EQ.ZERO) ANAME(N,JJ)=OX
      DO 41 J=1,30
      NJ = J
      IF(LLMT(J).EQ.0) GO TO 45
      IF(NAME(N,JJ).EQ.LLMT(J))GO TO 46
41 CONTINUE
45 L = NJ
      LLMT(L)=NAME(N,JJ)
46 DO 48 KK=1,101
      IF(ATOM(1,KK).EQ.ANAME(N,JJ))GO TO 50
48 CONTINUE
      L=0
      GO TO 20
50 RM=RM+ANUM(N,JJ)*ATOM(2,KK)
      V(NJ)=ATOM(3,KK)
      DATA(NJ)=DATA(NJ) + ANUM(N,JJ)
100 CONTINUE
C
C      ADD CONTRIBUTIONS TO WP(K), HPP(K), AM(K), BOP(I,K) AND RH(K)
C
101 PCWT=PECWT(N)
      TOUT1=-1.0
C**** WRITE(1,9988) N,TOUT1,DENS(N),PECWT(N),TOUT2
      IF(MOLES) PCWT=PCWT*RM
      PCWT2=DENS(N)*PCWT
      PCWSD(K)=PCWSD(K)+PCWT2
      IF(TWOESTG)PCWT=(1.0-DENS(N))*PCWT
      PCWET(K)=PCWET(K)+PCWT
      WP(K)=WP(K) + PCWT
      EM = ENTH(N)
      IF(NAME(N,5).NE.IZEPO)HPP(K)=HPP(K)+EM*PCWT/(RM*RR/4184.)
      HPP2(K)=HPP2(K)+EM*PCWT2/(RM*RR/4184.)
C**** WRITE(1,9988) K,PCWSD(K),PCWET(K),PCWT,HPP2(K)
9988 FORMAT(1X,20,(PCWSD(PCWT)PCWT HPP2,/,1X,I2,4(1X,F14.8))
      AM(K)=AM(K)+PCWT/RM
      DO 110 J=1,L
      BOP(J,K)=DATA(J)*PCWT/RM +BOP(J,K)
      BPP2(J,K)=BPP2(J,K)+DATA(J)*PCWT2/RM
      BOP2(J,K)=BOP2(J,K)+DATA(J)*PECWT(N)/RM
110 CONTINUE
      IF(TWOESTG)GO TO 117
      IF(DENS(N).NE.0.)GO TO 115
      GO TO 117
115 RH(K)=RH(K)+PCWT/DENS(N)

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```

REAC 990
REAC1000
REAC1010
REAC1020
REAC1030
REAC1040
REAC1050
REAC1060
REAC1070
REAC1080
REAC1090
REAC1100
REAC1110
REAC1120
REAC1130
REAC1140
REAC1150
REAC1160
REAC1170
REAC1180
REAC1190
REAC1200
REAC1210
REAC1220
REAC1230
REAC1240
REAC1250
REAC1260
REAC1270
REAC1280
REAC1290
REAC1300
REAC1310
REAC1320
REAC1330
REAC1340
REAC1350
REAC1360
REAC1370
REAC1380
REAC1390
REAC1400
REAC1410
REAC1420
REAC1430
REAC1440
REAC1450
REAC1460
REAC1470
REAC1480
REAC1490
REAC1500
REAC1510
REAC1520
REAC1530
REAC1540

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1	CONTINUE	HCAL 680
	GO TO 11	HCAL 690
3	CONTINUE	HCAL 700
C.....	END TWOSTG BLOCK	HCAL 710
	IF (AM(1).NE.0.0 .AND. AM(2).NE.0.0) GO TO 4	HCAL 720
	AM1= AM(2)	HCAL 730
	IF (AM(2).EQ.0.0) AM1= AM(1)	HCAL 740
	GO TO 9	HCAL 750
4	AM1=(OF+1.)*AM(1)*AM(2)/(AM(1)+OF*AM(2))	HCAL 760
9	TM = 0.	HCAL 770
	IF (PP.GT.0.) TM = DLOG(PP*DBLE(AM1))	HCAL 780
	SSUM(NPT) = 0.	HCAL 790
	HPP(1) = 0.	HCAL 800
	HPP(2) = 0.	HCAL 810
	HSUB0 = 0.	HCAL 820
	CPRI = 0.	HCAL 830
	ANN = (1.+OF)	HCAL 840
C		HCAL 850
C	LOOP ON REACTANTS.	HCAL 860
C	IF OXIDANT, K=1	HCAL 870
C	IF FUEL, K=2	HCAL 880
C		HCAL 890
11	CONTINUE	HCAL 900
	DO 900 N=1,NREAC	HCAL 910
	K=2	HCAL 920
	IF (FOX(N).EQ.OX)K=1	HCAL 930
	IF (NAME(N,5).NE.IZERO) GO TO 89	HCAL 940
	IF (.NOT.CALCH.AND.TT.NE.0.) GO TO 15	HCAL 950
	TT = RTEMP(N)	HCAL 960
C		HCAL 970
C	IS TT IN RANGE	HCAL 980
C		HCAL 990
15	IF (SHOCK) GO TO 16	HCAL1000
	IF (TT.LT. (TLOW/1.2) .OR. TT.GT. (THIGH*1.2)) GO TO 75	HCAL1010
16	J = NUM(N,5)	HCAL1020
	IF (J.NE.0) GO TO 50	HCAL1030
	DO 10 J=1,L	HCAL1040
	DATA(J)=0.	HCAL1050
10	CONTINUE	HCAL1060
C		HCAL1070
C	TEMPORARILY STORE STOICHIOMETRIC COEFFICIENTS IN DATA ARRAY.	HCAL1080
	DO 40 I=1,4	HCAL1090
	IF (ANUM(N,I).EQ.0.)GO TO 50	HCAL1100
	DO 20 J=1,L	HCAL1110
	JS=J	HCAL1120
	IF (LMT(J).EQ.NAME(N,I)) GO TO 30	HCAL1130
20	CONTINUE	HCAL1140
30	DATA(JS)=ANUM(N,I)	HCAL1150
40	CONTINUE	HCAL1160
50	IS=0	HCAL1170
C		HCAL1180
C	SEARCH FOR REACTANT IN THERMO SPECIES. STORE INDEX IN NUM(N,5).	HCAL1190
		HCAL1200
	DO 70 J= 1,NS	HCAL1210
	IF (IUSE(J).EQ.0)GO TO 55	HCAL1220
	IS = IS+1	HCAL1230

```

      IF (FAZ(N).EQ.A) GO TO 70
      IF (TT.GT.TEMP (IS,2).AND.TEMP (IS,2).NE.THIGH) GO TO 70
      IF (TT.LT.TEMP (IS,1).AND.TEMP (IS,1).NE.TLOW) GO TO 70
      GO TO 56
55  IF (FAZ(N).NE.AC.AND.FAZ(N).NE.BLK) GO TO 70
56  DO 6J I=1,L
      IF (A(I,J).NE.DATA(I)) GO TO 70
60  CONTINUE
      NUM(N,5) = J
      GO TO 90
70  CONTINUE
      GO TO 80
C
C      CALCULATE EN FOR REACTANT AND CALL CPHS TO CALCULATE PROPERTIES.
C
      89 KOD = 1
      90 CONTINUE
C.....TWO STG BLOCK....11/14/79
      IF (.NOT.TWO STG) GO TO 94
      PCWT=DENS(N)*PECWT(N)
      PCWT=(1.0-DENS(N))*PECWT(N)
      RM=RMW(N)
      IF (NAME(N,5).NE.IZERO) GO TO 92
      NSS =NSK
      NSK= J
      TLN = ALOG(TT)
      JS1=J
      CALL CPHS
      NSK= NSS
      IF (H0(J).GT.-.01 .AND. H0(J).LT..01) H0(J) = 0
      RTEMP(N) = TT
      ENTH(N)=H0(J)*RR*TT/4184.
92  CONTINUE
      EM = ENTH(N)
      HPP(K)=HPP(K)+EM*PCWT/(RM*RR/4184.)
      HPP2(K)=HPP2(K)+EM*PCWT2/(RM*RR/4184.)
      GO TO 900
C...END TWO STG BLOCK....
94  CONTINUE
      IF (MOLES) ENJ = PECWT(N)/WP(K)
      IF (.NOT.MOLES) ENJ = PECWT(N)/RMW(N)
      ENJ = ENJ/ANN
      IF (K.EQ.1) ENJ = ENJ*OF
      IF (NAME(N,5).NE.IZERO) GO TO 500
      NSS =NSK
      NSK= J
      TLN = ALOG(TT)
      IF (.NOT.CALCH) EN(NPT,J) = ENJ
      JS1=J
      CALL CPHS
      NSK= NSS
      IF (H0(J).GT.-.01 .AND. H0(J).LT..01) H0(J) = 0.
      RTEMP(N) = TT
      IF (VOL) H0(J)=V0(J)-1.
      ENTH(N)=H0(J)*RR*TT/4184.
C

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HCAL1240
HCAL1250
HCAL1260
HCAL1270
HCAL1280
HCAL1290
HCAL1300
HCAL1310
HCAL1320
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HCAL1370
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HCAL1400
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HCAL1460
HCAL1470
HCAL1480
HCAL1490
HCAL1500
HCAL1510
HCAL1520
HCAL1530
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HCAL1560
HCAL1570
HCAL1580
HCAL1590
HCAL1600
HCAL1610
HCAL1620
HCAL1630
HCAL1640
HCAL1650
HCAL1660
HCAL1670
HCAL1680
HCAL1690
HCAL1700
HCAL1710
HCAL1720
HCAL1730
HCAL1740
HCAL1750
HCAL1760
HCAL1770
HCAL1780
HCAL1790

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C      ADD CONTRIBUTION TO CP, H, AND S OF TOTAL REACTANT.
C
      CPR1 = CPR1 + CPSUM
      SSUM(NPT) = SSUM(NPT) + ENJ * (S(J)-DLOG(ENJ)-TM)
500  ER = ENTH(N)*E1J*4184./RR
      HSUB0 = HSUB0+EP
      HPP(K) = HPP(K)+ER
900  CONTINUE
      IF(TSAVE.NE.0.) TT=TSAVE
      GO TO 1000
75  WRITE(6,76)
76  FORMAT(5H0REACTANT TEMPERATURE OUT OF RANGE OF THERMO DATA )
      TT = 0.
      GO TO 1000
80  WRITE(6,85) N
85  FORMAT(9H0REACTANT,I2,22H IS NOT IN THERMO DATA )
      TT = 0.
1000 IF (KOD.EQ.1) CPR1 = 0.
      RETURN
      END
      SUBROUTINE MATRIX(FLAG)
C
C      LOGICAL SHOCK,MMHG,UV,DETN,SIUNIT,NSQM,CALCH
C      LOGICAL HP,SP,PP,NEW,IONS,MOLES,FROZ,EOL,PSIA,RKT,VOL,TV,SV
C      LOGICAL FA,ERATIO,FPCT,OTTO
C      LOGICAL NEQL,CONVG,LOGV,SFLG,AREA,FLAG
C
C      THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR
C      NON-CDC MACHINES
C
      DOUBLE PRECISION TTT,TM,PP,SIGMA,SIG,VLM1,VLM
      DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS,S0
      DOUBLE PRECISION G,X,S,EN,ENLN,H0,ENLS,ENN,EMM,SUMN
      DOUBLE PRECISION H,F,SS,PERM1,TERM,SSS,DXOUTP
C
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
1  ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
2  ,VLM(13),TOTN(13)
      COMMON/SOLUT/NSOL,ISOLN(3,16),SFLG,SUMSN,ENN5,ENLS
      COMMON/MISC/S0,ENN,SUMN,TT,ATOM(3,101),LLMT(30),B0(30),B0P(30,2)
1  ,TM,TLOW,TMID,THIGH,CPSUM,PP,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
2  ,HPP(2),PH(2),VMIN(2),VPLS(2),WP(2),DATA(30),NAME(30,5)
3  ,ANUM(30,5),PECWT(30),ENTH(30),FAZ(30),RTEMP(30),FOX(30),DENS(30)
4  ,RHOP,RM7(30),TLN,CR,OXF(30),ENNL,ENSAVE,ENLSAV,TRACE
      COMMON /DOUBLE/ G(60,61), X(60)
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,ISV, NPP, MOLES,NP,NT,NPT,NLM
1  ,N ,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEW,NSUB,NSUP,ITM,CPCVFR,CPCVEQ
2  ,IONS,NC,NSERT,JSO,JLID,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALGHM
3  ,IOAVE,ISAVE,JSUP,ISUB,ITNUM
      COMMON/NEQ/EN(30),ENM,SJQ,NQ1,NSK,NEOPT
      COMMON/NUM/NUMB1
      COMMON/MHDD/SSNEW,DX,DXI,XJY(26),AI(26),UE,NITER,NSTOP,SIG(26),IPPM
X  ,B7,XK,PIPP
      COMMON/SPECE1/NSPCMX,NCMAX,NELMX,TMP(175,2),SUB(600,3),S(1)
      COMMON/SPECE2/ENLN(1)

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HCAL1800
HCAL1810
HCAL1820
HCAL1830
HCAL1840
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HCAL1860
HCAL1870
HCAL1880
HCAL1890
HCAL1900
HCAL1910
HCAL1920
HCAL1930
HCAL1940
HCAL1950
HCAL1960
HCAL1970
HCAL1980
HCAL1990
MATR 10
MATR 20
MATR 30
MATR 40
MATR 50
MATR 60
MATR 70
MATR 80
MATR 90
MATR 100
MATR 110
MATR 120
MATR 130
MATR 140
MATR 150
MATR 160
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MATR 180
MATR 190
MATR 200
MATR 210
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MATR 230
MATR 240
MATR 250
MATR 260
MATR 270
MATR 280
MATR 290
MATR 300
MATR 310
MATR 320
MATR 330
MATR 340
MATR 350
MATR 360

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COMMON/SPECE3/K0(1) MATR 370
COMMON/SPECE5/IUSE(1) MATR 380
COMMON/DB5VEC/DXOUTP(1) MATR 390
COMMON/K04/EN(13,1) MATR 400
COMMON/STOIC/A(30,1) MATR 410
C... NSPCMX REFERS TO THE MAXIMUM NO. OF SPECIES ALLOWED MATR 420
C... NCNMAX REFERS TO THE MAXIMUM NO. OF CONDENSED SPECIES ALLOWED MATR 430
C THIS IS FIXED AND REFERS TO THE SIZE OF TEMP(N,2) IN COMMON MATR 440
C SPECI1.....MUST CHANGE THIS COMMON EVERYWHERE IF A LARGER SMATR 450
C IS NEEDED MATR 460
C... NELMX REFERS TO THE MAXIMUM NO. OF ELEMENTS ALLOWED MATR 470
C THIS IS FIXED AND REFERS TO THE SIZE OF XELMC(N) AND A(N,NSMATR 480
C .....MUST CHANGE COMMON TSTG AND STOIC EVERYWHERE IF MATR 490
C A LARGER SIZE IS NEEDED MATR 500
C MATR 510
C MATR 520
C EQUIVALENCE (NLM,L),(TP,TV),(SV,SP),(UV,HP) MATR 530
C EQUIVALENCE (OTTO,CPCVPR),(CPCVEQ,LOGV) MATR 540
C MATR 550
C DATA ISUBFL/0/ MATR 560
C MATR 570
C IF(CONVG)GO TO 210 MATR 580
C IF(IPP.NE.NEOPT)GO TO 213 MATR 590
C IF(NUMB1.NE.1)GO TO 210 MATR 600
C IF(ISUBFL.NE.0)GO TO 210 MATR 610
C IF(NS.EQ.NSK)GO TO 210 MATR 620
C ISUBFL=1 MATR 630
C SUMN=SUMN-EMM MATR 640
C ENN=ENN-EMM MATR 650
210 ENNEVM=ENN+EMM MATR 660
C IQ2 = IQ1+1 MATR 670
C IQ3 = IQ2 + 1 MATR 680
C IQ4=IQ1-1 MATR 690
C KMAT = IQ3 MATR 700
C IF(.NOT.CONVG.AND.TP) KMAT = IQ2 MATR 710
C IMAT = KMAT - 1 MATR 720
C MATR 730
C CLEAR MATRIX STORAGES TO ZERO MATR 740
C MATR 750
C IMAT1=IMAT MATR 760
C KMAT1=KMAT MATR 770
C IF(IPP.NE.NEOPT)GO TO 209 MATR 780
C IF(NUMB1.NE.1)GO TO 209 MATR 790
C IF(NS.EQ.NSK)GO TO 209 MATR 800
C KMAT1=KMAT1+NQ1 MATR 810
C IMAT1=IMAT1+NQ1 MATR 820
209 CONTINUE MATR 830
C DO 211 I=1,IMAT1 MATR 840
C DO 211 K=1,KMAT1 MATR 850
C G(I,K)= 0.000 MATR 860
211 CONTINUE MATR 870
C G(IQ2,IQ1) = 0. MATR 880
C IF(SFLG) G(IQ2,IQ4)=0. MATR 890
C SSS = 0. MATR 900
C ESUM(NPT) = 0. MATR 910
C MATR 920

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C BEGIN SET UP OF ITERATION MATRIX
C
KK = L
DO 65 J=1,NS
  (F(IUSE(J).LT.0) GO TO 65
  H=H0(J)*EN(NPT,J)
  IF(IUSE(J).GT.0 .AND. IUSE(J).LT.1000) GO TO 70
  F = (H0(J)-S(J)+ENLN(J)+TM)*EN(NPT,J)
  IF(IUSE(J).GT.1000) F=F-(ENLS+TM)*EN(NPT,J)
  SS = H-F
  TERM1 = H
  IF (KMAT.EQ.102) TERM1 = F
  DO 55 I = 1, L
C CALCULATE THE ELEMENTS R(I,K)
C
IF (A(I,J).EQ.0.) GO TO 55
TERM= A(I,J)*EN(NPT,J)
DO 15 K=I, L
  G(I,K)= G(I,K) + A(K,J)*TERM
15 CONTINUE
C
IF(IUSE(J).EQ.0) G(I,IQ1)=G(I,IQ1)+TERM
IF(IUSE(J).GT.1000) G(I,IQ4)=G(I,IQ4)+TERM
G(I,IQ2)=G(I,IQ2)+A(I,J)*TERM1
IF (CONVG.OR.TP) GO TO 55
G(I,IQ3)= G(I,IQ3)+A(I,J)*F
IF (SP) G(IQ2,I) = G(IQ2,I) + A(I,J)*SS
55 CONTINUE
IF (KMAT.EQ.102) GO TO 64
IF(CONVG.OR.HP) GO TO 59
IF(IUSE(J).EQ.0) G(IQ2,IQ1) = G(IQ2,IQ1) + SS
IF(IUSE(J).GT.1000) G(IQ2,IQ4) = G(IQ2,IQ4) + SS
G(IQ2,IQ2)=G(IQ2,IQ2)+H0(J)*SS
IF(IUSE(J).EQ.0) G(IQ2,IQ3) = G(IQ2,IQ3)+(S(J) - ENLN(J)-TM)*F
IF(IUSE(J).GT.1000) G(IQ2,IQ3)=G(IQ2,IQ3)+(S(J) - ENLN(J)+ENLS)*F
GO TO 62
59 G(IQ2,IQ2)=G(IQ2,IQ2)+H0(J)*H
IF (CONVG) GO TO 64
G(IQ2,IQ3)=G(IQ2,IQ3)+H0(J)*F
62 IF(IUSE(J).EQ.0) G(IQ1,IQ3)=G(IQ1,IQ3)+F
IF(IUSE(J).GT.1000) G(IQ4,IQ3)=G(IQ4,IQ3)+F
64 IF(IUSE(J).EQ.0) G(IQ1,IQ2)=G(IQ1,IQ2)+TERM1
IF(IUSE(J).GT.1000) G(IQ4,IQ2)=G(IQ4,IQ2)+TERM1
GO TO 65
C CONDENSED SPECIES
C
70 KK = KK + 1
DO 75 I = 1,L
  G(I,KK) = A(I,J)
  G(I,KMAT) = G(I,KMAT) - A(I,J)*EN(NPT,J)
75 CONTINUE
G(KK,IQ2) = H0(J)
G(KK,KMAT) = H0(J) - S(J)
HSUM(NPT) = HSUM(NPT)+ H

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MATR 930
MATR 940
MATR 950
MATR 960
MATR 970
MATR 980
MATR 990
MATR1000
MATR1010
MATR1020
MATR1030
MATR1040
MATR1050
MATR1060
MATR1070
MATR1080
MATR1090
MATR1100
MATR1110
MATR1120
MATR1130
MATR1140
MATR1150
MATR1160
MATR1170
MATR1180
MATR1190
MATR1200
MATR1210
MATR1220
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MATR1400
MATR1410
MATR1420
MATR1430
MATR1440
MATR1450
MATR1460
MATR1470
MATR1480

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      IF(.NOT.SP) GO TO 65
      S13 = SSS + S(J)*EN(NPT,J)
      G(IQ2,K1) = S(J)
65  CONTINUE
      DO 81 I=1,L
      G(I,IQ1)=G(I,IQ1)*ENN/(ENNEMM)
81  CONTINUE
      G(IQ2,IQ1)=G(IQ2,IQ1)*ENN/(ENNEMM)
      SSS=SSS+G(IQ2,IQ1)*(ENNEMM)/ENN
      IF(SFLG) SSS=SSS+G(IQ2,IQ4)
      IF(SFLG) HSUM(NPT)=HSUM(NPT)+G(IQ4,IQ2)
      HSUM(NPT) = HSUM(NPT) + G(IQ1,IQ2)
      G(IQ1,IQ1)=SUMN*ENN/(ENNEMM) -ENN
      IF(.NOT.SFLG) GO TO 701
      SUMSN=0.
      DO 702 J=1,NS
      IF(IUSE(J).LT.1000) GO TO 702
      SUMSN=SUMSN+EN(NPT,J)
702 CONTINUE
      G(IQ4,IQ4)=SUMSN-ENNS
      IF(CONVG) G(IQ4,IQ4) = 0.
C
C **** ADD NON-EQ CONTRIBUTION
C
701 IF(IPP.LT.NEQPT)GO TO 82
      NSP1=NS+1
      DO 83 J=NSP1,NSK
      IF(IUSE(J).LT.0)GO TO 83
      HSUM(NPT)=HSUM(NPT)+EN(NPT,J)*H0(J)
      SS=S(J)
      IF (IUSE(J).EQ.0)SS=SS-ENLN(J)-TM
      SSS=SSS+SS*EN(NPT,J)
83  CONTINUE
C
C REFLECT SYMMETRIC PORTIONS OF THE MATRIX
C
82 ISYM=IQ1
      IF(HP.OR.CONVG)ISYM=IQ2
      DO 102 I=1,ISYM
      DO 102 J=1,ISYM
      G(J,I)=G(I,J)
102 CONTINUE
      DO 104 J=1,L
      G(IQ1,J)=G(IQ1,J)*(ENNEMM4)/ENN
104 CONTINUE
      IF(HP.OR.CONVG)G(IQ2,IQ1)=G(IQ2,IQ1)*ENN/(ENNEMM)
C
C COMPLETE THE RIGHT HAND SIDE
C
      IF(.NOT.CONVG)GO TO 140
      IF(.NOT.LOCV) GO TO 175
C
C LOGV = .TRUE.-- SET UP MATRIX TO SOLVE FOR DLPVT
C
      G(IQ1,IQ2) = ENN
      IF(SFLG) G(IQ4,IQ2)=ENNS

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MATR1490
 MATR1500
 MATR1510
 MATR1520
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 MATR1920
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 MATR1940
 MATR1950
 MATR1960
 MATR1970
 MATR1980
 MATR1990
 MATR2000
 MATR2010
 MATR2020
 MATR2030
 MATR2040

IQ = IQ1 - 1	MATR2050
IF(SFLG) IQ=IQ-1	MATR2060
DO 135 I = 1,IQ	MATR2070
G(I,IQ2)=G(I,IQ1)*(ENNEMM)/ENN	MATR2080
135 CONTINUE	MATR2090
GO TO 175	MATR2100
140 DO 145 I=1,L	MATR2110
X(1)=F0(I)-G(I,IQ1)*(ENNEMM)/ENN-B0N(I)	MATR2120
IF(SFLG) X(1)=X(1)-G(I,IQ4)	MATR2130
G(I,KMAT) = G(I,KMAT)+X(1)	MATR2140
145 CONTINUE	MATR2150
G(IQ1,KMAT) = G(IQ1,KMAT)+ENN-SUMN	MATR2160
IF(SFLG) G(IQ4,KMAT)=G(IQ4,KMAT) + ENNS - SUMSN	MATR2170
C	MATR2180
C COMPLETE ENERGY ROW AND TEMPERATURE COLUMN	MATR2190
C	MATR2200
IF (KMAT .EQ. IQ2) GO TO 185	MATR2210
IF (SP)ENERGY = S0+ENN-SUMN - SSS	MATR2220
IF(SP.AND.SFLG) ENERGY=ENERGY+ENNS-SUMSN	MATR2230
IF(HP)ENERGY=HSUB0/TT - HSUM(NPT)	MATR2240
G(IQ2,IQ3)=G(IQ2,IQ3)+ ENERGY	MATR2250
175 G(IQ2,IQ2)= G(IQ2,IQ2)+CPSUM	MATR2260
185 RETURN	MATR2270
END	MATR2280
SUBROUTINE CONDOC(PFLAG)	COND 10
C	COND 20
C THIS IS A SUBROUTINE FOR THE NASA-LEWIS CHEMICAL EQUILIBRIUM CODE	COND 30
C OF S. GORDON AND B. MCBRIDE (NASA SP-273, 1971).	COND 40
C	COND 50
C IT WAS WRITTEN BY HOWARD D. COHEN (PHONE\ 617-253-3496),	COND 60
C ENERGY LABORATORY, MIT, IN OCTOBER 1976.	COND 70
C IT USES THE DEMETRIADES AND ARGYROPOULOS ALGORITHM (PHYS. FLUIDS,	COND 80
C 9, 2136 (1966)).	COND 90
C THIS VERSION USES THE AVERAGED CROSS SECTIONS REPORTED IN	COND 100
C 1) FE SPENCER AND AV PHELPS, PROC 15TH SYMP ENG ASP OF MHD,	COND 110
C PHILADELPHIA, PAPER IX.9, 1976.	COND 120
C 2) FE SPENCER, ET AL, IN RESEARCH IN COAL-BASED MHD,	COND 130
C MONTHLY TECHNICAL PROGRESS REPORT, PITTSBURGH ENERGY RESEARCH	COND 140
C CENTER, BY D. BIENSTOCK, JULY 1976.	COND 150
C	COND 160
C ONLY CHEMICAL SPECIES COMMONLY FOUND IN OPEN-CYCLE MHD GENERATORS	COND 170
C WITHOUT SLAG ARE INCLUDED IN THIS VERSION. ALL OTHER NEUTRAL	COND 180
C SPECIES WILL BE IGNORED. CROSS SECTIONS FROM 1700 TO 3000 K	COND 190
C HAVE BEEN TABULATED. OUTSIDE THIS RANGE VALUES WILL BE	COND 200
C EXTRAPOLATED.	COND 210
C	COND 220
C WHEN USING THIS SUBROUTINE, MAKE SURE THAT THE COMMON STATEMENTS	COND 230
C IN THIS SUBROUTINE ARE COMPATIBLE WITH THE VERSION OF THE NASA-	COND 240
C LEWIS PROGRAM THAT YOU ARE USING.	COND 250
C IT IS SUGGESTED THAT THIS SUBROUTINE BE CALLED JUST PRIOR TO THE	COND 260
C RETURN FROM THE OUT2 ENTRY POINT OF THE OUT1 SUBROUTINE.	COND 270
C	COND 280
C	COND 290
C DOUBLE PRECISION TTT,TM,PP,SIGMA,SIG,VLM1,VLM	COND 300
C DOUBLE PRECISION HSUM,SSIM,CPR,DLVTP,DLVPT,GAMMAS,S0	COND 310
C DOUBLE PRECISION G,X,S,EN,ENN,EMM,SUMN	COND 320

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C      PROGRAM NEOMHD(INPUT,OUTPUT,TAPE7,TAPE5=INPUT,TAPE6=OUTPUT)      MAIN 10      PAGE 0120

C
LOGICAL SHOCK,MMHG,UV,DETN,SIUNIT,NSQM,CALCH,PFLAG      COND 330
LOGICAL H+,SP,TP,NEWr,IONS,MOLES,PSIA,RKT,VOL,TV,SV      COND 340
LOGICAL FA,ERATIO,FPCT,OTTO      COND 350
LOGICAL NEOL,CONVG,LOGV      COND 360
C
COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)      COND 370
1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)      COND 380
2 ,VLE(13),TOTN(13)      COND 390
COMMON/MISC/S0,ENN,SUMN,TT,ATOM(3,101),LLMT(30),B0(30),B0P(30,2)      COND 400
1 ,TM,TLOW,TMID,THIGH,CPSUM,PP,OF,BORAT,FPCT,R,RR,HSUB0,AC(2),AM(2)      COND 410
2 ,HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(30),NAME(30,5)      COND 420
3 ,ANUM(30,5),PECWT(30),ETH(30),FAZ(30),RTEMP(30),FOX(30),DENS(30)      COND 430
4 ,RHOP,RMW(30),TLN,CR,OXF(30),ENNL,ENSAVE,ENLSAV,TRACE      COND 440
COMMON/DOUBLE/G(60,61),X(60)      COND 450
COMMON/INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM      COND 460
1 ,NS,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWr,NSUB,NSUP,ITM,CPCVFR,CPCVEQ      COND 470
2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH      COND 480
3 ,IQSAVE,LSAVE,ISUP,ISUB,ITNUM      COND 490
COMMON/OUT/FORMAT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)      COND 500
1 ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2      COND 510
2 ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0,FRHO(4)      COND 520
COMMON/CSIG/SIGMA(13)      COND 530
COMMON/SIGOUT/INEL(3),ANE(15),FIONS(3),AIONS(15),FSIGWO(4),      COND 540
XFSIG(4),SIGM(15),PFREQ(3),TOTAL(15)      COND 550
COMMON/NEO/B0N(30),EMM,SNEO,NQ1,NSK,NEOPT      COND 560
COMMON/SPECE1/NSPCMX,NCMAX,NELMX,TEMP(175,2),SUB(600,3),S(1)      COND 570
COMMON/KGM/EN(13,1)      COND 580
C... NSPCMX REFERS TO THE MAXIMUM NO. OF SPECIES ALLOWED      COND 590
C... NCMAX REFERS TO THE MAXIMUM NO. OF CONDENSED SPECIES ALLOWED      COND 600
C      THIS IS FIXED AND REFERS TO THE SIZE OF TEMP(N,2) IN COMMON      COND 610
C      SPECE1.....MUST CHANGE THIS COMMON EVERYWHERE IF A LARGER S      COND 620
C      IS NEEDED      COND 630
C... NELMX REFERS TO THE MAXIMUM NO. OF ELEMENTS ALLOWED      COND 640
C      THIS IS FIXED AND REFERS TO THE SIZE OF XELMC(N) AND A(N,NSCOND      COND 650
C      .....MUST CHANGE COMMON TSTG AND STOIC EVERYWHERE IF      COND 660
C      A LARGER SIZE IS NEEDED      COND 670
C
DIMENSION JSUBNQ(600,3),AN(15),BP(100),BN(100)      COND 680
1 ,ANEG(15),APOS(15),MAST(4),MSK(2)      COND 690
2 ,QN(15),A2QN(15),A5QN(15)      COND 700
C+++++IF THE SIZE OF THE SUB ARRAY IS CHANGED...CHANGE JSUB ALSO      COND 710
DIMENSION JSUB(600,3),TOTA(15)      COND 720
DIMENSION QK(14,3),QKOH(14,3),QN2(14,3),QOH(14,3)      COND 730
1 ,QCO(14,3),QCO2(14,3),QH2O(14,3)      COND 740
DIMENSION QS(14,3,16),IPT(15),X1(15),X2(15)      COND 750
DIMENSION QO(14,3),QO2(14,3),QH2(14,3),QAR(14,3),QNO(14,3),      COND 760
*QH(14,3),QSO2(14,3),QCS(14,3)      COND 770
DIMENSION WS1P(100,3),WS1N(100,3)      COND 780
EQUIVALENCE (JSUB(1,1),SUB(1,1))      COND 790
EQUIVALENCE (OTTO,CPCVFR),(CPCVEQ,LOGV)      COND 800
EQUIVALENCE (QS(1,1,1),QCO(1,1)),(QS(1,1,2),QCO2(1,1)),      COND 810
1(QS(1,1,3),QH2O(1,1)),(QS(1,1,4),QK(1,1)),(QS(1,1,5),QN2(1,1)),      COND 820
2(QS(1,1,6),QOH(1,1)),(QS(1,1,7),QH(1,1)),(QS(1,1,8),QKOH(1,1)),      COND 830
3(QS(1,1,9),QO2(1,1)),(QS(1,1,10),QO(1,1)),(QS(1,1,11),QH2(1,1)),      COND 840
4(QS(1,1,12),QNO(1,1)),(QS(1,1,13),QAR(1,1)),(QS(1,1,14),QCS(1,1)),      COND 850
COND 860
COND 870
COND 880

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5(QS(1,1,15),QSO2(1,1))
DATA QO /5.096,5.017,5.027,5.038,5.048,5.058
1 ,5.067,5.076,5.085,5.094,5.103,5.111,5.120,5.128 COND 890
2 ,.2152,.2155,.2159,.2162,.2164,.2167,.2170,.2173,.2176,.2179 COND 900
3 ,.2181,.2184,.2187,.2190 COND 910
4 ,1.337,1.337,1.338,1.339,1.340,1.340,1.341,1.342 COND 920
5 ,1.343,1.344,1.345,1.346,1.347,1.348/ COND 930
DATA QO2 /5.624,5.696,5.765,5.832,5.896,5.958 COND 940
1 ,6.018,6.075,6.129,6.181,6.231,6.278,6.322,6.364 COND 950
2 ,.2396,.2896,.2897,.2898,.2899,.2395,.2890,.2881,.2869 COND 960
3 ,.2855,.2837,.2816,.2793,.2763 COND 970
4 ,1.498,1.501,1.502,1.501,1.496,1.490,1.482,1.472 COND 980
5 ,1.460,1.447,1.433,1.419,1.404,1.388/ COND 990
DATA QH2 /13.916,14.098,14.272,14.434,14.596,14.747,14.890 COND 1000
1 ,15.026,15.156,15.279,15.396,15.507,15.612,15.712 COND 1010
2 ,.2914,.2911,.2905,.2897,.2888,.2876,.2863,.2849 COND 1020
3 ,.2833,.2816,.28799,.2780,.2761,.2741 COND 1030
4 ,1.500,1.495,1.489,1.482,1.475,1.467,1.460,1.452 COND 1040
5 ,1.444,1.435,1.427,1.418,1.410,1.401/ COND 1050
6 QH /32.778,32.362,31.964,31.581,31.214,30.861,30.521,30.193 COND 1060
7 ,29.876,29.570,29.274,28.988,28.710,28.440 COND 1070
8 ,.1120,.1095,.1072,.1051,.1031,.1012 COND 1080
9 ,.0993,.0976,.0959,.0942,.0926,.0910,.0894,.0879 COND 1090
A ,1.5,1.495,1.489,1.482,1.475,1.467,1.46,1.452,1.444 COND 1100
B ,1.435,1.427,1.418,1.410,1.401/ COND 1110
DATA QAR / .494,.526,.560,.596,.632,.669,.707,.745 COND 1120
1 ,.783,.821,.860,.899,.937,.976 COND 1130
2 ,.6356,.6574,.6723,.6822,.6882,.6913,.6924,.6919,.6904,.6880 COND 1140
3 ,.6851,.6819,.6784,.6749 COND 1150
4 ,3.085,3.062,3.033,3.000,2.965,2.930,2.896,2.863,2.832,2.803 COND 1160
5 ,2.775,2.750,2.727,2.705/ COND 1170
DATA QNO / 16.592,17.05,17.43,17.735,17.97,18.15,18.28, COND 1180
1 18.369,18.42,18.44,18.43,18.39,18.34,18.27 COND 1190
2 ,.4080,.3766,.3478,.3212,.2969,.2745,.2539,.2351,.2177 COND 1200
3 ,.2017,.1869,.1734,.1608,.1493 COND 1210
4 ,1.269,1.19,1.124,1.071,1.027,.991,.962,.938,.919,.904 COND 1220
5 ,.892,.883,.876,.871/ COND 1230
DATA QSO2 / 84.93,80.25,76.08,72.33,63.95,65.88,63.08 COND 1240
1 ,00.51,58.15,55.98,53.97,52.098,50.359,48.736 COND 1250
2 ,-.197,-.1957,-.1945,-.1934,-.1923,-.1914,-.1905,-.1897,-.1890 COND 1260
3 ,-.1884,-.1878,-.1872,-.1867,-.1863 COND 1270
4 ,2*.923,2*.922,.921,.920,.919,.918,.917,2*.916 COND 1280
5 ,2*.915,.914/ COND 1290
DATA QCS / 685.48,645.31,607.81,572.99,540.78 COND 1300
1 ,511.07,483.71,458.56,435.45,414.24,394.77,376.91 COND 1310
2 ,360.50,345.44 COND 1320
3 ,-.2116,-.2134,-.2520,-.2677,-.2306,-.2909,-.2989,-.3046,-.3080 COND 1330
4 ,.3100,-.3101,-.3035,-.3055,-.3012 COND 1340
5 ,.501,.539,.582,.625,.673,.720,.768,.815,.862 COND 1350
6 ,.907,.951,.994,1.03,1.073/ COND 1360
C+++ DATA FSIGWO/4H W/4HO T/4HNS 4H /,FFREQ/4HFREQ,4H (1/, COND 1370
C+++ 1 4FSEC /,FIONS/4HIONS,4HC DE,4HNS) / COND 1380
C+++ DATA FSIG /4HSIGM,4HA (M,4HMO/M,2H) /,FNEL/4HELEC,4H DEN, COND 1390
C+++ 1 4HS / COND 1400
DATA QCO/13.050,13.360,13.669,13.979,14.290,14.601,14.911, COND 1410
1 15.219,15.523,15.823,16.117,16.403,16.680,16.947, COND 1420
COND 1430
COND 1440
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      .3617,.3668,.3722, COND1450
3.3771,.3823,.3872,.3908,.3933,.3948 ,.3951,.3943, COND1460
4.3924,.3894,.3855, COND1470
5 1.771,1.800,1.23,1.840,1.850,1.851,1.844,1.829,1.807 COND1480
6 ,1.779,1.746,1.703,1.668,1.626/ COND1490
DATA QH2O/108.532,102.550,97.229,92.443,88.12,84.197,80.620,77.344 COND1500
1 ,74.333,71.555,68.985,66.598,64.377,62.305, COND1510
2 -.1968,-.1955,-.1942,-.1931,-.1921,-.1911,-.1903, COND1520
3 -.1895,-.1887,-.1881,-.1874,-.1869,-.1863,-.1859, COND1530
4 .923,.923,.922,.922,.921,.920,.919,.919,.918,.917, COND1540
5 .916,.916,.915,.915/ COND1550
DATA QK/300.143,284.791,271.027,258.609,247.345,237.076, COND1560
1 227.674,219.029,211.053,203.669,196.814,190.432, COND1570
2 194.477,178.906, COND1580
3 -.1679,-.1669,-.1661,-.1654,-.1648,-.1644,-.1640,-.1636,-.1633, COND1590
4 -.1630,-.1627,-.1624,-.1620,-.1616, COND1600
5 .921,.919,.917,.915,.914,.912,4*.911,.912,.913,.915,.917/ COND1610
DATA QCO2 /19.15,18.13,17.22,16.39,15.64,14.96,14.34,13.77,13.25 COND1620
1 ,12.77,12.33,11.92,11.55,11.20, COND1630
2 -.1802,-.1823,-.1836,-.1841,-.1840,-.1831,-.1816,-.1796, COND1640
3 -.1769,-.1738,-.1700,-.1658,-.1610,-.1558 COND1650
4 ,.857,.870,.883,.897,.911,.926,.942,.957,.974,.992 COND1660
5 ,1.010,1.029,1.049,1.070/ COND1670
DATA QKOH/355.0,335.0,313.0,303.0,289.0,276.0,264.0,253.0,243.0, COND1680
*234.0,225.0,217.0,210.0,203.0 COND1690
2 ,-.1994,-.1993,-.1992,5*-.1990,2*-.1991,-.1992,-.1993,-.1994 COND1700
3 ,-.1995 COND1710
4 ,2*.903,.902,2*.901,.900,.900,.899, 3*.898,3*.897/ COND1720
DATA QN2 / 9.00,9.178, 9.270,9.358,9.445,9.532 COND1730
1 ,9.620,9.710,9.804,9.903,10.007,10.115,10.229,10.349 COND1740
2 ,.2757,.2741,.2737,.2747,.2769 COND1750
3 ,.2804,.2852 ,.2911,.2980,.3058, COND1760
4 ,.3143,.3234,.3330,.3427 COND1770
5 ,1.428,1.444,1.467,1.495,1.529,1.568,1.611 COND1780
6 ,1.657,1.705,1.753,1.801,1.847,1.891,1.931/ COND1790
DATA QOH /87.00,82.19,77.90,74.05,70.58,67.42,64.54, COND1800
1 61.91,59.48,57.25,55.18,53.26,51.48,49.81 COND1810
2 ,-.1981,-.1969,-.1959,-.1948,-.1939,-.1930,-.1922,-.1914 COND1820
3 ,.1908,-.1901,-.1895,-.1889,-.1883,-.1878 COND1830
4 ,.921,3*.920,2*.919,2*.918,3*.917,3*.916/ COND1840
DATA IHE/4HE /,IHCO2/4HCO2 /,IHCO/4HCO /,IHK/4HK / COND1850
1 ,IHH2O,IHN2,IHOH,IHH,IHKOH,IHO2,IHNO,IHSO2,IHAR,IHCS COND1860
2 /3HH2O,2HN2,2HOH,1HH,3HKOH,2HO2,2HNO,3HSO2,2HAR,2HCS COND1870
3 , IHO,IHH2/IHO,2:HH2/ COND1880
DATA IPLS/1H+/,IMNS/1H-/ COND1890
COND1900
C IF(TT.EQ.0.)GO TO 1000 COND1910
I=NPT COND1920
10 SIGMA(I)=0. COND1930
DO 20 K=1,NSK COND1940
IF (JSUB(K,1).EQ. IHE) GO TO 30 COND1950
20 CONTINUE COND1960
GO TO 200 COND1970
30 KE=K COND1980
I=NPT COND1990
QN(I)=0.0 COND2000
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      A2QN(I)=0.0
      A5QN(I)=0.0
      APOS(I)=0.0
      ANEG(I)=0.0
      AITE = (TTT(I)-1700.)/100. +1.
      AITE=AMIN1(AITE,13.)
      AITE=-MAX1(AITE,1.)
      ITE(I)=AITE
      X1(I)=AITE-FLOAT(ITE(I))
      X2(I)=1.0 - X1(I)
40    CONTINUE
      INOQ = 0
      IWP=0
      IWN=0
      DO 170 N=1,NSK
      IF (N .NE. KE) GO TO 60
      J=NPT
      ANE(J) = EN(J,KE)*6.02252E23*1.E+6/VLM(J)
50    CONTINUE
      GO TO 170
60    CONTINUE
      J=NPT
      AN(J) = EN(J,N)*6.02252E23*1.E+6/VLM(J)
70    CONTINUE
      L=NPT
      IF (AN(L) .GT. 1.E15) GO TO 90
80    CONTINUE
      GO TO 170
90    CONTINUE
      DO 100 J=1,3
      MSK(1)=JSUB(N,J)
      DECODE(4,2000,MSK) MASK
2000  FORMAT(4A1)
      DO 100 JJ=1,4
      IF(MASK(JJ) .EQ. IPLS) GO TO 130
      IF(MASK(JJ) .EQ. IMNS) GO TO 150
100   CONTINUE
C     NEUTRAL SPECIES
      ISPEC=100
      IF (JSUB(N,1).EQ. ITCO ) ISPEC= 1
      IF (JSUB(N,1).EQ. IFCO2 ) ISPEC= 2
      IF (JSUB(N,1).EQ. IHH2O ) ISPEC= 3
      IF (JSUB(N,1).EQ. IHK ) ISPEC= 4
      IF (JSUB(N,1).EQ. IHN2 ) ISPEC= 5
      IF (JSUB(N,1).EQ. IHOH ) ISPEC= 6
      IF (JSUB(N,1).EQ. IHH ) ISPEC= 7
      IF (JSUB(N,1).EQ. IHHOH ) ISPEC= 8
      IF (JSUB(N,1).EQ. IHO2 ) ISPEC= 9
      IF (JSUB(N,1).EQ. IHO ) ISPEC= 10
      IF (JSUB(N,1).EQ. IHH2 ) ISPEC= 11
      IF (JSUB(N,1).EQ. IHHO ) ISPEC= 12
      IF (JSUB(N,1).EQ. IHAR ) ISPEC= 13
      IF (JSUB(N,1).EQ. IHCS ) ISPEC= 14
      IF (JSUB(N,1).EQ. IHSO2 ) ISPEC= 15
      IF (ISPEC .LT. 100) GO TO 110
      INOQ = INOQ+ 1
      COND2010
      COND2020
      COND2030
      COND2040
      COND2050
      COND2060
      COND2070
      COND2080
      COND2090
      COND2100
      COND2110
      COND2120
      COND2130
      COND2140
      COND2150
      COND2160
      COND2170
      COND2180
      COND2190
      COND2200
      COND2210
      COND2220
      COND2230
      COND2240
      COND2250
      COND2260
      COND2270
      COND2280
      COND2290
      COND2300
      COND2310
      COND2320
      COND2330
      COND2340
      COND2350
      COND2360
      COND2370
      COND2380
      COND2390
      COND2400
      COND2410
      COND2420
      COND2430
      COND2440
      COND2450
      COND2460
      COND2470
      COND2480
      COND2490
      COND2500
      COND2510
      COND2520
      COND2530
      COND2540
      COND2550

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      JSUBNQ(INOQ,1)=JSUB(N,1)          COND257#
      JSUBNQ(INOQ,2)=JSUB(N,2)          COND258#
      JSUBNQ(INOQ,3)=JSUB(N,3)          COND259#
      GO TO 17#                          COND260#
11# CONTINUE                            COND261#
C   NEUTRAL SPECIES                     COND262#
      J=NPT                              COND263#
      II=ITE(J)                          COND264#
      III=ITE(J)+1                       COND265#
      A2 = (QS(III,2,ISPEC)*X1(J) + QS(II,2,ISPEC)*X2(J)) COND266#
      A5 = (QS(III,3,ISPEC)*X1(J) + QS(II,3,ISPEC)*X2(J)) COND267#
      QNX = (QS(III,1,ISPEC)*X1(J) + QS(II,1,ISPEC)*X2(J))*AN(J)*1.E-2# COND268#
      QN(J) = QN(J) + QNX                COND269#
      A2QN(J) = A2QN(J) + QNX*A2         COND270#
      A5QN(J) = A5QN(J) + QNX*A5         COND271#
12# CONTINUE                            COND272#
      GO TO 17#                          COND273#
13# IWP=IWP+1                           COND274#
      WS1P(IWP,1)=SUB(N,1)               COND275#
      WS1P(IWP,2)=SUB(N,2)               COND276#
      WS1P(IWP,3)=SUB(N,3)               COND277#
C   POSITIVE ION                        COND278#
      J=NPT                              COND279#
14# APOS(J)=AN(J) + APOS(J)              COND280#
      BP(IWP)=AN(J)                      COND281#
      GO TO 17#                          COND282#
15# IWN=IWN+1                           COND283#
      WS1N(IWN,1)=SUB(N,1)               COND284#
      WS1N(IWN,2)=SUB(N,2)               COND285#
      WS1N(IWN,3)=SUB(N,3)               COND286#
C   NEGATIVE ION                       COND287#
      J=NPT                              COND288#
16# ANEG(J)=AN(J) + ANEG(J)              COND289#
      BN(IWN)=AN(J)                      COND290#
17# CONTINUE                            COND291#
      IF(PFLAG) WRITE(6,137) NPT         COND292#
137 FORMAT(/44X,45HION NUMBER DENSITY AND CONDUCTIVITY AT POINT , COND293#
      * I3/1(6X,34HION,9X,15HDENS (M-3),3X)) COND294#
      IF(PFLAG) WRITE(6,136) (IW,(WS1P(IW,JW),JW=1,3),BP(IW),IW=1,IWP) COND295#
      IF(PFLAG) WRITE(6,136) (IW,(WS1N(IW,JW),JW=1,3),BN(IW),IW=1,IWN) COND296#
136 FORMAT(/4(2X,I2,2X,3A4,1X,1PE9.3,3X)) COND297#
      J=NPT                              COND298#
      IF (ANE(J) .GT. 1.E1#) GO TO 18#   COND299#
      TOTAL(J)=#                         COND300#
      AIONS(J)=#                         COND301#
      SIGM(J)=#                          COND302#
      GO TO 19#                          COND303#
18# CONTINUE                            COND304#
      TT=TTT(J)                          COND305#
      SQRTT=DSQRT(TTT(J))                COND306#
      TOTA(J) = 8283.*SQRTT*QN(J)        COND307#
      AIONS(J) = APOS(J)+ANEG(J)          COND308#
      AIONS(J)=AMAX1(AIONS(J),ANE(J))     COND309#
      ALAM = 2.789E6 * SQRT(TT**3/AIONS(J)) COND310#
      ALNLAM = ALOG(ALAM)                 COND311#
      QEE = 4.386E-1#*ALNLAM/TT**2       COND312#

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ANUEE = 1.1714E4 * AIONS(J) * SQRTTT * QEE COND31300
TOTAL(J) = TOTA(J) + ANUEE COND31400
STAR = .4*(1.-1./(2.*ALNLM)) * ANUEE + A5QN(J) COND31500
ANU0 = A2QN(J) COND31600
DELTA = 2.5 * ANU0 ** 2 / STAR / TOTAL(J) COND31700
SIG = 2.818E-8 * ANE(J) / TOTAL(J) COND31800
FACT = 1. / (1. - DELTA) COND31900
SIGMA(J) = SIG * FACT COND32000
IF(PFLAG) WRITE(6,191) SIGMA(J) COND32100
191 FORMAT(16HCONDUCTIVITY = F10.4,2X,7H(MHO/M) //) COND32200
SIGM(J) = SIG * FACT * TOTAL(J) / TOTA(J) COND32300
1900 CONTINUE COND32400
2000 CONTINUE COND32500
C COND32600
10000 RETURN COND32700
END COND32800
SUBROUTINE NEWOF NEWO 100
C NEWO 200
C SAVES OR USES COMPOSITIONS FROM PREVIOUS POINT AS INITIAL ESTIMATES NEWO 300
C NEWO 400
C THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR NEWO 500
C NON-CDC MACHINES NEWO 600
C NEWO 700
C DOUBLE PRECISION TTT,TM,PP,SIGMA,SIG,VLM1,VLM NEWO 800
C DOUBLE PRECISION S,S0,ENN,SUMN NEWO 1000
C INTEGER SUB NEWO 1100
C NEWO 1200
C LOGICAL SHOCK,IMHG,UV,DETN,SIUNIT,NSOM,CALCH NEWO 1300
C LOGICAL HP,SP,TP,NEWR,IONS,MOLES,FROZ,EQL,PSIA,RKT,VOL,TV,SV NEWO 1400
C LOGICAL FA,OXFL,ERATIO,FPCT,OTTO NEWO 1500
C LOGICAL NEQL,CONVG,LOGV,AREA,TWOSTG NEWO 1600
C NEWO 1700
C NEWO 1800
COMMON/MISC/S0 ENN,SUMN,TT,ATOM(3,101),LLMT(30),B0(30),B0P(30,2) NEWO 1900
1 ,TM,TLOW,TMID,THIGH,CPSUM,PP,OF,EORAT,FPCT,R,RR,HSUB0,AC(2),AM(2) NEWO 2000
2 ,HPP(2),PH(2),VMIN(2),VPLS(2),WP(2),DATA(30),NAME(30,5) NEWO 2100
3 ,ANUM(30,5),PECWT(30),ENTH(30),FAZ(30),RTEMP(30),FOX(30),DENS(30) NEWO 2200
4 ,RHOP,RMW(30),TLN,CR,OXI(30),ENNL,ENSAVE,ENLSAV,TRACE,SIZE NEWO 2300
COMMON/INDX/ IDEBUG,CONVE,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM NEWO 2400
1 ,NS,KMAT,IMAT,IOI,NOF,NOMIT,IP,NEWR,NSUB,NSUP,ITM,CPCVFR,CPCVEO NEWO 2500
2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH NEWO 2600
3 ,ISAVE,LSAVE,ISUP,ISUB,ITNUM NEWO 2700
COMMON/MIWE4/PCVET(2),HPP2(2),PCWSD(2),B0P2(30,2) NEWO 2800
COMMON/SPCE1/NCPCMX,NCMAX,NELMX,TEMP(175,2),SUB(600,3),S(1) NEWO 2900
COMMON/TSTG/TWOSTG,ALPH,NLMI,XELMC(30),XMWC(1) NEWO 3000
C... NSPCM REFERS TO THE MAXIMUM NO. OF SPECIES ALLOWED NEWO 310
C... NCMAX REFERS TO THE MAXIMUM NO. OF CONDENSED SPECIES ALLOWED NEWO 320
C THIS IS FIXED AND REFERS TO THE SIZE OF TEMP(N,2) IN COMMON NEWO 330
C SPEC1.....MUST CHANGE THIS COMMON EVERYWHERE IF A LARGER SNEWO 340
C IS NEEDED NEWO 350
C... NELMX REFERS TO THE MAXIMUM NO. OF ELEMENTS ALLOWED NEWO 360
C THIS IS FIXED AND REFERS TO THE SIZE OF XELMC(N) AND A(N,NSNEWO 370
C .....MUST CHANGE COMMON TSTG AND STOIC EVERYWHERE IF NEWO 380
C A LARGER SIZE IS NEEDED NEWO 390
C NEWO 400

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EQUIVALENCE (A(1),JSOLS),(AC(2),JLIQS) NEWO 410
EQUIVALENCE (OTTO,CPCVFR),(CPCVEQ,LOGV) NEWO 420
C NEWO 430
C NEWO 440
C NEWO 450
C NEWO 460
C NEWO 470
WRITE(6,730) OF NEWO 480
730 FORMAT(6HOF = ,F10.6) NEWO 490
EQRAT = 0. NEWO 500
SUM = OF + 1. NEWO 510
IF(.NOT.TWOSTG)GO TO 735 NEWO 520
SUM=PCWFT(2)+OF*PCWFT(1) NEWO 530
735 CONTINUE NEWO 540
V2 = (OF*VMIN(1)+VMIN(2))/SUM NEWO 550
V1 = (OF*VPLS(1)+VPLS(2))/SUM NEWO 560
IF(V2.NE.0.) EQRAT=ABS(V1/V2) NEWO 570
IF (RH(1).NE.0. .AND. RH(2).NE.0.) GO TO 744 NEWO 580
RHOP = RH(2) NEWO 590
IF (RHOP.EQ.0.) RHOP = RH(1) NEWO 600
GO TO 745 NEWO 610
744 RHOP = (OF+1.)*RH(1)*RH(2)/(RH(1)+ OF *RH(2)) NEWO 620
745 DO 747 I=1,NLM NEWO 630
B0(I) = (OF *B0P(I,1)+ B0P(I,2))/SUM NEWO 640
IF(I.NE.1) GO TO 746 NEWO 650
BIGB = B0(1) NEWO 660
SMALB = B0(1) NEWO 670
GO TO 747 NEWO 680
746 IF(B0(I).EQ.0.) GO TO 747 NEWO 690
IF(B0(I).LT.SMALB) SMALB=B0(I) NEWO 700
IF(B0(I).GT.BIGB) BIGB=B0(I) NEWO 710
747 CONTINUE NEWO 720
NPT = 1 NEWO 730
IF(.NOT.CALCH) GO TO 750 NEWO 740
CALL HCALC NEWO 750
IF(TT.EQ.0.) RETURN NEWO 760
CALCH = .FALSE. NEWO 770
IF(TWOSTG)GO TO 750 NEWO 780
IF(OF.NE.0.) HPP(1)=SUM*HPP(1)/OF NEWO 790
HPP(2) = SUM*HPP(2) NEWO 800
GO TO 760 NEWO 810
750 HSUB0= (OF*HPP(1) + HPP(2))/SUM NEWO 820
760 CONTINUE NEWO 830
TEM = SMALB/BIGB NEWO 840
SIZE = 18.420681 NEWO 850
IF(TEM.LT.1.E-5) SIZE=ALOG(1000./TEM) NEWO 860
JSOL = 0 NEWO 870
JLIQ = 0 NEWO 880
WRITE (6,770) NEWO 890
770 FORMAT(1H ,25X,14HEFFECTIVE FUEL,10X,17HEFFECTIVE OXIDANT,12X,7HMINENTURE ) NEWO 900
1XTURE ) NEWO 910
IF(VOL) WRITE(6,772) NEWO 920
IF(.NOT.VOL) WRITE(6,774) NEWO 930
772 FORMAT(16H INTERNAL ENERGY,14X,6HHPP(2),19X,6HHPP(1),19X,5HHSUB0 ) NEWO 940
774 FORMAT(9H ENTHALPY,21X,6HHPP(2),19X,6HHPP(1),19X,5HHSUB0 ) NEWO 950
WRITE(6,776)HPP(2),HPP(1),HSUB0 NEWO 960
776 FORMAT(19H (KG-MOL)(DEG K)/KG,E21.3,E25.8 )

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WRITE(6,778)
778 FORMAT(12H0KG-ATOMS/KG,17X,8HB0P(I,2),17X,8HB0P(I,1),18X,5HB0(I))
780 FORMAT(7X,A4,4X,3E25.8)
WRITE(6,780)(LLMT(I), B0P(I,2),B0P(I,1),B0(I),I=1,NLM)
RETURN
END
C.....THIS PACKAGE CONTAINS THE FOLLOWING SUBROUTINES
C      (1) GAUSS
C      (2) VAREMT
C      (3) EFMT
C      (4) THERMP
C      (5) FUNCTION INTERP
C      (6) DEGOUT
C.....
SUBROUTINE GAUSS
C
C      SOLVE ANY LINEAR SET OF UP TO 60 EQUATIONS
C      NUMBER OF EQUATIONS = IMAT
C
C      DOUBLE PRECISION G,X,COEFX,SUM,Z
C
C      LOGICAL SHOCK,MMHG,UV,DETN,SIUNIT,NSQM,CALCH
C      LOGICAL HP,SP,TP,NEW,IONS,MOLES,PROZ,EQL,PSIA,RKT,VOL,TV,SV
C      LOGICAL FA,ERATIO,FPCT,OPTO,SPLG
C      LOGICAL NEQL,CONVG,LOGV,SFLG,AREA
C      DIMENSION COEFX(60)
C      COMMON/DOUBLE/ G(60,61), X(60)
C      COMMON/MIKE0/NNDUNY(3),IMPRNT,NMPATH,NUMIV,XINDP(1)
C      COMMON/INIX/ IDEBUG,CONVG,TP,HP,SP,ISV, NPP, MOLES,NP,NT,NPT,NLM
1  ,NS,KMAT,IMAT,IOI,NOF,NOMIT,IP,NEW,NSUB,NSUP,ITM,CPCVFR,CPCVEQ
2  ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCHGAUS
3  ,IQSAVE,LSAVE,ISUP,ISUB,ITNUM
C
C      EQUIVALENCE (OTTO,CPCVFR),(CPCVEQ,LOGV)
C
C      DATA BIGNO/1.E+30/
C
C      BEGIN ELIMINATION OF NNTH VARIABLE
C
C      IUSE1 = IMAT+1
6  DO 45 NN=1,IMAT
  IF(NN-IMAT) 8,83,8
83  IF(G(NN,NN))31,23,31
C
C      SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW
C
8  DO 18 I=NN,IMAT
  COEFX(I) = BIGNO
  IF(G(I,NN).EQ.0.) GO TO 18
  COEFX(I) = 0.
  DO 10 J=NN,IUSE1
    SUM = G(I,J)
    IF(SUM.LT.0.) SUM=-SUM
    IF(J.NE.NN) GO TO 9
    Z = SUM
  GO TO 10

```

```

NEW0 970
NEW0 980
NEW0 990
NEW01000
NEW01010
NEW01020
GAUS 10
GAUS 20
GAUS 30
GAUS 40
GAUS 50
GAUS 60
GAUS 70
GAUS 80
GAUS 90
GAUS 100
GAUS 110
GAUS 120
GAUS 130
GAUS 140
GAUS 150
GAUS 160
GAUS 170
GAUS 180
GAUS 190
GAUS 200
GAUS 210
GAUS 220
GAUS 230
GAUS 240
GAUS 250
GAUS 260
GAUS 270
GAUS 280
GAUS 290
GAUS 300
GAUS 310
GAUS 320
GAUS 330
GAUS 340
GAUS 350
GAUS 360
GAUS 370
GAUS 380
GAUS 390
GAUS 400
GAUS 410
GAUS 420
GAUS 430
GAUS 440
GAUS 450
GAUS 460
GAUS 470
GAUS 480
GAUS 490
GAUS 500

```

9	IF(SUM.GT.COEFX(I)) COEFX(I)=SUM	GAUS 510
10	CONTINUE	GAUS 520
	COEFX(I) = COEFX(I)/Z	GAUS 530
18	CONTINUE	GAUS 540
C		GAUS 550
C	LOCATE ROW WITH SMALLEST MAXIMUM COEFFICIENT	GAUS 560
C		GAUS 570
	TEMP = BIGNO	GAUS 580
	I=0	GAUS 590
20	DO 22 J=NN,IMAT	GAUS 600
	IF (COEFX(J)-TEMP) 87,22,22	GAUS 610
87	TEMP=COEFX(J)	GAUS 620
	I=J	GAUS 630
22	CONTINUE	GAUS 640
	IF(I) 28,23,28	GAUS 650
C		GAUS 660
C	INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH	GAUS 670
C	VARIABLE FROM THE REMAINING EQUATIONS	GAUS 680
C		GAUS 690
C	INTERCHANGE EQUATIONS I AND NN	GAUS 700
C		GAUS 710
28	IF(NN-I) 29,31,29	GAUS 720
29	DO 30 J=NN,IUSE1	GAUS 730
	Z=G(I,J)	GAUS 740
	G(I,J)=G(NN,J)	GAUS 750
	G(NN,J)=Z	GAUS 760
30	CONTINUE	GAUS 770
C		GAUS 780
C	DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH	GAUS 790
C	VARIABLE FROM THE REMAINING EQUATIONS	GAUS 800
C		GAUS 810
31	K = NN + 1	GAUS 820
	DO 36 J = K, IUSE1	GAUS 830
	IF(G(NN,NN).EQ.0.) GO TO 23	GAUS 840
	G(NN,J) = G(NN,J) / G(NN,NN)	GAUS 850
36	CONTINUE	GAUS 860
	IF(K-IUSE1) 88,45,88	GAUS 870
88	DO 44 I=K,IMAT	GAUS 880
40	DO 44 J = K, IUSE1	GAUS 890
	G(I,J) = G(I,J) - G(I,NN)*G(NN,J)	GAUS 900
44	CONTINUE	GAUS 910
45	CONTINUE	GAUS 920
C		GAUS 930
C	BACKSOLVE FOR THE VARIABLES	GAUS 940
C		GAUS 950
	K = IMAT	GAUS 960
47	J = K + 1	GAUS 970
	X(K) = 0.0D0	GAUS 980
	SUM = 0.0	GAUS 990
	IF(IMAT-J) 51,48,48	GAUS1000
48	DO 50 I=J,IMAT	GAUS1010
	SUM = SUM + G(K,I)* X(I)	GAUS1020
50	CONTINUE	GAUS1030
51	X(K) = G(K,IUSE1) - SUM	GAUS1040
	K = K - 1	GAUS1050
	IF (K) 47,151,47	GAUS1060

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23 NSERT=NN                                GAUS1070
   IF(I.NE.0)GO TO 151                    GAUS1080
   NUMDEG=1                               GAUS1090
   IF(IMPRNT.GE.0)CALL DBGOUT(IMAT,HP,SP,COEFX,NUMDEG) GAUS1100
151 RETURN                                GAUS1110
   END                                    GAUS1120
   SUBROUTINE VAREMT(V,NPT)                VARE 10
C                                          VARE 20
   DIMENSION V(13)                        VARE 30
C                                          VARE 40
   COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4) VARE 50
1   ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2 VARE 60
2   ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0 VARE 70
C                                          VARE 80
   DO 45 I=1,NPT                          VARE 90
   K= 2*I+3                               VARE 100
   FMT(K) = F4                             VARE 110
   IF (V(I).GE.10.) FMT(K) = F3            VARE 120
   IF (V(I).GE.100.) FMT(K) = F2          VARE 130
   IF (V(I).GE.10000.) FMT(K) = F1        VARE 140
   IF (V(I).GE.1000000.) FMT(K) = F0     VARE 150
45 CONTINUE                               VARE 160
   RETURN                                VARE 170
   END                                    VARE 180
   SUBROUTINE EFMT(NPT,AA,V)              EFMT 10
C                                          EFMT 20
   DIMENSION AA(3), V(13), W(13), NE(13), FRMT(7) EFMT 30
   COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4) EFMT 40
1   ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2 EFMT 50
2   ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0 EFMT 60
C                                          EFMT 70
   DATA FRMT/3H(1H,4H,3A4,4H,11X,4H,13(,4HF7.4,4H,I2),1H)/,F63/4HF6.3EFMT 80
1/,FI3/4H,I3)/,F74/4HF7.4/,FI2/4H,I2)/,F11X/4H,11X/,F2X/3H,2X/ EFMT 90
   DATA W/13*0./,NE/13*0/              EFMT 100
C                                          EFMT 110
   FRMT(5) = F74                          EFMT 120
   FRMT(6) = FI2                          EFMT 130
   J1 = 1                                EFMT 140
   FRMT(3) = F2X                          EFMT 150
   IF(FMT(4).NE.FMT9X) GO TO 130          EFMT 160
   J1 = 2                                EFMT 170
   FRMT(3) = F11X                         EFMT 180
130 DO 145 I=J1,NPT                      EFMT 190
   IF(V(I).NE.0.) GO TO 140              EFMT 200
   W(I) = 0.                             EFMT 210
   NE(I) = 0                             EFMT 220
   GO TO 145                             EFMT 230
140 EE = ALOG10(ABS(V(I)))               EFMT 240
   NE(I) = EE                             EFMT 250
   FE = NE(I)                             EFMT 260
   IF(ES.LE.0..AND.FE.NE.EE) NE(I)=NE(I)-1 EFMT 270
   IF(IABS(NE(I)).LT.10) GO TO 144        EFMT 280
   FRMT(5) = F63                          EFMT 290
   FRMT(6) = FI3                          EFMT 300
144 W(I) = V(I)/10.**NE(I)               EFMT 310
145 CONTINUE                             EFMT 320

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C	PROGRAM NEQMDH(INPUT,OUTPUT,TAPE7,TAPE5=INPUT,TAPE6=OUTPUT)	MAIN 10	PAGE 5130
	WRITE(6,FRMT) (AA(I),I=1,3),(W(J), NE(J),J=J1,NPT)	EFMT 330	
1000	RETURN	EFMT 340	
	END	EFMT 350	
	SUBROUTINE THERMP	THER 10	
C		THER 20	
C	THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR	THER 30	
C	NON-CDC MACHINES	THER 40	
C		THER 50	
	DOUBLE PRECISION TTT,TM,PP,SIGMA,SIG,VLM1,VLM	THER 60	
	DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS,S0	THER 70	
	DOUBLE PRECISION S,ENLN,H0,DELN,ENN,SUMN	THER 80	
C		THER 90	
	LOGICAL SHOCK,MMHG,UV,DETN,SIUNIT,NSQM,CALCH	THER 100	
	LOGICAL HP,SP,TP,NEWR,IONS,MOLES,FROZ,EQL,PSIA,RKT,VOL,TV,SV	THER 110	
	LOGICAL ERATIO,FPCT,OTTO,SFLG	THER 120	
	LOGICAL NEQL,CONVG,LOGV,SFLG,AREA	THER 130	
C		THER 140	
	DIMENSION VL(26)	THER 150	
C		THER 160	
	COMMON/MIKES/EXIN,BZOUT(13),BETOUT(13)	THER 170	
	COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)	THER 180	
	1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)	THER 190	
	2 ,VLH(13),TOTN(13)	THER 200	
	COMMON/MISC/S0,ENN,SUMN,TT,ATOM(3,101),LLMT(30),B0(30),B0P(30,2)	THER 210	
	1 ,TM,TLOW,TMID,THIGH,CPSUM,PP,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)	THER 220	
	2 ,HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(30),NAME(30,5)	THER 230	
	3 ,ANUM(30,5),PECWT(30),ENTH(30),FAZ(30),RTEMP(30),FOX(30),DENS(30)	THER 240	
	4 ,RHOP,RMW(30),TLN,CR,OXF(30),ENNL,ENSAVE,ENLSAV ,TRACE	THER 250	
	COMMON/INDEX/ IDEBUG,CONVG,TP,HP,SP,ISV, NPP, MOLES,NP,NT,NPT,NLM	THER 260	
	1 ,NS,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,NSUB,NSUP,ITM,CPCVFR,CPCVEQ	THER 270	
	2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH	THER 280	
	3 ,IQSAVE,LSAVE,ISUP,ISUB,ITNUM	THER 290	
	COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)	THER 300	
	1 ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2	THER 310	
	2 ,FRI,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0	THER 320	
C		THER 330	
	EQUIVALENCE (K,ISV),(VL(1),P(1)),(UV,HP),(TP,TV),(SP,SV)	THER 340	
C		THER 350	
	EQUIVALENCE (OTTO,CPCVFR),(CPCVEQ,LOGV)	THER 360	
C		THER 370	
	DATA FUU/4HU, C/	THER 380	
C		THER 390	
	IF(T(1).EQ.0.) T(1) = 3000.	THER 400	
C		THER 410	
	IOF = 0	THER 420	
95	IOF = IOF+1	THER 430	
	OF = OXF(IOF)	THER 440	
	CALL NEWOF	THER 450	
	IF(TT.EQ.0..AND.CALCH) RETURN	THER 460	
C		THER 470	
C	SET ASSIGNED P OR VOLUME	THER 480	
C		THER 490	
C	ADD SPECIAL HTLOSS TO HSUB0 FOR HP PROBLEM WHEN EXIN .LT. 0.0	THER 500	
C	THAT IS HTLOSS=-EXIN/1.987165	THER 510	
	IF(.NOT.HP)GO TO 901	THER 520	
	IF(EXIN.GE.0.0)GO TO 901	THER 530	
	HSUB0=HSUB0+EXIN/1.987165		

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901 CONTINUE                                THER 540
DO 903 IP=1,NP                              THER 550
PP = P(IP)                                  THER 560
C                                             THER 570
C SET ASSIGNED T                            THER 580
C                                             THER 590
DO 902 IT=1,NT                              THER 600
VLM(NPT) = VL(IP)                          THER 610
TT = T(IT)                                 THER 620
CALL EQLBRM(.TRUE.)                        THER 630
CALL CONDOC(.TRUE.)                        THER 640
IF(TT.NE.0.)GO TO 800                      THER 650
IF(NPT.EQ.0) GO TO 1000                    THER 660
800 K = 0                                    THER 670
IF(IP.EQ.NP.AND.IT.EQ.NT.OR.TT.EQ.0.) GO TO 360 THER 680
K = NPT                                     THER 690
IF(NPT.NE.11) GO TO 870                    THER 700
860 IF(.NOT.HP) WRITE(6,5)                  THER 710
5 FORMAT(1H1,41X,48HTHERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED THER 720
1)                                           THER 730
IF(HP) WRITE(6,6)                          THER 740
6 FORMAT(1H1,36X,59HTHERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES THER 750
1AT ASSIGNED )                             THER 760
IF(.NOT.VOL) GO TO 861                     THER 770
IF(UV) WRITE(6,10)                         THER 780
10 FORMAT(1H0,62X,7H VOLUME /)             THER 790
IF(TV) WRITE(6,11)                         THER 800
11 FORMAT(1H0,54X,22HTEMPERATURE AND VOLUME/) THER 810
IF(SV) WRITE(6,12)                         THER 820
12 FORMAT(1H0,56X,18HENTROPY AND VOLUME/)  THER 830
GO TO 862                                  THER 840
861 IF(HP) WRITE(6,20)                      THER 850
20 FORMAT(1H0,62X,10H PRESSURES /)         THER 860
IF(TP) WRITE(6,21)                         THER 870
21 FORMAT(1H0,53X,24HTEMPERATURE AND PRESSURE/) THER 880
IF(SP) WRITE(6,22)                         THER 890
22 FORMAT(1H0,55X,20HENTROPY AND PRESSURE/) THER 900
862 CALL OUT1                              THER 910
WRITE (6,863)                              THER 920
863 FORMAT (25H0THERMODYNAMIC PROPERTIES//) THER 930
IF(.NOT.VOL) GO TO 864                     THER 940
FMT(4) = FMT(6)                            THER 950
IF(.NOT.UV) GO TO 864                      THER 960
DO 63 I=1,NPT                              THER 970
FMT(2*I+3) = F2                             THER 980
V(I) = HSUB0*R                              THER 990
63 CONTINUE                                THER1000
WRITE(6,FMT) FUU,PH(2),F3,FB,(V(I),I=1,NPT) THER1010
864 CALL OUT2                              THER1020
CALL OUT3                                  THER1030
865 IF(K.EQ.0 .AND. IOF.EQ.NOF) GO TO 1000 THER1040
IF(IDEBUG.GT.1:) IDEBUG=IDEBUG-13          THER1050
WRITE(6,863)                               THER1060
868 FORMAT(1H1)                             THER1070
NPT = 0                                     THER1080
870 NPT = NPT + 1                          THER1090

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      IF(.NOT.TP.AND.TT.NE.0.) T(1)=TT
      IF(NT.EQ.1.AND.NP.EQ.1) GO TO 95
      IF(IP.EQ.1.AND.IT.EQ.1) ISV=-ISV
      IF(NT.EQ.1) GO TO 871
      IF(IT.EQ.NT.OR.TT.EQ.0.) ISV=0
871  CALL SAVE
902  CONTINUE
903  CONTINUE
      GO TO 95
1000 RETURN
      END
      REAL FUNCTION INTERP(XCC,X,Y,NDEG,NPTS,DINT,IER)
C
C
C  FUNCTION PERFORMS NEWTONS INTERPOLATION FOR DISCRETE DATA
C  AS A FUNCTION OF ONE VARIABLE
C
C
C  WHERE XC - INDEPENDENT VARIABLE AT WHICH THE INTERPOLATED VALUE
C            OF THE DEPENDENT VARIABLE IS DESIRED
C            X - TABLE OF INDEPENDENT VARIABLE VALUES IN INCREASING
C              ORDER
C            Y - CORRESPONDING TABLE OF DEPENDENT VARIABLE VALUES
C            NDEG - ORDER OF THE INTERPOLATING POLYNOMIAL USED (MAX - 10)
C            NPTS - NUMBER OF ENTRIES IN X AND Y
C            DINT - DERIVATIVE AT XC
C            IER - RETURN CODE:
C                  0 = INTERPOLATION WAS PERFORMED
C                 -1 = EXTRAPOLATION BELOW TABLE VALUES
C                  1 = EXTRAPOLATION ABOVE TABLE VALUES
C
C  ROUTINE MODIFIED FROM 'THE COMPUTING TECHNOLOGY CENTER NUMERICAL
C  ANALYSIS LIBRARY', O.R.N.L.
C
      DIMENSION X(1),Y(1),Y1(11),PI(12)
      INTEGER HI
      DATA PI/12*1./
C
      XC=XCC
      NFIT=NDEG + 1
      N=NFIT
      MFLAG=0
      IF(N.GT. NPTS) N=NPTS
      IF(XC-X(1)) 50,20,10
10  IF(XC.GT. X(NPTS)) GO TO 70
20  IER=0
      DO 30 I=1,NPTS
      IF(XC - X(I)) 40,120,30
120 XC=XC + .000001
      MFLAG=I
      CONTINUE
30  LOW=I - (N+1)/2
40  IF(LOW.LE. 0) GO TO 60
      HI=LOW + N - 1

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      IF(HI .GT. NPTS) GO TO 87
      GO TO 98
C
C   XC LT X(1)
C
58   IER=-1
68   HI=N
      LOW=1
      GO TO 98
C
C   XC GT X(NPTS)
C
78   IER=1
88   LOW=NPTS - N + 1
      HI=NPTS
C
C   INTERPOLATE
C
98   CON=1.
      DINT=8.
      Y1(1)=Y(LOW)
      INTERP=Y(LOW)
      IM=LOW - 1
      IL=LOW + 1
      DO 118 K=IL,HI
      VAL=INTERP
      IA=K - LOW
      IS=IA + 1
      Y1(IS)=Y(K)
      DO 188 I=1,IA
      IR=IM + I
      IF(X(IR).EQ.X(K))GO TO 188
      Y1(IS) = (Y1(I)-Y1(IS))/(X(IR)-X(K))
188  CONTINUE
      CON=CON*(XC-X(K-1))
      PI(IA+1)=CON
      CON1=PI(IA)
      IF(IA .LT. 2) GO TO 112
      DO 111 I=2,IA
      IF(PI(I).EQ.8.8)GO TO 111
      CON1=CON1 + CON*PI(I-1)/PI(I)
111  CONTINUE
112  DINT=DINT + CON1*Y1(IS)
118  INTERP=VAL + CON*Y1(IS)
      IF(MFLAG.NE.8)INTERP=Y(MFLAG)
      RETURN
      END
      SUBROUTINE DBGOUT(N,H,S,X,K)
      LOGICAL H,S
      DOUBLE PRECISION X
      DIMENSION X(1)
      DATA IH/8/,IS/8/
      IF(H)IH=1
      IF(S)IS=1
      WRITE(1,10) N,H,S,K
      WRITE(1,11)
      INTE 468
      INTE 478
      INTE 488
      INTE 498
      INTE 508
      INTE 518
      INTE 528
      INTE 538
      INTE 548
      INTE 558
      INTE 568
      INTE 578
      INTE 588
      INTE 598
      INTE 608
      INTE 618
      INTE 628
      INTE 638
      INTE 648
      INTE 658
      INTE 668
      INTE 678
      INTE 688
      INTE 698
      INTE 708
      INTE 718
      INTE 728
      INTE 738
      INTE 748
      INTE 758
      INTE 768
      INTE 778
      INTE 788
      INTE 798
      INTE 808
      INTE 818
      INTE 828
      INTE 838
      INTE 848
      INTE 858
      INTE 868
      INTE 878
      INTE 888
      INTE 898
      INTE 908
      INTE 918
      INTE 928
      DBGO 18
      DBGO 28
      DBGO 38
      DBGO 48
      DBGO 58
      DBGO 68
      DBGO 78
      DBGO 88
      DBGO 98

```

```

      DO 5 I=1,N
      WRITE(1,12) I,X(I)
      5 CONTINUE
10  FORMAT(1X,7(1H*),I3,19H DEBUG PTS. FOR HP=,I2,8H AND SP=,I2,
      *2X,15HDBG OUTPUT NO. ,I3,1X,7(1H*),/)
11  FORMAT(10X,6HNUMBER,10X,5HVALUE)
12  FORMAT(11X,I3,7X,G18.9)
      RETURN
      END
      SUBROUTINE DIFSUB(N,T,Y,SAVE,H,HMIN,HMAX,EPS,MF,YMAX,ERROR,KFLAG,
      1 JSTART,MAXDER,PW,IPS,PSCALE,ND)
      IMPLICIT DOUBLE PRECISION (A-H,Q-Z)
      REAL*4 XINDP,B0N,SNEQ
      LOGICAL XDXOU1,XDXOU2
C*****
C*
C* THIS SUBROUTINE INTEGRATES A SET OF N ORDINARY DIFFERENTIAL FIRST
C* ORDER EQUATIONS OVER ONE STEP OF LENGTH H AT EACH CALL. H CAN BE
C* SPECIFIED BY THE USER FOR EACH STEP, BUT IT MAY BE INCREASED OR
C* DECREASED BY DIFSUB WITHIN THE RANGE HMIN TO HMAX IN ORDER TO
C* ACHIEVE AS LARGE A STEP AS POSSIBLE WHILE NOT COMMITTING A SINGLE
C* STEP ERROR WHICH IS LARGER THAN EPS IN THE L-2 NORM, WHERE EACH
C* COMPONENT OF THE ERROR IS DIVIDED BY THE COMPONENTS OF YMAX.
C*
C* THE PROGRAM REQUIRES TWO SUBROUTINES NAMED
C*   DIFFUN(T,Y,DY)
C*   PEDERV(T,Y,PW,M)
C* THE FIRST, DIFFUN, EVALUATES THE DERIVATIVES OF THE DEPENDENT
C* VARIABLES STORED IN Y(1,I) FOR I = 1 TO N, AND STORES THE
C* DERIVATIVES IN THE ARRAY DY.
C* PEDERV IS USED ONLY IF MF IS 1, AND COMPUTES THE PARTIAL
C* DERIVATIVES OF THE DIFFERENTIAL EQUATIONS AS DESCRIBED UNDER THE
C* MF PARAMETER.
C*
C* THE PROGRAM USES DOUBLE PRECISION ARITHMETIC FOR ALL FLOATING
C* POINT VARIABLES EXCEPT THOSE STARTING WITH P. THE LATTER ARE
C* SINGLE PRECISION TO SAVE TIME AND SPACE.
C*
C* THE TEMPORARY STORAGE SPACE IS PROVIDED BY THE CALLER IN THE
C* ARRAYS PW, PSCALE, IPS, AND SAVE.
C* THE ARRAY PW IS USED ONLY TO HOLD THE MATRIX OF THE SAME NAME, BUT
C* SAVE IS USED TO HOLD SEVERAL ARRAYS. THE REGIONS USED ARE
C*   SAVE(J,I) 1.LE.J.LE.8 AND 1.LE.I.LE.N IS USED TO SAVE THE
C*             VALUES OF Y IN CASE A STEP HAS TO BE REPEATED.
C*   SAVE(9,I) IS USED MAINLY TO HOLD THE CORRECTION TERMS IN THE
C*             CORRECTOR LOOP.
C*   SAVE(10,I) IS USED TO SAVE THE VALUES OF THE SUMS OF ALL OF THE
C*             CORRECTION TERMS IN THE PREVIOUS STEP AFTER THEY
C*             HAVE BEEN ACCUMULATED IN THE ARRAY ERROR IN THE
C*             CURRENT STEP. THIS ENABLES THE BACKWARDS DIFFERENCE
C*             OF ERROR TO BE FORMED. IT IS USED TO ESTIMATE THE
C*             STEP SIZE FOR ONE ORDER HIGHER THAN CURRENT.
C*   SAVE(N1+I,1) IS USED TO STORE THE DERIVATIVES WHEN THEY ARE
C*             COMPUTED BY DIFFUN. IT IS ALSO ACCESSED AS
C*             SAVE(N2,1) AS A COMPLETE ARRAY.
C*   SAVE(N5+I,1) HOLDS THE DERIVATIVES DURING JACOBIAN EVALUATIONS.

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      DBGO 100
      DBGO 110
      DBGO 120
      DBGO 130
      DBGO 140
      DBGO 150
      DBGO 160
      DBGO 170
      DBGO 180
      DIFS 10
      DIFS 20
      DIFS 30
      DIFS 40
      DIFS 50
      DIFS 60
      *DIFS 70
      *DIFS 80
      *DIFS 90
      *DIFS 100
      *DIFS 110
      *DIFS 120
      *DIFS 130
      *DIFS 140
      *DIFS 150
      *DIFS 160
      *DIFS 170
      *DIFS 180
      *DIFS 190
      *DIFS 200
      *DIFS 210
      *DIFS 220
      *DIFS 230
      *DIFS 240
      *DIFS 250
      *DIFS 260
      *DIFS 270
      *DIFS 280
      *DIFS 290
      *DIFS 300
      *DIFS 310
      *DIFS 320
      *DIFS 330
      *DIFS 340
      *DIFS 350
      *DIFS 360
      *DIFS 370
      *DIFS 380
      *DIFS 390
      *DIFS 400
      *DIFS 410
      *DIFS 420
      *DIFS 430
      *DIFS 440
      *DIFS 450
      *DIFS 460
      *DIFS 470

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C*           IT IS REFERENCED AS SAVE(N6,1) AS A COMPLETE ARRAY. *DIFS 480
C* THE PARAMETERS TO THE SUBROUTINE DIFSUB HAVE *DIFS 490
C* THE FOLLOWING MEANINGS.. *DIFS 500
C* *DIFS 510
C* N THE NUMBER OF FIRST ORDER DIFFERENTIAL EQUATIONS. N *DIFS 520
C* MAY BE DECREASED ON LATER CALLS IF THE NUMBER OF *DIFS 530
C* ACTIVE EQUATIONS REDUCES, BUT IT MUST NOT BE *DIFS 540
C* INCREASED WITHOUT CALLING WITH JSTART = 0. *DIFS 550
C* T THE INDEPENDENT VARIABLE. *DIFS 560
C* Y AN 8 BY N ARRAY CONTAINING THE DEPENDENT VARIABLES AND *DIFS 570
C* THEIR SCALED DERIVATIVES. Y(J+1,I) CONTAINS *DIFS 580
C* THE J-TH DERIVATIVE OF Y(I) SCALED BY *DIFS 590
C* H**J/FACTORIAL(J) WHERE H IS THE CURRENT *DIFS 600
C* STEP SIZE. ONLY Y(1,I) NEED BE PROVIDED BY *DIFS 610
C* THE CALLING PROGRAM ON THE FIRST ENTRY. *DIFS 620
C* IF IT IS DESIRED TO INTERPOLATE TO NON MESH POINTS *DIFS 630
C* THESE VALUES CAN BE USED. IF THE CURRENT STEP SIZE *DIFS 640
C* IS H AND THE VALUE AT T + E IS NEEDED, FORM *DIFS 650
C* S = E/H, AND THEN COMPUTE *DIFS 660
C* NO *DIFS 670
C* Y(I)(T+E) = SUM Y(J+1,I)*S**J *DIFS 680
C* J=0 *DIFS 690
C* SAVE A BLOCK OF AT LEAST 12*N FLOATING POINT LOCATIONS *DIFS 700
C* USED BY THE SUBROUTINES. *DIFS 710
C* H THE STEP SIZE TO BE ATTEMPTED ON THE NEXT STEP. *DIFS 720
C* H MAY BE ADJUSTED UP OR DOWN BY THE PROGRAM *DIFS 730
C* IN ORDER TO ACHIEVE AN ECONOMICAL INTEGRATION. *DIFS 740
C* HOWEVER, IF THE H PROVIDED BY THE USER DOES *DIFS 750
C* NOT CAUSE A LARGER ERROR THAN REQUESTED, IT *DIFS 760
C* WILL BE USED. TO SAVE COMPUTER TIME, THE USER IS *DIFS 770
C* ADVISED TO USE A FAIRLY SMALL STEP FOR THE FIRST *DIFS 780
C* CALL. IT WILL BE AUTOMATICALLY INCREASED LATER. *DIFS 790
C* HMIN THE MINIMUM STEP SIZE THAT WILL BE USED FOR THE *DIFS 800
C* INTEGRATION. NOTE THAT ON STARTING THIS MUST BE *DIFS 810
C* MUCH SMALLER THAN THE AVERAGE H EXPECTED SINCE *DIFS 820
C* A FIRST ORDER METHOD IS USED INITIALLY. *DIFS 830
C* HMAX THE MAXIMUM SIZE TO WHICH THE STEP WILL BE INCREASED *DIFS 840
C* EPS THE ERROR TEST CONSTANT. SINGLE STEP ERROR ESTIMATES *DIFS 850
C* DIVIDED BY YMAX(I) MUST BE LESS THAN THIS *DIFS 860
C* IN THE EUCLIDEAN NORM. THE STEP AND/OR ORDER IS *DIFS 870
C* ADJUSTED TO ACHIEVE THIS. *DIFS 880
C* MF THE METHOD INDICATOR. THE FOLLOWING ARE ALLOWED.. *DIFS 890
C* 0 AN ADAMS PREDICTOR CORRECTOR IS USED. *DIFS 900
C* 1 A MULTI-STEP METHOD SUITABLE FOR STIFF *DIFS 910
C* SYSTEMS IS USED. IT WILL ALSO WORK FOR *DIFS 920
C* NON STIFF SYSTEMS. HOWEVER THE USER *DIFS 930
C* MUST PROVIDE A SUBROUTINE PEDERV WHICH *DIFS 940
C* EVALUATES THE PARTIAL DERIVATIVES OF *DIFS 950
C* THE DIFFERENTIAL EQUATIONS WITH RESPECT *DIFS 960
C* TO THE Y'S. THIS IS DONE BY CALL *DIFS 970
C* PEDERV(T,Y,PW,M). PW IS AN N BY N ARRAY *DIFS 980
C* WHICH MUST BE SET TO THE PARTIAL OF *DIFS 990
C* THE I-TH EQUATION WITH RESPECT *DIFS1000
C* TO THE J DEPENDENT VARIABLE IN PW(I,J). *DIFS1010
C* PW IS ACTUALLY STORED IN AN M BY M *DIFS1020
C* ARRAY WHERE M IS THE VALUE OF N USED ON *DIFS1030

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C*          THE FIRST CALL TO THIS PROGRAM. *DIFS1040
C*          2 THE SAME AS CASE 1, EXCEPT THAT THIS *DIFS1050
C*          SUBROUTINE COMPUTES THE PARTIAL *DIFS1060
C*          DERIVATIVES BY NUMERICAL DIFFERENCING *DIFS1070
C*          OF THE DERIVATIVES. HENCE PEDERV IS *DIFS1080
C*          NOT CALLED. *DIFS1090
C*          YMAX AN ARRAY OF N LOCATIONS WHICH CONTAINS THE MAXIMUM *DIFS1100
C*          OF EACH Y SEEN SO FAR. IT SHOULD NORMALLY BE SET TO *DIFS1110
C*          1 IN EACH COMPONENT BEFORE THE FIRST ENTRY. (SEE THE *DIFS1120
C*          DESCRIPTION OF EPS.) *DIFS1130
C*          ERROR AN ARRAY OF N ELEMENTS WHICH CONTAINS THE ESTIMATED *DIFS1140
C*          ONE STEP ERROR IN EACH COMPONENT. *DIFS1150
C*          KFLAG A COMPLETION CODE WITH THE FOLLOWING MEANINGS.. *DIFS1160
C*          +1 THE STEP WAS SUCCESSFUL. *DIFS1170
C*          -1 THE STEP WAS TAKEN WITH H = HMIN, BUT THE *DIFS1180
C*          REQUESTED ERROR WAS NOT ACHIEVED. *DIFS1190
C*          -2 THE MAXIMUM ORDER SPECIFIED WAS FOUND TO *DIFS1200
C*          BE TOO LARGE. *DIFS1210
C*          -3 CORRECTOR CONVERGENCE COULD NOT BE *DIFS1220
C*          ACHIEVED FOR H .GT. HMIN. *DIFS1230
C*          -4 THE REQUESTED ERROR IS SMALLER THAN CAN *DIFS1240
C*          BE HANDLED FOR THIS PROBLEM. *DIFS1250
C*          JSTART AN INPUT INDICATOR WITH THE FOLLOWING MEANINGS.. *DIFS1260
C*          -1 REPEAT THE LAST STEP WITH A NEW H *DIFS1270
C*          0 PERFORM THE FIRST STEP. THE FIRST STEP *DIFS1280
C*          MUST BE DONE WITH THIS VALUE OF JSTART *DIFS1290
C*          SO THAT THE SUBROUTINE CAN INITIALIZE *DIFS1300
C*          ITSELF. *DIFS1310
C*          +1 TAKE A NEW STEP CONTINUING FROM THE LAST. *DIFS1320
C*          JSTART IS SET TO NO, THE CURRENT ORDER OF THE METHOD *DIFS1330
C*          AT EXIT. NO IS ALSO THE ORDER OF THE MAXIMUM *DIFS1340
C*          DERIVATIVE AVAILABLE. *DIFS1350
C*          MAXDER THE MAXIMUM DERIVATIVE THAT SHOULD BE USED IN THE *DIFS1360
C*          METHOD. SINCE THE ORDER IS EQUAL TO THE HIGHEST *DIFS1370
C*          DERIVATIVE USED, THIS RESTRICTS THE ORDER. IT MUST *DIFS1380
C*          BE LESS THAN 8 FOR ADAMS AND 7 FOR STIFF METHODS. *DIFS1390
C*          PW A BLOCK OF AT LEAST N**2 FLOATING POINT LOCATIONS. *DIFS1400
C*          IPS A BLOCK OF N INTEGERS USED FOR MATRIX INVERSION. *DIFS1410
C*          PSCALE A BLOCK OF N FLOATING POINT LOCATIONS ALSO USED FOR *DIFS1420
C*          MATRIX INVERSION. *DIFS1430
C*          ND THE SIZE OF THE WORK ARRAYS. *DIFS1440
C***** *DIFS1450
C          DIMENSION DXOUTP(200) *DIFS1460
C          COMMON/SPHQPT/KBEGN(35),KIIJJ,XHINC,XFIX,XHNQPT,XHNMIN *DIFS1470
C          COMMON/NEQ/BON(30),EMM,SNEQ,NQ1,NSK,NEQPT *DIFS1480
C          COMMON/MIKE0/ITE1,ITE2,ITE3,IMPRNT,NMPATH,NUMIV,XINDP *DIFS1490
C          DIMENSION Y(8,ND),YMAX(ND),SAVE(10,ND),ERROR(ND),PW(ND,ND), *DIFS1500
C          1 A(8),PERTST(7,2,3),IPS(ND),PSCALE(ND) *DIFS1510
C***** *DIFS1520
C* THE COEFFICIENTS IN PERTST ARE USED IN SELECTING THE STEP AND *DIFS1530
C* ORDER. THEREFORE ONLY ABOUT ONE PERCENT ACCURACY IS NEEDED. *DIFS1540
C***** *DIFS1550
C          DATA PERTST /2.0,4.5,7.333,10.42,13.7,17.15,1.0, *DIFS1560
C          1 2.0,17.0,24.0,37.89,53.33,70.08,87.97, *DIFS1570
C          *DIFS1580
C          *DIFS1590

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2          3.0,6.0,9.157,12.5,15.98,1.0,1.0,      DIFS1600
3          12.0,24.0,37.89,53.33,70.03,87.97,1.0,    DIFS1610
4          1.0,1.0,5.0,1667,0.04133,0.008257,1.0,    DIFS1620
5          1.0,1.0,2.0,1.0,.3157,.07407,.0139/       DIFS1630
DATA A(2) /-1.00/                                     DIFS1640
DATA EPSDFS/1.D-10/,EPSBND/1.D-2/,RRMIN/1.D-12/,RRPURB/1.D-13/ DIFS1650
IRET = 1                                             DIFS1660
KFLAG = 1                                           DIFS1670
IF (JSTART.LE.0) GO TO 140                          DIFS1680
C*****DIFS1690
C* BEGIN BY SAVING INFORMATION FOR POSSIBLE RESTARTS AND CHANGING *DIFS1700
C* H BY THE FACTOR R IF THE CALLER HAS CHANGED H. ALL VARIABLES *DIFS1710
C* DEPENDENT ON H MUST ALSO BE CHANGED.             *DIFS1720
C* E IS A COMPARISON FOR ERRORS OF THE CURRENT ORDER NO. EUP IS *DIFS1730
C* TO TEST FOR INCREASING THE ORDER, EDWN FOR DECREASING THE ORDER. *DIFS1740
C* HNEW IS THE STEP SIZE THAT WAS USED ON THE LAST CALL. *DIFS1750
C*****DIFS1760
100 DO 110 I = 1,N                                  DIFS1770
      DO 110 J = 1,K                                  DIFS1780
110   SAVE(J,I) = Y(J,I)                            DIFS1790
      HOLD = HNEW                                     DIFS1800
      HSAV=0.0                                         DIFS1810
      IF (H.EQ.HOLD) GO TO 130                         DIFS1820
120   RACUM = H/HOLD                                  DIFS1830
      IF (H.LT.HOLD) HSAV=H                           DIFS1840
      IRET1 = 1                                         DIFS1850
      GO TO 750                                         DIFS1860
130   NQOLD = NO                                       DIFS1870
      TOLD = T                                          DIFS1880
      RACUM = 1.                                       DIFS1890
      IF (JSTART.GT.0) GO TO 250                       DIFS1900
      GO TO 170                                         DIFS1910
140   IF (JSTART.EQ.-1) GO TO 160                     DIFS1920
C*****DIFS1930
C* ON THE FIRST CALL, THE ORDER IS SET TO 1 AND THE INITIAL *DIFS1940
C* DERIVATIVES ARE CALCULATED.                       *DIFS1950
C*****DIFS1960
      NO = 1                                           DIFS1970
      N3 = N + 1                                       DIFS1980
      N1 = N*10                                        DIFS1990
      N2 = N1 + 1                                       DIFS2000
      N5 = N1 + N                                       DIFS2010
      N6 = N5 + 1                                       DIFS2020
      CALL DIFFUN(T,Y,SAVE(N2,1))                     DIFS2030
      IF (KBEGN(15).LT.0) RETURN                       DIFS2040
      DO 150 I = 1,N                                   DIFS2050
        N11 = N1 + I                                   DIFS2060
150   Y(2,I) = SAVE(N11,1)*H                           DIFS2070
      ENEW = H                                          DIFS2080
      K = 2                                             DIFS2090
      GO TO 100                                         DIFS2100
C*****DIFS2110
C* REPEAT LAST STEP BY RESTORING SAVED INFORMATION. *DIFS2120
C*****DIFS2130
160   IF (NO.EQ.NQOLD) JSTART = 1                     DIFS2140
      T = TOLD                                         DIFS2150

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[illegible]

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216 GO TO 230
  A(1) = -.3298611111111111D0
  A(3) = -1.1416666666666667D0
  A(4) = -.6250000000000000D0
  A(5) = -.1770833333333333D0
  A(6) = -.2500000000000000D-01
  A(7) = -.1388888888888889D-02
  GO TO 230
217 A(1) = -.3155919312169312D0
  A(3) = -1.2250000000000000D0
  A(4) = -.7518518518518519D0
  A(5) = -.2552083333333333D0
  A(6) = -.4861111111111111D-01
  A(7) = -.4861111111111111D-02
  A(8) = -.1984126984126984D-03
  GO TO 230
221 A(1) = -1.0000000000000000D0
  GO TO 230
222 A(1) = -.6666666666666667D0
  A(3) = -.3333333333333333D0
  GO TO 230
223 A(1) = -.5454545454545455D0
  A(3) = -.5454545454545455D0
  A(4) = -.9090909090909091D-01
  GO TO 230
224 A(1) = -.4800000000000000D0
  A(3) = -.7000000000000000D0
  A(4) = -.2000000000000000D0
  A(5) = -.2000000000000000D-01
  GO TO 230
225 A(1) = -.4379562043795620D0
  A(3) = -.8211678832116788D0
  A(4) = -.3102189781021898D0
  A(5) = -.5474452554744526D-01
  A(6) = -.3649635036496350D-02
  GO TO 230
226 A(1) = -.4081632653061225D0
  A(3) = -.9206349206349206D0
  A(4) = -.4166666666666667D0
  A(5) = -.9920634920634921D-01
  A(6) = -.1190476190476190D-01
  A(7) = -.5668934240362812D-03
230 K = NQ + 1
  IDOUB = K
  MTYP = (4 - MF)/2
  ENQ2 = .5/FLOAT(NQ + 1)
  ENQ3 = .5/FLOAT(NQ + 2)
  ENQ1 = .5/FLOAT(NQ)
  PEP SH = EPS
  EUP = (PERTST(NQ,MTYP,2)*PEP SH)**2
  E = (PERTST(NQ,MTYP,1)*PEP SH)**2
  EDWN = (PERTST(NQ,MTYP,3)*PEP SH)**2
  IF (EDWN.EQ.0) GO TO 780
C.... SPECIAL BOUNDS SET FOR NEQPT PROBLEMS
  IF (NEQPT.GE.7) GO TO 238
  BND = EPSBND*ENQ3/DBLE(FLOAT(N))

```

```

DIFS2720
DIFS2730
DIFS2740
DIFS2750
DIFS2760
DIFS2770
DIFS2780
DIFS2790
DIFS2800
DIFS2810
DIFS2820
DIFS2830
DIFS2840
DIFS2850
DIFS2860
DIFS2870
DIFS2880
DIFS2890
DIFS2900
DIFS2910
DIFS2920
DIFS2930
DIFS2940
DIFS2950
DIFS2960
DIFS2970
DIFS2980
DIFS2990
DIFS3000
DIFS3010
DIFS3020
DIFS3030
DIFS3040
DIFS3050
DIFS3060
DIFS3070
DIFS3080
DIFS3090
DIFS3100
DIFS3110
DIFS3120
DIFS3130
DIFS3140
DIFS3150
DIFS3160
DIFS3170
DIFS3180
DIFS3190
DIFS3200
DIFS3210
DIFS3220
DIFS3230
DIFS3240
DIFS3250
DIFS3260
DIFS3270

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      GO TO 248                                DIFS3288
238 CONTINUE                                DIFS3298
      BND = EPS*ENQ3/DBLE(FLOAT(N))           DIFS3308
248 IWEVAL = MF                               DIFS3318
      GO TO ( 258 , 688 ),IRET               DIFS3328
C*****DIFS3338
C* THIS SECTION COMPUTES THE PREDICTED VALUES BY EFFECTIVELY *DIFS3348
C* MULTIPLYING THE SAVED INFORMATION BY THE PASCAL TRIANGLE *DIFS3358
C* MATPIX. *DIFS3368
C*****DIFS3378
258 T = T + H                                DIFS3388
      DO 268 J = 2,K                          DIFS3398
        DO 268 J1 = J,K                      DIFS3408
          J2 = K - J1 + J - 1                DIFS3418
          DO 268 I = 1,N                     DIFS3428
            Y(J2,I) = Y(J2,I) + Y(J2+1,I)    DIFS3438
C*****DIFS3448
C* UP TO 3 CORRECTOR ITERATIONS ARE TAKEN. CONVERGENCE IS TESTED *DIFS3458
C* BY REQUIRING CHANGES TO B: LESS THAN BND WHICH IS DEPENDENT ON *DIFS3468
C* THE ERROR TEST CONSTANT. *DIFS3478
C* THE SUM OF THE CORRECTIONS IS ACCUMULATED IN THE ARRAY *DIFS3488
C* ERROR(I). IT IS EQUAL TO THE K-TH DERIVATIVE OF Y MULTIPLIED *DIFS3498
C* BY H**K/(FACTORIAL(K-1)*A(K)), AND IS THEREFORE PROPORTIONAL *DIFS3508
C* TO THE ACTUAL ERRORS TO THE LOWEST POWER OF H PRESENT. (H**K) *DIFS3518
C*****DIFS3528
      DO 278 I = 1,N                          DIFS3538
        ERROR(I) = 0.                        DIFS3548
278 NUMOUT=0                                DIFS3558
      DO 438 L = 1,3                          DIFS3568
        CALL DIFFUN (T,Y,SAVE(N2,1))         DIFS3578
        IF(KBEGN(35).LT.0)RETURN              DIFS3588
C*****DIFS3598
C* IF THERE HAS BEEN A CHANGE OF ORDER OR THERE HAS BEEN TROUBLE *DIFS3608
C* WITH CONVERGENCE, PW IS RE-EVALUATED PRIOR TO STARTING THE *DIFS3618
C* CORRECTOR ITERATION IN THE CASE OF STIFF METHODS. IWEVAL IS *DIFS3628
C* THEN SET TO -1 AS AN INDICATOR THAT IT HAS BEEN DONE. *DIFS3638
C*****DIFS3648
      IF (IWEVAL.LT.1) GO TO 358              DIFS3658
      IF (MF.EQ.2) GO TO 318                 DIFS3668
C+++ CALL PEDERV(T,Y,PW,N)                  DIFS3678
      R = A(1)*H                             DIFS3688
      DO 288 I = 1,N                         DIFS3698
        DO 288 J = 1,N                       DIFS3708
          PW(I,J) = PW(I,J)*R                DIFS3718
288                                          DIFS3728
C*****DIFS3728
C* ADD THE IDENTITY MATRIX TO THE JACOBIAN AND INVERT TO GET PW. *DIFS3738
C*****DIFS3748
298 DO 308 I = 1,N                          DIFS3758
308 PW(I,I) = 1.0 + PW(I,I)                 DIFS3768
      IWEVAL = -1                             DIFS3778
      DO 5 I = 1,N                           DIFS3788
        IPS(I) = I                           DIFS3798
        PRWNRM = 0.                          DIFS3808
        DO 2 J = 1,N                         DIFS3818
          IF(PRWNRM.LT. ABS(PW(I,J))) PRWNRM = ABS(PW(I,J)) DIFS3828
2          CONTINUE                          DIFS3838

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      IF(PRWNRM .EQ. 0.) GO TO 440
5     PSCALE(I) = 1./PRWNRM
      NM1 = N - 1
      DO 17 KK = 1,NM1
        PBIG = 0.
        DO 11 I = KK,N
          IP = IPS(I)
          PSIZE = ABS(PW(IP,KK))*PSCALE(IP)
          IF(PSIZE .LE. PBIG) GO TO 11
          PBIG = PSIZE
          IDXPIV = I
11        CONTINUE
        IF(PBIG .EQ. 0.) GO TO 440
        IF(IDXPIV .EQ. KK) GO TO 15
        J = IPS(KK)
        IPS(KK) = IPS(IDXPIV)
        IPS(IDXPIV) = J
15        KP = IPS(KK)
        PIVOT = PW(KP,KK)
        KP1 = KK + 1
        DO 16 I = KP1,N
          IP = IPS(I)
          PEM = -PW(IP,KK)/PIVOT
          PW(IP,KK) = -PEM
          DO 16 J = KP1,N
16            PW(IP,J) = PW(IP,J) + PEM*PW(KP,J)
17        CONTINUE
        KP = IPS(N)
        IF(PW(KP,N) .EQ. 0.) GO TO 440
        GO TO 350
C*****
C* EVALUATE THE JACOBIAN INTO PW BY NUMERICAL DIFFERENCING. R IS THE
C* CHANGE MADE TO THE ELEMENT OF Y. IT IS EPS RELATIVE TO Y WITH
C* A MINIMUM OF EPS**2.
C*****
310     DO 320 I = 1,N
320       SAVE(9,I) = Y(1,I)
        DO 340 J = 1,N
          R = EPS*DMAX1(EPSDFS,DABS(SAVE(9,J)))
          IF(KLEGN(J).LT.0)R=RRPURB
CZZZZ IF(KLEGN(J).LT.0)GO TO 340
          Y(1,J) = Y(1,J) + R
          D = A(1)*H/R
          CALL DIFFUN(T,Y,SAVE(N5,1))
          IF(KLEGN(35).LT.0)RETURN
          DO 330 I = 1,N
            N5I = N5 + I
            N1I = N1 + I
330           PW(I,J) = (SAVE(N5I,1) - SAVE(N1I,1))*D
340           Y(1,J) = SAVE(9,J)
          GO TO 290
350       IF(MF.NE.0) GO TO 370
          DO 360 I = 1,N
            N1I = N1 + I
360           SAVE(9,I) = Y(2,I) - SAVE(N1I,1)*H
          GO TO 410

```

```

DIFS3840
DIFS3850
DIFS3860
DIFS3870
DIFS3880
DIFS3890
DIFS3900
DIFS3910
DIFS3920
DIFS3930
DIFS3940
DIFS3950
DIFS3960
DIFS3970
DIFS3980
DIFS3990
DIFS4000
DIFS4010
DIFS4020
DIFS4030
DIFS4040
DIFS4050
DIFS4060
DIFS4070
DIFS4080
DIFS4090
DIFS4100
DIFS4110
DIFS4120
DIFS4130
DIFS4140
DIFS4150
DIFS4160
DIFS4170
DIFS4180
DIFS4190
DIFS4200
DIFS4210
DIFS4220
DIFS4230
DIFS4240
DIFS4250
DIFS4260
DIFS4270
DIFS4280
DIFS4290
DIFS4300
DIFS4310
DIFS4320
DIFS4330
DIFS4340
DIFS4350
DIFS4360
DIFS4370
DIFS4380

```

```

C* BEEN THREE FAILURES. IN THAT CASE THE DERIVATIVES ARE ASSUMED TO *DIFS5510
C* HAVE ACCUMULATED ERRORS SO A RESTART FROM THE CURRENT VALUES OF Y *DIFS5520
C* IS TRIED. *DIFS5530
C***** *DIFS5540
540 KFLAG = KFLAG - 2 *DIFS5550
    IF (H.LE.(HMIN*1.00001D0)) GO TO 740 *DIFS5560
    T = TOLD *DIFS5570
    IF (KFLAG.LE.-5) GO TO 720 *DIFS5580
C***** *DIFS5590
C* PR1, PR2, AND PR3 WILL CONTAIN THE AMOUNTS BY WHICH THE STEP SIZE *DIFS5600
C* COULD BE DIVIDED AT ORDER ONE LOWER, AT THIS ORDER, AND AT ORDER *DIFS5610
C* ONE HIGHER RESPECTIVELY. *DIFS5620
C***** *DIFS5630
550 PR2 = (D/E)**ENQ2*1.2 *DIFS5640
    PR3 = 1.E+20 *DIFS5650
    IF ((NQ.GE.MAXDER).OR.(KFLAG.LE.-1)) GO TO 570 *DIFS5660
    D = 0. *DIFS5670
    DO 560 I = 1,N *DIFS5680
560 D = D + ((ERROR(I) - SAVE(10,I))/YMAX(I))**2 *DIFS5690
    PR3 = (D/EUP)**ENQ3*1.4 *DIFS5700
570 PR1 = 1.E+20 *DIFS5710
    IF (NQ.LE.1) GO TO 590 *DIFS5720
    D = 0. *DIFS5730
    DO 580 I = 1,N *DIFS5740
580 D = D + (Y(K,I)/YMAX(I))**2 *DIFS5750
    PR1 = (D/EDWN)**ENQ1*1.3 *DIFS5760
590 CONTINUE *DIFS5770
    IF (PR2.LE.PR3) GO TO 650 *DIFS5780
    IF (PR3.LT.PR1) GO TO 660 *DIFS5790
600 R = 1.0/AMAX1(PR1,1.E-4) *DIFS5800
    NEWQ = NQ - 1 *DIFS5810
610 IDOUB = 10 *DIFS5820
    IF ((KFLAG.EQ.1).AND.(R.LT.1.1D0))GO TO 700 *DIFS5830
    IF (NEWQ.LE.NQ) GO TO 630 *DIFS5840
C***** *DIFS5850
C* COMPUTE ONE ADDITIONAL SCALED DERIVATIVE IF ORDER IS INCREASED. *DIFS5860
C***** *DIFS5870
    DO 620 I = 1,N *DIFS5880
620 Y(NEWQ+1,I) = ERROR(I)*A(K)/DBLE(FLOAT(K)) *DIFS5890
630 K = NEWQ + 1 *DIFS5900
    IF (KFLAG.EQ.1) GO TO 670 *DIFS5910
    RACUM = RACUM*R *DIFS5920
    IRET1 = 3 *DIFS5930
    GO TO 750 *DIFS5940
640 IF (NEWQ.EQ.NQ) GO TO 250 *DIFS5950
    NQ = NEWQ *DIFS5960
    GO TO 170 *DIFS5970
650 IF (PR2.GT.PR1) GO TO 600 *DIFS5980
    NEWQ = NQ *DIFS5990
    R = 1.0/AMAX1(PR2,1.E-4) *DIFS6000
    GO TO 610 *DIFS6010
660 R = 1.0/AMAX1(PR3,1.E-4) *DIFS6020
    NEWQ = NQ + 1 *DIFS6030
    GO TO 610 *DIFS6040
670 IRET = 2 *DIFS6050
    R = DMIN1(R,HMAX/DABS(H)) *DIFS6060

```

```

CADD NEXT 5 LINES AS WELL AS CHANGE COMMON AND FIX MHD
CCCCC IF(KBEGN(35).EQ.0)GO TO 672
CCCCC IF(R.LT.1.0D0)GO TO 672
CCCCC R=1.0D0
CCCCC GO TO 679
672 CONTINUE
H = H*R
IF(K.IIJJ.LE.0)GO TO 675
XIT=XHINC
IF(K.IIJJ.GT.30)XIT=XHNMIN
IF(H.LE.XIT)GO TO 679
R=(XIT/H)*R
H=XIT
GO TO 679
675 CONTINUE
677 CONTINUE
IF(R.LE.1.0D0)GO TO 679
IF(H.LE.XHNQPT)GO TO 679
H=H*XFIX
R=R*XFIX
679 CONTINUE
HNEW = H
IF (NO.EQ.NEWQ) GO TO 680
NO = NEWQ
GO TO 170
680 R1 = 1.
DO 690 J = 2,K
R1 = R1*R
DO 690 I = 1,N
690 Y(J,I) = Y(J,I)*R1
IDOU = K
700 DO 710 I = 1,N
710 YMAX(I) = DMAX1(YMAX(I),DABS(Y(1,I)))
JSTART = NO
RETURN
720 IF (NO.EQ.1) GO TO 780
CALL DIFFUN (T,Y,SAVE(N2,1))
IF(KBEGN(35).LT.0)RETURN
R = H/HOLD
DO 730 I = 1,N
Y(1,I) = SAVE(1,I)
N1I = N1 + I
SAVE(2,I) = HOLD*SAVE(N1I,1)
730 Y(2,I) = SAVE(2,I)*R
NO = 1
KFLAG = 1
GO TO 170
740 KFLAG = -1
HNEW = H
JSTART = NO
RETURN
C*****
C* THIS SECTION SCALES ALL VARIABLES CONNECTED WITH H AND RETURNS
C* TO THE ENTERING SECTION.
C*****
750 RACUM = DMAX1(DABS(HMIN/HOLD),RACUM)

```

```

DIFS6070
DIFS6080
DIFS6090
DIFS6100
DIFS6110
DIFS6120
DIFS6130
DIFS6140
DIFS6150
DIFS6160
DIFS6170
DIFS6180
DIFS6190
DIFS6200
DIFS6210
DIFS6220
DIFS6230
DIFS6240
DIFS6250
DIFS6260
DIFS6270
DIFS6280
DIFS6290
DIFS6300
DIFS6310
DIFS6320
DIFS6330
DIFS6340
DIFS6350
DIFS6360
DIFS6370
DIFS6380
DIFS6390
DIFS6400
DIFS6410
DIFS6420
DIFS6430
DIFS6440
DIFS6450
DIFS6460
DIFS6470
DIFS6480
DIFS6490
DIFS6500
DIFS6510
DIFS6520
DIFS6530
DIFS6540
DIFS6550
DIFS6560
DIFS6570
DIFS6580
DIFS6590
DIFS6600
DIFS6610
DIFS6620

```

```

      RACUM = DMIN1(RACUM,DABS(HMAX/HOLD))
      R1 = 1.
      DO 760 J = 2,K
        R1 = R1*RACUM
        DO 760 I = 1,N
          Y(J,I) = SAVE(J,I)*R1
760    H = HOLD*RACUM
        IF(HSAV.NE.0.000)HOLD=HSAV
        DO 770 I = 1,N
770    Y(1,I) = SAVE(1,I)
        IDOUB = K
        IF(NT.EQ.0)GO TO 775
        IF(IMPRNT.LT.2)GO TO 775
        WRITE(1,3000) NT,IDOUB,IRET1,BND
        NUMDBG=305
3000  FORMAT(1X,5H+ NT=,I3,7H IDOUB=,I3,7H IRET1=,I3,5H BND=,G13.5)
        CALL DEBOUT(NUMOUT,XDXOU1,XDXOU2,DXOUTP,NUMDBG)
775    CONTINUE
        KKIIJJ=KKIIJJ+NUMOUT/3
        NUMOUT=0
        GO TO ( 130 , 250 , 640 ),IRET1
780    KFLAG = -4
        GO TO 470
        END
        BLOCK DATA
C
      DOUBLE PRECISION TTT,TM,PP,SIGMA,SIG,VLMI,VLM,S0
      DOUBLE PRECISION ENN,SUMN
C
      LOGICAL SHOCK,MMHG,UV,DETN,SIUNIT,NSOM,CALCH
      LOGICAL HP,SP,TP,NEWI,IONS,MOLES,FROZ,EQL,PSIA,RKT,VOL,TV,SV
      LOGICAL EPATIO,FPCT,OTTO,SPLG
      LOGICAL NEQL,CONVG,LOGV,SPLG,AREA
C
C
C
      DIMENSION ATEM(3,50)
C
      COMMON/SIGOUT/FNEL(3),ANE(15),FIONS(3),AIONS(15),FSIGWO(4),
XFSIG(4),SIGM(15),FFREQ(3),TOTAL(15)
      COMMON/MISC/S0,ENN,SUMN,TT,ATOM(3,101),LLMT(30),B0(30),B0P(30,2)
      1 ,TM,TLOW,TMID,THIGH,CPSUM,PP,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
      2 ,HPP(2),PH(2), VMIN(2),VPLS(2),WP(2),DATA(30),NAME(30,5)
      3 ,ANUM(30.5),PECWT(30),ENTH(30),FAZ(30),RTEMP(30),FOX(30),DENS(30)
      4 ,RHOF,PMW(30),TLN,CR,OXF(30),ENNL,ENSAVE,ENLSAV ,TRACE,SIZE
      COMMON/OUT/EMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)
      1 ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2
      2 ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0,FRHO(4)
C
      EQUIVALENCE (ATOM(1,52),ATEM)
C
      DATA FSIGWO/4H W/,4HO IO,4HNS ,4H /,FFREQ/4HFREQ,4H (1/,
      1 4HSEC) /,FIONS/4HIONS,4HC DE,4HNS) /
      DATA FSIG /4HSIG,4HA (M 4HIO/4,2H) /,FNEL/4HELEC,4H DEN,
      1 4HS /
C

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DIFS6630
 DIFS6640
 DIFS6650
 DIFS6660
 DIFS6670
 DIFS6680
 DIFS6690
 DIFS6700
 DIFS6710
 DIFS6720
 DIFS6730

DIFS6740
 DIFS6750
 DIFS6760
 DIFS6770
 DIFS6780
 DIFS6790
 BLOC 10
 BLOC 20
 BLOC 30
 BLOC 40
 BLOC 50
 BLOC 60
 BLOC 70
 BLOC 80
 BLOC 90
 BLOC 100
 BLOC 110
 BLOC 120
 BLOC 130
 BLOC 140
 BLOC 150
 BLOC 160
 BLOC 170
 BLOC 180
 BLOC 190
 BLOC 200
 BLOC 210
 BLOC 220
 BLOC 230
 BLOC 240
 BLOC 250
 BLOC 260
 BLOC 270
 BLOC 280
 BLOC 290
 BLOC 300
 BLOC 310
 BLOC 320

C ATOMIC SYMBOLS, WEIGHTS, AND VALENCES

C

DATA ATOM/

A	2HH	, 1.00797	, 1.,	2HHE	, 4.0026	, 0.,	2HLI	, 6.939	, 1.,	BLOC 330
B	2HBE	, 9.0122	, 2.,	2HBI	, 10.811	, 3.,	2HCL	, 12.01115	, 4.,	BLOC 340
C	2HBN	, 14.0067	, 0.,	2HBO	, 15.9994	, -2.,	2HFC	, 18.9984	, -1.,	BLOC 350
D	2HNE	, 20.183	, 0.,	2HNA	, 22.9898	, 1.,	2HMG	, 24.312	, 2.,	BLOC 360
E	2HAL	, 26.9815	, 3.,	2HSI	, 28.086	, 4.,	2HP	, 30.9738	, 5.,	BLOC 370
F	2HS	, 32.064	, 4.,	2HCL	, 35.453	, -1.,	2HAR	, 39.948	, 0.,	BLOC 380
G	2HK	, 39.102	, 1.,	2HCA	, 40.080	, 2.,	2HSC	, 44.956	, 3.,	BLOC 390
H	2HTI	, 47.900	, 4.,	2HV	, 50.942	, 5.,	2HCR	, 51.996	, 3.,	BLOC 400
I	2HMM	, 54.9380	, 2.,	2HFE	, 55.847	, 3.,	2HCO	, 58.9332	, 2.,	BLOC 410
J	2HNI	, 58.710	, 2.,	2HCU	, 63.540	, 2.,	2HZN	, 65.370	, 2.,	BLOC 420
K	2HGA	, 69.720	, 3.,	2HGE	, 72.590	, 4.,	2HAS	, 74.9216	, 3.,	BLOC 430
L	2HSE	, 78.960	, 4.,	2HBR	, 79.909	, -1.,	2HKR	, 83.800	, 0.,	BLOC 440
M	2HRB	, 85.47	, 1.,	2HSR	, 87.520	, 2.,	2HY	, 88.905	, 3.,	BLOC 450
N	2H2R	, 91.220	, 4.,	2HNB	, 92.906	, 5.,	2HMO	, 95.94	, 6.,	BLOC 460
O	2HTC	, 99.000	, 7.,	2HRU	, 101.070	, 3.,	2HRH	, 102.905	, 3.,	BLOC 470
P	2HPD	, 106.400	, 2.,	2HAG	, 107.370	, 1.,	2HCD	, 112.400	, 2.,	BLOC 480
Q	2HIN	, 114.820	, 3.,	2HSN	, 118.690	, 4.,	2HSB	, 121.750	, 3.,	BLOC 490
R	2HTE	, 127.600	, 4.,	2HI	, 126.9044	, -1.,	2HXB	, 131.300	, 0.,	BLOC 500
S	2HCS	, 132.905	, 1.,	2HBA	, 137.340	, 2.,	2HLA	, 138.910	, 3.,	BLOC 510
T	2HCE	, 140.120	, 3.,	2HPR	, 140.907	, 3.,	2HND	, 144.240	, 3.,	BLOC 520
U	2HPM	, 145.000	, 3.,	2HSM	, 150.350	, 3.,	2HEU	, 151.960	, 3.,	BLOC 530
V	2HGD	, 157.250	, 3.,	2HTB	, 158.924	, 3.,	2HDY	, 162.500	, 3.,	BLOC 540
W	2HGO	, 164.930	, 3.,	2HER	, 167.260	, 3.,	2HTM	, 168.934	, 3.,	BLOC 550
X	2HYB	, 173.040	, 3.,	2HLU	, 174.397	, 3.,	2HBF	, 178.490	, 4.,	BLOC 560
Y	2HTA	, 180.948	, 5.,	2HW	, 183.850	, 6.,	2HRE	, 186.200	, 7.,	BLOC 570
Z	2HOS	, 190.200	, 4.,	2HIP	, 192.200	, 4.,	2HPT	, 195.090	, 4.,	BLOC 580
A	2HAU	, 196.967	, 3.,	2HGG	, 200.590	, 2.,	2HTL	, 204.370	, 1.,	BLOC 590
B	2HPB	, 207.190	, 2.,	2HBI	, 208.980	, 3.,	2HPO	, 210.000	, 2.,	BLOC 600
C	2HAT	, 210.000	, 0.,	2HRN	, 222.000	, 0.,	2HFR	, 223.000	, 1.,	BLOC 610
D	2HRA	, 226.000	, 2.,	2HAC	, 227.000	, 3.,	2HTH	, 232.038	, 4.,	BLOC 620
E	2HPA	, 231.000	, 5.,	2HU	, 238.030	, 6.,	2HVV	, 101.961	, 0.,	BLOC 630
F	2HPU	, 242.000	, 4.,	2HAM	, 243.000	, 3.,	2HYU	, 60.085	, 0.,	BLOC 640
G	2HBK	, 249.000	, 3.,	2HCF	, 251.000	, 3.,	2HES	, 254.000	, 0.,	BLOC 650
H	2HFM	, 253.000	, 0.,	2HD	, 2.014102	, 1. /				BLOC 660

C

C

C

INFORMATION USED IN VARIABLE OUTPUT FORMAT

DATA	FMT/3H(1H,4H,3A4,4H,A2,,3HF9,,2H0,,3HF9,,2H0,,3HF9,,2H0,,3HF9BLOC 730	
1.,2H0,,3HF9,,2H0,,3HF9,,2H0,,3HF9,,2H0,,3HF9,,2H0,,3HF9BLOC 740		
2.,2H0,,3HF9,,2H0,,3HF9,,2H0,,3HF9,,1H0,1H)/,FB,F0,F1,F2,F3,F4,F5/BLOC 750		
31H,,2H0,,2H1,,2H2,,2H3,,2H4,,2H5,,/FMT13/2H13/,FMT9X/3H9X/,FMTI9BLOC 760		
4/3HI9,/	BLOC 770	
DATA	FP/4HP, A,4HTM,2H,1H /	BLOC 780
1,FT/4HT, D,4NEG K,4H	2H /,FH/4HH, C,4HAL/G,2H,1H /	BLOC 790
2,FS/4HS, C,4HAL/(,4HG)(K,2H) /,FM/4HM, M,4HOL W,2HT,1H /		BLOC 800
3,FV/:H(DLV,4H/DLP,4H)T,2H /,FD/4H(DLV,4H/DLT,2H)P,1H /		BLOC 810
4,FC/ HCP, 4HCAL/,4I(G)(,2HK)/,FG/4HGAMM,4HA (S,2H),1H /		BLOC 820
5,FL/4HSON,4HVEL,4HM/SE,2HC /		BLOC 830
		BLOC 840

C

C

C

INFORMATION USED IN PERFORMANCE OUTPUT

DATA	FR1/4HPC/P/, FC1/2HCF/, FN/4HMACH,4H NUM,4HBER,1H /	BLOC 850
1,FR/4HCSTA,4HR, F,4HT/SE,2HC /,FI/4HISP,,4H LB-,4HSEC/,2HLB/		BLOC 860
		BLOC 870
		BLOC 880

C PROGRAM NEOMHD(INPUT,OUTPUT,TAPE7,"APES=INPUT,TAPE6=OUTPUT)

BLOC 890
BLOC 900

2,FA/:HIVAC,4H,LE-,4HSEC/,2HLE /,FA1/4HAE/A/,FA2/1HT/
END

APPENDIX D THERMO DATA (FORMAT AND LISTING)

The order and format of the input data cards in this appendix are given in the following table:

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 (90) to (92) (for upper temperature interval)	5(E15.8)	1 to 75
	Integer 2	I5	80
5	Coefficients in equations (90) to (92) (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 (90) to (92) (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

^aGaseous 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.

The program writes the THERMO data on a file, designated as Fortran Logical Unit 7, as the cards are read. The data are written on the file with the same format as the cards with one exception, that the THERMO code card is omitted.

A sample listing of a set of THERMO data cards appears as follows:

```

320.100 1000.000 5000.000
KALO2(S)      10/78 K  1AL  10  2  0S  300.000 1986.000      1
  0.17521160E 02  0.24013437E-01-0.63052099E-04  0.46093152E-07-0.10688797E-10      2
-0.13943850E 06-0.97563712E 02  0.10219235E 02-0.28796211E-01  0.14474083E-03      3
-0.22921600E-06  0.11709841E-09-0.13173960E 06-0.38574593E 02      4
KALO3(L)      11/78 K  1AL  10  2  0L  1986.000 3600.000      1
  0.15559841E 02  0.57600956E-04  0.29229841E-06-0.15502044E-09  0.21880338E-13      2
-0.13598709E 06-0.62554352E 02  0.00000000E 00  0.00000000E 00  0.00000000E 00      3
  0.00000000E 00  0.00000000E 00  0.00000000E 00  0.00000000E 00      4
KALO4(L)      10/78 K  1AL  1SI 10  4L  2010.000 3600.000      1
  0.18000197E 02  0.52222768E-02-0.18005340E-05  0.19045625E-09  0.39862861E-14      2
-0.20000000E 06-0.62554352E 02  0.00000000E 00  0.00000000E 00  0.00000000E 00      3
  0.20000000E 00  0.00000000E 00  0.00000000E 00  0.00000000E 00      4
KALO5(L)      10/78 K  1AL  1SI 20  6L  2019.000 3600.000      1
  0.18000197E 02  0.16019411E-02-0.18005340E-05  0.13000000E-09  0.27527134E-13      2
-0.20000000E 06-0.14163947E 03  0.00000000E 00  0.00000000E 00  0.00000000E 00      3
  0.00000000E 00  0.00000000E 00  0.00000000E 00  0.00000000E 00      4
KALO6(S)      GS4/76K  1AL  1SI 30  8S  300.000 1470.000      1
  0.34223747E 02  0.77212130E-03  0.53000000E-05-0.29784770E-08  0.61708505E-12      2
-0.40000000E 06-0.17173570E 03  0.27410522E 02-0.20009449E-01  0.90974543E-04      3
-0.20000000E 07  0.18934160E-10-0.48354369E 06-0.12557780E 03      4
KALO7(L)      10/78 K  1AL  1SI 30  8L  300.000 3600.000      1
  0.18000197E 02  0.49079363E-01-0.23200510E-04  0.43500000E-08-0.26349046E-12      2
-0.20000000E 06-0.23021680E 02  0.10000000E 02  0.62618423E-01-0.35634788E-04      3
-0.20000000E 08  0.70864425E-11-0.47500000E 06-0.42356102E 02      4
KALO8(L)      10/78 K  2SI  20  5  0L  1318.000 3600.000      1
  0.33567260E 02  0.84069210E-02-0.53500000E-05  0.14363750E-08-0.13949497E-12      2
-0.31599594E 06-0.18000000E 03  0.00000000E 00  0.00000000E 00  0.00000000E 00      3
  0.00000000E 00  0.00000000E 00  0.00000000E 00  0.00000000E 00      4
KALO9(L)      10/78 K  20  1  0  0L  1000.000 3600.000      1
  0.12000190E 02  0.12000000E-02-0.90211623E-05  0.27286782E-09-0.30453396E-13      2
-0.43594820E 05-0.54184000E 02  0.00000000E 00  0.23000000E 00  0.00000000E 00      3
  0.00000000E 00  0.00000000E 00  0.00000000E 00  0.00000000E 00      4
END

```


APPENDIX E

SYMBOLS

A	area, m^2
A_e/A_t	ratio of nozzle exit area to throat area
a	velocity of sound, m/sec
a_{ij}	stoichiometric coefficients, kg-atoms of element i per kg-mole of species j , $(kg\text{-atom})_i/(kg\text{-mole})_j$
$a_{ij}^{(k)}$	stoichiometric coefficients, kg-atoms of element i per kg-mole of reactant j (oxidant if $k = 1$, fuel if $k = 2$), $(kg\text{-atom})_i^{(k)}/(kg\text{-mole})_j^{(k)}$
$a_i (i=1 \text{ to } 7)$	least squares coefficients
B	magnetic field, Tesla
b_i	kg-atoms of element i per kg of mixture, $(kg\text{-atom})_i/kg$
$b_i^{(k)}$	assigned kg-atoms of element i per kilogram of total oxidant ($k = 1$) or total fuel ($k = 2$), $(kg\text{-atom})_i^{(k)}/kg^{(k)}$
b_i^0	assigned kg-atoms of element i per kg of total reactant, $(kg\text{-atom})_i/kg$
$(c_p^0)_j$	standard state constant pressure specific heat for species or reactant j , $J/(kg\text{-mole})_j(K)$
$(c_v^0)_j$	standard state constant volume specific heat for species j , $J/(kg\text{-mole})_j(K)$
c_p	constant pressure specific heat of mixture, $J/(kg)(K)$
c_v	constant volume specific heat of mixture, $J/(kg)(K)$
E_x	axial component of electric field, volts/m

E_y	transverse component of electric field, volts/m
F	force per unit volume, N/m^3
G	Gibbs free energy of mixture with constraints, J/kg
g	Gibbs free energy of mixture, J/kg
$(H_T^0)_j$	standard state enthalpy for species j , J/(kg-mole) $_j$
$(H_T^0)^{(k)}_j$	enthalpy of reactant j ($k = 1$ for oxidant, $k = 2$ for fuel), J/(kg-mole) $^{(k)}_j$
$(\Delta H_f^0)_T$	heat of formation at temperature T , J/(kg-mole)
$\mathcal{H}_0$	enthalpy of total reactant, kg-mole/kg
$\mathcal{H}^{(k)}$	enthalpy of total oxidant ($k = 1$) or total fuel ($k = 2$), (kg-mole/kg) k
h	enthalpy of mixture, J/kg
h_0	enthalpy of total reactants, J/kg
J_x	axial component of current density, amp/m 2
J_y	transverse component of current density, amp/m 2
K	load factor, dimensionless
$K_r(p)$	equilibrium constant for r -th reaction
k_{rf}	forward rate constant of r -th reaction in units of molecule-cc-sec
M	total moles of gaseous species which are rate controlled, kg-mole/kg
M_i	atomic weight of chemical element i , (kg/kg-atom) $_i$
M_0	molecular weight of total reactant, kg/kg-mole

$M^{(k)}$	molecular weight of total oxidant ($k = 1$) or total fuel ($k = 2$), (kg/kg-mole) ^(k)
$M_j^{(k)}$	molecular weight of reactant j (oxidant if $k = 1$, fuel if $k = 2$), (kg/kg-mole) _{j} ^(k)
$\mathcal{M}$	Mach number
N	total moles of gaseous species which are not rate controlled, kg-mole/kg
$N_j^{(k)}$	kg-moles of reactant j (oxidant if $k = 1$, fuel if $k = 2$), (kg-mole) _{j} ^(k)
n_c	total moles of liquid species in liquid solution, kg-mole/kg
n_g	total moles of gaseous species, kg-mole/kg
n_j	kg-moles of species j per kg of mixture, (kg-mole) _{j} /kg
$n_j^{(k)}$	kg-moles per kilogram of reactant j (oxidant if $k = 1$, fuel if $k = 2$), (kg-mole) _{j} ^(k) /kg ^(k)
O/F	oxidant to fuel weight (or mass) ratio
p	pressure, N/m ²
p_{atm}	pressure, atm
p_c/p_e	ratio of combustion pressure to exit pressure
p_0	assigned or initial pressure, N/m ²
q	energy per unit volume per second, J/m ³ -sec
R	universal gas constant, 8314.3 J/(kg-mole)(K)
r	equivalence ratio
S_j	entropy of species j , J/(kg-mole) _{j} (K)
$(S_T^0)_j$	standard state entropy for species j , J/(kg-mole)(K)

s	entropy of mixture, J/(kg)(K)
s_0	entropy of total reactants, J/(kg)(K)
T	temperature, K
u	velocity (m/sec)
v	specific volume, m^3/kg
v^+	positive oxidation state of total reactant
v^-	negative oxidation state of total reactant
$v^{+(k)}$	positive oxidation of total oxidant ($k = 1$) or total fuel ($k = 2$)
$v^{-(k)}$	negative oxidation state of total oxidant ($k = 1$) or total fuel ($k = 2$)
v_i^+	positive oxidation state of chemical element i
v_i^-	negative oxidation state of chemical element i
$w_j^{(k)}$	weight of reactant j (oxidant if $k = 1$, fuel if $k = 2$), $kg_j^{(k)}$
$\dot{w}_i$	production rate of i -th species due to chemical reactions, (kg-mole)/(m^3 -sec)
x	axial distance, m
y_i^F	mass fraction of i -th fuel reactant in total fuel
y_i^O	mass fraction of i -th oxidizer reactant in total oxidizer
α	fraction of condensed species rejected from the combustor first stage
β	Hall parameter, dimensionless
β_i	fraction of i -th oxidizer species injected in the combustor second stage
γ	ratio of specific heats
γ_s	isentropic exponent

$\gamma_{S,T}$	special isentropic exponent
θ_i	fraction of i-th fuel reactant injected in the combustor second stage
λ	control factor
λ_i	Lagrangian multiplier for chemical element i, J/(kg-atom) _i
μ_j	chemical potential of species j, J/(kg-mole) _j
μ_j^0	standard state chemical potential for species j, J/(kg-mole) _j
v_{ri}	stoichiometric coefficient of i-th product species in the r-th chemical reaction
v_{ri}	stoichiometric coefficient of i-th reactant species in the r-th chemical reaction
π_i	$-\lambda_i/RT$, Lagrangian multiplier for chemical element i, kg-mole/(kg-atom) _i
ρ	density of mixture, kg/m ³
σ	plasma conductivity, mho/m

Subscripts:

a	ambient
c	combustion, condensed
e	exit
g	gas
k	iteration k
m	melting temperature
0	total reactant; zero th iteration
t	throat
1,2,5	stations

Superscripts:

0 an assigned or initial condition
k 1 if oxidant, 2 if fuel

Indices:

ℓ number of chemical elements (if ions are considered,
 number of chemical elements plus one)
ME number of possible species which are not rate controlled,
 gaseous and condensed
NT number of possible species, gases and condensed
NREAC number of reactants
r number of chemical reactions