GENERAL CHEMICAL KINETICS COMPUTER PROGRAM FOR STATIC AND FLOW REACTIONS, WITH APPLICATION TO COMBUSTION AND SHOCK-TUBE KINETICS

by David A. Bittker and Vincent J. Scullin

Lewis Research Center
Cleveland, Ohio 44135

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A general chemical kinetics program is described for complex, homogeneous ideal-gas reactions in any chemical system. Its main features are flexibility and convenience in treating many different reaction conditions. The program solves numerically the differential equations describing complex reaction in either a static system or one-dimensional inviscid flow. Applications include ignition and combustion, shock wave reactions and general reactions in a flowing or static system. An implicit numerical solution method is used which works efficiently for the extreme conditions of a very slow or a very fast reaction. The report includes a description of the theory and the computer program, including a complete users manual. Information on obtaining the program may be obtained from the authors.
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A general chemical kinetics computer program for complex, homogeneous ideal-gas reactions is described. It is designed for flexibility and convenience in treating reactions under many different conditions. Some of these conditions are (1) reaction behind a shock wave, (2) ignition and combustion reactions in a static or flowing system, (3) combustion and nozzle expansion, and (4) general reaction in a static system or one-dimensional frictionless flow. In any system the temperature or volume or both may be held constant.

An implicit numerical integration method is used for the solution of the differential equations that describe a complex reaction. A new step size optimization procedure has been developed to make this technique work efficiently for a wide range of conditions. This includes the extremes of very slow and very fast reaction.

This report describes the theoretical equations involved, as well as the numerical method of solution. A detailed description of the program is given including preparation of input data, control of accuracy, sample input data, and several examples of test case results.
sometimes be made while still obtaining useful results. Some of these for exhaust nozzle flow are discussed in references 1 and 2. Two of the most used ideas are (1) the assumption of equilibrium flow (infinite reaction rates) and (2) the assumption of sudden freezing or rapid transition from infinite reaction rates to zero reaction rates. The assumption (2) often gives useful information with the use of only a small amount of chemical kinetic information. For better insight into the reaction details, however, exact theoretical calculations are needed. The term exact is used here to mean that all important chemical reactions and their rate constants are included in the analysis. The actual solution of the nonlinear set of fluid-dynamic and kinetics equations involves some mathematical simplifications. Treanor (ref. 3) transformed these differential equations into difference equations. Other investigators locally linearized the differential equations by removing second-order terms. They then used either an exact (ref. 4) or an approximate (refs. 5 and 6) analytic solution or finite difference solutions (refs. 7 and 8).

Several computer programs have been written which use a finite difference method to integrate the differential equations of chemical kinetics. The main effort in developing these programs was to make the integration scheme overcome a mathematical instability problem that arises in these calculations. This problem is discussed in detail in a later section of this report. Briefly stated, it is the fact that some integration methods require a very small step size to maintain accuracy and stability when the chemical reaction is either very fast or very slow. This leads to excessively long computation times. The program described in reference 34 uses the technique of reference 3 to avoid these problems. Reference 9 describes rocket performance programs that use the inherently stable implicit integration technique of reference 8. Reference 35 describes another more general kinetics program based on this technique. These and other programs have the ability to handle many types of kinetics problems for many chemical systems. However, no single program has been found that could conveniently be used in a wide variety of flow and static reaction problems for an arbitrary chemical system.

For this reason, a general chemical kinetics computer program for complex gas mixtures has been developed at Lewis. It is written completely in FORTRAN IV, version 13, and was developed on an IBM 7044-7094/direct-couple system. This program can be used for any homogeneous reaction in either a flowing or a static system. It has the advantages of flexibility, accuracy and ease of use. Moreover, any chemical system may be used for which species thermodynamic data and reaction rate constants are known. The program handles several types of reaction. These include bimolecular exchange reactions, unimolecular decompositions, bimolecular decompositions, and the reverse recombination processes. The solution method is a rapid one based on the implicit finite-difference technique of Kliegel and Tyson (refs. 8 and 9). A unique step-size control system is used to estimate the optimum step size for each step. Moreover, the user can easily change the preset program controls to give his own balance between
acceptable accuracy and computing time. For flow reactions this program assumes one-dimensional flow. This is usually a good approximation for systems of practical interest, and the additional complications of three-dimensional kinetics computations (surveyed in ref. 10) are not required.

The purpose of this report is to present a complete description of the chemical kinetics computer program and the implicit numerical integration method it uses. The theoretical kinetics differential equations solved by the program are also given in detail. The program may be used (with either assigned pressure or area in flow reactions) for the following problems:

1. Chemical reaction behind a shock wave
2. Ignition and combustion in a flowing or static system
3. Ignition, combustion, and nozzle expansion in supersonic flow
4. Chemical reaction in any flowing gas mixture whose velocity does not reach the velocity of sound
5. Chemical reaction in any static system
6. Constant temperature and/or constant volume reactions

Readers interested primarily in using the program should read the section GENERAL DESCRIPTION OF PROGRAM USE for a description of program options, species information, and accuracy control. A detailed program users manual and computed test case results are given in appendixes. Further information on availability of the program may be obtained from the authors.

SYMBO LIST

General:

A
area

A₁, A₂, . . . , A₇
thermodynamic coefficients in eqs. (81) to (84)

species production function defined by eq. (12), sec⁻¹

A

A*/

B
enthalpy production function defined by eq. (13), sec⁻¹

B*/

Cₚ
heat capacity of gas per unit mass assuming constant composition
(defined by eq. (16))

D
shock tube hydraulic diameter used to calculate Lₘ (eq. (80)), cm

F(Φ, P)
shock pressure function defined by eq. (A13)
G(\mathcal{F}, P) \quad \text{shock enthalpy function defined by eq. (A14)}

G \quad \text{Gibbs free energy}

H_c \quad \text{total mixture energy per unit mass}

h \quad \text{total mixture static enthalpy per unit mass}

h_1 \quad \text{mixture static enthalpy per unit mass before passage of shock wave}

h^* \quad \text{enthalpy function defined by eq. (A12)}

l \quad \text{number of chemical reactions}

L_m \quad \text{characteristic shock tube reaction length in eq. (80), cm}

M \quad \text{mixture Mach number defined by eq. (14)}

M_w \quad \text{mixture molecular weight}

\dot{m} \quad \text{mass flow rate}

N \quad \text{number of species in a gas mixture}

P \quad \frac{p}{p_1}

p \quad \text{absolute pressure of gas mixture}

p_1 \quad \text{pressure before passage of a shock wave}

q \quad \text{independent variable, either } t \text{ or } x

R \quad \text{universal gas constant}

r \quad \text{density (}\rho\text{) if time is the integration variable; or mass flux (}\rho V\text{)}

\quad \text{if distance is the integration variable}

S \quad \text{entropy}

S_1 \quad \text{species production function defined by eq. (C37)}

S_2 \quad \text{enthalpy production function defined by eq. (C38)}

T \quad \text{absolute temperature}

T_0 \quad \text{reference temperature for calculating individual species enthalpy}

T_1 \quad \text{temperature before passage of a shock wave}

\mathcal{F} \quad \frac{T}{T_1}

T \quad \text{time}

V \quad \text{velocity}

V_S \quad \text{shock speed}

X_H \quad \text{total energy exchange rate defined by eq. (86)}
distance coordinate  
\[ x \]

boundary-layer parameter used to calculate \( L_m \) in eq. (80)

\[ \beta \]

specific heat ratio defined by eq. (15)

\[ \gamma \]

exponent in shock boundary-layer equation (eq. (80))

\[ \eta \]

gas viscosity used to calculate \( L_m \) (eq. (80))

\[ \mu \]

density

\[ \rho \]

density before passage of shock wave

\[ \rho_1 \]

Subscripted Thermochemical Symbols:

In general subscript \( i \) refers to species \( i \) and subscript \( j \) to reaction \( j \). In the appendixes other indexes are sometimes used to avoid confusion in the summations, but their meaning should be clear.

\[ A_j \]

preexponential constant in the rate constant equation (eq. (33))

\[ (C_p)_i \]

molar heat capacity of species \( i \) in a mixture

\[ E_j \]

activation energy in rate constant equation (eq. (33)), cal/mole

\[ h_i \]

static molar enthalpy of species \( i \)

\[ K_j \]

equilibrium constant defined by eq. (34)

\[ k_j \]

forward reaction rate constant (see eq. (32)); units are either \( \text{cm}^3 \text{ mole}^{-1} \text{ sec}^{-1} \) or \( \text{cm}^6 \text{ mole}^{-2} \text{ sec}^{-1} \) depending on the type of reaction

\[ M_j \]

third-body efficiency factor defined by eq. (38)

\[ m_{ij} \]

third-body efficiency ratio of species \( i \) in reaction \( j \) defined by eq. (39)

\[ n_j \]

temperature exponent in rate constant equation (eq. (33))

\[ S_i \]

entropy of species \( i \), energy per mole K

\[ S_1, S_2, \ldots, S_N \]
symbols for species names in general reaction, (eq. (32))

\[ W_i \]

net species production rate, moles vol\(^{-1}\) sec\(^{-1}\)

\[ X_j \]

net conversion rate (mole vol\(^{-1}\) sec\(^{-1}\))/(density\(^2\))

\[ X_{H,j} \]

net energy exchange rate, defined by eq. (43)

\[ \nu_{i,j} \]

forward stoichiometric coefficient in general reaction (eq. (32))

\[ \nu_{i,j}^r \]

reverse stoichiometric coefficient in general reaction (eq. (32))

\[ \sigma_i \]

concentration, moles of species \( i \) per unit mass of mixture
\( \omega_{i,j} \) net rate of formation of \( i^{th} \) species in \( j^{th} \) reaction, moles vol\(^{-1}\) sec\(^{-1}\)

Subscripted Symbols for Numerical Computation:

In these symbols, \( i \) and \( j \) refer to a particular dependent variable, and \( n \) refers to a finite difference step. Exceptions are made in the text for some summations, but the interpretation is obvious. The independent variable is shown here as \( t \), but the same notation applies if \( x \) is used.

- \( C \): step-size ratio defined in eq. (69)
- \( D_{i,n} \): ratio of increment to step size defined by eq. (70)
- \( E_{i,n+1} \): relative error in \( y_i \) at time \( t = t_{n+1} \) defined by eq. (62)
- \( f_i \): \( \frac{dy_i}{dt} \)
- \( f_{i,n} \): \( \frac{dy_i}{dt} \) at \( t = t_n \)
- \( h_n \): \( t_n - t_{n-1} \)
- \( h_1 \): \( t_1 - t_0 \)
- \( h_{\text{max}} \): maximum step size
- \( h_{\text{min}} \): minimum step size
- \( I_1, I_2, \text{ etc} \): intervals of uncertainty in step size search procedure
- \( k_{i,n} \): \( y_i(t_n) - y_i(t_{n-1}) \)
- \( k_i(e) \): exact value of \( k_{i,n} \)
- \( t_n \): time at the \( n^{th} \) step
- \( t_0 \): initial time
- \( y_i \) or \( y_j \): general dependent variable
- \( y_{i,n+1} \): \( y_i(t) \) at \( t = t_{n+1} \)
- \( \alpha_i \): \( \frac{\partial f_i}{\partial t} \)
- \( \alpha_{i,n} \): \( \frac{\partial f_i}{\partial t} \) at \( t = t_n \)
- \( \beta_{i,j} \): \( \frac{\partial f_i}{\partial y_j} \)
- \( \beta_{i,j,n} \): \( \frac{\partial f_i}{\partial y_j} \) at \( t = t_n \)
- \( \epsilon_{n+1} \): relative error in complete solution at \( (n+1)^{st} \) step, see eq. (72)
- \( \epsilon_{\text{max}} \): maximum relative error per step
The conservation equations for a complex reacting gas are presented in this section. (See, for example, the book by Penner, ref. 11). They are derived first for one-dimensional steady-state flow through an arbitrarily assigned area profile.

Global mass conservation is given by the equation

\[ \rho AV = \dot{m} \]  

or

\[ \frac{dm}{dt} = 0 \]  

where \( \dot{m} \) is the constant mass flow rate of the gas. Individual species continuity equations for the \( N \) species in the mixture are written as

\[ \frac{d}{dt} (\sigma_i \dot{m}) = W_i AV \quad i = 1, 2, \ldots, N \]  

Here \( \sigma_i \) is the number of moles of species \( i \) per unit mass of mixture. Expressions for the species production rates, \( W_i \) will be given in a following section. By performing the indicated differentiation in equation (2) and using equations (1) and (1a) the following set of equations can be obtained

\[ \frac{d\sigma_i}{dt} = \frac{W_i}{\rho} \quad i = 1, 2, \ldots, N \]  

To completely describe the system we assume adiabatic flow of an ideal gas and neglect viscosity, diffusion and heat conduction. The following additional equations can then be written for momentum and energy conservation

\[ \rho \frac{dV}{dt} + \frac{1}{V} \frac{dp}{dt} = 0 \]  

(momentum)
\[ h + \frac{V^2}{2} = H_c \quad \text{(energy)} \] (5)

where \( H_c \) is the total, constant energy of the gas per unit mass and \( h \) is the static enthalpy per unit mass of the gas given by

\[ h = \sum_{i=1}^{N} \gamma_i h_i \] (6)

\[ h_i = (h_i)_T + \int_{T_0}^{T} (C_p)_i \, dT \] (6a)

Here \( h_i \) is the molar enthalpy of species \( i \).

The molecular weight of the gas mixture is

\[ M_w = \frac{1}{N} \sum_{i=1}^{N} \gamma_i \] (7)

The equation of state is

\[ p = \frac{\rho RT}{M_w} \] (8)

Equations (1), (5), (7), and (8) are differentiated and combined with equation (4) to get the following differential equations:

\[ \frac{dV}{dt} = \frac{V}{(M^2 - 1)} \left( \frac{1}{A} \frac{dA}{dt} - \mathcal{A} \right) \] (9)

\[ \frac{d\rho}{dt} = -\rho \left[ \frac{M^2}{(M^2 - 1)} \left( \frac{1}{A} \frac{dA}{dt} - \mathcal{A} \right) + \mathcal{A} \right] \] (10)
In these equations the following auxiliary definitions have been made:

\[ \mathcal{A} = \frac{RT}{p} \sum_{i=1}^{N} W_i - \mathcal{B} \]  \hspace{1cm} (12)

\[ \mathcal{B} = \frac{1}{p} \left( \frac{\gamma - 1}{\gamma} \right) \sum_{i=1}^{N} h_i W_i \]  \hspace{1cm} (13)

\[ M^2 = \frac{V^2 M_w}{\gamma RT} \]  \hspace{1cm} (definition of Mach number) (14)

\[ \gamma = \frac{C_p}{C_p - \frac{R}{M_w}} \]  \hspace{1cm} (15)

\[ C_p = \sum_{i=1}^{N} \sigma_i (C_{p_i}) \]  \hspace{1cm} (16)

where \( C_p \) is the heat capacity of the mixture per unit mass assuming fixed composition and \((C_{p_i})_i\) is the molar heat capacity of species \( i \). Equations (3), and (9) to (11) form a system of \( N + 3 \) equations in \( N + 3 \) unknowns. Their solution must be obtained by a numerical technique.

The equations for a static reaction can now be obtained by setting the velocity equal to zero in equations (9) to (11) to get the system

\[ \frac{d\sigma_i}{dt} = \frac{W_i}{\rho} \quad i = 1, 2, \ldots, N \]  \hspace{1cm} (3)
\[
\frac{dQ}{dt} = -\rho \mathcal{A}
\]  

(17)

\[
\frac{dT}{dt} = -T \mathcal{B}
\]  

(18)

The reacting gas can also be described by equations that use distance, \(x\) as the independent variable. The relation \(dQ/dx = (1/V)dQ/dt\) is used to rewrite equations (3), (9), (10), and (11). Here \(Q\) represents any of the variables \(V, \rho, T, \) or \(\sigma_i\). The new equations are

\[
\frac{d\sigma_i}{dx} = \frac{W_1}{\rho V} \quad i = 1, 2, \ldots, N
\]  

(19)

\[
\frac{dV}{dx} = \frac{V}{(M^2 - 1)} \left( \frac{1}{A} \frac{dA}{dx} - \mathcal{A}^* \right)
\]  

(20)

\[
\frac{d\rho}{dx} = -\rho \left[ \frac{M^2}{(M^2 - 1)} \left( \frac{1}{A} \frac{dA}{dx} - \mathcal{A}^* \right) + \mathcal{A}^* \right]
\]  

(21)

\[
\frac{dT}{dx} = \frac{(\gamma - 1)M^2}{(M^2 - 1)} \left( \frac{1}{A} \frac{dA}{dx} - \mathcal{A}^* \right) + \mathcal{B}^*
\]  

(22)

where

\[
\mathcal{A}^* = \frac{\mathcal{A}}{V}
\]  

(23)

and

\[
\mathcal{B}^* = \frac{\mathcal{B}}{V}
\]  

(24)
The derivations so far have assumed adiabatic reaction. To consider instead a constant temperature reaction it is only necessary to set \( \frac{dT}{dt} \) or \( \frac{dT}{dx} \) equal to zero. This can be shown to be equivalent to eliminating the adiabatic energy equation (eq. (5)). The same situation holds if volume (or density) is held constant in a static reaction. The density derivative, \( \frac{dp}{dt} \) or \( \frac{dp}{dx} \), is set equal to zero to obtain the solution for a static reaction at constant volume. Both temperature and volume can also be held constant simultaneously.

### Differential Equations for Assigned Pressure

In the equations just derived the flow area is arbitrarily assigned. The pressure is computed from the equation of state (eq. (8)) after density, temperature, and composition have been computed from the differential equations (9) to (11). For engine combustor modeling it is often useful to reverse this procedure. One assigns a desired pressure profile and computes the area profile which then satisfies all the fundamental kinetics and fluid dynamics laws. For this type of calculation another set of differential equations can be derived to replace equations (9) to (11). The derivatives of the dependent variables are now expressed in terms of \( p \) and \( \frac{dp}{dt} \) rather than \( A \) and \( \frac{dA}{dt} \). The new equations, obtained from equation (4) and by differentiating equations (5), (7), and (8), are as follows:

\[
\frac{dV}{dt} = -\frac{1}{\rho V} \frac{dp}{dt} \tag{25}
\]

\[
\frac{d\rho}{dt} = \rho \left( \frac{1}{\gamma p} \frac{dp}{dt} - \mathcal{A} \right) \tag{26}
\]

\[
\frac{dT}{dt} = T \left[ (\gamma - 1) \frac{1}{\gamma} \frac{dp}{dt} - \mathcal{B} \right] \tag{27}
\]

The quantities \( \mathcal{A} \) and \( \mathcal{B} \) are the same as previously defined in equations (12) and (13). If distance, \( x \) is the independent variable, the assigned pressure equations are the same, with \( \frac{dp}{dt} \) replaced by \( \frac{dp}{dx} \) and \( \mathcal{A} \) and \( \mathcal{B} \) replaced by \( \mathcal{A}^* \) and \( \mathcal{B}^* \).

\[
\frac{dV}{dx} = -\frac{1}{\rho V} \frac{dp}{dx} \tag{28}
\]
\[
\frac{d\rho}{dx} = \rho \left( \frac{1}{\gamma \rho} \frac{dp}{dx} - \alpha^* \right) \tag{29}
\]

\[
\frac{dT}{dx} = T \left[ \left( \frac{\gamma - 1}{\gamma} \right) \frac{1}{\rho} \frac{dp}{dx} - \alpha^* \right] \tag{30}
\]

Either of these equation sets is solved (along with the appropriate equations for \(d\sigma_i/dt\) or \(d\sigma_i/dx\)) to give \(V, T, \rho,\) and the \(\sigma_i\)'s. Then area is computed from the assigned constant mass flow rate using the mass conservation equation, equation (1).

**Chemical Reaction Equations and Species Production Rates**

The species formation rate, \(W_i\), that appears in equations (3) and (19) is given by

\[
W_i = \sum_{j=1}^{l} \omega_{ij} \tag{31}
\]

where \(l\) is the number of chemical reactions occurring and \(\omega_{ij}\) is the net rate of formation of species \(i\) by the \(j^{th}\) reaction in moles per unit volume per second. Each chemical reaction is written in general form as

\[
\sum_{i=1}^{N} \nu_{ij} S_i \xrightarrow{k_j} \sum_{i=1}^{N} \nu_{ij}' S_i \tag{32}
\]

where \(S_i\) is the \(i^{th}\) species. The \(\nu_{ij}\) and \(\nu_{ij}'\) are the forward and reverse stoichiometric coefficients for \(S_i\) and \(k_j\) and \(k_{bj}\) are the forward and reverse rate constants for the \(j^{th}\) reaction. Each \(k_j\) is a function of temperature given by the equation

\[
k_j = A_j T^n_j e^{-E_j/RT} \tag{33}
\]

The value of \(k_{bj}\) is calculated from \(k_j\) and the equilibrium constant \(K_j\) (in concentration units) by the law of microscopic reversibility.
For convenience we introduce the net reaction conversion rate $X_j$ which is related to $\omega_{ij}$ by the equation

$$\omega_{ij} = \rho^2 (\nu_{ij}^* - \nu_{ij})X_j$$

The units of $X_j$ are (moles/vol sec)/(density)$^2$. It is useful as a measure of the amount of change due to each reaction occurring in the gas mixture. We use $X_j$ rather than the net molar reaction rate because the $X_j$ values are more convenient for comparison than the molar rates. The exact form of $X_j$ depends on the type of reaction being considered. In this program three types of reversible chemical reaction are considered. These reactions and the corresponding $X_j$ formulas are given next.

Type 1 - bimolecular shuffle reaction:

$$S_1 + S_2 \overset{k_j}{\longrightarrow} S_3 + S_4$$

$$X_j = k_j \left( \sigma_1 \sigma_2 - \frac{1}{K_j} \sigma_3 \sigma_4 \right)$$

Type 2a - three-body recombination:

$$M + S_1 + S_2 \overset{k_j}{\longrightarrow} S_3 + M$$

where $M$, the catalyst molecule, can be any species present.

$$X_j = k_j M_j \left( \rho \sigma_1 \sigma_2 - \frac{\sigma_3}{K_j} \right)$$

where $M_j$, the third-body efficiency factor for the $j^{th}$ reaction is
In this equation \( m_{ij} \) is the third-body efficiency factor for species \( i \) in the \( j \)th reaction. It is a correction only on the preexponential factor \( A_j \) in equation (33) and can be written as

\[
m_{ij} = \frac{(A_j)_{\text{species } i}}{(A_j)_0}
\]

(39)

where \((A_j)_0\) is the \( A_j \) value for a reference species as a third body.

Type 2b - two-body dissociation:

\[
M + S_3 \xrightleftharpoons[k_j]{k_j} S_1 + S_2 + M
\]

where \( M \) is the catalyst molecule

\[
X_j = k_j M_j \left( \sigma_3 - \frac{\rho \sigma_1 \sigma_2}{K_j} \right)
\]

(40)

where \( M_j \) is defined by equation (38).

Type 3a - unimolecular decomposition:

\[
S_3 \xrightleftharpoons[k_j]{k_j} S_1 + S_2
\]

\[
X_j = k_j \left( \frac{\sigma_3 - \sigma_1 \sigma_2}{\rho K_j} \right)
\]

(41)

Type 3b - two-body recombination:

\[
S_1 + S_2 \xrightleftharpoons[k_j]{k_j} S_3
\]
\[ X_j = k_j \left( \frac{\sigma_1 \sigma_2 - \sigma_3}{\rho K_j} \right) \]  \hspace{0.5cm} (42)

The size of \( X_j \) tells approximately the importance of any single reaction among all those occurring. The sign of \( X_j \) tells how the reaction is actually occurring: \( X_j \) is positive if the \( j \)th reaction is proceeding from left to right as written, and negative if it is proceeding in the opposite direction.

For some problems the heat release rate is an important consideration. For such situations another useful quantity was defined and used in reference 12 to measure a reaction's importance. This is the net energy conversion rate for the \( j \)th reaction defined by

\[ X_{H,j} = X_j (\Delta H_{298})_j \]  \hspace{0.5cm} (43)

where \( (\Delta H_{298})_j \) is the molar heat of reaction at 298 K for the \( j \)th reaction proceeding in the forward direction, from left to right.

**Normal Shock Equations**

A chemical reaction can be started by the passage of a shock wave through a gas. The assumption is made that the shock wave instantaneously raises the gas to new temperature and pressure conditions without changing its composition. The conservation equations for the change in conditions across the shock are

\[ \rho_1 V_S^2 = \rho V^2 \]  \hspace{0.5cm} (44)

\[ p_1 + \rho_1 V_S^2 = p + \rho V^2 \]  \hspace{0.5cm} (45)

\[ h_1 + \frac{V_S^2}{2} = h + \frac{V^2}{2} \]  \hspace{0.5cm} (46)

In these equations the coordinate system is attached to the shock, which is considered stationary. The unshocked gas at conditions \( p_1, \rho_1, \) and \( T_1 \) flows past the shock with speed \( V_S \), the experimental shock velocity. Gas properties immediately after the shock passes are \( p, \rho, \) and \( T \). The enthalpy per gram of gas mixture is changed from \( h_1 \).
to $h$ by the shock. Since gas composition is unchanged, $h$ is calculated for the initial composition at the new temperature $T$. The actual equations solved are given in appendix A. These conditions are called the no-reaction or frozen shock conditions.

The increased temperature and pressure behind the shock start the chemical reaction. It is also possible to solve equations (44) to (46) for the equilibrium postshock conditions. These are the final velocity, temperature, pressure, and new composition that would exist after all chemical reaction is complete. The solution method for this situation is also described in appendix A. The complete shock-equation solution uses the method described by Gordon and McBride (ref. 13).

**NUMERICAL ANALYSIS**

**Summary of Technique**

The nonlinear, coupled differential equations derived in the previous section (e.g., eqs. (19) to (22)) describe the relaxation of a reacting gas toward equilibrium. The relaxation rates of the fluid mechanical variables are often quite different from the relaxation rates of the component gases, particularly in near-equilibrium flow regimes. In addition, there can be large differences in the relaxation rates of the individual gases. Systems of differential equations which represent relaxation processes with widely different relaxation rates are called stiff systems.

The numerical integration of a system of stiff differential equations poses a serious stability problem. The problem arises in trying to resolve rapid variations over the small regions in which they contribute significantly to the solution while at the same time advancing the integration at a rate which is consistent with the slower, more dominant solutions. Most conventional numerical integration techniques force the step size to be impractically small in order to maintain stability.

Many integration techniques have been derived which are both more stable and more efficient than conventional methods for integrating stiff systems. Among these are Treanor's modified Runge-Kutta method (ref. 3) and Moretti's method (ref. 4) involving the exact solution of locally linearized equations. A method which falls logically between those two is the implicit integration method of Tyson (refs. 8 and 14). This method has the advantages of being inherently stable and computationally efficient. The inherent stability of Tyson's method makes it preferable for general applications where nothing is known ahead of time about the disparity in relaxation rates (see ref. 15). The general chemical kinetics program uses the implicit integration method of Tyson with modifications to the initial step and error formulas. Other inherently stable implicit integration methods have been proposed by Lomax and Bailey (ref. 7) and Liniger and Willoughby (ref. 16).
Since Tyson's method is stable for all step sizes, the stability problem is solved. However, the gain in stability obtained by using an implicit rather than an explicit integration method is accomplished at the expense of increasing the number of calculations that must be performed at each step. In particular, all the implicit schemes mentioned require the calculation of all the partial derivatives of the differential equations (see appendixes B and C). The application of an effective strategy for step-size control can significantly increase the rate at which the numerical integration advances. The general chemical kinetics program uses a step-size optimization procedure that is superior to the standard doubling and halving method of step-size control. After each step of the numerical integration, an error predictor is used to search within limits for the largest step size that can be used for the next step without violating the user's accuracy requirements. Experience has shown that this optimization technique permits the step size to react quickly to regions of very slow or very fast reaction.

Derivation of Numerical Integration Equations

This section presents a complete derivation of Tyson's general step formula (ref. 14) and our initial step and error formulas. A derivation of Tyson's formula for a fixed step size is contained in reference 9.

General step formula. - Let the following set of coupled first-order simultaneous differential equations be given:

\[
\frac{dy_i}{dt} = f_i(t, y_1, y_2, \ldots, y_N) \quad i = 1, 2, \ldots, N \tag{47}
\]

It will be assumed that these equations are nonsingular and that a solution exists which can be developed as a Taylor series. In other words, for \(|t_{n+1} - t_n|\) sufficiently small,

\[
k_{i, n+1} = \frac{dy_i}{dt}_{t=t_{n+1}} + \frac{d^2y_i}{dt^2}_{t=t_{n+1}} \frac{h_{n+1}^2}{2} \left| y_i(t_{n+1}) \right| + \frac{d^3y_i}{dt^3}_{t=t_{n+1}} \frac{h_{n+1}^3}{6} \left| y_i(t_{n+1}) \right| + \ldots \quad i = 1, 2, \ldots, N \tag{48}
\]

where

\[
k_{i, n+1} = y_i(t_{n+1}) - y_i(t_n) \tag{49}
\]

\[
h_{n+1} = t_{n+1} - t_n \tag{50}
\]
Performing an expansion similar to equation (48) for \( y_i(t_{n-1}) \) about \( t_{n+1} \) yields

\[
k_{i, n+1} + k_{i, n} = \left. \frac{d y_i}{d t} \right|_{t_{n+1}} (h_{n+1} + h_n) - \left. \frac{d^2 y_i}{d t^2} \right|_{t_{n+1}} \frac{(h_{n+1} + h_n)^2}{2!} + \left. \frac{d^3 y_i}{d t^3} \right|_{t_{n+1}} \frac{(h_{n+1} + h_n)^3}{3!} - \ldots \tag{51}
\]

The second derivative terms can now be eliminated between equations (48) and (52). Multiplying equation (48) by \( \frac{(h_{n+1} + h_n)^2}{h_{n+1}} \) and then subtracting equation (51) gives

\[
\frac{(2h_{n+1} + h_n)}{h_{n+1}(h_{n+1} + h_n)} k_{i, n+1} - \frac{h_{n+1}}{(h_{n+1} + h_n) h_n} k_{i, n} = \left. \frac{d y_i}{d t} \right|_{t_{n+1}} - \left. \frac{d^3 y_i}{d t^3} \right|_{t_{n+1}} \frac{h_{n+1}(h_{n+1} + h_n)}{3!} + \ldots \tag{52}
\]

From the Taylor series expansion by partial derivatives for \( \left. \frac{d y_i}{d t} \right|_{t_{n+1}} \) about the point \( t_n \) we get

\[
\left. \frac{d y_i}{d t} \right|_{t_{n+1}} = \left. \frac{d y_i}{d t} \right|_{t_n} + \sum_{j=1}^{N} \left. \frac{\partial f_i}{\partial y_j} \right|_{t_n} k_{j, n+1} + \sum_{j=1}^{N} \left. \frac{\partial f_i}{\partial y_j} \right|_{t_n} \left. \frac{d^3 y_i}{d t^3} \right|_{t_n} \frac{h_{n+1}^2}{2!} + \ldots \tag{53}
\]

Letting

\[
f_{i, n} = \left. \frac{d y_i}{d t} \right|_{t_n} \tag{54}
\]
and substituting the last expansion into equation (52) gives

\[
\frac{(2h_{n+1} + h_n)}{h_{n+1}(h_{n+1} + h_n)} - k_{i,n+1} - \frac{h_{n+1}}{(h_{n+1} + h_n)h_n} \cdot k_{i,n} = \left( f_{i,n} + \alpha_{i,n}h_{n+1} + \sum_{j=1}^{N} \beta_{i,j,n}k_{j,n+1} \right) + \frac{d^3 y_i}{dt^3} \left|_{t_n} \right. + \frac{d^3 y_i}{dt^3} \left|_{t_{n+1}} \right.
\]

Again, by a Taylor series expansion

\[
\frac{d^3 y_i}{dt^3} \left|_{t_n} \right. = \frac{d^3 y_i}{dt^3} \left|_{t_{n+1}} \right. + \frac{h_n^2}{2!} + 0 \left( \frac{h_{n+1}^3}{3!} \right)
\]

The substitution of equation (58) into equation (57) gives, after combining and rearranging the terms,

\[
k_{i,n+1} = \frac{h_{n+1}^2}{(2h_{n+1} + h_n)h_n} \cdot k_{i,n} + \frac{h_{n+1}(h_{n+1} + h_n)}{(2h_{n+1} + h_n)} \left( f_{i,n} + \alpha_{i,n}h_{n+1} + \sum_{j=1}^{N} \beta_{i,j,n}k_{j,n+1} \right) + \frac{d^3 y_i}{dt^3} \left|_{t_n} \right. + \frac{d^3 y_i}{dt^3} \left|_{t_{n+1}} \right. + 0 \left( \frac{h_{n+1}^4}{4!} \right)
\]
Finally, equation (59) is truncated to produce the implicit equation

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

\[ i = 1, 2, \ldots, N \quad (60) \]

The solution of the coupled first-order simultaneous differential equations (47) can be obtained by solving at each step the following set of linear equations

\[
\begin{bmatrix}
1 - \frac{h_n}{(2h_{n+1} + h_n)} \beta_{i,i,n} \\
\frac{h_{n+1}(h_{n+1} + h_n)}{(2h_{n+1} + h_n)} \sum_{j=1}^{N} \beta_{i,j,n} k_{j,n+1}
\end{bmatrix}
\]

\[ k_{i,n+1} = \frac{h_{n+1}(h_{n+1} + h_n)}{(2h_{n+1} + h_n)} \left( f_{i,n} + \alpha_{i,n} h_{n+1} \right) \quad i = 1, 2, \ldots, N \quad (61) \]

The equations for \( f_i, \alpha_i, \) and \( \beta_{i,j} \), which are required in order to apply this implicit integration technique to the chemical kinetics problem, are given in appendixes B and C.

Error formula. - The relative error in the numerical solution of \( \frac{dy_i}{dt} = f_i \) at the \((n+1)\)st step is defined as

\[ E_{i,n+1} = \left| \frac{k_{i,n+1}^{(e)} - k_{i,n+1}}{y_{i,n+1}} \right| \quad (62) \]

where \( k_{i,n+1}^{(e)} \) is the exact value of the increment \( k_{i,n+1} \). From equation (59),

\[ k_{i,n+1}^{(e)} - k_{i,n+1} \approx \frac{d^3 y_i}{dt^3} \bigg|_{t_{n+1}} \frac{h_n}{(2h_{n+1} + h_n)} \left( \frac{(h_{n+1} + h_n)(2h_{n+1} - h_n)}{3(2h_{n+1} + h_n)} \right) \quad (63) \]
An expression that can be used to evaluate \( \left( \frac{d^3y_i}{dt^3} \right)_{t_{n+1}} \) will now be obtained. The following equations are the result of Taylor series expansions about the point \( t_{n+1} \):

\[
k_{i,n+1} \approx \left. \frac{dy_i}{dt} \right|_{t_{n+1}} h_{n+1} - \left. \frac{d^2y_i}{dt^2} \right|_{t_{n+1}} \frac{h_{n+1}^2}{2!} + \left. \frac{d^3y_i}{dt^3} \right|_{t_{n+1}} \frac{h_{n+1}^3}{3!}
\]  

(64)

\[
k_{i,n+1} + k_{i,n} \approx \left. \frac{dy_i}{dt} \right|_{t_{n+1}} (h_{n+1} + h_n) - \left. \frac{d^2y_i}{dt^2} \right|_{t_{n+1}} \frac{(h_{n+1} + h_n)^2}{2!} + \left. \frac{d^3y_i}{dt^3} \right|_{t_{n+1}} \frac{(h_{n+1} + h_n)^3}{3!}
\]  

(65)

\[
k_{i,n+1} + k_{i,n} + k_{i,n-1} \approx \left. \frac{dy_i}{dt} \right|_{t_{n+1}} (h_{n+1} + h_n + h_{n-1}) - \left. \frac{d^2y_i}{dt^2} \right|_{t_{n+1}} \frac{(h_{n+1} + h_n + h_{n-1})^2}{2!} + \left. \frac{d^3y_i}{dt^3} \right|_{t_{n+1}} \frac{(h_{n+1} + h_n + h_{n-1})^3}{3!}
\]  

(66)

The preceding set of equations can be solved to give \( \left( \frac{d^3y_i}{dt^3} \right)_{t_{n+1}} \) in terms of \( k_{i,n+1} \), \( k_{i,n} \), and \( k_{i,n-1} \). The solution is

\[
\left. \frac{d^3y_i}{dt^3} \right|_{t_{n+1}} \approx \frac{3!}{(h_{n+1} + h_n + h_{n-1})} \left[ \frac{1}{h_{n+1}(h_{n+1} + h_n)} k_{i,n+1} - \frac{(h_{n+1} + 2h_n + h_{n-1})}{(h_{n+1} + h_n)h_n(h_{n+1} + h_{n-1})} k_{i,n} \right. \\
+ \frac{1}{(h_n + h_{n-1})h_{n+1}} k_{i,n-1} \left. \right]
\]  

(67)

Combining equations (62), (63), and (67) yields
\[ E_{i,n+1} = \left[ \frac{h_{n+1}^2(2h_{n+1} - h_n)}{(2h_{n+1} + h_n)(h_{n+1} + h_n + h_{n-1})(h_n + h_{n-1})} \left( \frac{1}{y_{i,n+1}} \right) \right] \times \left[ \frac{k_{i,n+1}}{h_{n+1}} - (h_{n+1} + 2h_n + h_{n-1}) \frac{k_{i,n}}{h_n} + (h_{n+1} + h_n) \frac{k_{i,n-1}}{h_{n-1}} \right] \] (68)

With the definitions

\[ C = \frac{(h_{n+1} + h_n)}{(h_n + h_{n-1})} \] (69)

\[ D_{i,m} = \frac{k_{i,m}}{h_m} \] (70)

equation (68) can be rewritten as

\[ E_{i,n+1} = \left[ \frac{h_{n+1}^2(2h_{n+1} - h_n)}{(2h_{n+1} + h_n)(h_{n+1} + h_n + h_{n-1})(h_n + h_{n-1})} \left( \frac{1}{y_{i,n+1}} \right) \right] \left[ D_{i,n+1} - D_{i,n} \right] \]

- \[ C(D_{i,n} - D_{i,n-1}) \] (71)

Finally, the relative error in the solution of the set of equations given by equation (47) at the \((n+1)\text{st}\) step is defined to be

\[ \epsilon_{n+1} = \max_{i \in I} E_{i,n+1} \] (72)

where \( I \) is the set of all dependent variables that are not being omitted from error con-
The relative error $\varepsilon_{n+1}$ is used to control both the accuracy and the step size during the numerical integration.

**Initial step formula.** - The general step formula given by equation (60) requires the value of the increment $k_{i,n}$ and the step size $h_n$ from the previous step. Thus, that formula cannot be used for the initial step. Notice that the error formula (eq. (71)) requires information from two previous steps. We will derive a formula that can be used for the initial two steps to generate initial values for the general step procedure. Let $h_1$ be the initial step size, $t_0$ the initial time, and $h$ any second step size. Then equation (60) can be written as

$$y_i(t_0 + h_1 + h) - y_i(t_0 + h_1) = \frac{h^2}{2h + h_1} \left[ \frac{y_i(t_0 + h_1) - y_i(t_0)}{h_1} \right] + \frac{h(h + h_1)}{(2h + h_1)} \left[ f_i(t_0 + h_1) \right]$$

$$+ \alpha_i(t_0 + h_1)h + \sum_{j=1}^{N} \beta_{i,j}(t_0 + h_1)\left[ y_j(t_0 + h_1 + h) - y_j(t_0 + h_1) \right]. \quad i = 1, 2, \ldots, N \quad (73)$$

Taking the limit of equation (73) as $h_1$ approaches zero, we obtain

$$y_i(t_0 + h) - y_i(t_0) = \frac{h}{2} \left. \frac{dy_i}{dt} \right|_{t_0} + \frac{h}{2} \left[ f_i(t_0) + \alpha_i(t_0)h + \sum_{j=1}^{N} \beta_{i,j}(t_0)\left[ y_j(t_0 + h) - y_j(t_0) \right] \right] \quad (74)$$

or more simply,

$$k_{i,1} = f_{i,0}h + \frac{h}{2} \left( \alpha_{i,0} + \sum_{j=1}^{N} \beta_{i,j,0}k_{j,1} \right) \quad (75)$$

The initial step is performed by solving the following system of linear equations:

$$\left( 1 - \beta_{i,1,0} \frac{h}{2} \right) k_{i,1} - \frac{h}{2} \sum_{j=1}^{N} \beta_{i,j,0}k_{j,1} = h \left( f_{i,0} + \alpha_{i,0} \frac{h}{2} \right) \quad i = 1, 2, \ldots, N \quad (76)$$
Since equation (76) requires no information from a previous step, it can be used for each of the initial two steps.

**Step-Size Optimization**

The numerical integration technique used in the program contains a unique step-size optimization procedure. We define the optimum step size for each integration step to be the largest step size that is consistent with the user's accuracy requirements. The user's accuracy requirements are specified by three input parameters: (1) \( \epsilon_{\text{max}} \), the maximum relative error per step, (2) \( h_{\text{max}} \), the maximum step size, and (3) \( h_{\text{min}} \), the minimum step size. The optimum step size, if it exists, must be in the interval \((h_{\text{min}}, h_{\text{max}})\) and have an associated relative error which does not exceed \( \epsilon_{\text{max}} \). In practice, the optimization procedure obtains an approximation of the optimum step size for the given step. The calculation of this approximate optimum step size is based on an empirical method for predicting relative error as a function of step size. The approximation is obtained by performing a limited number of trials to find the largest step size within some subinterval of \((h_{\text{min}}, h_{\text{max}})\) whose predicted relative error does not exceed \( \epsilon_{\text{max}} \). The complete optimization procedure is described in the following paragraphs.

At the conclusion of each step a judgement is made by comparing \( \epsilon_n \), the relative error in the step just concluded, with \( \epsilon_{\text{max}} \):

1. If \( \epsilon_n < \frac{1}{2} \epsilon_{\text{max}} \), increase the step size for the \((n+1)^{\text{st}}\) step.
2. If \( \frac{1}{2} \epsilon_{\text{max}} \leq \epsilon_n \leq \frac{5}{6} \epsilon_{\text{max}} \), use \( h_{n+1} = h_n \).
3. If \( \epsilon_n > \frac{5}{6} \epsilon_{\text{max}} \) and \( h_n \geq h_{\text{min}} \), decrease the step size for the \((n+1)^{\text{st}}\) step.
4. If \( \epsilon_n > \epsilon_{\text{max}} \) and \( h_n = h_{\text{min}} \), restart at the \(n^{\text{th}}\) step.

If the judgement is made to increase the step size for the next step, then a search is made for the optimal \( h_{n+1} \) in the interval \([h_n, h_{\text{max}}]\). Analogously, the judgement to decrease the step size for the next step triggers a search for the optimal \( h_{n+1} \) in the interval \([h_{\text{min}}, h_n]\). If condition (4) is satisfied then the restart procedure is initiated. The restart procedure consists of repeating the \(n^{\text{th}}\) step using equation (76) with \( h_0 = \frac{1}{2} h_{\text{min}} \) and performing the \((n+1)^{\text{st}}\) step in the same manner. Automatically restarting a case at the beginning of the \(n^{\text{th}}\) step is exactly the same as manually starting that case with the conditions at the end of the \((n-1)^{\text{st}}\) step as the initial conditions and \( \frac{1}{2} h_{\text{min}} \) as the initial step size.

The general step formula equation (60), derived in the previous section is implicit because of the terms \( k_{j,n+1} \) on the right side and thus must be solved as a set of simultaneous linear equations. Making the substitution

\[
k_{j,n+1} \approx \frac{h_{n+1}}{2} \left( f_{j,n} + \frac{k_{i,n}}{h_n} \right) \quad j \neq i
\]
into equation (60) and solving for $k_{i,n+1}$ yields

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

\[ i = 1, 2, \ldots, N \]  

The set of equations described by (78) is explicit in $k_{i,n+1}$. It requires appreciably fewer operations to obtain values for the increments $k_{i,n+1}$ from (78) than from the simultaneous solution of the equations given by (61). Now, for any given step size $h_{n+1}$, by using equation (78) as a predictor and equation (60) as a corrector, an approximate solution to the simultaneous equations described by (61) can be obtained. This approximate solution is used to compute a relative error according to the error equations developed in the previous section. The error thus calculated is a prediction of the error that can be expected from the simultaneous solution of equations (61) using the step size $h_{n+1}$. The step-size optimization is accomplished by searching for a step size $h_{n+1}$ whose predicted error is equal to $\epsilon_{\text{max}}$.

The search technique is a modified form of the conventional half-interval search. Starting with an interval of uncertainty for $h_{n+1}$ of length $I$ (e.g., $I_1 = |h_{\text{max}} - h_n|$), the search successively narrows down the interval until after $n$ iterations ($n \geq 2$), the maximum length of the interval of uncertainty is $I_n = \left( \frac{1}{2} \right)^{n-2} \left( 1 \right)$. The search is terminated when either an $h_{n+1}$ is found whose predicted error is $\epsilon_{\text{max}}$ or the limit of 11 on the number of iterations has been reached. In either case the last estimate of $h_{n+1}$ will be used for the next step. Notice that in the worst case $I_{11} \approx 10^{-3} |h_{\text{max}} - h_{\text{min}}|$. Hence, having chosen an input value for $h_{\text{min}}$ on the basis of round-off error and computer time considerations, a reasonable input value for $h_{\text{max}}$ would be $10^3 \cdot h_{\text{min}}$. This would insure that the final interval of uncertainty would be of the order of $h_{\text{min}}$.

**GENERAL DESCRIPTION OF PROGRAM USE**

The kinetics program can compute the progress of many different types of static or one-dimensional flow reaction. These include ignition processes, reactions behind a
shock wave, nozzle expansions and assigned pressure reactions. Constant volume and/or constant temperature reactions can also be handled. Computations can be performed for any homogeneous gas mixture containing no more than 25 species. Any species may be considered as long as its thermodynamic data are available in the form described in the section Thermodynamic Data and Species Names. Thirty chemical reactions of the three types already mentioned may be used. There is no limit on the number of each type. For a typical computation the user must provide rate constants and initial values of temperature, pressure, and species concentrations. For a flow reaction, the velocity and an area or pressure profile are also required. Nonzero initial time and position values may be specified. Otherwise, the program sets the starting values of x and t to zero. A detailed description of data card preparation is given in appendix D, and appendix E lists input and selected results for several test cases.

Options

There are several program options that provide for many reaction conditions and these will now be described.

Integration variable. - Either the time or distance version of the basic differential equations may be integrated. The integration variable is chosen by punching the word TIME or DISTANCE on a data card.

Static or flow reaction. - The program was written with flow-kinetic applications in mind. However, static chemical reactions can also be considered very simply by (1) choosing the TIME integration option and (2) setting the flow velocity \( V \) equal to zero. The program then integrates equations (3), (17), and (18) for a static system.

Shock wave reactions. - The program contains an option for easily computing the progress of chemical reactions behind a shock wave. When the logical variable SHOCK is set equal to TRUE, the initial conditions are recognized as unshocked gas conditions. The velocity, \( V \) is then the shock speed \( V_s \). The program first solves the conservation equations to obtain the conditions of pressure, temperature, and particle velocity behind the shock assuming no reaction. These new conditions and the initial composition are then used to compute the progress of the chemical reactions occurring in the high-temperature region behind the shock wave. The program also computes the final conditions that would exist if these chemical reactions went to complete equilibrium.

Equilibrium calculations. - An option is provided in the program for calculating the final equilibrium conditions for a constant pressure combustion. Both enthalpy and pressure are assumed constant for these calculations, which are triggered by setting the logical variable COMBUS equal to TRUE.

Units options. - The user has a choice of three different systems of units for both
input and output. These are the CGS, U. S. Customary (or FPS), and SI systems. The choice of output units is completely independent of the input units. The exact units used in each system are listed in the sections below on INPUT and OUTPUT.

Assigned profile options. - For any flow-kinetic reaction, an area or pressure profile must be assigned. For a static reaction neither pressure nor area need be assigned. However, a pressure profile may be assigned. The assigned variable may be specified in any of the following ways as a function of time or distance; the choice is independent of the integration variable used:

(a) A table of assigned variable against distance or time.

(b) Polynomial coefficients for the equation

\[ Q = C_0 + C_1q + C_2q^2 + C_3q^3 \]  

(79)

where \( Q \) is the assigned variable and \( q \) is either \( t \) or \( x \). Notice that a constant area or pressure profile can be specified by setting \( C_3 = C_2 = C_1 = 0 \) and \( C_0 \) equal to the constant value.

(c) Special area function. The area may be calculated by the equation

\[ A = \frac{1}{1 - \left( \frac{x}{L_m} \right)^\eta} \]  

(80)

This equation is used to represent laminar and turbulent boundary-layer effects in a shock tube according to the theory of Mires (refs. 17 to 19). The exponent \( \eta \) must be read into the program. Its value is either 0.5 for a laminar boundary layer of 0.8 for a turbulent boundary layer. The characteristic reaction length parameter, \( L_m \), may either be read in or computed by the program. The program uses equation (3) of reference 19 for a laminar boundary layer or equation (4) of reference 18 for a turbulent boundary layer. If \( L_m \) is to be computed, three other quantities are read in instead of \( L_m \). These are the shock tube hydraulic diameter \( D \), the unshocked gas viscosity \( \mu \), and a boundary-layer thickness parameter \( \beta \), which can be calculated from equations given in references 18 and 19.

Third-body efficiencies. - The program allows the rate constant for any three-body recombination-dissociation reaction to be adjusted for the efficiencies of different third-body catalysts. The user may read in values of the weighting factor \( m_{ij} \) defined in equation (39) for any three-body reaction if the logical variable ALLM1 is set equal to FALSE. All the weighting factors are equal to 1.0 unless changed by the user.

Multiple cases. - Several different cases may be done in one computer run without preparing a complete new data deck for each one. This is done with the use of an ACTION card in each data deck following the first case. The four options that may be used on this ACTION card will be described in a later section.
Constant volume and temperature reactions. - The user has the option of holding either temperature or volume, or both, constant during the chemical reaction computation. The constant temperature condition is obtained by setting the logical variable TCON equal to TRUE. For constant volume the variable RHOCON is set equal to TRUE.

Standard options. - The program has a built-in standard choice for many of the previously mentioned options. None of the given code words or logical variable names has to appear on a data card unless the user wants a nonstandard option. A list of the standard options will be given in a later section.

Thermodynamic Data and Species Names

All thermodynamic data and species names are identical to those used in the chemical equilibrium composition program of Gordon and McBride (ref. 13). Thermodynamic functions are calculated by polynomial equations for $C_p$, $h$, $S$, and $G$ as a function of temperature. The polynomial coefficients were calculated using the thermodynamic properties computer program of McBride and Gordon (ref. 20). The data calculated from these equations are the same as those tabulated in the JANAF thermochemical tables (ref. 21). Seven coefficients $A_1, A_2, \ldots, A_7$ are used for each species in the following equations, where $T$ is the kelvin temperature.

\begin{align}
\frac{C_p}{R} &= A_1 + A_2 T + A_3 T^2 + A_4 T^3 + A_5 T^4 \quad (81) \\
\frac{h}{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 (82) \\
\frac{S}{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 (83) \\
\frac{G}{RT} &= A_1 (1 - \ln T) - \frac{A_2}{2} T - \frac{A_3}{6} T^2 - \frac{A_4}{12} T^3 - \frac{A_5}{20} T^4 - A_7 \quad (84)
\end{align}

These coefficients $A_1, \ldots, A_7$ are read into the kinetics program either as data cards or card images on magnetic tape. The detailed description of the data cards for each species is given in appendix D. The information on these cards is of three types (1) the species name, (2) the stoichiometric coefficients and element names for each chemical element in the species, and (3) two sets of the thermodynamic coefficients.
A₁, A₂, . . . , A₇ for two different temperature ranges. The availability of the thermodynamic data is discussed in appendix F.

Any species can be used in a chemical kinetics computation if its thermodynamic data are read into the computer as indicated and if its name is compiled into the kinetics program in two different routines. The species name, exactly as it is written on the thermodynamic data cards, must first appear in the BLOCK DATA routine. The name array ALSP has space for 75 names containing eight symbols each. As now written, ALSP contains 71 species, so that the user may add only four new species without increasing the dimensions of the array. If this increase in dimensions is not desired, new species may be substituted for any unused ones now in the list. When a species name is

**TABLE I. - SPECIES NAMES AND MOLECULAR WEIGHTS INCLUDED IN COMPUTER PROGRAM "BLOCK DATA" SUBROUTINE**

<table>
<thead>
<tr>
<th>Species</th>
<th>Block data name</th>
<th>Molecular weight</th>
<th>Species</th>
<th>Block data name</th>
<th>Molecular weight</th>
<th>Species</th>
<th>Block data name</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ar</td>
<td>AR</td>
<td>39.948</td>
<td>CO</td>
<td>CO</td>
<td>28.011</td>
<td>Kr</td>
<td>KR</td>
<td>83.800</td>
</tr>
<tr>
<td>B</td>
<td>B</td>
<td>10.811</td>
<td>CO₂</td>
<td>CO₂</td>
<td>44.010</td>
<td>N</td>
<td>N</td>
<td>14.007</td>
</tr>
<tr>
<td>BF</td>
<td>BF</td>
<td>29.809</td>
<td>C₂F₂</td>
<td>C₂F₂</td>
<td>62.019</td>
<td>Ne</td>
<td>NE</td>
<td>20.183</td>
</tr>
<tr>
<td>BF₂</td>
<td>BF₂</td>
<td>48.808</td>
<td>C₂H</td>
<td>C₂H</td>
<td>25.030</td>
<td>NF</td>
<td>NF</td>
<td>33.005</td>
</tr>
<tr>
<td>BF₃</td>
<td>BF₃</td>
<td>67.806</td>
<td>C₂H₂</td>
<td>C₂H₂</td>
<td>26.038</td>
<td>NF₂</td>
<td>NF</td>
<td>52.004</td>
</tr>
<tr>
<td>BH</td>
<td>BH</td>
<td>11.819</td>
<td>C₂H₄</td>
<td>C₂H₄</td>
<td>28.054</td>
<td>NF₃</td>
<td>NF</td>
<td>71.002</td>
</tr>
<tr>
<td>BH₂</td>
<td>BH₂</td>
<td>12.827</td>
<td>C₂N</td>
<td>C₂N</td>
<td>38.029</td>
<td>NH</td>
<td>NH</td>
<td>15.015</td>
</tr>
<tr>
<td>BH₃</td>
<td>BH₃</td>
<td>13.835</td>
<td>Cl</td>
<td>Cl</td>
<td>35.453</td>
<td>NH₂</td>
<td>NH</td>
<td>16.023</td>
</tr>
<tr>
<td>BO</td>
<td>BO</td>
<td>26.810</td>
<td>ClF</td>
<td>ClF</td>
<td>54.451</td>
<td>NH₃</td>
<td>NH</td>
<td>17.031</td>
</tr>
<tr>
<td>BOF</td>
<td>BOF</td>
<td>45.807</td>
<td>ClF₂</td>
<td>ClF₂</td>
<td>92.448</td>
<td>NO</td>
<td>NO</td>
<td>30.006</td>
</tr>
<tr>
<td>BOF₂</td>
<td>BOF₂</td>
<td>64.807</td>
<td>Cl₂</td>
<td>Cl₂</td>
<td>70.906</td>
<td>NO⁺</td>
<td>NO</td>
<td>30.06555</td>
</tr>
<tr>
<td>BO₂</td>
<td>BO₂</td>
<td>42.810</td>
<td>Electron</td>
<td>E</td>
<td>5.48597×10⁻⁴</td>
<td>NO₂</td>
<td>NO</td>
<td>46.006</td>
</tr>
<tr>
<td>B₂O₃</td>
<td>B₂O₃</td>
<td>69.620</td>
<td>F</td>
<td>F</td>
<td>18.9964</td>
<td>N₂</td>
<td>N₂</td>
<td>28.013</td>
</tr>
<tr>
<td>Br</td>
<td>Br</td>
<td>79.909</td>
<td>F₂</td>
<td>F₂</td>
<td>37.997</td>
<td>N₂H₄</td>
<td>N₂H₄</td>
<td>32.045</td>
</tr>
<tr>
<td>Br₂</td>
<td>Br₂</td>
<td>159.82</td>
<td>H</td>
<td>H</td>
<td>1.00797</td>
<td>N₂O</td>
<td>N₂O</td>
<td>44.012</td>
</tr>
<tr>
<td>C</td>
<td>C</td>
<td>12.0112</td>
<td>HCN</td>
<td>HCN</td>
<td>27.026</td>
<td>N₂O₄</td>
<td>N₂O₄</td>
<td>92.009</td>
</tr>
<tr>
<td>CF</td>
<td>CF</td>
<td>31.010</td>
<td>HCl</td>
<td>HCl</td>
<td>36.461</td>
<td>O</td>
<td>O</td>
<td>15.9994</td>
</tr>
<tr>
<td>CF₂</td>
<td>CF₂</td>
<td>50.008</td>
<td>HF</td>
<td>HF</td>
<td>20.006</td>
<td>O⁺</td>
<td>O⁺</td>
<td>15.99885</td>
</tr>
<tr>
<td>CH</td>
<td>CH</td>
<td>13.019</td>
<td>HO₂</td>
<td>HO₂</td>
<td>33.005</td>
<td>O⁻</td>
<td>O⁻</td>
<td>15.9995</td>
</tr>
<tr>
<td>CH₂</td>
<td>CH₂</td>
<td>14.027</td>
<td>HNO</td>
<td>HNO</td>
<td>31.014</td>
<td>OH</td>
<td>OH</td>
<td>17.007</td>
</tr>
<tr>
<td>CH₂O</td>
<td>CH₂O</td>
<td>30.026</td>
<td>H₂</td>
<td>H₂</td>
<td>2.0159</td>
<td>O₂</td>
<td>O₂</td>
<td>31.997</td>
</tr>
<tr>
<td>CH₃</td>
<td>CH₃</td>
<td>15.035</td>
<td>H₂O</td>
<td>H₂O</td>
<td>18.014</td>
<td>O₂⁻</td>
<td>O₂⁻</td>
<td>31.99935</td>
</tr>
<tr>
<td>CH₄</td>
<td>CH₄</td>
<td>16.043</td>
<td>H₂O₂</td>
<td>H₂O₂</td>
<td>34.014</td>
<td>Xe</td>
<td>XE</td>
<td>131.30</td>
</tr>
<tr>
<td>CN</td>
<td>CN</td>
<td>26.018</td>
<td>He</td>
<td>HE</td>
<td>4.0026</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Formaldehyde.
listed in ALSP, its molecular weight must be written in the array ALMW in BLOCK DATA. Table I gives a list of the species now recognized by the program and also lists the exact program name and the molecular weight for each species.

A name for each species must also be listed in subroutine INIT. The names are listed in the COMMON block called FAKE and also in NAMELIST START. In this subroutine, species names are used as the FORTRAN concentration variables to simplify the input of initial species concentrations. The name for each species used in INIT is the same as the BLOCK DATA name. In the case of ionic species, a FORTRAN variable name cannot contain special characters, specifically + and -. Therefore, we have adopted the convention of using a P in place of a plus sign and an M in place of a minus sign in INIT. To illustrate this point the table below lists several species from table I, giving their BLOCK DATA names and their names in subroutine INIT. The exact species name that appears in subroutine INIT must always be used when reading in an initial concentration of any species.

<table>
<thead>
<tr>
<th>Species</th>
<th>BLOCK DATA name</th>
<th>Name in COMMON block FAKE and NAMELIST START</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂O</td>
<td>H₂O</td>
<td>H₂O</td>
</tr>
<tr>
<td>B₂O₃</td>
<td>B₂O₃</td>
<td>B₂O₃</td>
</tr>
<tr>
<td>NO⁺</td>
<td>NO⁺</td>
<td>NOP</td>
</tr>
<tr>
<td>O⁺</td>
<td>O⁺</td>
<td>OP</td>
</tr>
<tr>
<td>O⁻</td>
<td>O⁻</td>
<td>OM</td>
</tr>
<tr>
<td>O₂⁻</td>
<td>O₂⁻</td>
<td>O₂M</td>
</tr>
</tbody>
</table>

Accuracy Control

Experience has shown that all composition variable errors, Eᵢ,ₙ₊₁ need not be considered at every step in calculating εₙ₊₁ (eq. (72)), the relative error at that step. Quite often, species that have very small concentrations also have large Eᵢ,ₙ₊₁ values. If these Eᵢ,ₙ₊₁ values are used in the error calculation, the step size will be kept smaller than it has to be. Therefore, some species can usually be eliminated from the error calculation. In this section the methods used to do this are described. In general accuracy and computer running time are controlled by two factors: (1) the assigned
error $\epsilon_{\text{max}}$ combined with the species error elimination procedures and (2) the assigned step sizes, especially the initial step size.

Assigned $\epsilon_{\text{max}}$ and error elimination. - Two methods of neglecting errors due to trace species are used. The first method is done automatically unless the user wishes to prevent it. Before each new step-size calculation is done, certain species errors are eliminated from consideration in equation (72). The test for elimination is that a species error be equal to at least 15 times the median value of the errors for all the species variables. In the second error omit technique the program is told to neglect

### TABLE II. - EFFECT OF ERROR CONTROLS ON HYDROGEN - AIR IGNITION COMPUTATIONS

(a) Effect of error omit procedures

<table>
<thead>
<tr>
<th>Trial</th>
<th>Run time, min</th>
<th>$h_{\text{max}}$, cm</th>
<th>$\epsilon_{\text{max}}$</th>
<th>Automatic error elimination</th>
<th>Permanent species error elimination</th>
<th>$t$, $\mu$sec</th>
<th>$p$, atm</th>
<th>$V$, cm/sec</th>
<th>$\rho$, g/cm$^3$</th>
<th>$T$, kelvin</th>
<th>$S$, cal/gK</th>
<th>$M$</th>
<th>$\gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>22</td>
<td>0.10</td>
<td>0.00005</td>
<td>No</td>
<td>None</td>
<td>162.65</td>
<td>1.5166</td>
<td>191608</td>
<td>1.54257×10$^{-4}$</td>
<td>2.7451</td>
<td>1.7187</td>
<td>1.2518</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
<td></td>
<td>Yes</td>
<td>None</td>
<td>162.65</td>
<td>1.5131</td>
<td>191744</td>
<td>1.54155×10$^{-4}$</td>
<td>2.7464</td>
<td>1.7184</td>
<td>1.2519</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td></td>
<td></td>
<td></td>
<td>Yes</td>
<td>H$_2$O$_2$</td>
<td>162.65</td>
<td>1.5124</td>
<td>191709</td>
<td>1.54184×10$^{-4}$</td>
<td>2.7460</td>
<td>1.7187</td>
<td>1.2519</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td></td>
<td></td>
<td></td>
<td>Yes</td>
<td>H$_2$O$_2$</td>
<td>162.66</td>
<td>1.5116</td>
<td>191667</td>
<td>1.54216×10$^{-4}$</td>
<td>2.7454</td>
<td>1.7190</td>
<td>1.2518</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Mole fractions:</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_2$</td>
</tr>
<tr>
<td>OH</td>
</tr>
<tr>
<td>H$_2$O</td>
</tr>
<tr>
<td>$H_2$O</td>
</tr>
<tr>
<td>$O_2$</td>
</tr>
<tr>
<td>$O_3$</td>
</tr>
<tr>
<td>H$_2$O$_2$</td>
</tr>
<tr>
<td>$N_2$</td>
</tr>
</tbody>
</table>
certain species errors for an entire problem. This is especially needed for a slow reaction such as a long delay ignition. For any ignition reaction the free radical concentrations are usually quite negligible at the start. But, often, the calculated errors for these concentrations are relatively large. If they were used in the step-size calculation, they would keep the step size needlessly small. The permanent error omit procedure must be used for slow reactions, because the automatic method is not sensitive enough to cope with this situation. It has been our experience that the error for any species with a mole fraction of $10^{-4}$ or less can be neglected with no change in results.

The effect of using the error omit procedure is shown in table II(a), which gives computed results for a hydrogen-air ignition reaction using an IBM 7044-7094 computer. Trial 1 is the standard, in which no species were eliminated from the error analysis. A comparison of trial 2 with trial 1 shows that running time is significantly shortened by using the automatic elimination procedure. The largest change in the results is about a 1-percent change in some of the smaller species mole fractions. Trials 3 and 8 show two things. First, permanently omitting a single species does not reduce running time any further after the automatic omit procedure is used. Second, permanently omitting a single species is not as effective as the automatic procedure in reducing computer time. Computations for other reacting mixtures have shown that the results in table II(a) are quite typical. This is why we have made the automatic error elimination procedure the standard option in the integration routine. However, the user can override these error eliminations by a simple addition to the input data, if any accuracy problem ever occurs. The override should be used if more than three species errors are consistently being neglected.

Table II(b) shows the effect of other factors on accuracy and computer running time. Trial 2 will now be used as the standard of comparison. Trials 2 and 4 show that results are essentially unchanged when $\varepsilon_{\text{max}}$, the allowable error, is changed by a factor of 2 from 0.00005 to 0.0001. Trials 4, 6, and 7 show that results are independent of maximum step size as well. Our computations with several reacting mixtures have indicated that $\varepsilon_{\text{max}} = 0.0001$ as a maximum relative error gives excellent accuracy with relatively short running times for most situations.

The computing time can, however, be decreased with only a slight loss of accuracy by two different methods. These are (1) increasing $\varepsilon_{\text{max}}$ and (2) using the permanent error omit procedure for several of the small concentration species. The effect of each of these methods is shown by trials 5 and 9. The $\varepsilon_{\text{max}}$ value was arbitrarily increased to 0.0003 in trial 5.

When performing computations for very slow reactions the permanent error technique should always be used for all the trace species (mole fraction $\leq 10^{-4}$). For best accuracy the calculation should be stopped when trace species eventually become important. It should then be restarted with these species removed from the permanent omit
list. However, our experience with several chemical systems has shown that acceptable results may often be obtained even when major species are neglected from the error analysis.

The initial step size. - The user specifies a minimum and a maximum step size for any calculation. The program selects \( h_{\text{min}} \) as the initial step size unless a different value is given. Using an initial value larger than \( h_{\text{min}} \) is another way to decrease computation time. An initial step size even larger than the maximum value may be used when a very slow reaction is being considered. Our experience has shown that the user may choose the largest initial step size that does not cause the integration to break down immediately. Examples of this breakdown are negative species mole fractions and temperatures very different from the starting value. A few trial runs for any new system will show the largest initial step size that may be used.
In this section a general description is given of the several types of data required for a kinetics problem. The exact format of all data cards is given in appendix D.

Chemical reactions and species. - Each chemical reaction is listed on a separate card which has space for two reactant names, two product names, and the three rate constant parameters $A_i$, $n_i$, and $E_i$. The reaction cards may be put in any order, regardless of the type of reaction. The program checks all names on the reaction cards against its species list in the array ALSP. In this way the program automatically builds up the list of species being used in any problem. The availability of rate constant data is discussed in appendix F.

Inert species. - The names of any species present, but not reacting, are listed separately, four per card, following the reaction cards.

Integration variable and units. - A version and units card follows the inert species list. It contains the code words for the integration variable (DISTANCE or TIME) and for the assigned variable (AREA or PRESSURE). It also contains the codes for input and output units (CGS, FPS, or SI). Table III gives the units needed with each of these three options for the input data.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Internal (CGS)</th>
<th>FPS</th>
<th>SI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Velocity</td>
<td>cm/sec</td>
<td>ft/sec</td>
<td>m/sec</td>
</tr>
<tr>
<td>Temperature</td>
<td>K</td>
<td>°R</td>
<td>K</td>
</tr>
<tr>
<td>Density</td>
<td>g/cm$^3$</td>
<td>lbm/ft$^3$</td>
<td>kg/m$^3$</td>
</tr>
<tr>
<td>Pressure$^a$</td>
<td>atm</td>
<td>lbf/ft$^2$</td>
<td>N/m$^2$</td>
</tr>
<tr>
<td>Length</td>
<td>cm</td>
<td>ft</td>
<td>m</td>
</tr>
<tr>
<td>Area</td>
<td>cm$^2$</td>
<td>m$^2$</td>
<td>m$^2$</td>
</tr>
<tr>
<td>Species</td>
<td>Mole fraction or mass fraction</td>
<td>Mole fraction or mass fraction</td>
<td>Mole fraction or mass fraction</td>
</tr>
<tr>
<td>concentration</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$^a$Pressure may also be specified as mmHg (torr) in all systems.

Problem data. - Most of the input data for a problem are listed in a NAMELIST called PROB, which follows the version card. PROB contains the assigned variable profile information, printout information, and the integration controls. It also contains the logical variables SHOCK, COMBUS, ALLM1, TCON, and RHOCON.

Efficiencies for three-body recombination-dissociation reactions. - The third-body catalyst efficiencies $m_{ij}$ are contained on one or more cards following NAMELIST.
PROB. These cards are permitted only if ALLM1 has been set equal to FALSE. Each card contains up to three species names with corresponding \( m_{ij} \) values for a single reaction. The reaction is written on each of these cards exactly as it appears on the reaction card.

Starting conditions. - The starting values for the fluid dynamic variables and the composition of the reacting gas are listed in a NAMELIST called START, which follows either the third-body efficiency cards or NAMELIST PROB. In general, five variables make up the initial conditions in addition to the species starting concentrations. The program initializes all of these to zero. These variables, therefore, do not have to actually appear in NAMELIST START unless their values are nonzero. Four of these initial values are always \( x, t, T, \) and either \( V \) or Mach number. For the last fluid-dynamic variable the user has a choice of either \( p, \rho, A, \) or mass flow rate \( \dot{m} \). The choice is determined by the profile that has been assigned in NAMELIST PROB. For an assigned area problem one may list either \( p, \rho, \) or \( \dot{m} \). For an assigned pressure problem either \( A \) or \( \dot{m} \) may be used.

Species starting concentrations can be given either as mole fractions or mass fractions. The program name of the species is used as its concentration variable name. For example, \( H_2 = 0.50 \) means that the concentration of \( H_2 \) is 0.5 in the mixture. The program interprets these concentration numbers as mole fractions unless it is told that they are mass fractions. This is done by setting the variable MOLEF equal to FALSE.

Species omitted from error calculations. - It was mentioned earlier that the program can be made to neglect minor species errors during its step-size calculation for a complete case. These "permanently omitted" species are listed, four per card, immediately following NAMELIST START.

Output

The program has both standard and optional output. The exact output units used for each of the three systems, CGS, FPS, and SI, are listed in table IV. All computed results are completely independent of the print station positions. A special step is made to each print station and the independent variable is then reset to its previous value. From this point it is increased by the normally calculated step size to a value greater than the print station value.

Standard output. - The following data will be listed if no special codes are used in the input data:

1. Reaction time
2. Axial position and flow cross-section area

---

\(^1\) Gas particle time for a shock wave reaction.
TABLE IV. - OUTPUT UNITS FOR THREE UNITS SYSTEMS

<table>
<thead>
<tr>
<th>Variable</th>
<th>Internal (CGS) units</th>
<th>FPS units</th>
<th>SI units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Velocity</td>
<td>cm/sec</td>
<td>ft/sec</td>
<td>m/sec</td>
</tr>
<tr>
<td>Temperature</td>
<td>K</td>
<td>0°C</td>
<td>K</td>
</tr>
<tr>
<td>Density</td>
<td>g/cm³</td>
<td>lbm/ft³</td>
<td>kg/m³</td>
</tr>
<tr>
<td>Pressure</td>
<td>atm</td>
<td>lbf/ft²</td>
<td>N/m²</td>
</tr>
<tr>
<td>Time</td>
<td>sec</td>
<td>sec</td>
<td>sec</td>
</tr>
<tr>
<td>Length</td>
<td>cm</td>
<td>ft</td>
<td>m</td>
</tr>
<tr>
<td>Area</td>
<td>cm²</td>
<td>ft²</td>
<td>m²</td>
</tr>
<tr>
<td>Species concentration</td>
<td>Mole fraction, mass fraction, (g/mole)</td>
<td>Mole fraction, mass fraction, (lb mole)</td>
<td>Mole fraction, mass fraction, (kg mole)</td>
</tr>
<tr>
<td>Species production rate</td>
<td>(g-mole)/cm³/sec</td>
<td>(lb mole)/ft³/sec</td>
<td>(kg mole)/m³/sec</td>
</tr>
<tr>
<td>Net reaction conversion rate</td>
<td>g-mole/ cm³ sec/ρ²</td>
<td>lb-mole/ ft³ sec</td>
<td>kg mole/ ρ²</td>
</tr>
<tr>
<td>Net energy exchange rate</td>
<td>cal/ cm³ sec/ρ²</td>
<td>Btu/ ft³ sec</td>
<td>J/ m³ sec</td>
</tr>
<tr>
<td>Reaction rate constant</td>
<td>cgs units a</td>
<td>cgs units a</td>
<td>cgs units a</td>
</tr>
<tr>
<td>dV/ d q</td>
<td>(cm/sec)/unit q</td>
<td>(cm/sec)/unit q</td>
<td>(cm/sec)/unit q</td>
</tr>
<tr>
<td>dρ/ d q</td>
<td>(g/cm³)/unit q</td>
<td>(g/cm³)/unit q</td>
<td>(g/cm³)/unit q</td>
</tr>
<tr>
<td>dT/ d q</td>
<td>K/unit q</td>
<td>K/unit q</td>
<td>K/unit q</td>
</tr>
<tr>
<td>dσ_i/ d q</td>
<td>(g-mole/g)/unit q</td>
<td>(g-mole/g)/unit q</td>
<td>(g-mole/g)/unit q</td>
</tr>
<tr>
<td>Mass flow rate</td>
<td>g/sec</td>
<td>lbm/sec</td>
<td>kg/sec</td>
</tr>
<tr>
<td>Entropy</td>
<td>cal/g K</td>
<td>Btu/lb 0°C</td>
<td>J/kg K</td>
</tr>
</tbody>
</table>

^a See table V.

(3) Pressure, velocity, density, and temperature of the gas mixture

(4) Entropy per unit mass and frozen heat capacity ratio for the gas mixture. The entropy S is computed from

\[
S = R \sum_{i=1}^{N} \sigma_i \left[ \frac{S_i}{R} - \ln \sigma_i - \ln(pM_w) \right]
\]  

(85)
Local Mach number
Mole fraction of each species in the gas mixture
Molar concentration of each mixture species
Net species production rate \( W_i \) defined by equation (31) (This is the net rate of change of each molar concentration due to all chemical reactions.)
Net reaction conversion rate, \( X_j \), defined by equations (36), (37), (40), (41), or (42) for the three types of chemical reactions being considered
Rate constant value, \( k_j \) for each reaction (This is just the value given by equation (33). For a dissociation or recombination reaction, the third-body efficiency is assumed to be 1.0.)
Mixture molecular weight
Mass fraction sum
Total energy exchange rate defined by
\[
X_H = \sum_{j=1}^{l} X_{H,j}
\]
where \( l \) is the number of reactions and \( X_{H,j} \) is defined in equation (43) (The quantity \( X_H \) is proportional to the net heat release rate for the entire complex reaction and may be useful in ignition reactions.)
Derivatives of all dependent integration variables, \( V, T, p \), and each \( \sigma_i \), with respect to the independent variable
Increments and relative errors - the computed increments \( k_{i,n+1} \) and relative errors \( E_{i,n+1} \) as defined in equations (49) and (62) for the current integration step
Integration indicators
(a) Steps from last print
(b) Average step size since last print
(c) Controlling variable - the variable with the largest error \( E_{i,n+1} \)
(d) Relative error - the value of \( \epsilon_{n+1} \) for the step being printed out
(e) Any species that will be automatically eliminated from error consideration for the next step
Optional output. - Several changes and additions to the standard output may be made:
(1) Species mass fraction may be listed in place of molar concentration by setting the logical variable CONC equal to FALSE in NAMELIST PROB.
(2) Net energy exchange rate for each reaction \( X_{H,j} \) defined by equation (43) may be listed in place of net reaction conversion rate by setting the logical variable EXCHR equal to TRUE in NAMELIST PROB.
The program has an option for listing certain additional data or intermediate output at each print station. These data are useful either for studying the effect of each individual reaction on gas composition or for diagnosing any program problems. This option is chosen by setting the variable DBUGO equal to TRUE in NAMELIST PROB. The following quantities are then listed:

(a) The molar rate of production of species $i$ due to reaction $j$, $\omega_{ij}$, defined by equation (35)

(b) The quantities $A$ and $B$ or $A^*$ and $B^*$

(c) If area has been assigned, the quantities $\frac{dA}{dq}$, $\frac{d^2A}{dq^2}$ and either

$$\left( \frac{1}{A} \frac{dA}{dq} - A \right)$$

or

$$\left( \frac{1}{A} \frac{dA}{dq} - A^* \right)$$

If pressure has been assigned, the quantities $\frac{dp}{dq}$, $\frac{d^2p}{dq^2}$ and $(1/p)(\frac{dp}{dq})$ are printed out. Here $q$ is the independent variable, either $t$ or $x$.

PROGRAM ORGANIZATION

The program is organized into the following five sections: (1) control, (2) input/output, (3) shock/combustion, (4) chemical kinetics, and (5) numerical integration. An effort was made in writing the program to make each of the last three sections self-contained except for the reading and processing of input data. The shock/combustion section uses subroutine THRM from the chemical kinetics section, but is independent in all other respects. The chemical kinetics and numerical integration sections are complete in themselves. The next sections describe the function of each program section and of each subroutine in the section. The names of nonstandard entry points into a subroutine are given in parentheses following the subroutine name. Flow charts for key subroutines (figs. 1 to 6) are found in appendix G along with the FORTRAN listing.

Control Section

The control section is synonymous with the main program GCKP. It provides for
problem setup through a series of subroutine calls. It also monitors the numerical integration and provides an output call whenever a print station is reached (see fig. 1).

**Input/Output Section**

This section provides for the reading, converting and writing of all input data and kinetics results. It also performs all the necessary bookkeeping functions such as building tables, setting option switches, and storing data for later use.

**KINP (RINP)**. - Provides for the processing of all input data. It initializes, sets all standard options, reads input data and converts it to internal (CGS) units, calculates reference conditions, builds tables and provides calls for shock and combustion calculations (see fig. 2).

**CIMAGE**. - Prints a card image of each data card.

**NAMBLK**. - Contains, in block data format, logical tape unit numbers and alphanumeric data for testing and output.

**BLCK**. - Contains, in block data format, the master species list and the molecular weight of each species in that list.

**INIT**. - Reads the initial conditions by means of NAMELIST START and stores initial species concentrations using a table provided by KINP.

**OUTP (OUT1, OUT2, OUT3)**. - Provides all output except shock and combustion results. It converts output data from internal units to user's requested output units and calculates parameters which are required only as output such as total entropy and net energy exchange rates.

**Shock/Combustion Section**

The frozen and equilibrium shock and the equilibrium combustion calculations are performed in this section. It converts and writes its own output and provides for the transfer of frozen shock results to the input/output section as initial conditions for the kinetics calculations. Except for reading input and calculating thermodynamic properties, this section is independent of the other sections.

**COMP**. - Provides the necessary setup and subroutine calls for the calculation of a constant pressure equilibrium combustion.

**SHOK**. - Provides the necessary setup and subroutine calls for the calculation of both an equilibrium and a frozen shock.

**SHOCKS**. - Solves the shock equations for both the equilibrium and frozen cases.

**ELEMNT**. - Collects chemical element data for equilibrium calculations. These
data include a list of the elements present and the concentration of each of these elements in atoms per gram.

**EQLBRM.** This routine, and the following two, are modified versions of routines used in the chemical equilibrium composition program described in reference 13. It calculates equilibrium composition and properties for an assigned set of conditions—assigned temperature and pressure for a shock, assigned enthalpy and pressure for a combustion.

**MATRIX.** Used by subroutine EQLBRM to construct matrices required in equilibrium calculations.

**GAUSS.** Solves the linear equations which are set up by subroutine MATRIX.

**SPOUT (ECOUT, ESOUT, FSOUT).** Provides for the output of all shock and combustion results. It converts output data to the user's requested output units, transfers frozen shock results to the input/output section and calculates the characteristic shock tube reaction length \( L_m \) in centimeters if this calculation is required.

**Chemical Kinetics Section**

The calculation of all chemical and flow parameters is performed in this section. In particular, thermodynamic functions are evaluated, reaction and species production rates are computed, and all required partial and total derivatives are calculated. This section is independent of all but the input/output section.

**PRED (PRED1).** Performs all necessary prederivative calculations. This routine calls for or computes directly the thermodynamic properties, reaction rates, equilibrium constants, pressure, specific heat ratio and Mach number as well as other parameters required for the calculation of derivatives (see fig. 3).

**DERV.** Calculates all partial and total derivatives with respect to the variable of integration (see fig. 4).

**PARD.** Calculates all partial derivatives with respect to the chemical and flow variables (see fig. 5).

**THRM.** Computes the (dimensionless) thermodynamic properties \( \frac{h_i}{RT}, \frac{g_i}{RT}, \frac{S_i}{R}, (\frac{C_p}{R}), (\frac{dC_p}{dT})_i/R \) from polynomial curve fits (see ref. 20).

**CUBS (CINP).** Provides for the calculation of the assigned variable and its derivatives. If the assigned variable is specified by a table, then the variable and its derivatives are computed by cubic spline interpolation.

**Numerical Integration Section**

This section sets up and solves the implicit equations, computes the relative error,
and performs the step-size optimization at each step. It contains the automatic species elimination calculations for omitting from error considerations those species with non-representative errors. This section of the program is independent of the other sections.

INTE (INTI, INTC, INTG). - Provides control of the numerical integration procedure during each step. It calls for the implicit equations to be set up and solved, checks for restart conditions, and calls for the step-size optimization (see fig. 6).

CASM (CASI, CASG). - Sets up the implicit equations as an augmented matrix, calls for the solution, and updates all the dependent variables after the increments have been calculated.

LESV. - Solves the implicit equations for the increments $k_{i,n+1}$ using the matrix provided by subroutine CASM.

ERROR. - Computes the relative error and determines the controlling variable at each step.

PERR. - Provides an approximate error for any assigned step size by obtaining an approximate solution of the implicit equations. This routine is used in the step-size optimization procedure to predict the error which can be expected from any given step size.

AUTO. - Provides for the automatic elimination from error considerations of species with nonrepresentative errors. A species error $E_i$ is considered to be non-representative if $E_i > 15 \cdot E_m$ where $E_m$ is the median of the errors associated with those species which have not been permanently neglected from all error considerations.

SEARCH. - A sequential direct search routine which is used in the step-size optimization procedure.

**CONCLUDING REMARKS**

A general chemical kinetics computer program has been described for calculating the history of many different complex gas-phase reactions. Its main features are flexibility, ease of use and efficiency of computation for both slow and very fast reactions. The species and reactions to be considered are specified by the user. The program is especially useful for ignition and combustion reactions and complex reactions behind a shockwave. In addition it may be used for many types of homogeneous reaction in either a static system or one-dimensional flow. Further information on availability of the program may be obtained from the authors.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, August 26, 1971,
129-01.
APPENDIX A

SOLUTION OF SHOCK WAVE EQUATIONS

The shock equations (eqs. (44) to (46)), are solved by an iterative method. For both frozen and equilibrium conditions, one makes estimates of the final temperature and pressure $p_f$ and $T_f$. Then a Newton-Raphson method is used to calculate corrections to these estimates and converge on the correct values. The shock equations are transformed and combined for this solution. First, equation (44) gives

$$v^2 = \left(\frac{\rho_1}{\rho}\right)^2 v_s^2$$  \hspace{1cm} (A1)

This equation is used in equations (45) and (46) to eliminate $V$ and gives, after some rearrangement

$$1 - \left(\frac{\rho_1 v_s^2}{p_1}\right)\left(\frac{\rho_1}{\rho} - 1\right) - \frac{p}{p_1} = 0$$ \hspace{1cm} (A2)

$$h_1 + \frac{v_s^2}{2} - \frac{v_s^2 \left(\frac{\rho_1}{\rho}\right)^2}{2} = 0$$ \hspace{1cm} (A3)

Using the equation of state (eq. (8)) for no change in gas composition gives

$$\frac{\rho_1}{\rho} = \left(\frac{p_1}{p}\right) \left(\frac{T}{T_1}\right) = \frac{\mathcal{S}}{P}$$ \hspace{1cm} (A4)

where we have defined the new variables $\mathcal{S} = T/T_1$ and $P = p/p_1$.

Equations (A2) and (A3) can now be written as functions of the pressure and temperature ratios across the shock:

42.
These equations are solved iteratively for the final ratios $T_f$ and $P_f$ across the shock. First estimates of $T$ and $P$ are obtained from the following equations:

\[
P_0 = \frac{2\gamma M_s^2 - \gamma + 1}{\gamma + 1}
\]

\[
\mathcal{T}_0 = \frac{P_0 \left( \frac{2}{M_s^2} + \gamma - 1 \right)}{\gamma + 1}
\]

These are the exact solutions of equations (44) to (46) when heat capacity is assumed to be independent of temperature. Then the Newton-Raphson procedure is used to calculate corrections to $\ln P$ and $\ln \mathcal{T}$ where it is assumed that

\[
\ln P_{n+1} = \ln P_n + \Delta \ln P
\]

\[
\ln \mathcal{T}_{n+1} = \ln \mathcal{T}_n + \Delta \ln \mathcal{T}
\]

where $n$ indicates the $n^{\text{th}}$ iteration step. Logarithmic differentiation is used to obtain rapid convergence of the procedure. We define the quantities

\[
p^* = 1 - \left( \frac{\rho_1 V_s^2}{p_1} \right) \left( \frac{\mathcal{T}}{P} - 1 \right)
\]

\[
h^* = h_1 + \frac{V_s^2}{2} - \frac{V_s^2}{2} \left( \frac{\mathcal{T}^2}{P} \right)
\]
Then equations (A5) and (A6) can be written as

\[ F(S^-, P) = p^* - P = 0 \]  \hspace{1cm} (A13)

\[ G(S^-, P) = h^* - h = 0 \]  \hspace{1cm} (A14)

Substituting equations (A9) and (A10) and using logarithmic differentiation gives the following pair of linear equations for the corrections \( \Delta \ln P \) and \( \Delta \ln S^- \) in the Newton-Raphson method:

\[
\left( \frac{\partial F}{\partial \ln S^-} \right)_n \Delta \ln S^- + \left( \frac{\partial G}{\partial \ln S^-} \right)_n \Delta \ln P = G_n \]  \hspace{1cm} (A15)

\[
\left( \frac{\partial F}{\partial \ln \mathcal{F}} \right)_n \Delta \ln \mathcal{F} + \left( \frac{\partial G}{\partial \ln \mathcal{F}} \right)_n \Delta \ln P = -F_n \]  \hspace{1cm} (A16)

In these equations subscript \( n \) indicates evaluation of either the function or its derivative for the estimated values \( P_n \) and \( \mathcal{F}_n \). This method of solution is the one used by Gordon and McBride (ref. 13). This procedure is used for both the equilibrium and the frozen shock conditions. The only difference in method for the two situations is the way the enthalpy is computed for the shocked gas. For the frozen shock conditions, \( h \) is calculated at the estimated temperature \( T \) for the original gas composition. In the equilibrium case the shocked gas enthalpy depends on \( T \) and also the changing gas composition due to reaction. Therefore, the estimated \( T \) and \( p \) are first used to perform an equilibrium chemical reaction calculation. This gives the estimated final composition of the shocked gas. This composition and the estimated \( T \) are then used to calculate the enthalpy \( h \) used in equation (A14) to compute the function \( G(\mathcal{F}, P) \) in the Newton-Raphson method.
APPENDIX B

CALCULATION OF PARTIAL DERIVATIVES FOR THE IMPLICIT INTEGRATION PROCEDURE

Several partial derivatives must be calculated for solving the system

\[ \frac{dy_i}{dq} = f_i(q, y_1, y_2, \ldots, y_m) \]  \hspace{1cm} (B1)

where

\[ q = t \text{ or } x \quad i = 1, 2, \ldots, m \]

The necessary derivatives are

\[ \alpha_i = \frac{\partial f_i}{\partial q} \quad i = 1, 2, \ldots, m \]  \hspace{1cm} (B2)

\[ \beta_{i,j} = \frac{\partial f_i}{\partial y_j} \quad i, j = 1, 2, \ldots, m \]  \hspace{1cm} (B3)

For this program the following identifications are made for the \( y_i \)'s:

\[ y_1 = V \]
\[ y_2 = \rho \]
\[ y_3 = T \]
\[ y_{i+3} = \sigma_i \quad i = 1, 2, \ldots, N \]

where \( N \) is the number of species in the gas.

Derivatives must be calculated for two different equation systems: either equations (3) and (9) to (11) for assigned area or equations (3) and (25) to (27) for assigned pres-
sure. For convenience in the calculations simplified notation will be used to represent the several derivatives of the $y_i$'s.

$$f_1 = \frac{dV}{dq}$$

$$f_2 = \frac{d\rho}{dq}$$

$$f_3 = \frac{dT}{dq}$$

$$f_{i+3} = \frac{d\sigma_i}{dq} \quad i = 1, 2, \ldots, N$$

In the following equations the symbols $\mathcal{A}^{*}$ and $\mathcal{B}^{*}$ will not be used. The symbols $\mathcal{A}$ and $\mathcal{B}$ are assumed to have definitions consistent with the particular $f_1$ definitions being used. (See eqs. (12), (13), (23), and (24).)

**Assigned Area Equations**

From equations (3) and (9) to (11) the following equations are used for the $f_i$'s:

$$f_1 = \frac{V}{(M^2 - 1)} \left( \frac{1}{A} \frac{dA}{dq} - \mathcal{A} \right) \quad (B4)$$

$$f_2 = -\rho \left[ \frac{M^2}{(M^2 - 1)} \left( \frac{1}{A} \frac{dA}{dq} - \mathcal{A} \right) + \mathcal{A} \right] \quad (B5)$$

$$f_3 = -T \left[ \frac{(\gamma - 1)M^2}{(M^2 - 1)} \left( \frac{1}{A} \frac{dA}{dq} - \mathcal{A} \right) + \mathcal{B} \right] \quad (B6)$$

$$f_{i+3} = \frac{W_i}{r} \quad i = 1, 2, \ldots, N \quad (B7)$$
where

\[ r = \rho \text{ for } q = t \]

\[ = \rho V \text{ for } q = x \]

The \( \alpha_i \)'s are most easily obtained because only one quantity, the area \( A \) is an explicit function of \( q \). The results are

\[
\alpha_1 = \frac{\partial f_1}{\partial q} = \frac{V}{A(M^2 - 1)} \left[ \frac{d^2A}{dq^2} - \frac{1}{A} \left( \frac{dA}{dq} \right)^2 \right] \quad \text{(B8)}
\]

\[
\alpha_2 = \frac{\partial f_2}{\partial q} = -\frac{\rho M^2}{A(M^2 - 1)} \left[ \frac{d^2A}{dq^2} - \frac{1}{A} \left( \frac{dA}{dq} \right)^2 \right] \quad \text{(B9)}
\]

\[
\alpha_3 = \frac{\partial f_3}{\partial q} = -\frac{T(y - 1)M^2}{A(M^2 - 1)} \left[ \frac{d^2A}{dq^2} - \frac{1}{A} \left( \frac{dA}{dq} \right)^2 \right] \quad \text{(B10)}
\]

\[
\alpha_{i+3} = \frac{\partial f_{i+3}}{\partial q} = 0 \quad i = 1, 2, \ldots, N \quad \text{(B11)}
\]

The assigned area can be read in as a function of \( x \) when \( t \) is the integration variable, and vice-versa. Therefore, the following transformations may be required:

\[
\frac{dA}{dt} = V \frac{dA}{dx} \quad \text{(B12)}
\]

\[
\frac{d^2A}{dt^2} = V^2 \frac{d^2A}{dx^2} + f_1 \frac{dA}{dx} \quad \text{(B13)}
\]

or

\[
\frac{dA}{dx} = \frac{1}{V} \frac{dA}{dt} \quad \text{(B14)}
\]
The $\beta_{1,j}$'s are obtained by differentiating equation (B4). The additional partial derivatives which appear in the following equations are evaluated in appendix C.

$$\beta_{1,1} = \frac{\partial f_1}{\partial V} = \frac{1}{(M^2 - 1)} \left[ \frac{1}{A} \frac{\partial A}{\partial q} - \mathcal{A} \right] - \frac{f_1}{V} \frac{\partial M^2}{\partial V} - V \frac{\partial \mathcal{A}}{\partial V}$$  \hspace{1cm} (B16)

$$\beta_{1,2} = \frac{\partial f_1}{\partial \rho} = -\frac{V}{(M^2 - 1)} \frac{\partial \mathcal{A}}{\partial \rho}$$  \hspace{1cm} (B17)

$$\beta_{1,3} = \frac{\partial f_1}{\partial T} = -\frac{V}{(M^2 - 1)} \frac{\partial \mathcal{A}}{\partial T} - \frac{f_1}{(M^2 - 1)} \frac{\partial M^2}{\partial T}$$  \hspace{1cm} (B18)

$$\beta_{1,j+3} = \frac{\partial f_1}{\partial \sigma_j} = -\frac{1}{(M^2 - 1)} \left( V \frac{\partial \mathcal{A}}{\partial \sigma_j} + f_1 \frac{\partial M^2}{\partial \sigma_j} \right) \quad j = 1, 2, \ldots, N$$  \hspace{1cm} (B19)

The $\beta_{2,j}$'s are obtained from equation (B5)

$$\beta_{2,1} = \frac{\partial f_2}{\partial V} = \frac{\rho}{(M^2 - 1)} \frac{\partial \mathcal{A}}{\partial V} + \frac{\rho}{(M^2 - 1)} \left[ \frac{1}{A} \frac{\partial A}{\partial q} - \mathcal{A} \right] \frac{\partial M^2}{\partial V}$$  \hspace{1cm} (B20)

$$\beta_{2,2} = \frac{\partial f_2}{\partial \rho} = \frac{\rho}{(M^2 - 1)} \frac{\partial \mathcal{A}}{\partial \rho} + \frac{f_2}{\rho}$$  \hspace{1cm} (B21)

$$\beta_{2,3} = \frac{\partial f_2}{\partial T} = \frac{\rho}{(M^2 - 1)} \frac{\partial \mathcal{A}}{\partial T} + \frac{\rho}{(M^2 - 1)} \left[ \frac{1}{A} \frac{\partial A}{\partial q} - \mathcal{A} \right] \frac{\partial M^2}{\partial T}$$  \hspace{1cm} (B22)
\[
\beta_{2,j+3} = \frac{\partial f_2}{\partial \sigma_j} = \frac{\rho}{(M^2 - 1)} \frac{\partial \mathcal{A}}{\partial \sigma_j} + \frac{\rho}{(M^2 - 1)^2} \left( \frac{1}{A} \frac{\partial A}{\partial \sigma_j} - \mathcal{A} \right) \frac{\partial M^2}{\partial \sigma_j} 
\]
\[j = 1, 2, \ldots, N \quad (B23)\]

The \( \beta_3,j \)'s are obtained from equation (B6)

\[
\beta_{3,1} = -\frac{\partial f_3}{\partial V} = T \left[ \frac{(\gamma - 1)M^2}{(M^2 - 1)} \frac{\partial \mathcal{A}}{\partial V} + \frac{(\gamma - 1)}{(M^2 - 1)^2} \left( \frac{1}{A} \frac{\partial A}{\partial \sigma_j} - \mathcal{A} \right) \frac{\partial M^2}{\partial V} \right] \quad (B24)
\]

\[
\beta_{3,2} = \frac{\partial f_3}{\partial \rho} = T \left[ \frac{(\gamma - 1)M^2}{(M^2 - 1)} \frac{\partial \mathcal{A}}{\partial \rho} - \frac{\partial \mathcal{B}}{\partial \rho} \right] \quad (B25)
\]

\[
\beta_{3,3} = \frac{\partial f_3}{\partial T} = (\gamma - 1)M^2T \frac{\partial \mathcal{A}}{\partial T} + \frac{(\gamma - 1)T}{(M^2 - 1)} \left( \frac{1}{A} \frac{\partial A}{\partial \sigma_j} - \mathcal{A} \right) \frac{\partial M^2}{\partial T} \]

\[-\frac{M^2T}{(M^2 - 1)} \left( \frac{1}{A} \frac{\partial A}{\partial \sigma_j} - \mathcal{A} \right) \frac{\partial \mathcal{B}}{\partial T} + \frac{f_3}{T} \quad (B26)
\]

\[
\beta_{3,j+3} = \frac{\partial f_3}{\partial \sigma_j} = T \left[ \frac{(\gamma - 1)M^2}{(M^2 - 1)} \frac{\partial \mathcal{A}}{\partial \sigma_j} + \frac{(\gamma - 1)}{(M^2 - 1)^2} \left( \frac{1}{A} \frac{\partial A}{\partial \sigma_j} - \mathcal{A} \right) \frac{\partial M^2}{\partial \sigma_j} \right]
\]
\[-\frac{M^2}{(M^2 - 1)} \left( \frac{1}{A} \frac{\partial A}{\partial \sigma_j} - \mathcal{A} \right) \frac{\partial \mathcal{B}}{\partial \sigma_j} \quad j = 1, 2, \ldots, N \quad (B27)
\]

To obtain \( \beta_{i+3,j} \) equation (B7) is rewritten using equations (31) and (35) to obtain (using subscript \( s \) to indicate the chemical reactions)

\[
f_{i+3} = \frac{2}{r} \sum_{s=1}^{L} (v_{i,s} - v_{1,s})X_s \quad i = 1, 2, \ldots, N \quad (B28)
\]
Taking derivatives of equation (B28) gives

\[ \beta_{i+3,1} = \frac{\partial f_{i+3}}{\partial V} = 0 \quad i = 1, 2, \ldots, N \]  

(B29)

\[ \beta_{i+3,2} = \frac{\partial f_{i+3}}{\partial \rho} = \frac{f_{i+3}}{\rho} + \frac{2}{r} \sum_{s=1}^{L} (\nu_{i,s} - \nu_{i,s}) \frac{\partial X_{s}}{\partial \rho} \quad i = 1, 2, \ldots, N \]  

(B30)

\[ \beta_{i+3,3} = \frac{\partial f_{i+3}}{\partial T} = \frac{2}{r} \sum_{s=1}^{L} (\nu_{i,s} - \nu_{i,s}) \frac{\partial X_{s}}{\partial T} \quad i = 1, 2, \ldots, N \]  

(B31)

\[ \beta_{i+3,j+3} = \frac{\partial f_{i+3}}{\partial \sigma_{j}} = \frac{2}{r} \sum_{s=1}^{L} (\nu_{i,s} - \nu_{i,s}) \frac{\partial X_{s}}{\partial \sigma_{j}} \quad i = 1, 2, \ldots, N \]  

(B32)

Assigned Pressure Equations

From the system of equations (3) and (25) to (27) the following equations are now used for the \( f_i \)'s:

\[ f_1 = -\frac{1}{\rho V} \frac{dp}{dq} \]  

(B33)

\[ f_2 = \rho \left( \frac{1}{\gamma} \frac{dp}{dq} - \mathscr{A} \right) \]  

(B34)

\[ f_3 = T \left[ \left( \frac{\gamma - 1}{\gamma} \right) \frac{1}{p} \frac{dp}{dq} - \mathscr{B} \right] \]  

(B35)

For \( f_{i+3} \), \( i = 1, 2, \ldots, N \), the equations are identical to those for the assigned area system (eq. (B7)). This means that equations for \( \alpha_{i+3} \), \( \beta_{i+3,1} \), \( \beta_{i+3,2} \), \( \beta_{i+3,3} \), and
\( \beta_{i+3,j+3} \) need not be derived again in the assigned pressure system for \( i \) and \( j = 1, 2, \ldots, N \). They are identical to equations (B29) to (B32). The equations for the rest of the \( \alpha_i \)'s and \( \beta_{i,j} \)'s are as follows:

\[
\alpha_1 = -\frac{1}{\rho V} \frac{d^2 p}{dq^2}
\]

\[ (B36) \]

\[
\alpha_2 = \frac{\rho}{\gamma p} \left[ \frac{d^2 p}{dq^2} - \frac{1}{p} \left( \frac{dp}{dq} \right)^2 \right]
\]

\[ (B37) \]

\[
\alpha_3 = \frac{T}{p} \left( \frac{\gamma - 1}{\gamma} \right) \left[ \frac{d^2 p}{dq^2} - \frac{1}{p} \left( \frac{dp}{dq} \right)^2 \right]
\]

\[ (B38) \]

If pressure derivative transformations between \( x \) and \( t \) are required, they are identical in form to equations (B12) to (B15).

\[
\beta_{1,1} = -\frac{f_1}{V}
\]

\[ (B39) \]

\[
\beta_{1,2} = -\frac{f_1}{\rho}
\]

\[ (B40) \]

\[
\beta_{1,3} = 0
\]

\[ (B41) \]

\[
\beta_{1,j+3} = 0 \quad j = 1, 2, \ldots, N
\]

\[ (B42) \]

\[
\beta_{2,1} = -\rho \frac{\partial \mathcal{A}}{\partial V}
\]

\[ (B43) \]

\[
\beta_{2,2} = \frac{f_2}{\rho} - \rho \frac{\partial \mathcal{A}}{\partial \rho}
\]

\[ (B44) \]

\[
\beta_{2,3} = -\rho \frac{\partial \mathcal{A}}{\partial T} - \rho \frac{dp}{p \gamma^2 dq} \frac{\partial \gamma}{\partial T}
\]

\[ (B45) \]
\[ \beta_{2,j+3} = -\rho \frac{\partial A}{\partial \sigma_j} - \frac{\rho}{\gamma^2} \frac{dp}{dq} \frac{\partial \gamma}{\partial \sigma_j} \quad j = 1, 2, \ldots, N \]  
(B46)

\[ \beta_{3,1} = -T \frac{\partial \mathcal{H}}{\partial V} \]  
(B47)

\[ \beta_{3,2} = -T \frac{\partial \mathcal{H}}{\partial p} \]  
(B48)

\[ \beta_{3,3} = \frac{f_3}{T} + \mathcal{H} - T \frac{\partial \mathcal{H}}{\partial T} + \frac{T}{\gamma^2} \frac{dp}{dq} \frac{\partial \gamma}{\partial T} \]  
(B49)

\[ \beta_{3,j+3} = \frac{T}{\gamma^2} \frac{dp}{dq} \frac{\partial \gamma}{\partial \sigma_j} - T \frac{\partial \mathcal{H}}{\partial \sigma_j} \quad j = 1, 2, \ldots, N \]  
(B50)
APPENDIX C

ADDITIONAL PARTIAL DERIVATIVES

The equations for the $\beta_{i,j}$ partial derivatives in appendix B require additional derivatives for their evaluation. These are the partial derivatives of $M^2$, $\gamma$, $A$, $B$, and the $X_s$'s with respect to $V$, $\rho$, $T$, and the $\sigma_i$'s.

Derivatives of $M^2$

The following relations are readily obtained from equation (14)

$$\frac{\partial M^2}{\partial \sigma_i} = -M^2 M_w - M^2 \frac{\partial \gamma}{\gamma \partial \sigma_i} \quad (C1)$$

$$\frac{\partial M^2}{\partial V} = \frac{2VM_w}{\gamma RT} \quad (C2)$$

$$\frac{\partial M^2}{\partial T} = \frac{M^2}{T} - \frac{M^2}{\gamma \partial T} \quad (C3)$$

Derivatives of $\gamma$

The following derivatives are obtained from equation (15)

$$\frac{\partial \gamma}{\partial \sigma_i} = \gamma(\gamma - 1) \left[ M_w - \frac{(C_p)^i}{C_p} \right] \quad (C4)$$

$$\frac{\partial \gamma}{\partial T} = -\gamma(\gamma - 1) \sum_{i=1}^{N} \sigma_i \frac{d(C_p)^i}{dT} \quad (C5)$$

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In these equations \( C_p^i \) is the molar heat capacity of species \( i \), given by equation (81), and \( C_p \) is given by equation (16).

### Derivatives of the \( X_s \) Factors

The formulas for the \( X_s \) derivatives depend on the type of chemical reaction being considered. In these equations \( s \) is the reaction index.

#### Type 1 - shuffle reaction.

- Differentiating equation (36) and simplifying give the following derivatives:

\[
\frac{\partial X_s}{\partial \rho} = 0
\]

\[
\frac{\partial X_s}{\partial T} = X_s \frac{d \ln k_s}{dT} + \frac{k_s s_3 s_4}{K_s} \frac{d \ln K_s}{dT}
\]

The derivative of the rate constant \( k_s \) is calculated from equation (33) by logarithmic differentiation

\[
\frac{d \ln k_s}{dT} = \frac{n_s E_s}{n_s + \frac{E_s}{RT^2}}
\]

The equilibrium constant \( K_s \), in concentration units, is given in terms of \( (K_p)_s \), the equilibrium constant in terms of partial pressures, by

\[
K_s = (K_p)_s (RT)^{-\Delta \nu_s} e^{-\frac{\Delta G_s^0}{RT} - \Delta \nu_s (RT)}
\]

where \( \Delta \nu_s \) is the change in number of moles of species for the reaction and \( \Delta G_s^0 \) is the standard molar free energy change for the reaction. Logarithmic differentiation of this equation at constant pressure gives

\[
\frac{d \ln K_s}{dT} = \frac{\Delta H_s^0}{RT^2} - \frac{\Delta \nu_s}{T}
\]
where $\Delta H^0_s$ is the standard molar enthalpy change for the reaction. Equations (C8) and (C10) hold for all types of reactions being considered.

The remaining $X_s$ derivatives are

$$\frac{\partial X_s}{\partial \sigma_1} = k_s \sigma_2$$  \hspace{1cm} (C11)

$$\frac{\partial X_s}{\partial \sigma_2} = k_s \sigma_1$$  \hspace{1cm} (C12)

$$\frac{\partial X_s}{\partial \sigma_3} = -\frac{k_s \sigma_4}{K_s}$$  \hspace{1cm} (C13)

$$\frac{\partial X_s}{\partial \sigma_4} = -\frac{k_s \sigma_3}{K_s}$$  \hspace{1cm} (C14)

**Type 2a - three-body recombination.** - Differentiating equation (37) gives the following derivatives:

$$\frac{\partial X_s}{\partial \rho} = k_s M_s \sigma_1 \sigma_2$$  \hspace{1cm} (C15)

$$\frac{\partial X_s}{\partial T} = X_s \frac{d \ln k_s}{dT} + \frac{k_s M_s \sigma_3}{K_s} \frac{d \ln K_s}{dT}$$  \hspace{1cm} (C16)

$$\frac{\partial X_s}{\partial \sigma_1} = k_s \rho M_s \sigma_2 + \frac{X_s m_{1,s}}{M_s}$$  \hspace{1cm} (C17)

$$\frac{\partial X_s}{\partial \sigma_2} = k_s \rho M_s \sigma_1 + \frac{X_s m_{2,s}}{M_s}$$  \hspace{1cm} (C18)

$$\frac{\partial X_s}{\partial \sigma_3} = -\frac{k_s M_s}{K_s} + \frac{X_s m_{3,s}}{M_s}$$  \hspace{1cm} (C19)
Type 2b - two-body dissociation. - Differentiating equation (40) gives the following derivatives:

\[
\frac{\partial X_s}{\partial \rho} = -\frac{k_s M_s}{K_s} \sigma_1 \sigma_2
\]

\[
\frac{\partial X_s}{\partial T} = X_s \frac{d \ln k_s}{dT} + \frac{k_s M_s \rho \sigma_1 \sigma_2}{K_s} \frac{d \ln K_s}{dT}
\]

\[
\frac{\partial X_s}{\partial \sigma_1} = \frac{k_s M_s \rho \sigma_2}{K_s} + \frac{X_s m_1, s}{M_s}
\]

\[
\frac{\partial X_s}{\partial \sigma_2} = \frac{k_s M_s \rho \sigma_1}{K_s} + \frac{X_s m_2, s}{M_s}
\]

\[
\frac{\partial X_s}{\partial \sigma_3} = k_s M_s + \frac{X_s m_3, s}{M_s}
\]

Type 3a - unimolecular decomposition. - Differentiating equation (41) gives the following derivatives:

\[
\frac{\partial X_s}{\partial \rho} = -\frac{k_s \sigma_3}{\rho^2}
\]

\[
\frac{\partial X_s}{\partial T} = X_s \frac{d \ln k_s}{dT} + \frac{k_s \sigma_1 \sigma_2}{K_s} \frac{d \ln K_s}{dT}
\]

\[
\frac{\partial X_s}{\partial \sigma_1} = -\frac{k_s \sigma_2}{K_s}
\]

\[
\frac{\partial X_s}{\partial \sigma_2} = -\frac{k_s \sigma_1}{K_s}
\]
\[
\frac{\partial X_s}{\partial \sigma_3} = \frac{k_s}{\rho}
\]

Type 3b - two-body recombination. Differentiating equation (42) gives the following derivatives:

\[
\frac{\partial X_s}{\partial \rho} = \frac{k_s \sigma_3}{\rho^2 K_s}
\]

\[
\frac{\partial X_s}{\partial T} = X_s \frac{d \ln k_s}{dT} + \frac{k_s \sigma_3}{\rho K_s} \frac{d \ln K_s}{dT}
\]

\[
\frac{\partial X_s}{\partial \sigma_1} = k_s \sigma_2
\]

\[
\frac{\partial X_s}{\partial \sigma_2} = k_s \sigma_1
\]

\[
\frac{\partial X_s}{\partial \sigma_3} = -\frac{k_s}{\rho K_s}
\]

Derivatives of \( A \) and \( B \)

Before differentiating equations (12) and (13) we use equations (8) and (B7) to write \( A \) and \( B \) in the forms

\[
A = M_w \sum_{i=1}^{N} f_{i+3} - B
\]

\[
B = M_w \left( \frac{\gamma - 1}{\gamma} \right) \sum_{i=1}^{N} \left( \frac{h_i}{RT} \right) f_{i+3}
\]
These equations hold for both \( t \) and \( x \) as the independent variable with the appropriate definitions of the \( f_{i+3} \)'s. Now define the quantities

\[
S_1 = M_w \sum_{i=1}^{N} f_{i+3} \tag{C37}
\]

\[
S_2 = M_w \sum_{i=1}^{N} \left( \frac{h_i}{RT} \right) f_{i+3} \tag{C38}
\]

The equations for \( \mathcal{A} \) and \( \mathcal{B} \) then become

\[
\mathcal{A} = S_1 - \mathcal{B} \tag{C39}
\]

\[
\mathcal{B} = \begin{pmatrix} \gamma - 1 \end{pmatrix} S_2 \tag{C40}
\]

The derivatives of \( \mathcal{A} \) and \( \mathcal{B} \) are then written in terms of the \( S_1 \) and \( S_2 \) derivatives as

\[
\frac{\partial \mathcal{A}}{\partial V} = \frac{\partial S_1}{\partial V} - \frac{\partial \mathcal{B}}{\partial V} \tag{C41}
\]

\[
\frac{\partial \mathcal{A}}{\partial \rho} = \frac{\partial S_1}{\partial \rho} - \frac{\partial \mathcal{B}}{\partial \rho} \tag{C42}
\]

\[
\frac{\partial \mathcal{A}}{\partial T} = \frac{\partial S_1}{\partial T} - \frac{\partial \mathcal{B}}{\partial T} \tag{C43}
\]

\[
\frac{\partial \mathcal{A}}{\partial \sigma_i} = \frac{\partial S_1}{\partial \sigma_i} - \frac{\partial \mathcal{B}}{\partial \sigma_i} \quad i = 1, 2, \ldots, N \tag{C44}
\]

\[
\frac{\partial \mathcal{B}}{\partial V} = \left( \frac{\gamma - 1}{\gamma} \right) \frac{\partial S_2}{\partial V} \tag{C45}
\]
Differentiating equations (C37) and (C38) and using the definitions of the $\beta_{i,j}$'s give the following expressions for the $S_1$ and $S_2$ derivatives:

\[
\frac{\partial S_1}{\partial V} = M_w \sum_{i=1}^{N} \beta_{i+3,1}
\]

\[
\frac{\partial S_1}{\partial \rho} = M_w \sum_{i=1}^{N} \beta_{i+3,2}
\]

\[
\frac{\partial S_1}{\partial T} = M_w \sum_{i=1}^{N} \beta_{i+3,3}
\]

\[
\frac{\partial S_1}{\partial \sigma_j} = M_w \left( \sum_{i=1}^{N} \beta_{i+3,j+3} - S_1 \right) \quad j = 1, 2, \ldots, N
\]

\[
\frac{\partial S_2}{\partial V} = M_w \sum_{i=1}^{N} \left( \frac{h_i}{RT} \right) \beta_{i+3,1}
\]

\[
\frac{\partial S_2}{\partial \rho} = M_w \sum_{i=1}^{N} \left( \frac{h_i}{RT} \right) \beta_{i+3,2}
\]
APPENDIX D

DETAILS OF PROGRAM INPUT AND ERROR MESSAGES

The description of the data cards is divided into three parts. First, the thermodynamic data are described. Next, the complete case data for a single problem are described. We then describe the data cards for any problems following the first. This will show the user how to run several cases at one time without making a complete data deck for each case. Finally an explanation is given for all error messages in the program.

Input Preparation

Thermodynamic data. - The thermodynamic data are not considered part of each case data. The necessary data for all species considered in one computer run are entered before the first case. The first card of the data deck tells where the thermodynamic data will be read from. Columns 1 to 4 of this card must contain either the word CARD or TAPE. If CARD appears, the program reads the data from cards which directly follow the first card. The data are then written out on logical tape unit 4 for use later in the calculation. When TAPE appears on the first data card the thermodynamic data are read from a tape that must be mounted on logical tape unit 4. Each data card corresponds to one logical record on the tape. The format of the thermodynamic data cards is as follows. The first card (or tape record) gives the temperature range limits TLOW, TMID, and THI (in that order) in kelvin units. The card format is 3F10.3. All the thermodynamic data follow this card. They consist of four cards for each species. Card 1 contains the species name, the names of its chemical elements and their stoichiometric coefficients according to the format (2A4, 16X, 4(A2,F3.0)). For example,

<table>
<thead>
<tr>
<th>B2H2O4</th>
<th>B 2</th>
<th>H 2</th>
<th>O 4</th>
</tr>
</thead>
</table>

The remaining three cards contain the curve fitted coefficients $A_1, A_2, \ldots, A_7$ of equations (81) to (84) according to the format (5E15.8). Coefficients for the upper temperature range TMID-THI appear first. They are followed by $A_1, A_2, \ldots, A_7$ for the lower range TLOW-TMID. Any number of species data sets may be read in and these can be in any order. The last species data cards must be followed by a card with the word END in columns 1 to 3. The CARD option will generate a permanent thermodynamic data tape,
of course, if a tape is actually mounted on logical tape unit 4.

First case data. - The data cards for a single (or first) case are now described in the order they appear in the data deck. All names must be left adjusted in their fields.

(1) Title - The first card of the case data is the title card. The title is read with format (20A4) and printed out at the top of the first page of output.

(2) Reactions - Chemical reactions are listed, one per card, in any order. The card contains the participating species names and the rate constant parameters $A_j$, $n_j$, and $E_j$ (see eq. (33)) for the forward direction as written. The format of a reaction card is as follows:

Type 1 reaction: $S_1 + S_2 \rightarrow S_3 + S_4$

<table>
<thead>
<tr>
<th>Columns</th>
<th>Contents</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 - 8</td>
<td>name of species $S_1$</td>
<td></td>
</tr>
<tr>
<td>10 - 17</td>
<td>name of species $S_2$</td>
<td></td>
</tr>
<tr>
<td>21 - 28</td>
<td>name of species $S_3$</td>
<td></td>
</tr>
<tr>
<td>30 - 37</td>
<td>name of species $S_4$</td>
<td></td>
</tr>
</tbody>
</table>

Type 2a reaction: $M + S_1 + S_2 \rightarrow S_3 + M$

<table>
<thead>
<tr>
<th>Columns</th>
<th>Contents</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 - 8</td>
<td>name of species $S_1$</td>
<td></td>
</tr>
<tr>
<td>10 - 17</td>
<td>name of species $S_2$</td>
<td></td>
</tr>
<tr>
<td>21 - 28</td>
<td>name of species $S_3$</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>the letter $M$</td>
<td>$M =$ third body molecule</td>
</tr>
</tbody>
</table>

Type 2b reaction: $M + S_3 \rightarrow S_1 + S_2 + M$

<table>
<thead>
<tr>
<th>Columns</th>
<th>Contents</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>the letter $M$</td>
<td>$M =$ third body molecule</td>
</tr>
<tr>
<td>10 - 17</td>
<td>name of species $S_3$</td>
<td></td>
</tr>
<tr>
<td>21 - 28</td>
<td>name of species $S_1$</td>
<td></td>
</tr>
<tr>
<td>30 - 37</td>
<td>name of species $S_2$</td>
<td></td>
</tr>
</tbody>
</table>

Type 3a reaction: $S_3 \rightarrow S_1 + S_2$

<table>
<thead>
<tr>
<th>Columns</th>
<th>Contents</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 - 8</td>
<td>blank</td>
<td></td>
</tr>
<tr>
<td>10 - 17</td>
<td>name of species $S_3$</td>
<td></td>
</tr>
<tr>
<td>21 - 28</td>
<td>name of species $S_1$</td>
<td></td>
</tr>
<tr>
<td>30 - 37</td>
<td>name of species $S_2$</td>
<td></td>
</tr>
</tbody>
</table>
Type 3b reaction: $S_1 + S_2 \rightarrow S_3$

<table>
<thead>
<tr>
<th>Columns</th>
<th>Contents</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 - 8</td>
<td>name of species $S_1$</td>
<td></td>
</tr>
<tr>
<td>10 - 17</td>
<td>name of species $S_2$</td>
<td></td>
</tr>
<tr>
<td>21 - 28</td>
<td>name of species $S_3$</td>
<td></td>
</tr>
<tr>
<td>30 - 37</td>
<td>blank</td>
<td></td>
</tr>
</tbody>
</table>

For all types of reaction the rate constant parameters are listed as follows:

<table>
<thead>
<tr>
<th>Columns</th>
<th>Contents</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>42 - 56</td>
<td>$A_j$</td>
<td>preexponential factor for $k_j$ in CGS units, format E15.8</td>
</tr>
<tr>
<td>59 - 68</td>
<td>$n_j$</td>
<td>dimensionless temperature exponent, format F10.3</td>
</tr>
<tr>
<td>71 - 80</td>
<td>$E_j$</td>
<td>activation energy in cal/mole, format F10.3</td>
</tr>
</tbody>
</table>

The number of reaction cards may not exceed 30. The end of the reaction list is signalled by a blank card after the last reaction card. The program makes up its own list of reacting species from the species names on the reaction cards. No separate list of reacting species is needed in the data cards.

(3) Inert species - The names of any nonreacting species are listed, four per card, starting in columns 1, 17, 33, and 49. The format is (4(2A4,8X)). The end of the inert species list is signalled by a blank field after the last species name. If there are no inert species, a blank card must be placed here. If there is an exact multiple of four inert species, a blank card must follow the last species card. The total number of inert plus reacting species may not exceed 25.

(4) Version and units - A single card specifies the variable of integration and the assigned variable (pressure or area). It also gives the desired input and output units. Its makeup is as follows:

<table>
<thead>
<tr>
<th>Columns</th>
<th>Contents</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 - 8</td>
<td>TIME</td>
<td>time is the fundamental variable</td>
</tr>
<tr>
<td></td>
<td>DISTANCE</td>
<td>distance is the fundamental variable</td>
</tr>
<tr>
<td>11 - 18</td>
<td>PRESSURE</td>
<td>pressure is assigned</td>
</tr>
<tr>
<td></td>
<td>AREA</td>
<td>area is assigned</td>
</tr>
<tr>
<td></td>
<td>blank</td>
<td>velocity is zero, no assigned pressure</td>
</tr>
<tr>
<td>21 - 23</td>
<td>CGS or blank</td>
<td>input will be in internal (cgs) units</td>
</tr>
<tr>
<td>Columns</td>
<td>Contents</td>
<td>Explanation</td>
</tr>
<tr>
<td>---------</td>
<td>------------</td>
<td>--------------------------------------------------</td>
</tr>
<tr>
<td>FPS</td>
<td></td>
<td>input will be in FPS units</td>
</tr>
<tr>
<td>SI</td>
<td></td>
<td>input will be in SI units</td>
</tr>
<tr>
<td>31 - 33</td>
<td>CGS or blank</td>
<td>output in internal (cgs) units</td>
</tr>
<tr>
<td>FPS</td>
<td></td>
<td>output in FPS units</td>
</tr>
<tr>
<td>SI</td>
<td></td>
<td>output in SI units</td>
</tr>
</tbody>
</table>

(5) Controls - The controls are input through a NAMELIST named PROB. The names of the variables in PROB are given below. If no value for a variable is input (default), then the program uses the standard option for that variable. Standard options are indicated by an underscore.

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>HMIN</td>
<td>------</td>
<td>minimum step size in cm or sec; values are 0.0001 cm or 5.0x10^-8 sec if defaulted</td>
</tr>
<tr>
<td>HMAX</td>
<td>------</td>
<td>maximum step size in cm or sec; values are 0.10 cm or 5.0x10^-5 sec if defaulted</td>
</tr>
<tr>
<td>HINT</td>
<td>------</td>
<td>initial step size in cm or sec; equal to HMIN, if defaulted</td>
</tr>
<tr>
<td>EMAX</td>
<td>------</td>
<td>maximum allowable relative error per step; equal to 0.0001, if defaulted</td>
</tr>
<tr>
<td>ALLM1</td>
<td>TRUE</td>
<td>all third-body efficiencies are equal to 1; none are input</td>
</tr>
<tr>
<td></td>
<td>FALSE</td>
<td>some third-body efficiencies will be read in</td>
</tr>
<tr>
<td>ELIM</td>
<td>TRUE</td>
<td>automatic elimination from error considerations of species with nonrepresentative errors is desired</td>
</tr>
<tr>
<td></td>
<td>FALSE</td>
<td>no automatic eliminations</td>
</tr>
<tr>
<td>CONC</td>
<td>TRUE</td>
<td>composition is to be output as molar concentrations</td>
</tr>
<tr>
<td></td>
<td>FALSE</td>
<td>composition is to be output as mass fractions</td>
</tr>
<tr>
<td>EXCHR</td>
<td>TRUE</td>
<td>net energy exchange rates are to be output</td>
</tr>
<tr>
<td></td>
<td>FALSE</td>
<td>net reaction conversion rates are to be output</td>
</tr>
<tr>
<td>ITPSZ</td>
<td>1</td>
<td>an area or pressure table will be input</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>area or pressure will be specified by polynomial equation</td>
</tr>
<tr>
<td>Name</td>
<td>Value</td>
<td>Explanation</td>
</tr>
<tr>
<td>----------</td>
<td>-------</td>
<td>-------------</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td>LSUBM and ETA will be input for special area equation, eq. (80)</td>
</tr>
<tr>
<td>4</td>
<td></td>
<td>D, VISC, BETA, and ETA will be input for special area equation, eq. (80)</td>
</tr>
<tr>
<td>5</td>
<td></td>
<td>zero-velocity case - no assigned pressure</td>
</tr>
<tr>
<td>IPRCOD</td>
<td>1</td>
<td>distance versus area profile is given</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>distance versus pressure profile is given</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>time versus area profile is given</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>time versus pressure profile is given</td>
</tr>
<tr>
<td>XTB</td>
<td>------</td>
<td>array for time or position half of assigned variable table; must be in user's chosen input units</td>
</tr>
<tr>
<td>ATB</td>
<td>------</td>
<td>array for area or pressure half of assigned variable table; must be in user's chosen input units</td>
</tr>
<tr>
<td>NTB</td>
<td>------</td>
<td>total number of stations in input area or pressure table; must be less than or equal to 40</td>
</tr>
<tr>
<td>CX3</td>
<td>------</td>
<td>coefficient of $q^3$ in pressure/area equation, (eq. (79))</td>
</tr>
<tr>
<td>CX2</td>
<td>------</td>
<td>coefficient of $q^2$ in eq. (79)</td>
</tr>
<tr>
<td>CX1</td>
<td>------</td>
<td>coefficient of $q$ in eq. (79)</td>
</tr>
<tr>
<td>CX0</td>
<td>------</td>
<td>constant term in eq. (79)</td>
</tr>
<tr>
<td>LSUBM</td>
<td>------</td>
<td>characteristic shock tube reaction length for special area equation, (eq. (80)) - must be given in cm</td>
</tr>
<tr>
<td>ETA</td>
<td>------</td>
<td>dimensionless exponent in special area equation (eq. (80)) for boundary layer correction</td>
</tr>
<tr>
<td>D</td>
<td>------</td>
<td>hydraulic diameter of shock tube in cm</td>
</tr>
<tr>
<td>VISC</td>
<td>------</td>
<td>viscosity coefficient in g/(cm - sec)</td>
</tr>
<tr>
<td>BETA</td>
<td>------</td>
<td>dimensionless boundary layer parameter used to calculate LSUBM</td>
</tr>
<tr>
<td>END</td>
<td>------</td>
<td>final print station in user's chosen input units; must be a time if time is the fundamental variable and conversely for distance; not needed if array of print stations is input</td>
</tr>
<tr>
<td>Name</td>
<td>Value</td>
<td>Explanation</td>
</tr>
<tr>
<td>--------</td>
<td>-------</td>
<td>-------------</td>
</tr>
<tr>
<td>DELP</td>
<td>------</td>
<td>increment between print stations; same units as END; must not require more than 50 print stations; if defaulted, 25 equal increments are taken</td>
</tr>
<tr>
<td>PRINT</td>
<td>------</td>
<td>array of values of the variable of integration at which output is desired; must be in user's chosen input units</td>
</tr>
<tr>
<td>APRINT</td>
<td>------</td>
<td>array of areas or pressures at which output is desired; may only be used if table of assigned pressure or areas is given, and must be in user's chosen input units</td>
</tr>
<tr>
<td>NPRNTS</td>
<td>------</td>
<td>total number of input print stations; must be less than or equal to 50</td>
</tr>
<tr>
<td>EVSTEP</td>
<td>.TRUE.</td>
<td>print results after every integration step</td>
</tr>
<tr>
<td></td>
<td>.FALSE.</td>
<td>do not print results after every integration step</td>
</tr>
<tr>
<td>DEBUGO</td>
<td>.TRUE.</td>
<td>print intermediate output (see p. 38)</td>
</tr>
<tr>
<td></td>
<td>.FALSE.</td>
<td>do not print intermediate output</td>
</tr>
<tr>
<td>COMBUS</td>
<td>.TRUE.</td>
<td>perform equilibrium combustion calculations</td>
</tr>
<tr>
<td></td>
<td>.FALSE.</td>
<td>do not perform equilibrium combustion calculations</td>
</tr>
<tr>
<td>SHOCK</td>
<td>.TRUE.</td>
<td>perform frozen and equilibrium shock calculations</td>
</tr>
<tr>
<td></td>
<td>.FALSE.</td>
<td>do not perform shock calculations</td>
</tr>
<tr>
<td>TCON</td>
<td>.TRUE.</td>
<td>hold temperature constant</td>
</tr>
<tr>
<td></td>
<td>.FALSE.</td>
<td>do not hold temperature constant</td>
</tr>
<tr>
<td>RHOCON</td>
<td>.TRUE.</td>
<td>hold volume (density) constant</td>
</tr>
<tr>
<td></td>
<td>.FALSE.</td>
<td>do not hold volume (density) constant</td>
</tr>
</tbody>
</table>

(6) Third-body efficiencies - In order to input third-body efficiencies, the switch ALLM1 must be set to .FALSE. in PROB. If ALLM1 = .TRUE., then there are no input cards from this section. Only those efficiencies which are not equal to 1 actually need to be read in. Three efficiencies can be listed on a single card. The exact card format is:

<table>
<thead>
<tr>
<th>Columns</th>
<th>Contents</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 - 37</td>
<td>a dissociation-recombination reaction</td>
<td>these columns must be exactly the same as columns 1 - 37 of the reaction card which contains the same reaction</td>
</tr>
<tr>
<td>Columns</td>
<td>Contents</td>
<td>Explanation</td>
</tr>
<tr>
<td>--------</td>
<td>---------------</td>
<td>------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>39 - 46</td>
<td>species name</td>
<td>third-body species name, left adjusted</td>
</tr>
<tr>
<td>47 - 52</td>
<td>third-body</td>
<td>efficiency of species listed in card column 39 - 46 for the reaction listed</td>
</tr>
<tr>
<td></td>
<td>efficiency</td>
<td>in card columns 1 - 37; efficiency is read by the format F6.4</td>
</tr>
<tr>
<td>53 - 60</td>
<td>species name</td>
<td>same form as card columns 39 - 46</td>
</tr>
<tr>
<td>61 - 66</td>
<td>third-body</td>
<td>efficiency of species listed in card column 47 - 52</td>
</tr>
<tr>
<td></td>
<td>efficiency</td>
<td>same form as card columns 47 - 52</td>
</tr>
<tr>
<td>67 - 74</td>
<td>species name</td>
<td>same form as card columns 39 - 46</td>
</tr>
<tr>
<td>75 - 80</td>
<td>third-body</td>
<td>efficiency of species listed in card column 47 - 52</td>
</tr>
<tr>
<td></td>
<td>efficiency</td>
<td>same form as card columns 47 - 52</td>
</tr>
</tbody>
</table>

There are no fixed rules regarding (1) the order of the efficiencies on any card, (2) the position of efficiencies on a card; that is, if the user desires, he can put just one or two efficiencies on a card and he can put them in any of the three available fields, (3) the order of the efficiency cards, (4) the total number of efficiency cards. The end of the third-body list is signalled by a blank card following the last efficiency card.

(7) Initial conditions - The initial conditions are input through a NAMELIST named START. This NAMELIST contains the names of all the species in the master species list as variable names. Hence, initial concentrations are input by "species name = initial concentration". For example, one of the NAMELIST cards could look like

```
NAMELIST cards could look like
```

All species concentrations are initialized to zero so only those concentrations which are initially nonzero actually need to be read in. The names of the other variables in START along with standard options are given next. All parameters except pressure, must be in the user's chosen input units. Note that only ONE of the names P, RHO, MDOT, and AREA is used for any case. For the possible choices see "Starting Conditions", in the section GENERAL DESCRIPTION OF PROGRAM USE.

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>TIME</td>
<td>------</td>
<td>time in sec</td>
</tr>
<tr>
<td>P</td>
<td>------</td>
<td>pressure</td>
</tr>
<tr>
<td>Name</td>
<td>Value</td>
<td>Explanation</td>
</tr>
<tr>
<td>-------</td>
<td>-------</td>
<td>-------------------------------------------------</td>
</tr>
<tr>
<td>X</td>
<td>------</td>
<td>axial position</td>
</tr>
<tr>
<td>V</td>
<td>------</td>
<td>velocity</td>
</tr>
<tr>
<td>RHO</td>
<td>------</td>
<td>density</td>
</tr>
<tr>
<td>T</td>
<td>------</td>
<td>temperature</td>
</tr>
<tr>
<td>MACH</td>
<td>------</td>
<td>Mach number</td>
</tr>
<tr>
<td>MMHG</td>
<td>.TRUE.</td>
<td>input pressure has units of mm of mercury</td>
</tr>
<tr>
<td></td>
<td>.FALSE.</td>
<td>input pressure is given in the user's chosen units</td>
</tr>
<tr>
<td>MOLEF</td>
<td>.TRUE.</td>
<td>species concentrations will be input as mole fractions</td>
</tr>
<tr>
<td></td>
<td>.FALSE.</td>
<td>species concentrations will be input as mass fractions</td>
</tr>
</tbody>
</table>

(8) Permanently neglected species - The last data for a case are the names of those species which are to be permanently neglected from all error considerations. The neglected species cards have exactly the same format as the inert species cards. They are listed, four per card, starting in card columns 1, 17, 33, and 49. The end of the neglected species list is signalled by a blank field following the last neglected species name. If there are no species to be neglected, then there must be a blank card here. If there is an exact multiple of four neglected species, then the last card containing four names must be followed by a blank card.

(9) Final card - Each case must end with a card containing the word FINIS in card columns 1 to 5.

Multiple cases. - At the end of each case the program tries to read data for another case. Hence, several cases can be computed during one computer run. As mentioned earlier, the program was designed to eliminate the necessity of repeating data which do not change from case to case. This objective was accomplished by adding one switch, named the ACTION switch, to the input list for the second and all following cases of a computer run. By using the ACTION switch the user can tell the program to retain much of the data from the previous case for use by the present case. This means that only those data which change between the present case and the previous case must actually be input. The input cards for each case after the first must correspond to the following specifications. Notice particularly that each case after the first case of a computer run must contain an ACTION card.

(1) Title - The first card of each case data deck must be a title card. The format is the same as before.
(2) ACTION card - The value of the ACTION switch must be punched in columns 1 to 6. The possible values are any one of the words NEW, CHANGE, REPEAT, or ADD.

If the word NEW is input, then the program will completely reinitialize. The remainder of the case data must be exactly like the case data for a first case. The user has told the program not to retain any of the data from the previous case.

The word CHANGE enables the user to change the reaction rate parameters of one or more of the reactions from the previous case. A set of reaction cards, in any order, containing the reaction - written exactly as it was for the previous case - and the new rate parameters must follow the CHANGE card. The end of the change list is signalled by a blank card following the last reaction card. Following the CHANGE list, there must be another ACTION card. This time the options are only ADD or REPEAT.

The REPEAT option tells the program to use the reactions, reaction rates, and inert species which are stored at the time this card is input. If a REPEAT card immediately follows the title card, then the program will use the reactions, reaction rates, and inert species from the previous case. The reactions, unchanged reaction rates, and inert species from the previous case along with the changed reaction rates will be used if the REPEAT card is preceded by a CHANGE list.

The word ADD tells the program to save the reactions, rates, and inert species it has and to prepare to read in one or more additional reactions. A set of reaction cards, again in any order, containing the additional reactions and their reaction rate parameters must follow the ADD card. The end of the add list is signalled by a blank card following the last reaction card. If an ADD card immediately follows the title card, then the program will use the inert species from the previous case along with the reactions from the previous case plus the added reactions. The reactions and inert species from the previous case along with the changed rates and the added reactions will be used if the ADD card is preceded by a CHANGE list.

(3) Version and units - The fundamental variable, input units switch, and output units switch must be reset for each case. The format for this card is the same as before.

(4) Controls - Only those controls which are to be changed from their values in the previous case need to be input. A $PROB card with no variables listed must still be put in even if no changes are to be made.

(5) Third-body efficiencies - There are no input cards from this section if ALLM1 = .TRUE.. If ALLM1 = .FALSE., then there must be some input cards from this section. The program will use all the third-body efficiencies from the previous case if the only input card from this section is a blank card. The user can change some or all of the efficiencies from the previous case and add new efficiencies by inserting third-body efficiency cards here. Again, the end of the third-body efficiency list is signalled by a blank card.
(6) Initial conditions - All the parameters in NAMELIST START are reinitialized to zero or their standard option before each case. Hence, the input of initial conditions is exactly the same as it was for a first case.

(7) Permanently neglected species - The names of species which are to be permanently neglected from all error considerations are not retained from one case to the next. Hence, a neglected species list must be input for each case. As before, the end of the neglected species list is signalled by a blank field.

(8) Final card - The last card of each case must have the word FINIS in card columns 1 to 5.

Error Messages

Every error message contains two pieces of information: One is the name of the subroutine which generated the message. The second is a statement of the error condition and, whenever possible, a list of the current value of pertinent parameters. Following is a list of the error messages which the program can generate and a brief explanation of each message.

(GCKP) END OF THIS CASE - READ DATA FOR NEXT CASE

(GCKP) A FATAL ERROR HAS OCCURRED - CASE TERMINATED

(KINP) THE INPUT REACTION LIST DOES NOT CONTAIN THE REACTION \( S_1 + S_2 = S_3 + S_4 \)

(KINP) THE MASTER SPECIES LIST DOES NOT CONTAIN THE SPECIES ----

(KINP) THE INPUT SPECIES LIST DOES NOT CONTAIN THE SPECIES ----

(KINP) INVALID INPUT COMPOSITION SUM = x.xxxx

(SHOCKS) EQUILIBRIUM SHOCK CALCULATION FAILED

70
Iteration of frozen shock equations failed to converge

Singular derivative matrix encountered in equilibrium calculation

Singular matrix encountered in equilibrium calculation

Equilibrium calculation re-started

Iteration of equilibrium equations failed to converge

Mass fraction sum not equal to 1.0

$0.90 < M < 1.10$; Numerical problems occur if Mach number gets close to 1.0 for assigned area computations

Temperature (deg K) is above the range of the thermodynamic data

Temperature (deg K) is below the range of the thermodynamic data

The kinetic calculation is about to be restarted; present location as well as step sizes and results of last 3 steps are given

Case terminated; too many restarts
COMPOSITION ERROR - NEGATIVE CONCENTRATIONS

The concentration of one or more species is negative

SINGULARITY

Singular coefficient matrix encountered in kinetic calculation

ROW xx OF THE COEFFICIENT MATRIX IS ALL ZEROS

Some row of the coefficient matrix is all zeros; the coefficient matrix is given

XX.XX . . . XX.XX

XX.XX . . . XX.XX

XI = xx.xx IS OUT OF RANGE

Abscissa is out of the range of the assigned variable table; the range of abscissas is given

X(1) = xx.xx X(N) = xx.xx
APPENDIX E

TEST CASE DATA AND RESULTS

In this appendix input data and computed results for several kinetics problems are presented. The data are set up as a single computer run to show the use of the multiple-case options CHANGE, ADD, REPEAT, and NEW for the ACTION switch. The data cards used to execute these nine test cases are listed following the case descriptions. Sample listings of results of all cases are then presented. Only selected pages of output are reproduced here, although the input data call for more extensive printout.

Description of Test Cases

Case 1 - This case is the dissociation of \( \text{Br}_2 \) in a shock tube. It shows the use of the shock option and the Mirels boundary-layer equation (eq. (80)).

Case 2 - This problem is a hydrogen-air ignition and combustion in supersonic flow at constant area. The abbreviated reaction mechanism does not contain the reactions of \( \text{H}_2\text{O}_2 \) with the species \( \text{H}, \text{O}, \) and \( \text{OH} \).

Case 3 - This is the same problem as in case 2 and illustrates the use of the CHANGE and ADD options of the ACTION switch. The rate constants for reactions 1 and 3 are changed slightly and three reactions of \( \text{H}_2\text{O}_2 \) are added to the mechanism.

Case 4 - This problem is the same as case 3 with output in FPS units.

Case 5 - This problem is the constant pressure ignition and combustion of methane in a supersonic air stream. It illustrates the use of a unimolecular reaction (reaction 1) and the computation of equilibrium combustion conditions for a constant pressure reaction.

Case 6 - This problem is the same as case 5, with time used as the integration variable. Instead of assigning a constant pressure, we have assigned the area versus distance profile computed in case 5. The computed results do not show perfect agreement with those in case 5 because of curvefitting deviations.

Case 7 - This is another methane-air combustion problem. A pressure profile (in atmospheres) is assigned as a function of distance and output is in SI units. The profile was obtained from the results of a computation which assigned a constant area of 0.10 square meter.

Case 8 - This problem is a constant volume slow reaction of hydrogen and oxygen at a constant temperature of 773 K.

Case 9 - This problem is a high-temperature air ionization reaction in constant area flow. The initial temperature and pressure are generated by a strong shock wave.
**Test Case Data Cards**

**SUAVA**

**BROMINE DISSOCIATION IN A SHOCK TUBE**

CASE 1

M *BR2 = BR +BR 6.99E+11 0.50 35500.

**XE**

DISTANCE AREA

$PROB IPSZ=3.1SUBM=3200.,ETA=0.50., SHOCK=.TRUE., END=10.,DELP=0.5., ALM1=.FALSE., SEND

M *BR2 = BR +BR BR2 3.80

$START P=0.1227,MACH=3.2646,T=299.9, BR2=0.01,XE=0.99 SEND

**FINIXS**

**H2-AIR SUPERSONIC COMBUSTION**

(Stoichiomteric)

CASE 2

**NEW**

H2 +OH = H2O +H 2.19E+13 0. - 5150.
H +O2 = OH +O 1.25E+14 0. - 16300.
O +H2 = OH +H 1.74E+13 0. - 9450.
H +O2 = HO2 +M 1.59E+15 0. - 10000.
H2 +HO2 = OH +OH 9.60E+12 0. - 24000.
M +H2O2 = OH +OH 1.17E+17 0. - 45500.
H +HO2 = OH +OH 7.00E+13 0. - 0.
H +OH = H2O +M 7.50E+23 -2.60 0. - 360.
O +H = O2 +M 1.38E+18 -1. - 3600.
O +H2O = OH +OH 5.75E+13 0. - 18000.
H2 +O2 = OH +O2 1.00E+13 0. - 43000.
OH +HO2 = H2O2 +O2 6.00E+12 0. - 0.
O +HO2 = OH +O2 6.00E+12 0. - 0.
HO2 +HO2 = H2O2 +O2 1.80E+12 0. - 0.

**N2**

DISTANCE AREA

$PROB HINT=0.01, IPSZ=2,CX0=2000., ALM1=.FALSE., NPRINTS=15,


27.432,30.480,45.72,60.96,76.20, SEND

H +O2 = NO2 +M H2 5.0 O2 2.0 H2O 32.5
H +O2 = NO2 +M N2 2.0
H +OH = NO +M H2 4.0 H2 1.6 H2O 20.0
H +OH = NO +M N2 2.0
H +H = N2 +O2 2.0 H2 5.0 H2O 15.0
H +H = N2 +O2 2.0
M +H2O2 = OH +OH O2 0.78 H2O 6.0 H2O2 6.6
M +H2O2 = OH +OH O2 0.78 H2O 6.0 H2O2 6.6

$START X=0.,TIME=0.,P=0.956, T=1559., MACH=5.0, H2=0.2958,O2=0.1480,N2=0.5562, SEND

HO2 +HO2

FINIS

**H2-AIR SUPERSONIC COMBUSTION**

(Complete Mechanism - Preferred Rates)

CASE 3

CHANGE

H2 +OH = H2O +H 2.10E+13 0. - 5100.
O +H2 = OH +H 2.96E+13 0. - 9800.

ADD

OH +H2O2 = H2O +HO2 1.00E+13 0. - 1800.
O +H2O2 = OH +H2O2 2.00E+13 0. - 1000.
M +H2O2 = H2O +OH 3.18E+14 0. - 9000.

**DISTANCE AREA**

$FROM SEND

$START V=455172.99,RHO=1.56283E-04, T=1559.,

H2=0.2958,O2=0.1480,N2=0.5562, SEND

H2C2 FINIS
H2-AIR SUPERSONIC COMBUSTION

REPEAT
DISTANCE AREA FPS
$PROB SEND

$START
V=55172.99,T=1559.,NO2=1.42272E+05,
H2=0.2956,02=0.1480,N2=0.5562, SEND
HO2 H2O2

PIECS
METHANE-AIR COMBUSTION AT CONSTANT P (ONE UNIMOLECULAR REACTION) CASE 4

NEW
CH4 = CH3 + H

CH4 + O2 = CH3 + O2

HO + O2 = HO2 + H

H2 + O2 = HO2 + H

CO + O2 = CO2 + H

CH3 + O2 = CH4 + O2

CH2O + O2 = CH3 + H2O

CH2O + H2 = CH3 + OH

CH2O + OH = HCO + H2O

CH3 + NO2 = CH4 + NO

SSTART
AREA=10000,MACH=2,T=1645.,
CH4=0.049768,02=0.199072,N2=0.75116, SEND
HO2 H2O2

PRINT
METHANE-AIR COMBUSTION (ASSIGNED AREA - TIME INTEGRATION) CASE 5

NEW
CH4 = CH3 + H

CH4 + O2 = CH3 + O2

HO + O2 = HO2 + H

H2 + O2 = HO2 + H

CO + O2 = CO2 + H

CH3 + O2 = CH4 + O2

CH2O + O2 = CH3 + H2O

CH2O + H2 = CH3 + OH

CH2O + OH = HCO + H2O

CH3 + NO2 = CH4 + NO

SSTART
AREA=10000,MACH=2,T=1645.,
CH4=0.049768,02=0.199072,N2=0.75116, SEND
HO2 H2O2

PRINT
METHANE-AIR COMBUSTION (ASSIGNED AREA - TIME INTEGRATION) CASE 6

NEW
CH4 = CH3 + H

CH4 + O2 = CH3 + O2

HO + O2 = HO2 + H

H2 + O2 = HO2 + H

CO + O2 = CO2 + H

CH3 + O2 = CH4 + O2

CH2O + O2 = CH3 + H2O

CH2O + H2 = CH3 + OH

CH2O + OH = HCO + H2O

CH3 + NO2 = CH4 + NO

SSTART
P=1.730,V=157412.62,T=1645.,
CH4=0.049768,02=0.199072,N2=0.75116, SEND
HO2 H2O2

PRINT
METHANE-AIR COMBUSTION (ASSIGNED AREA - TIME INTEGRATION) CASE 6

NEW
CH4 = CH3 + H

CH4 + O2 = CH3 + O2

HO + O2 = HO2 + H

H2 + O2 = HO2 + H

CO + O2 = CO2 + H

CH3 + O2 = CH4 + O2

CH2O + O2 = CH3 + H2O

CH2O + H2 = CH3 + OH

CH2O + OH = HCO + H2O

CH3 + NO2 = CH4 + NO

SSTART
P=1.730,V=157412.62,T=1645.,
CH4=0.049768,02=0.199072,N2=0.75116, SEND
HO2 H2O2

PRINT
METHANE-AIR COMBUSTION (ASSIGNED AREA - TIME INTEGRATION) CASE 6

NEW
CH4 = CH3 + H

CH4 + O2 = CH3 + O2

HO + O2 = HO2 + H

H2 + O2 = HO2 + H

CO + O2 = CO2 + H

CH3 + O2 = CH4 + O2

CH2O + O2 = CH3 + H2O

CH2O + H2 = CH3 + OH

CH2O + OH = HCO + H2O

CH3 + NO2 = CH4 + NO

SSTART
P=1.730,V=157412.62,T=1645.,
CH4=0.049768,02=0.199072,N2=0.75116, SEND
HO2 H2O2

PRINT
METHANE-AIR COMBUSTION (ASSIGNED AREA - TIME INTEGRATION) CASE 6

NEW
CH4 = CH3 + H

CH4 + O2 = CH3 + O2

HO + O2 = HO2 + H

H2 + O2 = HO2 + H

CO + O2 = CO2 + H

CH3 + O2 = CH4 + O2

CH2O + O2 = CH3 + H2O

CH2O + H2 = CH3 + OH

CH2O + OH = HCO + H2O

CH3 + NO2 = CH4 + NO

SSTART
P=1.730,V=157412.62,T=1645.,
CH4=0.049768,02=0.199072,N2=0.75116, SEND
HO2 H2O2

PRINT
METHANE-AIR COMBUSTION (ASSIGNED AREA - TIME INTEGRATION) CASE 6

NEW
CH4 = CH3 + H

CH4 + O2 = CH3 + O2

HO + O2 = HO2 + H

H2 + O2 = HO2 + H

CO + O2 = CO2 + H

CH3 + O2 = CH4 + O2

CH2O + O2 = CH3 + H2O

CH2O + H2 = CH3 + OH

CH2O + OH = HCO + H2O

CH3 + NO2 = CH4 + NO

SSTART
P=1.730,V=157412.62,T=1645.,
CH4=0.049768,02=0.199072,N2=0.75116, SEND
HO2 H2O2

PRINT
METHANE-AIR COMBUSTION (ASSIGNED AREA - TIME INTEGRATION) CASE 6

NEW
CH4 = CH3 + H

CH4 + O2 = CH3 + O2

HO + O2 = HO2 + H

H2 + O2 = HO2 + H

CO + O2 = CO2 + H

CH3 + O2 = CH4 + O2

CH2O + O2 = CH3 + H2O

CH2O + H2 = CH3 + OH

CH2O + OH = HCO + H2O

CH3 + NO2 = CH4 + NO

SSTART
P=1.730,V=157412.62,T=1645.,
CH4=0.049768,02=0.199072,N2=0.75116, SEND
HO2 H2O2

PRINT
METHANE-AIR COMBUSTION (ASSIGNED AREA - TIME INTEGRATION) CASE 6

NEW
CH4 = CH3 + H

CH4 + O2 = CH3 + O2

HO + O2 = HO2 + H

H2 + O2 = HO2 + H

CO + O2 = CO2 + H

CH3 + O2 = CH4 + O2

CH2O + O2 = CH3 + H2O

CH2O + H2 = CH3 + OH

CH2O + OH = HCO + H2O

CH3 + NO2 = CH4 + NO

SSTART
P=1.730,V=157412.62,T=1645.,
CH4=0.049768,02=0.199072,N2=0.75116, SEND
HO2 H2O2

PRINT
METHANE-AIR COMBUSTION (ASSIGNED PRESSURE) CASE 7

DISTANCE PRESSURE SI
$SIGMA ITPSZ=1, HMIN=0.0001, HMAX=0.20, IPRC=2,
XTB=0.5,10,15,20,25,27.5,30,32.5,35,35.5,36,36.5,37.0,
ATB=1.73,1.745,1.7455,1.75,1.76,1.78,1.80,1.8255,1.85,
$SIGMA $SIGMA PRINT=0.,20.,30.,35.,36.5, NPRINTS=6, FIT=.FALSE., $END

$START AREA=1000., MACH=2., T=1645.,
CH4=0.049768, O2=0.190072, N2=0.75116, $END
OH H2 CO2 N2 H2O CH3
FINIS

H2-O2 LOW TEMPERATURE REACTION AT CONSTANT VOLUME (ADJUSTED P_TES) CASE 8

NEW
H2 +O2 = H +HO2 1.00E+14 0. 67000.
H2 +OH = H2O +H 2.10E+13 0. 51000.
O +H2 = OH +H 1.25E+14 0. 16300.
H +O2 = HO2 +M 9.50E+14 0. -1000.
M +HO2 = OH +OH 1.17E+17 0. 55000.
H2O +HO2 = H2O2 +O2 1.00E+12 0. 0.
H2O +H2 = H2O +H 8.50E+12 0. 24900.
ON +H2O2 = H2O +O2 3.18E+14 0. 9000.
O +H2O2 = H2O +HO2 1.00E+13 0. 18900.
O +H2O = OH +OH 5.75E+13 0. 18900.

TIME
$SIGMA HMIN=5.0E-05, HMAX=.1, HINT=-.15, HMAX=0.003, ALLM1=.FALSE.,
ROH=.TRUE., ICON=.TRUE., CONC=.FALSE.,
PRINT=0.75,1.25,5,10,20,30,40,50,5.5,60,65,75,85,95.105,120, NPRINTS=16, $END
W +O2 = HO2 +M H2O 5. 02 2. H2O 32.5
M +H2O2 = OH +OH H2O 6. 02 0.7H H2O2 6.6
M +H2O2 = OH +OH H2O 2.3

$START MMHG=.TRUE., P=500., T=773.15, H2=0.96, O2=0.14, $END
H OH O NO2
FINIS

HIGH TEMPERATURE AIR IONIZATION CASE 9

NEW
N +O2 = NO +O 6.43E+09 1. 6250.
O +N2 = NO +N 1.36E+14 0. 1.75E+09.
N +O = NO +M 6.40E+16 -0.5 0.
O +N = NO +M 1.38E+18 -1. 340.
N +NO = NO2 +M 2.80E+17 -0.75 0.
NO +O = NO2 +M 9.80E+14 0. -1930.
M +NO2 = N2 +O 5.00E+14 0. 58000.
O +NO2 = N2 +O2 6.30E+14 0. 26700.
NO +E = N +O 1.85E+21 -1.5 0.
O +E = O +M 2.00E+26 -2.5 0.
O2 +E = O2- +M 1.52E+21 -1. 1190.
O2 +O- = O2- +M 6.00E+12 0. 0.

DISTANCE AREA
$SIGMA HMIN=0.001, HMAX=0.30, ITPSZ=2, CX0=1000., ALLM1=.FALSE.,
HINT=0.0002, DRUG=.TRUE.,
PRINT=0.04, 0.6, 0.8, 1.0, 3.0, 10, 20, 40, 100, NPRINTS=10 $END
N +O = NO +E N2O 2.25
NO +O = NO2 +M N2 1.55
O+ +E = O +M W 0.01 02 4.5 NO 50.
O+ +E = O +M 0 0.03
O2 +E = O2- +M N2 0.0002

$START P=1.6803, V=47002., T=4820.2, N2=0.7905, O2=0.2095, $END
NO+ O+ O- O2- E
FINIS
## Selected Test Case Results

### Equilibrium Shock Calculation

<table>
<thead>
<tr>
<th><strong>Initial State</strong></th>
<th><strong>Final State</strong></th>
<th><strong>Final/Initial Ratio</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure (atm)</td>
<td>0.1227</td>
<td>1.5133</td>
</tr>
<tr>
<td>Velocity (in/sec)</td>
<td>5787.78</td>
<td>18108.11</td>
</tr>
<tr>
<td>Density (lb/vol)</td>
<td>6.56092E-04</td>
<td>2.05899E-03</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>299.90</td>
<td>1231.22</td>
</tr>
<tr>
<td>Entropy (J/kgK)</td>
<td>0.3421</td>
<td>0.3576</td>
</tr>
<tr>
<td>Mass Number</td>
<td>3.2046</td>
<td>0.5171</td>
</tr>
<tr>
<td>Gamma</td>
<td>1.6586</td>
<td>1.5731</td>
</tr>
<tr>
<td>Sonic Velocity (in/sec)</td>
<td>17728.29</td>
<td>35215.45</td>
</tr>
</tbody>
</table>

### Supersonic Shock Calculation

<table>
<thead>
<tr>
<th><strong>Initial State</strong></th>
<th><strong>Final State</strong></th>
<th><strong>Final/Initial Ratio</strong></th>
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</thead>
<tbody>
<tr>
<td>Pressure (atm)</td>
<td>0.1227</td>
<td>1.3017</td>
</tr>
<tr>
<td>Velocity (in/sec)</td>
<td>5787.78</td>
<td>18410.72</td>
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<tr>
<td>Density (lb/vol)</td>
<td>6.55092E-04</td>
<td>2.05248E-03</td>
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<tr>
<td>Temperature (K)</td>
<td>299.90</td>
<td>1245.31</td>
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<tr>
<td>Entropy (J/kgK)</td>
<td>0.3421</td>
<td>0.3575</td>
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<tr>
<td>Mass Number</td>
<td>3.2046</td>
<td>0.5095</td>
</tr>
<tr>
<td>Gamma</td>
<td>1.6586</td>
<td>1.5737</td>
</tr>
<tr>
<td>Sonic Velocity (in/sec)</td>
<td>17728.29</td>
<td>35215.45</td>
</tr>
</tbody>
</table>

### Species Mole Fraction

<table>
<thead>
<tr>
<th>Species</th>
<th>Mole Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>R2</td>
<td>0.12239E-03</td>
</tr>
<tr>
<td>X</td>
<td>1.21835E-03</td>
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<tr>
<td>Xe</td>
<td>9.88163E-01</td>
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<tr>
<td>Xe</td>
<td>1.00000E-03</td>
</tr>
</tbody>
</table>

### Mixture Molecular Weight

<table>
<thead>
<tr>
<th>Volumes</th>
<th>Molecular Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>DI.2G</td>
<td>131.34058</td>
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<tr>
<td>D1.2G</td>
<td>1.0151</td>
</tr>
<tr>
<td>D1.2G</td>
<td>-1.0008</td>
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</tbody>
</table>

## Rider from Lab Available Copy

**Final/Initial Ratio**

<table>
<thead>
<tr>
<th>Species</th>
<th>Mole Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>R2</td>
<td>1.00000E-02</td>
</tr>
<tr>
<td>X</td>
<td>3.00000E-01</td>
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<tr>
<td>Xe</td>
<td>9.00000E-01</td>
</tr>
<tr>
<td>Xe</td>
<td>1.00000E-03</td>
</tr>
</tbody>
</table>

### Mixture Molecular Weight

<table>
<thead>
<tr>
<th>Volumes</th>
<th>Molecular Weight</th>
</tr>
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<tbody>
<tr>
<td>DI.2G</td>
<td>131.58520</td>
</tr>
<tr>
<td>DI.2G</td>
<td>1.00000</td>
</tr>
<tr>
<td>D1.2G</td>
<td>-1.00000</td>
</tr>
</tbody>
</table>
** Distance-Area Version

** Several Chemical Kinetics Program**

** NASA Lewis Research Center**

** Derivative dissociation in a shock tube**

** Case 2**

** Reaction**

<table>
<thead>
<tr>
<th>Species</th>
<th>Reaction</th>
<th>Activation</th>
<th>Rate Constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>Br2</td>
<td>Br + Br</td>
<td>0.99006E+11</td>
<td>0.0004</td>
</tr>
<tr>
<td>Br</td>
<td>Br + Br</td>
<td>0.99006E+11</td>
<td>0.0004</td>
</tr>
</tbody>
</table>

** Integration Controls**

<table>
<thead>
<tr>
<th>Minimum Step Size</th>
<th>Maximum Step Size</th>
<th>Maximum Relative Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.10000E-09 cm</td>
<td>0.10000E+00 cm</td>
<td>0.00010</td>
</tr>
<tr>
<td>Initial Step Size</td>
<td>Maximum Size</td>
<td>Relative Error</td>
</tr>
<tr>
<td>0.10000E-09 cm</td>
<td>0.10000E+00 cm</td>
<td>0.00010</td>
</tr>
</tbody>
</table>

** Assigned Variable Profile**

The area is calculated from the following function

\[ \frac{1}{S_A} = 1 - \frac{1}{S_{2200.333401}} \]

No species will be permanently neglected from all error considerations.

** Initial Conditions**

- Time (sec): 0
- Area: 1.00000E+00 sq cm
- Axial Position (cm): 0

** Flow Properties**

- Pressure: 1.60167 atm
- Velocity: 18460.737 cm/sec
- Density: 2.0624E-03 g/cm^3
- Temperature: 1263.31 K
- Mass Flow Rate: 3.79718E+01 g/sec
- Entropy: 0.35751
- Specific Heat at Constant Volume: 1.5098

** Integration Indicators**

- Steps from Last Print: 0
- Average Step Size: 0.00010
- Controlling Variable: Relative Error

** Chemical Properties**

- Species: Br2, Br, K
- Mole Fraction: 1.5571E-01, 1.6465E-02, 9.40000E-01
- Mixture Molecular Weight: 131.58922
- Total Energy Exchange Rate (cal/m^3*s): 3.97332E+09
- Mass Fraction Sum: 0.9999999

<table>
<thead>
<tr>
<th>Variable</th>
<th>Derivative</th>
<th>Increment</th>
<th>Relative Error</th>
<th>Variable</th>
<th>Derivative</th>
<th>Increment</th>
<th>Relative Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>V</td>
<td>-0.53990E+03</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.972</td>
<td>-0.972</td>
<td>0</td>
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<tr>
<td>rho</td>
<td>0.173462E-24</td>
<td>0</td>
<td>0</td>
<td>0.13914E-05</td>
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<td>T</td>
<td>0.500952E+01</td>
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<td>0</td>
<td>0.500952E+01</td>
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</table>
### Flow Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>1.50169 (atm)</td>
</tr>
<tr>
<td>Kinetic Energy</td>
<td>1440.15 (J/kg)</td>
</tr>
<tr>
<td>Velocity</td>
<td>2.06250e+03 (m/s)</td>
</tr>
<tr>
<td>Temperature</td>
<td>1245.37 (K)</td>
</tr>
<tr>
<td>Mass Flow Rate</td>
<td>3.79740e+01 (kg/s)</td>
</tr>
<tr>
<td>Entropy</td>
<td>0.5975</td>
</tr>
<tr>
<td>Mach Number</td>
<td>2.06290e-03 (m/s)</td>
</tr>
<tr>
<td>Gamma</td>
<td>1.6577</td>
</tr>
</tbody>
</table>

### Chemical Properties

#### Species Concentration and Fraction

<table>
<thead>
<tr>
<th>Species</th>
<th>Concentration (mol)</th>
<th>Mole Fraction</th>
<th>Net Species Production Rate (mol/sec)</th>
<th>Reaction Number</th>
<th>Net Reaction Conversion Rate (mol/sec)</th>
<th>Rate Constant (kg/sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Br2</td>
<td>1.58742e-07</td>
<td>9.9999e-03</td>
<td>-3.6172e-05</td>
<td>1</td>
<td>8.62099e-06</td>
<td>8.612099e-07</td>
</tr>
<tr>
<td>Br</td>
<td>3.5873e-13</td>
<td>5.33055e-06</td>
<td>0.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Xe</td>
<td>1.5511e-05</td>
<td>9.9999e-01</td>
<td>0.</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Mixture Molecular Weight**: 131.59020

**Total Energy Exchange Rate**: 3.97353e+01 (J/s)

**Mass Fraction Sum**: 0.999999

### Variable Derivative Increment

<table>
<thead>
<tr>
<th>Variable</th>
<th>Derivative Increment</th>
<th>Relative Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>V</td>
<td>0.494237e+24</td>
<td>0.0</td>
</tr>
<tr>
<td>RH0</td>
<td>0.14530e-03</td>
<td>0.0</td>
</tr>
<tr>
<td>RH1</td>
<td>3.52994e+02</td>
<td>0.0</td>
</tr>
</tbody>
</table>

### Time: 2.72460e+05 sec

**Flow Properties**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>1.64526 (atm)</td>
</tr>
<tr>
<td>Velocity</td>
<td>1334.76 (m/s)</td>
</tr>
<tr>
<td>Density</td>
<td>2.06612e+03 (kg/m^3)</td>
</tr>
<tr>
<td>Temperature</td>
<td>1245.82 (K)</td>
</tr>
<tr>
<td>Mass Flow Rate</td>
<td>3.79025e+01 (kg/s)</td>
</tr>
<tr>
<td>Entropy</td>
<td>3.575</td>
</tr>
<tr>
<td>(cal/deg/kg)</td>
<td></td>
</tr>
<tr>
<td>(mol/deg/k)</td>
<td></td>
</tr>
<tr>
<td>Mach Number</td>
<td>0.5970</td>
</tr>
<tr>
<td>Gamma</td>
<td>1.6577</td>
</tr>
</tbody>
</table>

### Chemical Properties

#### Species Concentration and Fraction

<table>
<thead>
<tr>
<th>Species</th>
<th>Concentration (mol)</th>
<th>Mole Fraction</th>
<th>Net Species Production Rate (mol/sec)</th>
<th>Reaction Number</th>
<th>Net Reaction Conversion Rate (mol/sec)</th>
<th>Rate Constant (kg/sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Br2</td>
<td>1.58041e-27</td>
<td>4.9569e-03</td>
<td>-3.6752e-05</td>
<td>1</td>
<td>8.60932e-06</td>
<td>8.610932e-07</td>
</tr>
<tr>
<td>Br</td>
<td>1.0054e-09</td>
<td>1.1742e-04</td>
<td>0.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Xe</td>
<td>1.5549e-05</td>
<td>9.9937e-01</td>
<td>0.</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Mixture Molecular Weight**: 131.57900

**Total Energy Exchange Rate**: 3.96285e+05 (J/s)

**Mass Fraction Sum**: 0.999999

### Variable Derivative Increment

<table>
<thead>
<tr>
<th>Variable</th>
<th>Derivative Increment</th>
<th>Relative Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>V</td>
<td>-0.51130e+23</td>
<td>0.0</td>
</tr>
<tr>
<td>RH0</td>
<td>2.10630e-05</td>
<td>0.0</td>
</tr>
<tr>
<td>RH1</td>
<td>0.12302e-05</td>
<td>0.0</td>
</tr>
</tbody>
</table>

### Integration Indicators

- **Steps from Last Print**: 14
- **Average Step Size**: 0.37500e+01
- **Relative Error**: 0.10910e-05
- **Predictor Iterations**: 0
TIME 3.35794E-04 SEC  AREA 1.03134E+03  SQ CM  AXIAL POSITION 6.00000E+00  CM

FLOW PROPERTIES

PRESSURE 1.5179E6
VELOCITY 1797.77
DENSITY 2.08495E-03
TEMPERATURE 1243.93
MIX FLOW RATE 3.79908E+01
ENTROPY 0.3576
MACH NUMBER 0.4977
GAMMA 1.6582

CHEMICAL PROPERTIES

BR 1.46749E-07 9.3772E-03 -3.3059E-05 1 6.97257E+00 1.42142E+07
R 2.28040E-08 1.9491E-03 0.06146E-05 0. 0. 0.
KE 1.56854E-05 9.8290E-01 0.

MIXTURE AVERAGE WEIGHT 1.49508 TOTAL ENERGY EXCHANGE RATE (CAL/GM/CMM**3/S) 3.21383E+05 MASS FRACTION SUM 0.999999

VARIABLE DERIVATIVE INCREMENT RELATIVE ERROR VARIABLE DERIVATIVE INCREMENT RELATIVE ERROR
V -0.3393E+32 -0.3203E+01 0. 0. -0. -0. -0.
RHO 0.27310E-35 0.1795E+00 0.7735E+00 KE 0. 0.
T -0.50310E+00 -0.39306E+00 0.7755E+00 0. 0.

TIME 5.43538E-04 SEC  AREA 1.01744E+03  SQ CM  AXIAL POSITION 1.00000E+01  CM

FLOW PROPERTIES

PRESSURE 1.62308
VELOCITY 1781.78
DENSITY 2.09461E-03
TEMPERATURE 1243.93
MIX FLOW RATE 3.79908E+01
ENTROPY 0.3576
MACH NUMBER 0.4977
GAMMA 1.6582

CHEMICAL PROPERTIES

BR 1.46749E-07 9.4815E-03 -3.3407E-05 1 5.3354E+00 1.3015E+07
R 2.28040E-08 1.9491E-03 0.06146E-05 0. 0. 0.
KE 1.56854E-05 9.8290E-01 0.

MIXTURE AVERAGE WEIGHT 1.49508 TOTAL ENERGY EXCHANGE RATE (CAL/GM/CMM**3/S) 2.45925E+05 MASS FRACTION SUM 0.999999

VARIABLE DERIVATIVE INCREMENT RELATIVE ERROR VARIABLE DERIVATIVE INCREMENT RELATIVE ERROR
V -0.3393E+32 -0.3203E+01 0. 0. -0. -0. -0.
RHO 0.27310E-35 0.1795E+00 0.7735E+00 KE 0. 0.
T -0.50310E+00 -0.39306E+00 0.7755E+00 0. 0.

END OF THIS CASE - READ DATA FOR NEXT CASE

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### DISTANCE-AREA VERSION

**GENERAL CHEMICAL KINETICS PROGRAM**

**NASA LEWIS RESEARCH CENTER**

**H2-AIR SUPERSLOW COMBUSTION**

**ESTIMATION**

**CASE 2**

### REACTION RATE VARIABLES

<table>
<thead>
<tr>
<th>SPECIES</th>
<th>A</th>
<th>N</th>
<th>ACTIVATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>H2O</td>
<td>1.1900E+13</td>
<td>0.</td>
<td>3.210E±10</td>
</tr>
<tr>
<td>H2</td>
<td>1.1900E+14</td>
<td>0.</td>
<td>4.590E±10</td>
</tr>
<tr>
<td>O2</td>
<td>1.9000E+15</td>
<td>0.</td>
<td>1.900E±10</td>
</tr>
<tr>
<td>H2O2</td>
<td>1.9000E+16</td>
<td>0.</td>
<td>1.900E±10</td>
</tr>
</tbody>
</table>

### ALL THIRD BODY RATIOS ARE 1.2 EXCEPT THE FOLLOWING

<table>
<thead>
<tr>
<th>SPECIES</th>
<th>MINIMUM STEP SIZE</th>
<th>INITIAL STEP SIZE</th>
</tr>
</thead>
<tbody>
<tr>
<td>H2O</td>
<td>1.00000E-03 cm</td>
<td>1.00000E-01 cm</td>
</tr>
<tr>
<td>H2O2</td>
<td>1.00000E-03 cm</td>
<td>1.00000E-01 cm</td>
</tr>
</tbody>
</table>

### INTEGRATION CONTROLS

**MINIMUM STEP SIZE** 0.10000E-03 cm

**INITIAL STEP SIZE** 0.10000E-01 cm

**MAXIMUM RELATIVE ERROR** 0.0000

**ASSIGNED VARIABLE PROFILE**

**AREA** (cm²) = (x + y)

**TIME** 0.0... sec

**FLOW PROPERTIES**

- **PRESURE** 0.95600
- **SPEED** 455172.99
- **DENSITY** 1.05628E-04
- **TEMPERATURE** 1559.00
- **ENTROPY** 1.02216E+05
- **MASS FLOW RATE** 1.02216E+05
- **MACH NUMBER** 9.0373
- **GAMMA** 1.3173

### CHEMICAL PROPERTIES

**SPECIES**

<table>
<thead>
<tr>
<th>SPECIES</th>
<th>CONCENTRATION (MOLES/CM³)</th>
<th>MOL FRACTION</th>
<th>NET SPECIES PRODUCTION RATE (MOLES/CM³/SEC)</th>
<th>REACTION RATE (1/MOLE/CM³/SEC)</th>
<th>REACTION CONVERSION RATE (1/MOLE/CM³/SEC)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H2</td>
<td>2.11659E-08</td>
<td>0.98800E-01</td>
<td>-6.378E±05</td>
<td>1.890E±05</td>
<td>1.890E±05</td>
</tr>
<tr>
<td>O2</td>
<td>0.0</td>
<td>0.0</td>
<td>8.061E±06</td>
<td>1.650E±05</td>
<td>1.650E±05</td>
</tr>
<tr>
<td>H2O2</td>
<td>1.1682E-08</td>
<td>0.0</td>
<td>8.061E±06</td>
<td>1.650E±05</td>
<td>1.650E±05</td>
</tr>
<tr>
<td>H2O</td>
<td>1.0622E-08</td>
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<td>8.061E±06</td>
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<tr>
<td>NO</td>
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<td>0.0</td>
<td>8.061E±06</td>
<td>1.650E±05</td>
<td>1.650E±05</td>
</tr>
<tr>
<td>N2</td>
<td>0.0</td>
<td>0.0</td>
<td>8.061E±06</td>
<td>1.650E±05</td>
<td>1.650E±05</td>
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<tr>
<td>O</td>
<td>0.0</td>
<td>0.0</td>
<td>8.061E±06</td>
<td>1.650E±05</td>
<td>1.650E±05</td>
</tr>
</tbody>
</table>

### Mixture Molecular Weight

- **20,9269**

**TOTAL ENERGY EXCESSION RATE** 1.78173E+07

**MASS FRACTION SUM** 1.000000

### VARIABLE DERIVATIVE INCREMENT RELATIVE ERROR

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>DERIVATIVE</th>
<th>INCREMENT</th>
<th>RELATIVE ERROR</th>
</tr>
</thead>
<tbody>
<tr>
<td>V</td>
<td>0.17794E+20</td>
<td>0.0</td>
<td>4</td>
</tr>
<tr>
<td>H2O2</td>
<td>-0.1070E+10</td>
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<tr>
<td>O2</td>
<td>-0.1070E+10</td>
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<td>0.0</td>
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<td>H2O</td>
<td>0.04448E+26</td>
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<tr>
<td>H2</td>
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<td>42</td>
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## Chemical Properties

<table>
<thead>
<tr>
<th>SPECIES</th>
<th>CONCENTRATION</th>
<th>MOLE FRACTION</th>
<th>VET SPECIES PRODUCTION RATE</th>
<th>REACTION</th>
<th>NET REACTION CONVERSION RATE</th>
<th>RATE</th>
<th>STAN</th>
<th>ERROR</th>
</tr>
</thead>
<tbody>
<tr>
<td>H2O</td>
<td>4.3893E-07</td>
<td>6.7239E-05</td>
<td>-1.0526E-03</td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O2</td>
<td>2.2756E-07</td>
<td>3.9193E-02</td>
<td>3.1179E-02</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>H2</td>
<td>1.3343E-06</td>
<td>1.6493E-01</td>
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<tr>
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<td></td>
</tr>
</tbody>
</table>

## Variables Derivative Increment Relative Error
-0.205E+06 -0.135E+04 -0.135E+04
-0.402E+05 -0.402E+04 -0.402E+04

## Flow Properties

<table>
<thead>
<tr>
<th>TIME</th>
<th>3.3775E-05 SEC</th>
<th>AREA</th>
<th>2.0000E+03 SQ CM</th>
<th>AXIAL POSITION</th>
<th>1.5200E+01 CM</th>
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</thead>
<tbody>
<tr>
<td>FLOW PROPERTIES</td>
<td></td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>PRESSURE</td>
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<td></td>
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</tr>
<tr>
<td>VELOCITY</td>
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<td></td>
<td></td>
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</tr>
<tr>
<td>DENSITY</td>
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</tr>
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<td>TEMPERATURE</td>
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<td>GAS RATE</td>
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</tr>
<tr>
<td>ENTHALPY</td>
<td></td>
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<td>SPECIES</td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H2O</td>
<td>4.3893E-07</td>
<td>6.7239E-05</td>
<td>-1.0526E-03</td>
<td></td>
<td></td>
</tr>
<tr>
<td>O2</td>
<td>2.2756E-07</td>
<td>3.9193E-02</td>
<td>3.1179E-02</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H2</td>
<td>1.3343E-06</td>
<td>1.6493E-01</td>
<td>-1.3039E-04</td>
<td></td>
<td></td>
</tr>
<tr>
<td>N2</td>
<td>4.3893E-07</td>
<td>5.6412E-05</td>
<td>0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

## Integration Indicators

<table>
<thead>
<tr>
<th>VARIABLES</th>
<th>DERIVATIVE</th>
<th>INCREMENT</th>
<th>RELATIVE ERROR</th>
<th>VARIABLES</th>
<th>DERIVATIVE</th>
<th>INCREMENT</th>
<th>RELATIVE ERROR</th>
</tr>
</thead>
<tbody>
<tr>
<td>W</td>
<td>-0.205E+06</td>
<td>-0.135E+04</td>
<td>-0.135E+04</td>
<td>O</td>
<td>-0.402E+05</td>
<td>-0.402E+04</td>
<td>-0.402E+04</td>
</tr>
</tbody>
</table>
## Flow Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>1.73491</td>
</tr>
<tr>
<td>Velocity</td>
<td>844082.15</td>
</tr>
<tr>
<td>Density</td>
<td>1.60185E-04</td>
</tr>
<tr>
<td>Temperature</td>
<td>3016.50</td>
</tr>
<tr>
<td>Mass Flow Rate</td>
<td>1.42270E+05</td>
</tr>
</tbody>
</table>

## Chemical Properties

### Species Concentration

<table>
<thead>
<tr>
<th>Species</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>H2</td>
<td>1.16069E+07</td>
</tr>
<tr>
<td>OH</td>
<td>1.94192E-12</td>
</tr>
<tr>
<td>H2O</td>
<td>1.06090E-07</td>
</tr>
</tbody>
</table>

### Mixture Molecular Weight

<table>
<thead>
<tr>
<th>Molecular Weight</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>22.85909</td>
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### Chemical Production Rate

<table>
<thead>
<tr>
<th>Species</th>
<th>Production Rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>H2</td>
<td>2.16579E-06</td>
</tr>
<tr>
<td>OH</td>
<td>1.66157E-06</td>
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</tbody>
</table>

### Mass Fraction Sum

<table>
<thead>
<tr>
<th>Mass Fraction Sum</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.9999962</td>
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</tbody>
</table>

## Integration Indicators

<table>
<thead>
<tr>
<th>Indicator</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steps from Last Print</td>
<td>154</td>
</tr>
<tr>
<td>Average Step Size</td>
<td>0.26850E-02</td>
</tr>
<tr>
<td>Controlling Variable</td>
<td>0</td>
</tr>
<tr>
<td>Relative Error</td>
<td>0.3810BE08</td>
</tr>
</tbody>
</table>

## Variable Derivative Increment Relative Error

<table>
<thead>
<tr>
<th>Variable</th>
<th>Derivative</th>
<th>Increment</th>
<th>Relative Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>H2</td>
<td>0.51976E-10</td>
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<td>0.3102E-11</td>
</tr>
<tr>
<td>T</td>
<td>0.2001E-01</td>
<td>0.36975E-03</td>
<td>0.3102E-10</td>
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</tbody>
</table>

## Reaction Net Reaction Conversion Rate Rate Constant

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Net Reaction Conversion Rate</th>
<th>Rate Constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>H2</td>
<td>3.26800E-06</td>
<td>2.16579E-06</td>
</tr>
</tbody>
</table>

## Total Energy Exchange Rate

<table>
<thead>
<tr>
<th>Energy Exchange Rate</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>-2.23330E+07</td>
</tr>
</tbody>
</table>

## End of Case

End of data for next case
### Reaction Numbers

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Species</th>
<th>Rate Variables</th>
<th>Activation Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>H₂ + J₃</td>
<td>2.10000E+13</td>
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</tr>
<tr>
<td>2</td>
<td>H + O₂</td>
<td>1.20000E+14</td>
<td>0.0</td>
</tr>
<tr>
<td>3</td>
<td>O + O₂</td>
<td>1.95000E+13</td>
<td>0.0</td>
</tr>
<tr>
<td>4</td>
<td>H + O₂</td>
<td>1.19000E+13</td>
<td>0.0</td>
</tr>
<tr>
<td>5</td>
<td>H₂ + J₃</td>
<td>1.50000E+13</td>
<td>0.0</td>
</tr>
<tr>
<td>6</td>
<td>H₂ + O₂</td>
<td>1.19000E+13</td>
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</tr>
<tr>
<td>7</td>
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<tr>
<td>9</td>
<td>H₂ + J₃</td>
<td>1.19000E+13</td>
<td>0.0</td>
</tr>
<tr>
<td>10</td>
<td>O + O₂</td>
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<tr>
<td>11</td>
<td>H₂ + J₃</td>
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<td>0.0</td>
</tr>
<tr>
<td>12</td>
<td>H₂ + O₂</td>
<td>1.19000E+13</td>
<td>0.0</td>
</tr>
<tr>
<td>13</td>
<td>H + O₂</td>
<td>1.19000E+13</td>
<td>0.0</td>
</tr>
</tbody>
</table>

### Integration Controls

- **Minimum Step Size**: 0.00000E+00 cm
- **Initial Step Size**: 0.00000E+00 cm
- **Maximum Step Size**: 0.00000E+00 cm
- **Maximum Relative Error**: 0.00000

### Initial Conditions

- **Time**: 0.0 sec
- **Area**: 0.00000E+05 sq cm
- **Axial Position**: 0.0 cm

### Pressure Properties

- **Temperature**: 0.0 atm
- **Velocity**: 4000.0 m/s
- **Dissociation Energy**: 1.5600E+04 J/mol
- **Mass Flow Rate**: 1.3427E+05 g/s
- **Entropy**: 2.5099 J/K
- **Mach Number**: 5.375
- **Gamma**: 1.3173

### Chemical Properties

<table>
<thead>
<tr>
<th>Species</th>
<th>Concentration (Moles/Cm³)</th>
<th>Mole Fraction</th>
<th>Reaction Number</th>
<th>Reaction Rate Conversion Rate (Moles/Cm³/Sec)</th>
<th>Rate Constant (1/sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1.31655E-06</td>
<td>2.48960E-01</td>
<td>1</td>
<td>-1.2040E-05</td>
<td>9.7200E+13</td>
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<tr>
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<td>2.20000E-01</td>
<td>2</td>
<td>1.1840E-05</td>
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<tr>
<td>O₂</td>
<td>3.25000E-06</td>
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<td>9.0000E+12</td>
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<tr>
<td>O₃</td>
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<td>1.60000E-01</td>
<td>4</td>
<td>1.2400E-05</td>
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**All Third Body Ratios are 1.0 Except the Following**

- **MN₂**: 41 = 5.00000
- **MN₂**: 51 = 5.00000
- **MN₂**: 71 = 6.00000
- **MN₂**: 101 = 1.80000
- **MN₂**: 151 = 1.80000
- **MN₂**: 171 = 1.80000
- **MN₂**: 191 = 1.80000

**Schematic Diagram**

- **Area Calculation**
  - $$A = \pi \times r^2$$
  - $$A = \pi \times (0.00000E+05)^2$$

**Reaction Rate Equations**

- $$H₂ + O₂ = H₂O + O$$
- $$O₂ + O₂ = O₃$$

**Integration Indicators**

- **Steps from Last Print**: 0
- **Average Step Size**: 0.0
- **Controlling Variable**: 0.0
- **Relative Error**: 0.0
- **Predictor Iterations**: 0
### Mixture 4: Molecular Weight 20.91269

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<th>RELATIVE ERROR</th>
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Total Energy Exchange Rate: 1.7917E+07  
Mass Fraction Sum: 1.0000000

| TIME | 4.39393E-08 SEC | AREA | 2.00000E+03 SQ CM | AXIAL POSITION | 2.00000E-02 CM |

#### Flow Properties
- Pressure: 0.95500
- Velocity: 655172.99
- Density: 1.56283E-06
- Temperature: 225K
- Mass Flow Rate: 1.9227E+05
- Mach Number: 1.3173

#### Chemical Properties
- Species Concentration: 2.21055E-06
- Mole Fraction: 2.95900E-01
- Net SPECIES Production Rate: -3.7921E-05
- Reaction Net Reaction Conversion Rate: 2.3191E-07

| TIME | 6.39481E-06 SEC | AREA | 2.00000E+03 SQ CM | AXIAL POSITION | 3.04800E+00 CM |

#### Flow Properties
- Pressure: 0.95300
- Velocity: 655172.99
- Density: 1.56283E-06
- Temperature: 225K
- Mass Flow Rate: 1.9227E+05
- Mach Number: 1.3173

#### Chemical Properties
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- Mole Fraction: 2.95900E-01
- Net SPECIES Production Rate: -3.7921E-05
- Reaction Net Reaction Conversion Rate: 2.3191E-07
### CHEMICAL PROPERTIES

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<th>SPECIES PRODUCTIION RATE (MOLE/CM**3/SEC)</th>
<th>REACTION</th>
<th>NET REACTION CONVERSION RATE (MOLE/CM**3/SEC)</th>
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### FLOW PROPERTIES

- **PRESSURE:** 1.42491
- **VELOCITY (CM/SEC):** 43502.09
- **DENSITY (GM/CM**3):** 1.5850E+04
- **TEMPERATURE:** 2400.17
- **MIXTURE VISCOSITY (CM**2/SEC):** 2.8019
- **MACH NUMBER:** 1.2776

### INTEGRATION INDICATORS

- **STEPS FROM LAST PRINT:** 16
- **AVERAGE STEP SIZE:** 0.9454E-01
- **CONTROLLING VARIABLE:** T
- **RELATIVE ERROR:** 0.9043E-05
- **PREDICTER ITERATIONS:** 0

### CHEMICAL PROPERTIES (CONT.)

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- **CONTROLLING VARIABLE:** T
- **RELATIVE ERROR:** 0.9043E-05
- **PREDICTER ITERATIONS:** 0

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87
### Chemical Properties

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<tr>
<th>SPECIES</th>
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### Flow Properties

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### Integration Indicators

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### Integration Controls

- **Minimum Step Size:** 0.10000E-05 s
- **Initial Step Size:** 0.10000E-01 s
- **Maximum Step Size:** 0.10000E+00 s
- **Maximum Relative Error:** 1.0000E-04

### Initial Conditions

- **Flow Properties:**
  - Pressure: 2.02300E+03 atm
  - Velocity: 1.49932E+04 ft/s
  - Density: 9.75977E-03 g/cm³
  - Temperature: 2.00000E+00 K
  - Mass Flow Rate: 3.13552E+02 lb/s
  - Enthalpy: 2.68889E+00 Btu/lbm
  - Mach Number: 5.03723E+00
  - Gamma: 1.33919E+00

- **Chemical Properties:**
  - **Species:**
    - H2: 0.38058E+04
    - O2: 0.51608E-01
    - H2O: 0.33058E+04
    - H: 0.33058E+04
    - OH: 0.33058E+04
    - O: 0.33058E+04
    - H2O2: 0.33058E+04
    - H2: 0.33058E+04
  - **Concentration (mol/ft³):**
    - H2: 1.38058E+04
    - O2: 0.51608E-01
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    - OH: 0.33058E+04
    - O: 0.33058E+04
    - H2O2: 0.33058E+04
    - H2: 0.33058E+04
  - **Reactivity:**
    - **Reaction:**
      - Number: 1
        - Reaction: 1
          - H2 + O2
            - Energy: 2.10000E+13
              - Activation: 0°
              - Constant: 1.00000
  - **Chemical Reactions:**
    - **Reaction:**
      - Number: 1
        - Reaction: 1
          - H2 + O2
            - Energy: 2.10000E+13
              - Activation: 0°
              - Constant: 1.00000

**ALL THIRD BODY RADIi ARE 1.0 EXCEPT THE FOLLOWING:**

- **Species:**
  - H2O: 0.33058E+04
  - H2O2: 0.33058E+04
  - OH: 0.33058E+04
  - O: 0.33058E+04
  - H2: 0.33058E+04
  - H: 0.33058E+04
  - O2: 0.51608E-01
  - H2O: 0.33058E+04

**ASSIGNED VARIABLE PROFILES:**

- **Area:**
  - Calculation from the following polynomial:
    - \( A(x) = (x^4 + 2x^3 + 1)x^3 \)

**Chemical Properties**

- **Species:**
  - **Concentration (mol/ft³):**
    - H2: 1.38058E+04
    - O2: 0.51608E-01
    - H2O: 0.33058E+04
    - H: 0.33058E+04
    - OH: 0.33058E+04
    - O: 0.33058E+04
    - H2O2: 0.33058E+04
    - H2: 0.33058E+04

**Reaction Rate:**

- **Number:**
  - 1
  - Reaction: 1
    - H2 + O2
      - Energy: 2.10000E+13
        - Activation: 0°
        - Constant: 1.00000

**Chemical Reaction:**

- **Number:**
  - 1
  - Reaction: 1
    - H2 + O2
      - Energy: 2.10000E+13
        - Activation: 0°
        - Constant: 1.00000

**Chemical Properties:**

- **Species:**
  - **Concentration (mol/ft³):**
    - H2: 1.38058E+04
    - O2: 0.51608E-01
    - H2O: 0.33058E+04
    - H: 0.33058E+04
    - OH: 0.33058E+04
    - O: 0.33058E+04
    - H2O2: 0.33058E+04
    - H2: 0.33058E+04
### Mixture Molecular Weight

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### Chemical Properties

**Species** | **Concentration (Moles/Ft³)** | **Mole Fraction** | **Net Species Production Rate (Mole/FT*3/SEC)** | **Reaction Number** | **Net Reaction Conversion Rate (Mole/FT*3/SEC)** | **Rate Constant** (CGS Units)
---|---|---|---|---|---|---
H2 | 1.3600E-04 | 0.5464 | 0.9960E-03 | 1 | 1.032E-03 | 4.04E+08 |
OH | 1.04499E-10 | 0.0134 | 2.196E-07 | 1 | 3.41E-03 | 1.0E+08 |
H2O | 0.0000E+00 | 0.0000 | 0.0000E+00 | 1 | 0.0000E+00 | 0.0000E+00 |

### Mass Fraction Sum

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### Flow Properties

**Flow Properties**

- **Pressure** (LB/FT²): 2.0230E+03
- **Velocity** (FT/SEC): 1.4932E+07
- **Density** (LB/FT³): 2.196E-03
- **Temperature** (DEG R): 2.811E+03
- **Mass Flow Rate** (LB/SEC): 0.039699-11
- **Entropy** (BTU/FT²/deg R): 1.032E-03

**Chemical Properties**

**Species** | **Concentration (Moles/Ft³)** | **Mole Fraction** | **Net Species Production Rate (Mole/FT*3/SEC)** | **Reaction Number** | **Net Reaction Conversion Rate (Mole/FT*3/SEC)** | **Rate Constant** (CGS Units)
---|---|---|---|---|---|---
H2 | 1.3600E-04 | 0.5464 | 0.9960E-03 | 1 | 1.032E-03 | 4.04E+08 |
OH | 1.04499E-10 | 0.0134 | 2.196E-07 | 1 | 3.41E-03 | 1.0E+08 |
H2O | 0.0000E+00 | 0.0000 | 0.0000E+00 | 1 | 0.0000E+00 | 0.0000E+00 |

**Flow Properties**

- **Pressure** (LB/FT²): 2.0230E+03
- **Velocity** (FT/SEC): 1.4932E+07
- **Density** (LB/FT³): 2.196E-03
- **Temperature** (DEG R): 2.811E+03
- **Mass Flow Rate** (LB/SEC): 0.039699-11
- **Entropy** (BTU/FT²/deg R): 1.032E-03

**Chemical Properties**

**Species** | **Concentration (Moles/Ft³)** | **Mole Fraction** | **Net Species Production Rate (Mole/FT*3/SEC)** | **Reaction Number** | **Net Reaction Conversion Rate (Mole/FT*3/SEC)** | **Rate Constant** (CGS Units)
---|---|---|---|---|---|---
H2 | 1.3600E-04 | 0.5464 | 0.9960E-03 | 1 | 1.032E-03 | 4.04E+08 |
OH | 1.04499E-10 | 0.0134 | 2.196E-07 | 1 | 3.41E-03 | 1.0E+08 |
H2O | 0.0000E+00 | 0.0000 | 0.0000E+00 | 1 | 0.0000E+00 | 0.0000E+00 |
** EQUILIBRIUM COMBUSTION **

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** SPECIES **

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** MIXTURE MOLECULAR WEIGHT **

| MIXTURE MOLECULAR WEIGHT | 27.96144 |

** DIL. VOLUME/LOG T **

| AT CONSTANT P | 1.00593 |

** DIL.2 VOL/LOG P **

| AT CONSTANT T | -1.0097 |
**DISTANCE-PRESSURE VERSION**

**SEVERAL CHEMICAL KINETICS PROGRAM**

**NASA LEWIS RESEARCH CENTER**

**METHANE-AIR COMBUSTION AT CONSTANT P (THE UNIMOLECULAR REACTION) CASE 9**

### Reaction Rates

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### Integration Controls

- **Minimum Step Size**: 0.10000E+00 cm
- **Initial Step Size**: 0.20000E+01 cm
- **Maximum Step Size**: 0.20000E+00 cm
- **Maximum Relative Error**: 0.00010

**Assumed Variable Profile**

The pressure is calculated from the following polynomial:

\[P = \text{constant} \times (1 + 1.2 \times 10^{-6})\]

The following species will be neglected from all error considerations:

- CO2
- OH
- H2O2
- NO2

---

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**CHEMICAL PROPERTIES**

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**MIXTURE MOLECULAR WEIGHT**

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>DERIVATIVE</th>
<th>INCREMENT</th>
<th>RELATIVE ERROR</th>
<th>DERIVATIVE</th>
<th>INCREMENT</th>
<th>RELATIVE ERROR</th>
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<td>0.0</td>
<td>0.0</td>
<td>-0.9325E+00</td>
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<tr>
<td>T</td>
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<tr>
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<tr>
<td>CH3</td>
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<tr>
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<tr>
<td>H2O</td>
<td>0.1219E+08</td>
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**TOTAL ENERGY EXCHANGE RATE**

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<th>RELATIVE ERROR</th>
<th>DERIVATIVE</th>
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<tr>
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<td>-0.2605E+01</td>
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<td>-0.0894E+07</td>
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<tr>
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TIE 2.41E-04 £ SEC AREA 1.1214E+03 SQ CM AXIAL POSITION 3.8000E+01 CM

FLOES PROPERTIES

PRESSURE 1.73000
VELOCITY 157412°62
DENSITY 3.25025E-04
TEMPERATURE 151.16
MASS FLOW RATE 5.99139E+04

CHEMICAL PROPERTIES

SPECIES CONCENTRATION (CALES/CM**3)
CH4 1.76755E+06
CH3 7.1995E+06
H 1.3955E+06
O2 1.09955E+06
H2O 5.8242E+06
CO 1.23593E+06
CO2 9.2113E+06
OH 1.29359E+06
H2 2.16627E+06
H2O2 1.91727E-07

MIXTURE MOLECULAR WEIGHT 28.03260

TGT. NET SPECIES PRODUCTION RATE (CALES/CM**3/SEC)
CH4 2.0727E+07
CH3 4.5879E+07
H 1.4031E+07
O2 1.1235E+07
H2O 5.0876E+07
CO 7.7006E+07
CO2 8.2752E+07
OH 7.9378E+07
H2 1.2106E+07
H2O2 1.9172E-07

TOTAL ENERGY EXCHANGE RATE (CAL/GM**3/SEC)
-7.9949E+20

VARIABLE DERIVATIVE RELATIVE ERROR VARIABLE DERIVATIVE RELATIVE ERROR
V 0. 0.
PHD -0.10227E-04 0.9792E+06 0. 0.
H 0. 0.
NO 0. 0.
O2 0. 0.
H2O 0. 0.
CO 0. 0.

DERIVATIVE INCENTIVE RELATIVE ERROR DERIVATIVE INCENTIVE RELATIVE ERROR
V 0. 0.
PHD -0.10227E-04 0.9792E+06 0. 0.
H 0. 0.
NO 0. 0.
O2 0. 0.
H2O 0. 0.
CO 0. 0.

RELATIVE ERRORS SUM 0.09999977

Reproduced from best available copy.
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<th>INTEGRATION INDICATORS</th>
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<tr>
<td></td>
<td>AXIAL POSITION</td>
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**SPECIES CONCENTRATION (MOLES/CM**3)**

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<th>CONCENTRATION (MOLES/CM**3)</th>
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<tbody>
<tr>
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<tr>
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<td>1.14211E-09</td>
</tr>
<tr>
<td>CH2O</td>
<td>3.98939E-09</td>
</tr>
<tr>
<td>CH2</td>
<td>9.95371E-09</td>
</tr>
<tr>
<td>H2</td>
<td>6.02836E-06</td>
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<tr>
<td>HDO</td>
<td>5.69220E-07</td>
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<tr>
<td>H2O2</td>
<td>4.90419E-09</td>
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<tr>
<td>HDO2</td>
<td>1.82114E-12</td>
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<tr>
<td>N2</td>
<td>7.93875E-06</td>
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</tbody>
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**CHEMICAL PROPERTIES**

<table>
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<tr>
<th>SPECIES</th>
<th>CONCENTRATION (MOLES/CM**3)</th>
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<td>HDO2</td>
<td>1.82114E-12</td>
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**MIXTURE MOLECULAR WEIGHT** 27.72139

**TOTAL ENERGY EXCHANGE RATE** -3.05072E+10

**VARIABLE DERIVATIVE DERIVATIVE INCREMENT RELATIVE ERROR**

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<tr>
<th>VARIABLE</th>
<th>DERIVATIVE</th>
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<th>RELATIVE ERROR</th>
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<tbody>
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<td>-0.0.049225E-06</td>
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<tr>
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**CHEMICAL PROPERTIES**

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<tr>
<th>SPECIES</th>
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<th>MOL. FRACTION</th>
<th>VET SPECIES PRODUCTION RATE (MOLES/L*SEC)</th>
<th>REACTION NUMBER</th>
<th>VET REACTION CONVERSION RATE (SEC)</th>
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**MIXTURE MOLECULAR WEIGHT**

27.4431

**TOTAL ENERGY EXCHANGE RATE (CAL/CM**3**/SEC)**

-5.19424E+10

**MIXTURE MASS FRACTION SUM**

1.00000000
TIME-AREA VERSION

GENEERAL CHEMICAL KINETICS PROGRAM

NASA LEWIS RESEARCH CENTER

METHANE-AIR COMBUSTION

(ASSIGNED AREA - TIME INTEGRATION) CASE 6

REACTION NUMBER

REACTION

CH4 + O2 → CH3 + H

REACTION RATE VARIABLES

E

A

N

1

3,00000E+14

0

0

2

1,00000E+13

0

0

3

1,50000E+15

0

0

4

1,00000E+13

0

0

5

7,50000E+10

0

0

6

5,50000E+13

0

0

7

1,00000E+13

0

0

8

1,00000E+13

0

0

9

2,50000E+13

0

0

10

2,10000E+13

0

0

11

4,20000E+11

0

0

12

1,00000E+13

0

0

13

2,00000E+13

0

0

14

7,00000E+10

0

0

15

4,00000E+11

0

0

16

1,00000E+11

0

0

17

1,00000E+12

0

0

18

1,00000E+12

0

0

19

2,00000E+13

0

0

20

1,00000E+11

0

0

21

1,00000E+11

0

0

22

1,00000E+12

0

0

23

1,00000E+12

0

0

24

6,00000E+12

0

0

25

1,10000E+12

0

0

26

1,10000E+12

0

0

27

1,50000E+18

0

0

28

2,75000E+19

0

0

29

4,75000E+13

0

0

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(CH4) = 5.00000

M(O2) = 2.00000

M(H2O) = 6.00000

M(N2) = 1.50000

INTERPOLATION CONTROLS

MINIMUM STEP SIZE 0.250000E+09 SEC

MAXIMUM STEP SIZE 0.125000E-08 SEC

INITIAL STEP SIZE 0.125000E-06 SEC

MAXIMUM RELATIVE ERROR 0.00010

ASSIGNED VARIABLE PROFILE

THE AREA IS CALCULATED BY INTERPOLATION FROM THE FOLLOWING TABLE

STATION

AXIAL DISTANCE (CH)

AREA (CM2)

1

0.0

1.00000E+03

2

5.00000E+00

1.00465E+03

3

1.00000E+01

1.02025E+03

4

1.50000E+01

1.04636E+03

5

2.00000E+01

1.07246E+03

6

2.50000E+01

1.09852E+03

7

3.00000E+01

1.12459E+03

8

3.50000E+01

1.15057E+03

9

4.00000E+01

1.17655E+03

10

4.50000E+01

1.20253E+03

11

5.00000E+01

1.22849E+03

12

5.50000E+01

1.25445E+03

13

6.00000E+01

1.28041E+03

14

6.50000E+01

1.30636E+03

15

7.00000E+01

1.33231E+03

16

7.50000E+01

1.35826E+03

THE FOLLOWING SPECIES WILL BE NEGLECTED FROM ALL ERROR CONSIDERATIONS

CO2

H

OH

H2O

HCO
**INITIAL CONDITIONS**

**FLOW PROPERTIES**

- **Pressure**: 1.73000
- **Velocity**: 157612.62
- **Density**: 3.6159E-04
- **Temperature**: 1645.00
- **Mass Flow Rate**: 5.69199E+04

**INTEGRATION INDICATORS**

- **Steps from Last Print**: 0
- **Average Step Size**: 0
- **Controlling Variable**: 
- **Relative Error**: 0
- **Predictor Iterations**: 0

**CHEMICAL PROPERTIES**

<table>
<thead>
<tr>
<th>SPECIES</th>
<th>CONCENTRATION (MOLES/CM<strong>3</strong>)</th>
<th>MOLE FRACTION</th>
<th>NET SPECIES PRODUCTION RATE (MOLES/CM**3*/SEC)</th>
<th>REACTION NUMBER</th>
<th>NET REACTION CONVERSION RATE (MOLES/CM**3*/SEC)</th>
<th>RATE CONSTANT (CGS UNITS)</th>
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**MIXTURE MOLECULAR WEIGHT**: 28.21038

**TOTAL ENERGY EXCHANGE RATE**: 4.05133E+06

**MASS FRACTION SUM**: 0.999999989
**FLOW PROPERTIES**

- **Pressure (ATM):** 1.72995
- **Velocity (CM/SEC):** 1.69078

**Chemical Properties**

- **Species:**
  - CH4: 5.35915E-07
  - CH3: 7.65772E-09
  - NO: 2.39460E-06
  - H2O: 4.19129E-10
  - CO: 5.24659E-06
  - CO2: 5.24659E-06
  - N2: 5.37957E-08
  - H2O2: 5.45223E-13

**Absorbers**

- **Species Production Rate (MOLES/CM^3/SEC):**
  - CH4: 5.0354E-07
  - NO: 2.1531E-06
  - H2O: 1.2103E-05
  - CH2O: 1.3208E-07
  - OH: 3.6287E-08

**Mass Flow Rate (GM/SEC):** 5.6915E+04

**Energy (CAL/CM^3/SEC):** 2.1540

**Mach Number:** 1.6970

**Gamma:** 1.2763

**Integration Indicators**

- **Steps from Last Print:** 51
- **Average Step Size:** 0.1241E+05
- **Controlling Variable:** CO
- **Relative Error:** 0.15667E+04
- **Predictor Iterations:** 0

**CHEMICAL PROPERTIES**

- **Species:**
  - CH4: 5.35915E-07
  - NO: 2.39460E-06
  - H2O: 4.19129E-10
  - CO: 5.24659E-06
  - CO2: 5.24659E-06
  - N2: 5.37957E-08
  - H2O2: 5.45223E-13

- **Derivative Increment Relative Error:**
  - CH4: 0.1653E-07
  - NO: 0.2349E-06
  - H2O: 0.4061E-05
  - CO: 0.8268E-04

- **Integral Increment Relative Error:**
  - CH4: 0.1653E-07
  - NO: 0.2349E-06
  - H2O: 0.4061E-05
  - CO: 0.8268E-04

**Reproduced from best available copy.**
### Chemical Properties

<table>
<thead>
<tr>
<th>Species</th>
<th>Concentration</th>
<th>Mol Fraction</th>
<th>Vol Species Production Rate</th>
<th>Reaction</th>
<th>VET Reaction Conversion Rate</th>
<th>Rate Constant</th>
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<tbody>
<tr>
<td>CH₄</td>
<td>2.7307E+03</td>
<td>1.00</td>
<td>1.8169E+03</td>
<td>1</td>
<td>6.9059E+04</td>
<td>8.2533E+02</td>
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<tr>
<td>CH₃OH</td>
<td>9.4182E+03</td>
<td>0.90</td>
<td>1.8290E+03</td>
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<td>6.2293E+03</td>
<td>1.2540E+03</td>
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<tr>
<td>N₂</td>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>1.3040E+03</td>
</tr>
</tbody>
</table>

### Flow Properties

- Pressure: 1.3753 kPa
- Temperature: 273.15 K
- Density: 4.7394e-04 kg/m³
- Mass Flow Rate: 5.29535e-04 kg/s
- Entropy: 2.189 J/kgK
- Gamma: 1.6753
- Excess Pressure: 0.0006 kg/m³

### Integration Indicators

- Steps from Last Print: 47
- Average Step Size: 0.0006 kg/m³
- Controlling Variable: PHa
- Relative Error: 0.7203e-04
- Predicted Iterations: 5

### Mixture Molecular Weight

<table>
<thead>
<tr>
<th>Variable</th>
<th>Derivative</th>
<th>Increcuent</th>
<th>Relative Error</th>
<th>Variable</th>
<th>Derivative</th>
<th>Increcuent</th>
<th>Relative Error</th>
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</thead>
<tbody>
<tr>
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### Chemical Properties

- Species: CH₄, CH₃OH, N₂
- Concentration: 2.7307e+03, 9.4182e+03, 3.4270e+03
- Mol Fraction: 1.00, 0.90, 0.0
- Vol Species Production Rate: 1.8169e+03, 1.8290e+03, 0.0
- Reaction: 1
- VET Reaction Conversion Rate: 6.9059e+04, 6.2293e+03, 1.3040e+03
- Rate Constant: 8.2533e+02, 1.2540e+03, 1.3040e+03

---

### Time: 2.1450e+04 sec

- Area: 1.2988e+03 sq cm
- Axial Position: 1.0002e+03 cm

---

### Chemical Properties

- Species: CH₄, CH₃OH, N₂
- Concentration: 2.7307e+03, 9.4182e+03, 3.4270e+03
- Mol Fraction: 1.00, 0.90, 0.0
- Vol Species Production Rate: 1.8169e+03, 1.8290e+03, 0.0
- Reaction: 1
- VET Reaction Conversion Rate: 6.9059e+04, 6.2293e+03, 1.3040e+03
- Rate Constant: 8.2533e+02, 1.2540e+03, 1.3040e+03
<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>DERIVATIVE</th>
<th>INCREMENT</th>
<th>RELATIVE ERROR</th>
<th>VARIABLE</th>
<th>DERIVATIVE</th>
<th>INCREMENT</th>
<th>RELATIVE ERROR</th>
</tr>
</thead>
<tbody>
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**Assigned Variable Profile**

The pressure is calculated by interpolation from the following table:

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<th>Pressure (atm)</th>
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The following species will be neglected from all flame considerations:

- CO
- H
- O
- H2O
- CH4
- C2H2
- C2H4
- O2
- He
- N2
- Ar

**Initial Conditions**

- Time (sec): 0
- Area: 1.00000001
- Flow Rate: 1.00000001
- Axial Position: 0

**Flow Properties**

- Pressure: 1.7670E+00 atm
- Velocity: 1.7450E+00 m/s
- Enthalpy: 3.6359E+01 kJ/kg
- Temperature: 3.6750E+00 K
- Total Energy: 1.0500E+00 kJ/kg
- Mass Flow Rate: 5.0693E+01 kg/s
- Species: H2O, CO, CH4
- Initial Volume: 7.0000E+00 m3

**Integration Indicators**

- Steps from last print: 0
- Average Step Size: 0
- Controlling Variable: 0
- Relative Error: 0
- Prediction Iterations: 0

**Minimum/Maximum Step Size**

| Minimum Step Size | 0.100000E-03 m |
| Maximum Step Size | 0.200000E+00 cm |

**Minimum/Maximum Relative Error**

| Minimum Relative Error | 0.000000 |
| Maximum Relative Error | 0.000000 |
### Chemical Properties

<table>
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<tr>
<th>Species</th>
<th>Concentration (Moles/%)</th>
<th>Mole Fraction</th>
<th>Wet Species Production Rate (Mole/%)(sec)</th>
<th>Reaction</th>
<th>Wet Reaction Conversion Rate (Mole/%)(sec)</th>
<th>Mass Constant</th>
<th>Rate Constant</th>
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</table>

### Physical Properties

- **Species Properties**
  - **Species**: CH4, CH3, H2, O2, H2O2, CO, CO2, N2
  - **Concentration (Moles/%)**: 1.37 x 10^-20, 0, 0, 2.55 x 10^-00, 2.55 x 10^-00, 0, 0, 0
  - **Mole Fraction**: 0, 0.01, 0, 0.01, 0.01, 0, 0, 0

- **Chemical Reactions**
  - **Reaction 1**: CH4 + H2O2 = CH3 + H2O2
  - **Rate Constant**: 1.98 E-05

- **Mass Constant**: 7.61 E-05

### Additional Data

- **Area**: 1.000099 E+00
- **Axial Position**: 3.310000 E+01
- **Time**: 1.010000 E+00
- **Total Energy Exchange Rate**: 0.194000 E+00
- **Mass Fraction Sum**: 0.099999

---

**Note:** The data provided is for illustrative purposes and does not represent real-world chemical properties or reactions. The values are placeholders and should not be used for scientific or educational purposes without further validation.
## Mixture Molecular Weight

### Total Energy Exchange Rate

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>DERIVATIVE</th>
<th>INCREMENT</th>
<th>RELATIVE ERROR</th>
</tr>
</thead>
<tbody>
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### Total Energy Exchange Rate

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<tr>
<th>VARIABLE</th>
<th>DERIVATIVE</th>
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</tr>
<tr>
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### Total Energy Exchange Rate

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<tr>
<td>V</td>
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<tr>
<td>O2</td>
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<tr>
<td>CH4</td>
<td>0.120</td>
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<td>0.562</td>
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<tr>
<td>H</td>
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### Total Energy Exchange Rate

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<tr>
<td>CO</td>
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### Chemical Kinetics Program

#### H2-32 Low Temperature Reaction at Constant Volume (Adjusted Rates) Case 8

#### Reaction Variables

<table>
<thead>
<tr>
<th>Reaction Number</th>
<th>Reactants</th>
<th>Products</th>
<th>Rate Constant $\dot{A} = N_Ae^\Delta H/RT$</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>H2$ + 32$</td>
<td>H$ + H2$</td>
<td>$1.00000E+14$</td>
</tr>
<tr>
<td>2</td>
<td>H2$ + OH$</td>
<td>H2$ + 3$</td>
<td>$2.10000E+13$</td>
</tr>
<tr>
<td>3</td>
<td>H$ + 32$</td>
<td>H$ + 0$</td>
<td>$1.25000E+10$</td>
</tr>
<tr>
<td>4</td>
<td>O$ + H2$</td>
<td>OH$ + H2$</td>
<td>$2.35000E+10$</td>
</tr>
<tr>
<td>5</td>
<td>H$ + H2$</td>
<td>OH$ + H2$</td>
<td>$8.35000E+10$</td>
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<tr>
<td>6</td>
<td>H$ + H2$</td>
<td>OH$ + H2$</td>
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<tr>
<td>7</td>
<td>M$ + H2$2</td>
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<td>10</td>
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<td>H$ + 0$</td>
<td>$3.10000E+10$</td>
</tr>
<tr>
<td>11</td>
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<td>12</td>
<td>O$ + H2$</td>
<td>OH$ + H2$</td>
<td>$5.70000E+10$</td>
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</tbody>
</table>

#### Integration Controls

- Minimum Step Size: $0.50000E+04$ sec
- Initial Step Size: $0.15000E+00$ sec
- Maximum Step Size: $0.10000E+00$ sec
- Maximum Relative Error: $0.0030$

#### Assigned Variable Profile

This is a vanadium problem - an assigned variable is not required.

The following species will be neglected from all error considerations:

- H
- OH
- H2

The volume (density) will be held constant for this case.

The temperature will be held constant for this case.

#### Initial Conditions

- Time: $0.0$ sec
- Flow Properties:
  - Pressure: $0.65789$ atm
  - Density: $6.44320E-05$ g/cm$^3$
  - Temperature: $773.15$ K
  - Mass Flow Rate: $0.0$
  - Entropy: $8.7684$
  - Mach Number: $0.0$
  - Gamma: $1.3810$

#### Chemical Properties

<table>
<thead>
<tr>
<th>Species</th>
<th>Mass Fraction</th>
<th>Mole Fraction</th>
<th>Net Species Production Rate</th>
<th>Reaction Number</th>
<th>Reaction Conversion Rate</th>
<th>Rate Constant</th>
<th>CGS Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>H2</td>
<td>2.79028E-01</td>
<td>8.60000E-01</td>
<td>-1.48939E-16</td>
<td>1</td>
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<tr>
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<tr>
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<td>4.93803E+08</td>
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</tbody>
</table>
The image contains a page from a scientific document, possibly related to chemical engineering, thermodynamics, or fluid dynamics. The text is technical and includes various tables and data points, such as molecular weight, exchange rates, energy terms, and chemical properties. The data is presented in a structured format, typical of scientific journals or reports. The pages also include graphical representations of integration indicators, area, and axial position measurements, among other data points.
<table>
<thead>
<tr>
<th>SPECIES</th>
<th>MASS FRACTION</th>
<th>MOLE FRACTION</th>
<th>VET SPECIES PRODUCTION RATE</th>
<th>REACTION NUMBER</th>
<th>VET REACTION CONVERSION RATE</th>
<th>RATE CONSTANT</th>
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<tr>
<td>H2</td>
<td>0.197099E-01</td>
<td>0.299721E-02</td>
<td>-1.17987E-09</td>
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<tr>
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**MIXTURE MOLECULAR WEIGHT** 6.30756
**TOTAL ENERGY EXCHANGE RATE** -1.63402E+05
**MIXTURE MOLECULAR WEIGHT** 6.30756

**MIXTURE Vapor DERIVATIVE INCREMENT RELATIVE ERROR**

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**READ DATA FOR NEXT CASE**

*01= UNITS, 02= GRID*
### Case 1

#### Reaction Number

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Reaction Rate Variables</th>
<th>Activation</th>
<th>( E_r ) (kcal/mol)</th>
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<tbody>
<tr>
<td>1</td>
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<tr>
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<td>3</td>
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<tr>
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<tr>
<td>5</td>
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<tr>
<td>6</td>
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<td>7</td>
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<tr>
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<td>( 2.2 \times 10^{42} )</td>
<td>-1.5797</td>
</tr>
</tbody>
</table>

#### Integration Controls

- Minimum Step Size: 0.020000-02 cm
- Maximum Step Size: 0.300000-04 cm
- Initial Step Size: 0.200000-02 cm
- Maximum Relative Error: 0.000000

**Initial Conditions**

- \( 1.101 = 0.000000 \)
- \( 0.131 = 0.500000 \)
- \( 0.124 = 0.900000 \)
- \( 0.000000 \)
- \( 0.000000 \)

**Flow Properties**

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<th>Property</th>
<th>Value</th>
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**Chemical Properties**

<table>
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<tr>
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**Chemical Weight**

- Molecular Weight: 28.0165
- Total Energy Exchange Rate: 7.1E+04
- Mass Fraction Sum: 1.00000000

**Integration Indicators**

- Steps from Last Print: 0
- Average Step Size: 0.0
- Controlling Variable: 0
- Relative Error: 0.0
- Prediction Iterations: 0

**Variables**

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**Relative Error**

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- \( \Delta N = 0.000000 \)
- \( \Delta O2 = 0.000000 \)
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**Mixture**

- Molecular Weight: 28.0165
- Total Energy Exchange Rate: 7.1E+04
- Mass Fraction Sum: 1.00000000
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### INTEGRATION INDICATORS

- **Steps from Last Print:** 32
- **Average Step Size:** 0.2000E-03
- **Controlling Variable:** No
- **Relative Error:** 0.1992E-05
- **Projection Iterations:** 3
- **Eliminated Species:** O2, N2

### Mixture Molecular Weight

18.64043

### Total Energy Exchange Rate

5.780776E+11

### Mass Fraction Sum

1.0000042
### MEGA(J,J) RATE OF PRODUCTION OF SPECIES I BY REACTION J

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### CHEMICAL PROPERTIES

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### INTEGRATION INDICATORS

| STEPS FROM initial TIME | AVERAGE STEP SIZE | CONTROLLING VARIABLE | RELATIVE ERROR |
|------------------------|-------------------|----------------------|----------------|----------------|
| 6                      | 0.36542E-02       | N₂O                  | 0.48714E-04    | 0              |

### CHEMICAL PROPERTIES

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</tr>
<tr>
<td>O2-</td>
<td>0.10601E-01</td>
<td>O</td>
<td>-0.33416E-03</td>
</tr>
<tr>
<td>O-</td>
<td>0.10601E-01</td>
<td>O</td>
<td>-0.33416E-03</td>
</tr>
<tr>
<td>N</td>
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<td>O</td>
<td>-0.11017E-01</td>
</tr>
<tr>
<td>O2</td>
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<td>-0.2974E-08</td>
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<tr>
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<td>O</td>
<td>0.21581E-06</td>
</tr>
<tr>
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<td>0.10601E-01</td>
<td>O</td>
<td>0.30166E-05</td>
</tr>
<tr>
<td>NO2</td>
<td>0.10601E-01</td>
<td>O</td>
<td>0.36688E-03</td>
</tr>
<tr>
<td>NO3</td>
<td>0.10601E-01</td>
<td>O</td>
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</tr>
<tr>
<td>O2-</td>
<td>0.10601E-01</td>
<td>O</td>
<td>-0.33416E-03</td>
</tr>
<tr>
<td>O-</td>
<td>0.10601E-01</td>
<td>O</td>
<td>-0.33416E-03</td>
</tr>
</tbody>
</table>

### Flow Properties

- **Pressure**: 1.72894 atm
- **Velocity**: 3951.28 m/s
- **Density**: 1.49559E+04 kg/m³
- **Temperature**: 3815.97 K
- **Mass Flow Rate**: 5.76044E+03 kg/s
- **Entropy**: 2.4937 kJ/kg-K
- **Gamma**: 1.3013

### Chemical Properties

- **Species Concentration**:
  - N: 1.54073E-09 mol/m³
  - O2: 6.56714E-07 mol/m³
  - NO: 3.70374E-07 mol/m³
  - O: 2.71558E-07 mol/m³
  - N2: 3.91337E-06 mol/m³
  - NO2: 2.9304A-11 mol/m³
  - NO3: 4.9860E-11 mol/m³
  - O: 0.10716E-01 mol/m³
  - O2: 0.10601E-01 mol/m³
  - O: 0.10601E-01 mol/m³
  - N: 0.10716E-01 mol/m³

- **Mixture Molecular Weight**: 27.08972
- **Total Energy Exchange Rate**: 1.58710E+14 kJ/kg
- **Mass Fraction Sum**: 1.00000E+00
### Rate of Production of Species i by Reaction j

<table>
<thead>
<tr>
<th>SPECIES</th>
<th>RATE OF PRODUCTION</th>
<th>REACTION</th>
<th>NET PRODUCTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>O</td>
<td>0.636E-03</td>
<td></td>
<td>-0.1692E-04</td>
</tr>
<tr>
<td>O2</td>
<td>0.579E-03</td>
<td></td>
<td>0.2680E-08</td>
</tr>
<tr>
<td>NO</td>
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<td></td>
<td>-0.1692E-04</td>
</tr>
<tr>
<td>N2</td>
<td>0.636E-03</td>
<td></td>
<td>-0.1692E-04</td>
</tr>
<tr>
<td>NO2</td>
<td>0.636E-03</td>
<td></td>
<td>-0.1692E-04</td>
</tr>
<tr>
<td>O+</td>
<td>0.636E-03</td>
<td></td>
<td>-0.1692E-04</td>
</tr>
<tr>
<td>NO+</td>
<td>0.636E-03</td>
<td></td>
<td>-0.1692E-04</td>
</tr>
<tr>
<td>E</td>
<td>0.636E-03</td>
<td></td>
<td>-0.1692E-04</td>
</tr>
<tr>
<td>O2-</td>
<td>0.636E-03</td>
<td></td>
<td>-0.1692E-04</td>
</tr>
<tr>
<td>O-</td>
<td>0.636E-03</td>
<td></td>
<td>-0.1692E-04</td>
</tr>
</tbody>
</table>

### Flow Properties

- Pressure: 1.757E3
- Temperature: 36937.72
- Density: 1.859E-04
- Mass Flow Rate: 5.760E3
- Entrainment Rate: 2.424E3
- Mach Number: 1.034E4

### Chemical Properties

#### Specie Concentration (Moles/CM^3)

- N: 1.430e-09
- O2: 9.277E-07
- NO: 3.721E-07
- N2: 9.277E-07
- NO2: 5.179E-11
- NO+: 3.794E-12
- E: 3.657E-12
- O+: 1.209E-18
- O2-: 8.338E-15
- O-: 1.337E-13

#### Reaction Net Production Rate (Molecules/CM^3/SEC)

- N: -9.650E-04
- O2: 9.037E-04
- NO: -5.099E-04
- N2: 7.024E-04
- NO2: -4.998E-04
- NO+: -7.677E-04
- E: 6.974E-04
- O+: 2.069E-04
- O2-: 1.264E-04
- O-: 1.815E-04

### Integration Indicators

- Steps from Last Print: 57
- Average Step Size: 0.1057E+00
- Controlling Variable: NO2
- Relative Error: 0.284E-06
- Predictor Iterations: 11

### Mass Fraction of Species

- N: 0.719E-4
- O2: 0.832E-6
- NO: 0.329E-14
- N2: 0.752E-08
- NO2: 0.327E-07
- O+: 0.347E-07
- O2-: 0.617E-06
- O-: 0.617E-06

### Mixture Molecular Weight

25.67907
<table>
<thead>
<tr>
<th>SPECIES</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>0.77572E-05</td>
<td>-0.27572E-05</td>
<td>0.25563E-07</td>
<td>-0.</td>
<td>0.</td>
<td>0.44575E-10</td>
<td>0.</td>
<td>0.</td>
</tr>
<tr>
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<td>0.</td>
<td>-0.43746E-05</td>
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<td>0.</td>
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<td>0.</td>
<td>-0.45513E-08</td>
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</tr>
<tr>
<td>O</td>
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<td>0.25563E-07</td>
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<td>0.</td>
<td>0.22117E-10</td>
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<td>N2O</td>
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<td>-0.27572E-05</td>
<td>0.25563E-07</td>
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<td>0.</td>
<td>0.</td>
<td>0.</td>
<td>0.</td>
</tr>
<tr>
<td>NO+</td>
<td>0.77572E-05</td>
<td>-0.27572E-05</td>
<td>0.25563E-07</td>
<td>-0.</td>
<td>0.</td>
<td>0.</td>
<td>0.</td>
<td>0.</td>
</tr>
<tr>
<td>E</td>
<td>0.43845E-15</td>
<td>0.43845E-15</td>
<td>-0.11878E-11</td>
<td>-0.</td>
<td>0.</td>
<td>0.</td>
<td>0.</td>
<td>0.</td>
</tr>
<tr>
<td>D</td>
<td>0.43845E-15</td>
<td>0.43845E-15</td>
<td>-0.11878E-11</td>
<td>-0.</td>
<td>0.</td>
<td>0.</td>
<td>0.</td>
<td>0.</td>
</tr>
</tbody>
</table>

END OF THIS CASE - READ DATA FOR NEXT CASE
APPENDIX F

AVAILABILITY OF THERMODYNAMIC AND RATE CONSTANT DATA

Thermodynamic Data

The form of the thermodynamic data equations has already been discussed under the heading Thermodynamic Data and Species Names in the section GENERAL DESCRIPTION OF PROGRAM USE. Curve fitted coefficients $A_1, A_2, \ldots, A_7$ have been calculated for 415 species by Gordon and McBride. The complete list of coefficients has been published in reference 13. Two sets of coefficients are given for each species. The first listed set was obtained for the temperature range 1000 to 5000 K. The second set was curve fitted for the temperature range 300 to 1000 K. The high-range equation can be extrapolated beyond the high temperature limit to 6000 K and the low range equation can be used down to 100 K. These coefficients will be available as part of the chemical kinetics program.

Rate Constant Data

No set of "standard" reaction rate constants can be given analogous to the sets of coefficients for thermodynamic properties of the species. Rate constant data are much less precisely known. In general, the choice of rate constant for any reaction is left to the user. For the convenience of the reader a short list of rate constant equations is presented in table V. These rate constants are not to be taken necessarily as "best" values but only as reasonable values to use in performing kinetics calculations. Additional rate constant data are found in the sample case data listed in appendix E. Further kinetics information may be found in references 22 to 28 and 30.
**TABLE V. - REACTION RATE CONSTANTS$^a$**

\[ k_j = A_j \ T^{n_j} \ \exp(-E_j/RT). \]

<table>
<thead>
<tr>
<th>Reaction number</th>
<th>Reaction</th>
<th>$A_j$</th>
<th>$n_j$</th>
<th>$E_j$, cal/mole</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$H + O_2 \rightarrow OH + O$</td>
<td>$1.25 \times 10^{14}$</td>
<td>0</td>
<td>16 300</td>
<td>29</td>
</tr>
<tr>
<td>2</td>
<td>$O + H_2 \rightarrow OH + H$</td>
<td>$2.96 \times 10^{13}$</td>
<td>-</td>
<td>9 800</td>
<td>29</td>
</tr>
<tr>
<td>3</td>
<td>$H_2 + OH \rightarrow H_2O + H$</td>
<td>$2.1 \times 10^{13}$</td>
<td>-</td>
<td>5 100</td>
<td>29</td>
</tr>
<tr>
<td>4</td>
<td>$O + H_2O \rightarrow OH + OH$</td>
<td>$5.75 \times 10^{13}$</td>
<td>-</td>
<td>18 000</td>
<td>22</td>
</tr>
<tr>
<td>5</td>
<td>$H_2 + HO_2 \rightarrow H_2O_2 + H$</td>
<td>$9.6 \times 10^{12}$</td>
<td>-</td>
<td>24 000</td>
<td>23</td>
</tr>
<tr>
<td>6</td>
<td>$H + HO_2 \rightarrow OH + OH$</td>
<td>$7.0 \times 10^{13}$</td>
<td>-</td>
<td>0</td>
<td>30</td>
</tr>
<tr>
<td>7</td>
<td>$OH + HO_2 \rightarrow H_2O + O_2$</td>
<td>$6.0 \times 10^{12}$</td>
<td>-</td>
<td>0</td>
<td>30</td>
</tr>
<tr>
<td>8</td>
<td>$O + HO_2 \rightarrow OH + O_2$</td>
<td>$6.0 \times 10^{12}$</td>
<td>-</td>
<td>0</td>
<td>30</td>
</tr>
<tr>
<td>9</td>
<td>$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$</td>
<td>$1.8 \times 10^{12}$</td>
<td>-</td>
<td>0</td>
<td>30</td>
</tr>
<tr>
<td>10</td>
<td>$H + H_2O_2 \rightarrow H_2O + OH$</td>
<td>$3.18 \times 10^{14}$</td>
<td>-</td>
<td>9 000</td>
<td>23</td>
</tr>
<tr>
<td>11</td>
<td>$OH + H_2O_2 \rightarrow H_2O + HO_2$</td>
<td>$1.0 \times 10^{13}$</td>
<td>-</td>
<td>1 800</td>
<td>23</td>
</tr>
<tr>
<td>12</td>
<td>$H + O_2 + Ar \rightarrow HO_2 + Ar$</td>
<td>$1.59 \times 10^{15}$</td>
<td>-</td>
<td>-1 000</td>
<td>23</td>
</tr>
<tr>
<td>13</td>
<td>$H_2O_2 + N_2 \rightarrow OH + OH + N_2$</td>
<td>$1.17 \times 10^{17}$</td>
<td>-</td>
<td>45 500</td>
<td>23</td>
</tr>
<tr>
<td>14</td>
<td>$H + HO_2 \rightarrow H_2 + O_2$</td>
<td>$2.3 \times 10^{13}$</td>
<td>-</td>
<td>0</td>
<td>29</td>
</tr>
<tr>
<td>15</td>
<td>$H + H + Ar \rightarrow H_2 + Ar$</td>
<td>$1.0 \times 10^{18}$</td>
<td>-1.0</td>
<td>0</td>
<td>31</td>
</tr>
<tr>
<td>16</td>
<td>$O_2 + Ar \rightarrow O + O + Ar$</td>
<td>$2.55 \times 10^{18}$</td>
<td>-1.0</td>
<td>118 700</td>
<td>32</td>
</tr>
<tr>
<td>17</td>
<td>$H + OH + Ar \rightarrow H_2O + Ar$</td>
<td>$7.5 \times 10^{23}$</td>
<td>-2.6</td>
<td>0</td>
<td>33</td>
</tr>
<tr>
<td>18</td>
<td>$CO + OH \rightarrow CO_2 + H$</td>
<td>$4.2 \times 10^{11}$</td>
<td>0</td>
<td>1 000</td>
<td>29</td>
</tr>
<tr>
<td>19</td>
<td>$CO + O_2 \rightarrow CO_2 + O$</td>
<td>$1.6 \times 10^{13}$</td>
<td>0</td>
<td>41 000</td>
<td>29</td>
</tr>
<tr>
<td>20</td>
<td>$H_2 + O_2 \rightarrow OH + OH$</td>
<td>$1.0 \times 10^{13}$</td>
<td>0</td>
<td>43 000</td>
<td>(b)</td>
</tr>
<tr>
<td>21</td>
<td>$N + O + N_2 \rightarrow NO + N_2$</td>
<td>$6.4 \times 10^{16}$</td>
<td>0.5</td>
<td>0</td>
<td>24</td>
</tr>
<tr>
<td>22</td>
<td>$N + O_2 \rightarrow NO + O$</td>
<td>$6.4 \times 10^{9}$</td>
<td>1.0</td>
<td>6 250</td>
<td>24</td>
</tr>
<tr>
<td>23</td>
<td>$O + N_2 \rightarrow NO + N$</td>
<td>$1.36 \times 10^{14}$</td>
<td>0</td>
<td>75 400</td>
<td>24</td>
</tr>
<tr>
<td>24</td>
<td>$NO_2 + O \rightarrow NO + O_2$</td>
<td>$1.0 \times 10^{13}$</td>
<td>0</td>
<td>600</td>
<td>25</td>
</tr>
<tr>
<td>25</td>
<td>$NO + O + Ar \rightarrow NO_2 + Ar$</td>
<td>$1.05 \times 10^{15}$</td>
<td>0</td>
<td>-1 870</td>
<td>25</td>
</tr>
<tr>
<td>26</td>
<td>$NO_2 + H \rightarrow NO + OH$</td>
<td>$7.2 \times 10^{14}$</td>
<td>1</td>
<td>1 930</td>
<td>30</td>
</tr>
<tr>
<td>27</td>
<td>$NO + HO_2 \rightarrow NO_2 + OH$</td>
<td>$1.0 \times 10^{13}$</td>
<td>0</td>
<td>0</td>
<td>28</td>
</tr>
</tbody>
</table>

$^a$Units of bimolecular and two-body dissociation reaction rate constants are \( \text{cm}^3 \ \text{mole}^{-1} \ \text{sec}^{-1} \). Units of three-body recombination reaction rate constants are \( \text{cm}^6 \ \text{mole}^{-2} \ \text{sec}^{-1} \).

$^b$Authors' estimate.
APPENDIX G

FORTRAN PROGRAM LISTING AND FLOW CHARTS

$1HFTC GCKP DECK

C GENERAL CHEMICAL KINETICS PROGRAM

LOGICAL NEXT,EVSTEP

REAL IVAR

COMMON/COND/DUM1(4),IVAR,Y(28),DUM2(2),NEXT
COMMON/SINT/HMIN,HINT,HPI,HMAX,AVH,EMAX,RRP,JCV,KOUNT,ERRP
COMMON/PORE/PK(28),OK(28),BK(28),E(28)
COMMON/PRIN/PRINT(50),NPRINTS,END,EVSTEP

C READ AND CONVERT INPUT, PERFORM PRE-KINETIC CALCULATIONS
CALL KINP
1 IF (NEXT) GO TO 1000

C PRINT REACTIONS, ASSIGNED VARIABLE PROFILE, INTEGRATION CONTROLS
CALL OUT1

C COMPUTE (NON-INPUT) INITIAL CONDITIONS
CALL PRED1

C PRINT ALL INITIAL CONDITIONS
CALL OUT2
IF (NEXT) GO TO 1000

C INITIAL INTEGRATION STEPS
CALL INT1
NH = 2
AVH = HINT
CALL OUT3
IF (NEXT) GO TO 1000
IF (.NOT. EVSTEP) GO TO 3

2 NH = 0
PREV = IVAR
CALL INTG
NH = NH + 1
AVH = NH
IF (NH .NE. 1) AVH = (IVAR - PREV)/FLOAT(NH)
CALL OUT3
IF (NEXT) GO TO 1000
HTOP = END - IVAR
IF (HTOP .LE. 0.) GO TO 100
IF ((HTOP-HPI) .LT. 0.) HPI = HTOP
GO TO 2

C LOCATE FIRST PRINT STATION
3 DO 4 I=1,NPRINTS
IF (PRINT(I) .GT. IVAR) GO TO 5
4 CONTINUE
C ** INTEGRATION - PRINT RESULTS AT PRINT STATIONS
DO 10 I=NS,NPRNTS
   NH = 0
   PREV = IVAR
C SET NEXT PRINT STATION
   PRNT = PRINT(I)
C INTEGRATE TO PRINT STATION
6 HTOP = PRNT - IVAR
   IF (HTOP .LE. HNPI) GO TO 7
   CALL INTG
   NH = NH + 1
   IF (NEXT) GO TO 8
   GO TO 6
C SPECIAL STEP TO PRINT STATION
7 CALL CASG (HN,QK,HTOP,RK)
   ERRN = ERROR(Y,RK,E,JCV,HTOP)
   CALL PRED
   NH = NH + 1
   8 AVH = (IVAR - PREV)/FLOAT(NH)
   CALL OUT3
   IF (NEXT) GO TO 1000
   CALL INTO
10 CONTINUE
100 WRITE (6,101)
101 FORMAT (7H0 (GCKP) ,5X,*HEND OF THIS CASE - READ DATA FOR NEXT CASE*)
   CALL PINF
   GO TO 1
1000 WRITE (6,1001)
1001 FORMAT (7H0 (GCKP) ,5X,*FATAL ERROR HAS OCCURRED - CASE TERMINATED*)
   CALL PINF
   GO TO 1
END
$1HFTC
KINPP DECK
SUBROUTINE KINP
C INPUT CAN BE ACCEPTED IN (1) INTERNAL (CGS) UNITS, (2) FPS UNITS,
C (3) SI UNITS
C THE FOLLOWING UNITS ARE USED INTERNALLY
C * DISTANCE CM *
C * AREA CM**2 *
C * MASS FLOW RATE GM/SEC *
C * PRESSURE ATM *
C * TIME SEC *
C * VELOCITY CM/SEC *
C * DENSITY GM/CC *
C * TEMPERATURE DEG K *
C * CONCENTRATION MOLE(1)/MASS *
C INTERNAL CORRESPONDENCE
C * DVAR - DEPENDENT VARIABLE *
C * IVAR - INDEPENDENT VARIABLE *

120
THE FOLLOWING LOGICAL TAPE UNITS ARE REQUIRED
* LTHM(_) FOR THERMODYNAMIC DATA *
* LDAT(7) FOR TEMPORARY STORAGE OF DATA CARDS *

LOGICAL TAPE UNIT ASSIGNMENTS ARE SPECIFIED IN 'NAMBLK'

DOUBLE PRECISION DSP,DSPP,DSPM,DALSP

LOGICAL ALIM,CONC,DBGUO,ELIM,FVSTRP,EXCHR,MOLEP,MMHG

LOGICAL COMBUS,RHOCON,SHOCK,TCON

LOGICAL NEWPRT,NEXT

REAL MDOT,IVAR,M,MW,N,LSUBM,MIXMW,M2,NEW

DIMENSION ISS(25),TBR(3),CXTB(40),CATB(40),APPRINT(50),THMC(7,2)
DIMENSION SP(2,4),DSP(4),SPP(2,3),DSPM(2,27),DSPM(27)
DIMENSION SFS(2,7),LNT(4),SBS(4),C(25),CK(4)
DIMENSION CUA(2),FUA(2),SHA(2),CUPL(1),CUPL2(25),FUL(2),SUP(2)

COMMON/LTUS/LTHM,LDAT
COMMON/OPTS/VERSI,TIMEV,VERS,AR FAY,ELIM,TCON,RHOCON,IPPCOD
COMMON/COND/DVAR,REA,MDOT,P,IVAR,V,I_HO,T,SIGMA(255),LS,LSP3,NEXT
COMMON/REAC/LSB(2,30),XX(30),RATE(30),LKEO(30),DLKEO(30),MM(30),LP
COMMON/RAT/A(30),N(30),EACT(30),B(30),M(25,30),ALLZ
COMMON/AFUN/CN(1,25),ITPSZ,LSUPH,ETA,D,VISC,HETA
COMMON/SBEC/SNAM(2,305),MW(25),W(25),STOIC(25,30),OMEGA(25,30)
COMMON/SINT/HMIN,HMAX,HINT,EMAX,ERRN,JCV,KOUNT,BRPP
COMMON/TCOF/TC(7,2,25),TL0W,TMI0D,
COMMON/PRIN/PRINT(50),NP,CEND,FVSTP
COMMON/XVSA/XTB(40),ATS(40),NT,XX,AU(2),CX3,CX2,CX1,CX0
COMMON/SNMW/DALSP(75),ALMW(75)
COMMON/KOUT/TITLE(20),UNIT,UNITO,CONC,EXCHR,DELT,STDBGUO
COMMON/GHSC/GPT(25),RBT(25),SP(25),CPR(25),DCPR(25)
COMMON/PORE/PK(28),OK(28),KE(28),EK(28)
COMMON/SKIP/NEGL(25),I1,I2,IT
COMMON/NECC/BR,MIXMW,M2,GAMMA,TCPR,R
COMMON/MISC/TP,HP,CP90,HRO,ENN,SUMN,ENNL,LLMT(15),BO(15)
COMMON/INDX/TP,HP,NS,IC1,CONV,KMAT,IMAT

EQUIVALENCE (C,SIGMA), (SPM,DSPM), (SP,DSP), (SPP,DSPP), (SPT,SP)
EQUIVALENCE (SPM,SNAM(1,4)), (EFFM,SPM(1,26)), (BLANK,SPM(1,27))

EQUIVALENCE (CUX,EX)

DATA CU,FU,SU/2HCM,2HFT,2HM/

NAMELIST/PROB/HMIN,HMAX,HINT,EMAX,ALLM,ELIM,CONC,EXCHR
* IPPCOD,ITPSZ,XTB,ATB,NTH,CK3,CK2,CK1,CK0,LSUBM,ETA,D,VISC,BETA
* END,DLRP,PRINT,ENRNTS,APPRINT,FVSTRP,CEUGO
* COMBUS,SHOCK,TCON,RHOCON

* THERMODYNAMIC DATA WILL BE INPUT FROM "UNIT"
READ (5,99) UNIT
99 FORMAT (20A4)
    IF (UNIT .NE. CARDS) GO TO 3
 98 FORMAT (3FI0.3)
    WRITE (LTHM,98) TLOW,TMID,THI
    READ (5,97) (SPT(I),I=I,2}, (LMT{I) ,SUBS(I),I=I,4)
 97 FORMAT (2A4,16X,_(A2,F3.0))
     _FND' CARD SIGNALS END OF THERMODYNAMIC DATA
    IF (SET(1) .EQ. TAPEND) GO TO 2
 96 FORMAT (5E15.8)
    WRITE (LTHM,96) ((THMC(K,I) ,K=I,7) ,I=1,2)
 95 FORMAT (A)
    GO TO I
 94 FORMAT (A)
    WRITE (LTHM,94) TAPEND
    REWIND LTHM
 93 FORMAT (A)
    CALL CIMAGE
    READ OUTPUT
    TITLE
    READ (LDAT,99) TITLE
    ACTION = NEW
    GO TO 4
 92 FORMAT (A)
    ENTRY RINP
    NEXT = .FALSE.
    CALL CIMAGE
 91 FORMAT (A)
    READ NEW OUTPUT TITLE
    READ (LDAT,99) TITLE
    C READ ACTION SWITCH
    READ (LDAT,99) ACTION
    IF (ACTION .NE. NEW) GO TO 9
 90 FORMAT (A)
    SET STANDARD OPTIONS
    CONC = .TRUE.
    EXCHR = .FALSE.
    COMBUS = .FALSE.
    SHOCK = .FALSE.
    TCON = .FALSE.
    RHOCON = .FALSE.
    ELIM = .TRUE.
    ESTEP = .FALSE.
    DEBUG = .FALSE.
    EMAX = 0.0001
    ITPSZ = 5
    ALM1 = .TRUF.
    DO 5 I=1,25
    DO 5 J=1,30
    5 M(I,J) = 1.
 89 FORMAT (A)
    INITIALIZE
    NEXT = .FALSE.
    HINT = 0.
    NLM = 0
    NS = 0
    LS = 0
    LR = 0
    NT = 0
    DO 6 I=1,40
    XTP(I) = 0.
    CXT(I) = 0.
    ATB(I) = 0.
6 CATB(I) = 0.
UNCEND = 0.
CEND = 0.
NP = 0.
DO 7 I = 1,50
7 PRINT(1) = 0.
DO 8 I = 1,25
DO J = 1,30
8 STOIC(I,J) = 0.
LSTUBM = 0.
ETA = 0.
D = 0.
VISC = 0.
BETA = 0.
CX3 = 0.
CX2 = 0.
CX1 = 0.
CX0 = 0.
GO TO 14
9 IF (ACTION .NE. CHANGE) GO TO 13
C READ REACTION AND (CHANGED) REACTION RATE
10 READ (LDAT,95) ((SP(K,I),K=1,2),I=1,4),TA,TN,TEA
95 FORMAT (2(2A4,1X),1X,2(1X,2A4),8X,F15.5,2(2X,F10.5))
C BLANK CARD SIGNALS END OF REACTION LIST
C IF (SP(1,2).EQ.BLANK) GO TO 12
C SEARCH INPUT REACTION LIST
DO 11 J = 1,LR
N1 = LSR(1,J)
N2 = LSR(2,J)
N3 = LSR(3,J)
IF (N1 .EQ. 0) N1 = 26
IF (N1 .LT. 0) N1 = 27
IF (DSPNM(N1).NE.DSP(1).OR.DSPNM(N2).NE.DSP(2).OR.DSPNM(N3).NE.DSP(3)) GO TO 11
A(J) = TA
N(J) = TN
EACT(J) = TEA
GO TO 10
11 CONTINUE
C ERROR MESSAGE - NO MATCH FOUND
WRITE (6,101) ((SP(K,I),K=1,2),I=1,4)
101 WRITE (6,101) ((SP(K,I),K=1,2),I=1,4)
C IF (ACTION .EQ. REPEAT) GO TO 33
12 READ (LDAT,99) ACTION
C READ (NEW OR ADDED) REACTION AND REACTION RATE
15 READ (LDAT,95) ((SP(K,I),K=1,2),I=1,4),TA,TN,TEA
C BLANK CARD SIGNALS END OF NEW OR ADD REACTION LIST
IF (SP(1,2).EQ.BLANK) GO TO 21
LN = LR + 1
A(LR) = TA
N(LR) = TN
EACT(LR) = TEA
DO 20 I = 1,4
IF (SP(1,I).EQ.EFFM) GO TO 19
IF (SP(1,I).EQ.BLANK) GO TO 219
IF (LS .EQ. 0) GO TO 17
18
MATCH INPUT SPECIES AGAINST INPUT SPECIES LIST
DO 16 II=1,LS
IF (DSPNM(II) .NE. DSP(I)) GO TO 16
LSR(I,LR) = II
GO TO 20
16 CONTINUE
MATCH INPUT SPECIES AGAINST MASTER SPECIES LIST
17 DO 18 II=1,75
IF (DALSP(II) .NE. DSP(I)) GO TO 18
LS = LS + 1
LSR(I,LR) = LS
SPNM(1,LS) = SP(1,I)
SPNM(2,LS) = SP(2,I)
MW(LS) = ALMW(II)
ISS(LS) = II
GO TO 20
18 CONTINUE
ERROR MESSAGE - NO MATCH FOUND
WRITE (6,102) (SP(K,I),K=1,2)
102 FORMAT (7H0(KINP),SX,5_HTHE MASTER SPECIES LIST DOES NOT CONTAIN T
*HE SPECIES ,2A4)
RUN TERMINATED - ERROR IN INPUT REACTION LIST
STOP
19 LSR(I,LR) = 0
GO TO 20
219 LSR(I,LR) = -1
20 CONTINUE
GO TO 15
21 IF (ACTION .NE. NEW) GO TO 25
READ INERT SPECIES (4 PER CARD)
22 READ (LDAT,94) ((SP(K,I),K=1,2),I=1,4)
94 FORMAT (4(2A_,8X))
DO 24 I=1,4
FLANK FIELD SIGNALS END OF INERT SPECIES LIST
IF (SP(1,I) .EQ. BLANK) GO TO 25
SEARCH MASTER SPECIES LIST
23 DO 24 II=1,75
IF (DALSP(II) .NE. DSP(I)) GO TO 23
LS = LS + 1
SPNM(1,LS) = SP(1,I)
SPNM(2,LS) = SP(2,I)
MW(LS) = ALMW(II)
ISS(LS) = II
GO TO 24
23 CONTINUE
ERROR MESSAGE - NO MATCH FOUND
WRITE (6,102) (SP(K,I),K=1,2)
NEXT = .TRUE.
LS = LS + 1
MW(LS) = 1.
24 CONTINUE
GO TO 22
25 IF (LS .EQ. LSOLD) GO TO 30

124
C GET THERMODYNAMIC COEFFICIENTS FROM TAPE
LSP = LSOLD + 1
II = LSOLD
READ (LTHM,98) TLOW,TMID,THI
26 READ (LTHM,97) (SPT(I),I=1,2)
   IF (SPT(1) .EQ. TAPEND) GO TO 29
   READ (LTHM,96) ((THMC(K,I),K=1,7),I=1,2)
   DO 28 I=LSP,LS
      IF (DSPNH(I) .NE. DSP(1)) GO TO 28
   DO 27 KK=I,2
      DO 27 K=1,7
         TC(K,KK,I) = THHC(K,KK)
      DO 28 II = II + I
      IF (II .LT. LS) GO TO 26
   GO TO 230
28 CONTINUE
GO TO 26
C ERROR MESSAGE - END OF THERMO TAPE REACHED
29 WRITE (6,103)
103 FORMAT (7H0(KINP),SX,_2HFND OF THESMO TAPE - NOT ALL SPECIES FOUND AB282
   *)
   NEXT = .TRUE.
230 REWIND LTHM
C DETERMINE STOICHIOMETRIC COEFFICIENTS
30 LRP = LRPDLD + 1
   DO 31 I=1,LS
      DO 31 J=LRP,LR
         STOC = 0.
            IF (LSR(1,J) .EQ. I) STOC = STOC - 1.
            IF (LSR(2,J) .EQ. I) STOC = STOC - 1.
            IF (LSR(3,J) .EQ. I) STOC = STOC + 1.
            IF (LSR(4,J) .EQ. I) STOC = STOC + 1.
      31 STOIC(I,J) = STOC
GET SPECIES ENTHALPY AT REFERENCE T
TREF = 298.15
CALL THERM (TREF,0.)
TRAL = TREF*1.987165
   DO 32 J=LRP,LR
      N1 = LSR(1,J)
      N2 = LSR(2,J)
      N3 = LSR(3,J)
      N4 = LSR(4,J)
      N5 = N6 = N7 = N8 = N9 = 0
      IF (N1 .GT. 0) DELH(J) = DELH(J) - HRT(N1)
      IF (N4 .GT. 0) DELH(J) = DELH(J) + HRT(N4)
      32 DELH(J) = DELH(J)*TRAL
LSP3 = LS + 3
C RESET STANDARD OPTIONS
33 MOLFF = .TRUE.
   MMHG = .FALSE.
   NEWPRT = .FALSE.
C INITIALIZE
END = 0.
DELP = 0.
NTB = 0
NPNNTS = 0
DO 34 I=I,5
34 APRINT(I) = 0.
AREA = 0.
MDOT = 0.
P = 0.
V = 0.
RHO = 0.
T = 0.
HN = 0.
ERRN = 0.
NH = 0
AV = 0.
JCV = 30
KOUNT = 0
DO 35 I=I,28
35 E(I) = 0.
IT = 0.
I2 = 0

C READ NAME OF INDEPENDENT VARIABLE, NAME OF ASSIGNED VARIABLE,
C INPUT UNITS, OUTPUT UNITS
READ (LDAT,92) VERSI, VERSA, UNITI, UNITO
92 FORMAT (4(A4,6X))
IF (VERSA .EQ. BLANK) VERSA = AR_AV
IF (ACTION .NE. NEW) GO TO 80

C INITIALIZE STEP SIZE LIMITS
IF (VERSI .EQ. TIMEV) GO TO 78
HMIN = 0.0001
HMAX = 0.1000
IPRCOD = 2
GO TO 79
78 HMIN = 0.500E-07
HMAX = 0.500E-04
IPRCOD = 4
79 IF (VFRSA .EQ. AREAV) IPRCOD = IPRCOD - 1

C READ INTEGRATION CONTROLS, PROFILE OPTIONS,
C PRINT OPTIONS, SPECIALTY SWITCHES
80 READ (LDAT,FROB)
IF (.NOT. ALLM1) GO TO 36
DO 77 I=1,25
DO 77 J=1,30
77 M(I,J) = 1.
GO TO 40

C READ THIRD BCDY RATIOS
36 READ (LDAT,91) ((SP(K,I),K=1,2),I=1,4),((SPP(K,I),K=1,2),TBR(I),
* I=1,3)
91 FORMAT (2(2A4,1X),1X,2(1X,2A4),1X,3(2A4,F6.4))
C BLANK CARD SIGNALS END OF THIRD BCDY RATIO LIST
IF (SP(1,2) .EQ. BLANK) GO TO 40
C SEARCH INPUT REACTION LIST
DO 39 J=1,LR
N1 = LSP(1,J)
N2 = LSP(2,J)
N3 = LSP(3,J)
IF (N1 .EQ. 0) N1 = 26
IF (N1 .LT. 0) N1 = 27
IF (DSPNM(N1) .NE. DSP(1) .OR. DSPNM(N2) .NE. DSP(2) .OR. DSPNM(N3) .NE. DSP(3)) GO TO 39
DO 38 I=1,3
IF (SPP(I) .EQ. Blank) GO TO 38
C SEARCH INPUT SPECIES LIST
DO 37 II=I,LS
IF (DSPNM(II) .NE. DSP(I)) GO TO 37
M(II,J) = TSR(I)
GO TO 38
37 CONTINUE
C ERROR MESSAGE - NO MATCH FOUND
WRITE (6,104) (SPP(K,I),K=1,2)
NEXT = .TRUE.
38 CONTINUE
GO TO 36
39 CONTINUE
C ERROR MESSAGE - NO MATCH FOUND
WRITE (6,104) (DSP(K,I),K=1,2)
NEXT = .TRUE.
GO TO 36
GET INITIAL CONDITIONS
40 CALL INIT (ISS,MHG,MOLEF)
C READ SPECIES TO BE NEGLLECTED FROM ERROR CONSIDERATIONS (4 PER CARD)
41 READ (LDAT,94) ((SP(K,I),K=1,2),I=1,4)
DO 43 I=1,4
C FLANK FIELD SIGNALS END OF NEGLLECTED SPECIES LIST
IF (SP(I,I) .EQ. Blank) GO TO 42
C SEARCH INPUT SPECIES LIST
DO 42 II=I,LS
IF (DSPNM(II) .NE. DSP(I)) GO TO 42
II = II + 1
NEGL(II) = II
GO TO 43
42 CONTINUE
C ERROR MESSAGE - NO MATCH FOUND
WRITE (6,104) (DSP(K,I),K=1,2)
NEXT = .TRUE.
43 CONTINUE
GO TO 41
44 IT = I1
C CHECK INPUT COMPOSITION
CSUM = 0.
DO 47 I=1,LS
C SUM = CSUM + C(I)
IF (ABS(1.-CSUM) .LT. .001) GO TO 48
WRITE (6,105) CSUM,((DSPNM(K,I),K=1,2),C(I),I=1,LS)
105 FORMAT (7H0(KINP),5X,33HINVALID INPUT COMPOSITION SUM = .F11.6//
* (12X,2A4,E20.5))
NEXT = .TRUE.
RETURN

C SET INITIAL STEP SIZE
48 HI = HINT
IF (HINT .EQ. 0.) HI = HMIN

IF (ITPSZ .GT. 2) GO TO 53
IF (ITPSZ .EQ. 1 .AND. NTB .EQ. 0) GO TO 53
COV = 1.
CON2 = 1.
IF (VERSA .NE. AREAV) GO TO 203
XU = CU
AU(1) = CUA(1)
AU(2) = CUA(2)

C CONVERT AREA PROFILE TO INTERNAL UNITS
IF (UNITI .NE. FPS) GO TO 201
XU = FU
AU(1) = FUA (1)
AU(2) = FUA(2)
CONV = 30.48
GO TO 202

201 IF (UNITI .NE. SI) GO TO 206
XU = SU
AU(1) = SUA (1)
AU(2) = SUA(2)
CONV = 100.

202 CON2 = CONV*CONV
GO TO 206

203 XU = CU
AU(1) = CUP2(1)
AU(2) = CUP2(2)

C CONVERT PRESSURE PROFILE TO INTERNAL UNITS
IF (UNITI .NE. FPS) GO TO 204
XU = FU
AU(1) = FUP (1)
AU(2) = FUP(2)
CONV = 30.48
CON2 = 1./2116.2
GO TO 205

204 IF (UNITI .NE. SI) GO TO 205
XU = SU
AU(1) = SUP (1)
AU(2) = SUP(2)
CONV = 100.
CON2 = 1./1.01325E+05

205 IF (.NOT. MMHG) GO TO 206
AU(1) = CUP1(1)
AU(2) = CUP1(2)
CON2 = 1./760.

206 IF (VERSI .EQ. TIMEV) CONV = 1
IF (ITPSZ .EQ. 2) GO TO 208
DO 207 I=1,NTB
CXTB(I) = XTB(I)*CONV
207 CXTB(I) = ATB(I)*CON2
GO TO 53
208 DO 209 I=1,4
209 \text{CN(I)} = \text{CX(I)} \times \text{CON2}

53 \text{IF ((NPRTS \ .NE. 0) .OR. (DELP .NE. 0.) .OR. (END .NE. 0.)) NEWPRT = TRUE.}
\text{IF (.NOT. NEWPRT) GO TO 59}
\text{IF (END .NE. 0.) UNCEMD = END}

54 \text{PRINT(1) = IVAR + DELP}
\text{DO 55 I=2,50}
\text{PRINT(I) = PRINT(I-1) + DELP}
\text{IF (PRINT(I) .GE. UNCEMD) GO TO 56}
\text{55 CONTINUE}

56 \text{NP = I}
\text{PRINT(NP) = UNCEMD}
\text{GO TO 59}

57 \text{NP = NPRTS}
\text{IF (APRINT(1) .EQ. 0.) GO TO 59}
\text{CONV = 1.}
\text{IF (IPRCOD .EQ. 2 .OR. IPRCOD .EQ. 4) GO TO 210}
\text{IF (UNITI .EQ. PPS) CONV = 30.48}
\text{IF (UNITI .EQ. SI) CONV = 100.}
\text{CON2 = CONV*CONV}
\text{GO TO 213}

210 \text{CON2 = 1.}
\text{IF (UNITI .NE. PPS) GO TO 211}
\text{CONV = 30.48}
\text{CON2 = 1./2116.2}
\text{GO TO 212}

211 \text{IF (UNITI .NE. SI) GO TO 212}
\text{CONV = 100.}
\text{CON2 = 1./1.01325E+05}

212 \text{IF (MMHG) CON2 = 1./760.}

213 \text{IF (VERSI .EQ. TIMEV) CONV = 1.}
\text{CALL CUBS (CATB,CXTB,NT)}
\text{DO 58 I=1,NPRTS}
\text{APRINT(I) = APRINT(I) \times CON2}
\text{CALL CINP (APRINT(I),PRINT(I),DUM1,DUM2)}
\text{58 PRINT(I) = PRINT(I)/CONV}

59 \text{IF (ITPSZ .EQ. 1) CALL CUBS (CXTB,CATB,NT)}
\text{IF (UNITI .NE. PPS) GO TO 63}
\text{CONVERT FROM PPS UNITS TO INTERNAL (CGS) UNITS}
\text{IF (VERSI .NE. TIMEV) GO TO 60}
\text{DVAR = DVAR*30.48}
\text{GO TO 61}

60 \text{IVAR = IVAR*30.48}

61 \text{IF (MMHG) P = P*2.7845}
\text{P = P/2116.2}
\text{AREA = APEA*929.0304}
\text{MDOT = MDOT*453.59237}
\text{V = V*30.48}
\text{RHO = RHO/62.43}
\text{T = T*1.8}
\text{IF (.NOT. NEWPRT) .OR. VFPSI .EQ. TIMEV) GO TO 68}
\text{CEND = UNCEMD*30.48}
\text{DO 62 I=1,NP}
62 PRINT(I) = PRINT(I)*30.48
GO TO 68
63 IF (UNITT .NE. SI) GO TO 67
C CONVERT FROM SI UNITS TO INTERNAL (CGS) UNITS
IF (VERSI .NE. TIMEV) GO TO 64
DVAR = DVAR*100.
GO TO 65
64 IVAR = IVAR*100.
65 IF (MMHG) P = P*133.3224
AREA = AREA*10000.
MDOT = MDOT*10000.
V = V*100.
RHO = RHO*.001
IF (.NOT. NEWP_T) CEND = UNCEND*100.
DO 66 I=1,NP
66 PRINT(I) = PPINT(I)*100.
GO TO 68
67 CEND = UNCEND
IF (MMHG) P = P/760.
68 MIXMW = 0.
IF (.NOT. MOLEF) GO TO 71
C MOLE FRACTION TO MOLES(I)/MASS(MIXTURE)
DO 69 I=1,LS
69 MIXMW = MIXMW + C(I)*MW(I)
DO 70 I=1,LS
70 SIGMA(I) = C(I)/MIXMW
GO TO 73
C MASS FRACTION TO MOLES(I)/MASS(MIXTURE)
71 DO 72 I=1,LS
SIGMA(I) = C(I)/MW(I)
72 MIXMW = MIXMW + SIGMA(I)
MIXMW = 1./MIXMW
C UNIVERSAL GAS CONSTANT IN ATM-CC/MOLE-DEG K
73 RR = 82.056
C UNIVERSAL GAS CONSTANT IN ERGS/MOLE-DEG K
R = 8.3143E+07
IF (M2 .EQ. 0. .AND. .NOT. (CCMBUS .OR. SHOCK)) GO TO 81
CALL TMRM (T,1.)
CPR0 = 0.
DO 74 I=1,LS
74 CPR0 = CPR0 + CPR(I)*SIGMA(I)
GAMMA = CPR0/(CPR0 - 1./MIXMW)
IF (V .NE. 0.) GO TO 81
V = SQRT(M2*R/MIXMW*GAMMA*T)
81 IF (P .EQ. 0.) GO TO 82
RHO = P*MIXMW/(RR*T)
GO TO 75
82 IF (RHO .EQ. 0.) GO TO 83
P = RHO*RR*T/MIXMW
GO TO 75
83 IF (IPRCOD .GT. 2) GO TO 84
     X = IVAR
     IF (VERSI .EQ. TIMEV) X = DVAR
     CALL CINP (X,AVAR,DUM1,DUM2)
     GO TO 85
84  TIME = DVAR
     IF (VERSI .EQ. TIMEV) TIME = IVAR
     CALL CINP (TIME,AVAR,DUM1,DUM2)
85  IF (VERSA .EQ. AREAV) GO TO 86
     P = AVAR
     GO TO 81
86  AREA = AVAR
     RH0 = MDOT/(AREA*V)
     GO TO 82
75  IF (MDOT .EQ. 0.) MDOT = RH0*ARFA*V

     IF (.NOT. (COMBUS .OR. SHOCK)) RETURN
     HR0 = 0.
     DO 76 I=1,LS
     HR0 = HR0 + HRT(I)*SIGMA(I)
     M2 = V/R*V/T*MIXKM/GAMMA
     C EQUILIBRIUM COMBUSTION
     IF (COMBUS) CALL COMB
     C EQUILIBRIUM AND FROZEN SHOCK
     IF (SHOCK) CALL SHOK
     RETURN
END
$IRFTC INITT DECK
SUBROUTINE INIT (ISS,MMHGS,MOLEFS)

C READ INITIAL CONDITIONS
LOGICAL MMHG,MOLEF,MMHGS,MOLEFS

REAL IVAR,MDOT,M2,MACH
REAL N,NF,NF2,NF3,NH2,NH3,NO,NO2,N2,N2H4,N2O,N2O4,NE,KR,NH,NOP

DIMENSION ISS(25),TINP(75)

COMMON/LTUS/LTHM,LDAT
COMMON/OPTS/VERSI,TIMEV,DUM1(6)
COMMON/COND/AREA,MDOT,P,IVAP,V,RH0,T,CONC(25),LS,DUM2(2)
COMMON/NECC/DUM3(2),M2,DUM4(3)
COMMON/FAKE/
1 AR,BF,BF2,BF3,BH,BH2,BH3,BO,BOF,BOF2,B02,B203,Br,BR2,C,CF,CF2,
2 CH,CH2,CH3,CH4,CN,CO,C02,C2F2,C2H,C2H2,C2H4,C2N,Cl,CLF,CLF3,CL2,
3 F,F2,H,HCN,HCl,HF,H02,H2,H20,H2O2,HE,N,NF,NF2,NF3,NH2,NH3,NO,NO2,
4 N2,N2H4,N2O,N2O4,NE,O,OH,O2,HR0,KR,XE,NH,HCO,CH20,NOP,OP,OM,O2M,E

EQUIVALENCE (TINP(1),AR)
NAMELIST/START/X,AREA,MDOT,P,TIME,V,RH0,T,MACH, MMHG,MOLEF,
1 AR,BF,BF2,BF3,BH,BH2,BH3,BO,BOF,BOF2,B02,B203,Br,BR2,C,CF,CF2,
2 CH,CH2,CH3,CH4,CN,CO,C02,C2F2,C2H,C2H2,C2H4,C2N,Cl,CLF,CLF3,CL2,
3 F,F2,H,HCN,HCl,HF,H02,H2,H20,H2O2,HE,N,NF,NF2,NF3,NH2,NH3,NO,NO2,
4 N2,N2H4,N2O,N2O4,NE,O,OH,O2,HR0,KR,XE,NH,HCO,CH20,NOP,OP,OM,O2M,E
\[
\begin{align*}
X &= 0, \\
\text{TIME} &= 0, \\
\text{MACH} &= 0, \\
\text{DO} &\ 1 \ \text{II}=1,75 \\
1 \ \text{TINP}(\text{II}) &= 0, \\
\text{MMHG} &= \text{MMHGS} \\
\text{MOLEF} &= \text{MOLEFS} \\
\text{READ} &\ (\text{LDAT}, \text{START}) \\
\text{MMHGS} &= \text{MMHG} \\
\text{MOLEFS} &= \text{MOLEF} \\
\text{IF} &\ (\text{VERSI} \ . \ \text{EQ.} \ \text{TIMEV}) \ \text{GO} \ \text{TO} \ 2 \\
\text{IVAR} &= \text{X} \\
\text{DVAR} &= \text{TIME} \\
\text{GO} \ \text{TO} \ 3 \\
2 \ \text{IVAR} &= \text{TIME} \\
\text{DVAR} &= \text{X} \\
3 \ \text{M2} &= \text{MACH} \times \text{MACH} \\
\text{DO} &\ 4 \ \text{II}=1,\text{LS} \\
\text{JJ} &= \text{ISS(II)} \\
4 \ \text{CONC}(\text{II}) &= \text{TINP(JJ)} \\
\text{RETURN} \\
\text{END}
\end{align*}
\]
REWIND LDAT
RETURN
END
$IEFTC NAMBLK DECK
BLOCK DATA

C ALPHANUMERIC DATA FOR TESTING AND OUTPUT
COMMON/LTUS/LTHM, LDAT
COMMON/OPTS/DUM1, TIME, DUM2, AREA, DUM3(4)
COMMON/SPEC/SNAM(2, 3), DUM(2), EFFM(2), BLANK(2), DUM5(25, 62)
COMMON/KOUT/DUM6(54), FPS, SI, DUM7

C LOGICAL TAPE UNIT ASSIGNMENTS
DATA LTHM, LDAT/4, 7/

C ALPHANUMERIC DATA
DATA TIME, AREA/4HTIME, 4HAREA/
DATA SNAM, EFFM, BLANK/IHV, IH, 3HPHO, IH, IHT, IH, 1H, 1H, 1H /
DATA FPS, SI/3HFPS, 2HSI/
END
$IEFTC BLCK DECK
BLOCK DATA

C SPECIES NAMES AND MOLECULAR WEIGHTS
COMMON/SNMW/ALSP(2, 75), ALMW(75)

DATA ALSP/
* 4HAR , 4H , 4HB , 4H , 4HBF , 4H , 4HBF2 , 4H
* 4HBF3 , 4H , 4HBFH , 4H , 4HBOF2 , 4H , 4HBO2 , 4H
* 4HCF , 4H , 4HCF2 , 4H , 4HCCH , 4H , 4HCH2 , 4H
* 4HCH3 , 4H , 4HCH4 , 4H , 4HCN , 4H , 4HCO , 4H
* 4HCO2 , 4H , 4HBF2 , 4H , 4HBH3 , 4H
* 4HBF , 4H , 4HCCF2 , 4H , 4HBP2 , 4H , 4HCH2 , 4H
* 4HCH4 , 4H , 4HCCF2 , 4H , 4HCL , 4H
* 4HCL3 , 4H , 4HCL2 , 4H , 4HFP , 4H
* 4H , 4H , 4HHCN , 4H , 4HHCCL , 4H
* 4HHO2 , 4H , 4HH2O , 4H
* 4HHE , 4H
* 4HNF3 , 4H , 4HNF2 , 4H
* 4HNO2 , 4H , 4HN2O4 , 4H
* 4H2O2 , 4H
* 4HCO , 4H
* 4H , 4H , 4HHNO , 4H
* 4HNN , 4H
* 4HFO- , 4H
* 6*0 , /

DATA ALMW/
* 39.948 , 10.811 , 29.309
* 67.806 , 11.819 , 12.827
* 26.810 , 45.807 , 64.007
* 69.620 , 79.909 , 159.02
* 31.010 , 50.008 , 13.019
* 15.035 , 16.043 , 26.018
* 44.012 , 62.019 , 25.030
* 28.054 , 38.029 , 35.453
* 92.448 , 70.406 , 18.998
* 1.00797 , 27.026 , 36.461
* 48.948
* 13.030
* 42.810
* 12.012
* 14.027
* 28.011
* 26.038
* 54.451
* 37.997
* 20.006

133
C EQUILIBRIUM COMBUSTION CALCULATIONS

DOUBLE PRECISION EN, ENLN, DELN

LOGICAL TP, HP

COMMON/COND/DVAR, AREA, MDOT, P, IVAR, V, RHO, T, SIGMA (25), LS, LSP3, NEXT
COMMON/SPEC/DUM1 (6), SPNM (2, 27), DUM2 (25, 62)
COMMON/SPECIES/EN (25), ENLN (25), DELN (25), A (15, 25)
COMMON/INDX/TP, HP, DUM3 (6)
COMMON/MISC/TT, PP, CPR0, HR0, ENN, DUM4 (32)

TP = .FALSE.
HP = .TRUE.

CALL ELEMNT (LS, SPNM, SIGMA)
ENI = 0.1/FLOAT(LS)
ENIL = ALOG (ENI)
DO 3 I=1, LS
EN (I) = ENI
ENLN (I) = ENIL
ENN = 0.1

TT = 3800.
PP = P
CALL EQLRM
CALL EQLRM

RETURN

END

$IBFTC COMBB DECK
SUBROUTINE COMB

C EQUILIBRIUM COMBUSTION CALCULATIONS

DOUBLE PRECISION EN, ENLN, DELN

LOGICAL TP, HP

COMMON/COND/DVAR, AREA, MDOT, P, IVAR, V, RHO, T, SIGMA (25), LS, LSP3, NEXT
COMMON/SPEC/DUM1 (6), SPNM (2, 27), DUM2 (25, 62)
COMMON/SPECIES/EN (25), ENLN (25), DELN (25), A (15, 25)
COMMON/INDX/TP, HP, DUM3 (6)
COMMON/MISC/TT, PP, CPR0, HR0, ENN, DUM4 (32)

TP = .FALSE.
HP = .TRUE.

CALL ELEMNT (LS, SPNM, SIGMA)
ENI = 0.1/FLOAT(LS)
ENIL = ALOG (ENI)
DO 3 I=1, LS
EN (I) = ENI
ENLN (I) = ENIL
ENN = 0.1

TT = 3800.
PP = P
CALL EQLRM
CALL EQLRM

RETURN

END

$IBFTC SHOKK DECK
SUBROUTINE SHOK

C EQUILIBRIUM AND FROZEN SHOCK CALCULATIONS

DOUBLE PRECISION EN, ENLN, DELN
DOUBLE PRECISION DLVTP, DLVPT

LOGICAL TP, HP, EOL

REAL MIXMW

COMMON/COND/DVAR, AREA, MDOT, P, IVAR, V, RHO, T, SIGMA (25), LS, LSP3, NEXT
COMMON/NECC/PP, MIXMW, M2, GAMMA, TCRP, R
COMMON/SPEC/DUM1 (6), SPNM (2, 27), DUM2 (25, 62)
COMMON/SPECIES/EN (25), ENLN (25), DELN (25), A (15, 25)
COMMON/POINTS/DLVTP, DLVPT, GMM, WM
COMMON/INDX/TP, HP, DUM3 (6),
COMMON/MISC/TT, PP, CPR0, HR0, ENN, DUM4 (32)

134
C INITIALIZE
TP = .TRUE.
HP = .FALSE.

C EQUILIBRIUM SHOCK
CALL ELEMNT (LS,SPNM,SIGHA)
GAM = GAMMA
ENI = 0.1/FLOAT(LS)
ENIL = ALOG(ENI)
DO 2 I=1,LS
EN(I) = ENI
ENLN(I) = ENIL
ENN = 0.1
EQL = .TRUE.
CALL SHOCKS (EQL)
CALL ESOUT

2 ENLN(I) = ENIL
EN(I) = ENI
END

C FROZEN SHOCK
WM = HIXMW
DLVTP = 1.D0
DLVPT = -1.D0
GAM = GAMMA
DO 3 I=1,LS
3 EN(I) = SIGMA(I)
EQL = .FALSE.
CALL SHOCKS (EQL)
CALL FSOUT

RETURN
END

$IDFTC SHCNS DECK
SUBROUTINE SHOCKS (EQL)
C SHOCK EQUATIONS
DOUBLE PRECISION A,Y,AA
DOUBLE PRECISION SIGHA,ENLN,DELN
DOUBLE PRECISION DLVTP,DLVPT
LOGICAL EQL,NEXT
REAL MIXMW,M2

DIMENSION A(2,3),Y(3)

COMMON/COND/DVAR,AREA,MDOT,P,IVAR,V,RHO,T,DUM1(25),LS,LSP3,NEXT
COMMON/NECC/R,MIXMW,M2,DUM2,TCPR,R
COMMON/GHSC/GRT(25),HRT(25),SR(25),CPR(25),DCPR(25)
COMMON/SPECES/SIGMA(25),ENLN(25),DELN(25),AAA(15,25)
COMMON/POINTS/DLVTP,DLVPT,GAMMA,WM
COMMON/MISC/TT,PP,CPR0,HR0,DUM3(33)

C INITIAL ESTIMATE OF PRESSURE AND TEMPERATURE RATIOS
P21 = (2.*GAMMA*M2 - GAMMA + 1.)/(GAMMA + 1.)
T21 = P21*(2./M2 + GAMMA - 1.)/(GAMMA + 1.)
IF (EQL .AND. T*T21 .GT. 2000.) T21 = 0.7*T21 + 600./T

CONST = MIXMW*V/R*V/T
P21L = ALOG(P21)
T21L = ALOG(T21)
ITERATE ON PRESSURE AND TEMPERATURE RATIOS

DO 4 K = 1, R
PF = P21*P
TT = T21*T
IF (FCL) CALL EOLBRM
CALL THR (TT, 1.)
IF (NEXT) GC TO 5
TCPR = 0.
THR = 0.
DO 2 I = 1, LS
TCPR = TCPR + CPR(I) * SIGMA(I)
THR = THR + HT(I) * SIGMA(I)
RHO12 = T21/P21*MMWM
AA = RHO12*CONST
A(1,1) = -AA*DLVPT - P21
A(1,2) = -AA*DLVTP
A(1,3) = P21 - 1. + CONST*(RHO12 - 1.)
AA = (V*RHO12)**2/R
A(2,1) = -AA*DLVPT + TT*(DLVTP - 1.) / WM
A(2,2) = -AA*DLVTP - TT*TCPR
A(2,3) = THR - HRO - V**2*(1. - RHO12*RHO12)/(2.*R)
Y(1) = A(1,1)*A(2,2) - A(1,2)*A(2,1)
Y(2) = (A(1,1)*A(2,3) - A(2,1)*A(1,3))/Y(3)
Y(3) = (A(1,3)*A(2,2) - A(2,3)*A(1,2))/Y(3)
Y1 = DABS(Y(1))
Y2 = DABS(Y(2))
IF (Y2 .GT. Y1) Y1 = Y2
IF (Y1 .LT. 0.5E-04) RETURN
Y1 = Y1/0.000000452
IF (Y1 .LE. 1.) GO TO 3
Y(1) = Y(1)/Y1
Y(2) = Y(2)/Y1
3 P21L = P21L + Y(1)
T21L = T21L + Y(2)
P21 = EXP(P21L)
T21 = EXP(T21L)
4 CONTINUE
5 IF (.NOT. EQL) GO TO 6
WRITE (6, 100)
100 FORMAT (9HO(SHOCKS),5X,36HEQUILIBRIUM SHOCK CALCULATION FAILED)
NEXT = .FALSE.
RETURN
6 WRITE (6, 101)
101 FORMAT (9HO(SHOCKS),5X,31HFROZEN SHOCK CALCULATION FAILED)
NEXT = .TRUE.
RETURN
END

$IEFTC ELEMENT DECK
SUBROUTINE ELEMENT (LS, DSPEC, SIGMA)

COLLECT ELEMENT DATA FOR EQUILIBRIUM SHOCK OR COMBUSTION
DOUBLE PRECISION DSPEC, DSP
DOUBLE PRECISION EN, ENLN, DELN
DIMENSION DSPEC(25), SIGMA(25), SP(2), LMT(4), SUBS(4)
COMMON/LTUS/LTHM, LDAT
COMMON/SPECIES/EN(25), EMLN(25), DELN(25), A(15,25)
COMMON/MISC/DUM1(7), LLMT(15), B0(15)
COMMON/INDEX/TP, HP, NLM, NS, IQ1, DUM2(3)

EQUIVALENCE (DSP, SP(1))

IF (LS .EQ. NS) GO TO 10

C CONSTRUCT LIST OF ELEMENTS PRESENT
READ (LTHM,99) DUMMY
NSP = NS + 1
2 READ (LTHM,99) (SP(K),K=1,2), (LMT(K),SUBS(K),K=1,4), DUMM1, DUMM2, DUMM3
DO 8 I=NSP,LS
IF (DSPEC(I) .NE. DSP) GO TO 8
DO 3 L=1,15
3 A(L,I) = 0.
IF (NLM .NE. 0) GO TO 4
NLM = 1
LLMT(NLM) = LMT(1)
4 DO 6 K=1,4
IF (SUBS(K) .EQ. 0.) GO TO 7
DO 5 L=1,NLM
IF (LLMT(L) .NE. LMT(K)) GO TO 5
A(L,I) = SUBS(K)
GO TO 6
5 CONTINUE
NLM = NLM + 1
LLMT(NLM) = LMT(K)
A(NLM,I) = SUBS(K)
6 CONTINUE
7 NS = NS + 1
IF (NS .LT. LS) GO TO 2
GO TO 9
8 CONTINUE
GO TO 2
9 REWIND LTHM

C COMPUTE ELEMENT CONCENTRATION IN GM-ATOMS/GM
10 DO 11 L=1,NLM
B0(L) = 0.
DO 11 I=1,LS
11 B0(L) = B0(L) + A(L,I)*SIGMA(I)
I01 = NLM + 1
RETURN
END

$IBFTC EQUIL DECK
SUBROUTINE E0LBRM

C CALCULATE EQUILIBRIUM COMPOSITION AND PROPERTIES
DOUBLE PRECISION G,X,SUM
DOUBLE PRECISION EN,EMLN,DELT
DOUBLE PRECISION DLVTP,DLVPT
LOGICAL CONVG,ISING,LOGV,TP,NEXT
DIMENSION P_OW (18)  
COMMON/POINTS/DLVTP,DLVPT,GAMMA,WM  
COMMON/SPCES/EN (25),ENLN(25),DELN (25),A(15,25)  
COMMON/HSC/TT,PP,CPR0,HSUB0,ENN,SUMN,ENN,LMT(15),B0 (15)  
COMMON/INDEX/TP,HP,NS,IP1,CONV,NMAT,IMAT  
COMMON/GHSC/GPT (25),HPT (25),SP (25),CPP (25),DCPP (25)  
COMMON/MATX/XT(28,28),X (28)  
COMMON/COND/DM1 (4),DM2  
COMMON/INDX/TP, HP, NL, NS, IQ1, CONV, NMAT, IMAT  
COMMON/GHSC/GPT (25), HPT (25), SP (25), CPP (25), DCPP (25)  
COMMON/COND/DM3 (35), NEXT  

C  
INITIALIZE  
SMALNO = 1.0E-06  
SMNOL = -13.815511  
SIZE = 18.5  
SIZEF = 0.  
CONVG = .FALSE.  
ISING = .FALSE.  
LOGV = .FALSE.  
ITN = 35  
ITNUMB = ITN  
TLN = ALOG (TT)  
TM = ALOG (PP/ENN)  
ENNL = ALOG (ENN)  
CALL THR (TT,1.)  
CPSUM = 0.  
DO 2 I = 1, NS  
   CPSUM = CPSUM ÷ CPR (I) * EN(I)  
2  
C BEGIN ITERATION  
43 CALL MATRIIX  
NUMB = ITN - (ITNUMB - 1)  
IQ2 = IQ1 + 1  
IF (.NOT. CONVG) GO TO 67  
IF (LOGV) GO TO 63  
DO 182 L = 1, NLN  
182 PROW(L) = G(IQ1,L)  
GO TO 72  
C  
LOGV = .TRUE. --- SET UP MATRIX TO SOLVE FOR DLVPT  
63 G (IQ1, IQ2) = ENN  
IQ = IQ1 - 1  
DO 777 I = 1, IQ  
777 G (I, IQ2) = G (I, IQ1)  
72 IMAT = IMAT - 1  
67 ITST = IMAT  
CALL GAUSS  
IF (ITST .NE. IMAT) GO TO 778  
IF (.NOT. CONVG) GO TO 85  
IF (LOGV) GO TO 171  
SUM = 0.  
DO 175 L = 1, NLN  
175 SUM = SUM ÷ PBOW(L) * X(L)  
DLVTP = 1. ÷ (G(IQ2, IQ1) - SUM) ÷ ENN - X(IQ1)  
CCPR = G (IQ2, IQ2)  
DO 176 I = 1, IQ1  
176 CCPR = CCPR - G (IQ2, I) * X(I)  
LOGV = .TRUE.  
GO TO 43  

C SINGULAR MATRIX

774 IF (.NOT. CONVG) GO TO 871
WRITE (6,172)
172 FORMAT (HO(EQLB),5X,26HDERIVATIVE MATRIX SINGULAR)
GO TO 1171
871 WRITE (6,7_)
7_ FORMAT (HO(EQLB),5X,15H SINGULAR MATRIX)
ISING = .TRUE.
DO 970 I=I,NS
IF (EN(I) .NE. 0.) GO TO 970
EN(I) = SMALLNO
ENLN(I) = SMNOL
970 CONTINUE
WRITE (6,776)
776 FORMAT HO(EQLB),7HRESTAPT)
GO TO 43

85 ITNUM = ITNUM - 1
C OBTAIN CORRECTIONS TO THE ESTIMATES
IF (TP) X(IQ2) = 0.
DLNT = X(IQ2)
SUM = X(IQ1)
DO 101 I=I,NS
DELN(I) = HRT(I) *DLNT - HPT(I) + (SP(I) - ENLN(I) - TM) + SUM
DO 99 L =I,NLM
99 DELN(I) = DELN(I) + A(L,I) *X(I)
101 CONTINUE
AMBDA = 1.
AMBDA1 = 1.
SUM = DABS(X(IQ11))
AMBD = ABS(DLNT)
SUM = AMBD
DO 917 I=I,NS
AMBD1 = AMBD
SUM = AMBD1
IF (EN(I) .GT. 0. .AND. DELN(I) .GT. SUM) SUM = DELN(I)
IF (EN(I) .NE. 0. .OR. DELN(I) .LE. 0.) GO TO 917
SUM1 = (-9.212 - ENLN(I) + ENNL)/(DELN(I) - X(IQ1))
SUM1 = ABS(SUM1)
917 CONTINUE
IF (SUM .GT. 2.) AMBD = 2. /SUM
IF (AMBDA1 .LT. AMBD) AMBD = AMBDA1

C APPLY CORRECTIONS TO ESTIMATES
SUM = 0.
DO 113 I=I,NS
ENLN(I) = ENLN(I) + AMBD*DELN(I)
EN(I) = 0.
IF (ENLN(I) .GT. ENTITY + SIZE) .LF. 0.) GO TO 113
EN(I) = EXP(ENLN(I))
SUM = SUM + EN(I)
113 CONTINUE
SUMN = SUM
IF (TP) Go To 115
TLN = TLN + AMBD*DLNT
TT = EXP(TLN)
CALL THRML (TT,1.)
CP = 0.
DO 3 I=I,NS
CP = CP + CPR(I) *EN(I)
3 CP = CP + CPR(I) *EN(I)
115 ENNL = ENNL + AMBD*K(IQ)
ENNL = EXP(ENNL)
TM = ALOG(P/P/ENN)

139
C TEST FOR CONVERGENCE
IF (ITNUMB .EQ. 0) GO TO 13
IF (AMBDA .LT. 1.) GO TO 43
SUM = (ENN - SUMN)/ENN
SUM = DABS(SUM)
IF (SUM .GT. 0.5E-05) GO TO 43
DO 130 I=I,NS
AA = ABS(DELN(I)/SUMN) * EN(I)
IF (AA .GT. 0.5E-05) GO TO 43
130 CONTINUE
13 CONVG = .TRUE.
IF (ITNUMB .NE. 0) GO TO 160
WRITE (6,973) ITN
973 FORMAT (9H0(EQUBRM),5X,I2,R2H,ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREMENTS)
GO TO 873
160 IF (.NOT. (TP .AND. CONVG)) GO TO 143
CALL THRM (TT, I.)
CPSUM = 0.
DO 4 I=1,NS
4 CPSUM = CPSUM + CPR(I)*FN(I)
143 ITNUMB = ITN
GO TO 43
C CALCULATE EQUILIBRIUM PROPERTIES
171 DLVPT = -1.
DLVTP = 1.
CCPR = CPSUM
GO TO 199
171 SUM = 0.
DO 179 L=1,NLM
179 SUM = SUM + PROW(L) *X(L)
DLVPT = -2. + SUM/ENN + X(I21)
199 GAMMA = -1./(DLVPT + DLVTP**2*ENN/CCPP)
WM = 1./ENN
DO 872 I=1,NS
872 EN(I) = EXP(ENLN(I))
RETURN
873 WRITE (6,900)
900 FORMAT (9H0(EQUBRM),5X,3H,HEQULIBRUM CALCULATIONS ABANDONED)
NEXT = .TRUE.
GO TO 171
END
$IEFTC SOUT DECK
SUBROUTINE SPOUT
C SPECIAL OUTPUT
DOUBLE PRECISION EN,ENLN,DELN
DOUBLE PRECISION DLVTP,DLVPT
LOGICAL FROZ
REAL MIXMW,M2,MACHI,MACHF,M21,LSUBM
COMMON/KORT/DUM1(21),UNITO,DUM2(32),FPS,ST,DEUGO
COMMON/COND/DVAR,AREA,MDCT,P,IVAR,V,PHO,T,SIGMA(25),LS,LSP3,NEXT
COMMON/NECC/RE,MIXMW,M2,GAMMA,TCPP,R
COMMON/GHSC/GRT(25),HRT(25),SP(25),CPR(25),DCPP(25)
COMMON/SPEC/DUM3(6),SPM=(2,27),DUM4(25,62)
COMMON/AFIN/CX3,CX2,CX1,CX0,ITPSZ,LSUPV,ETA,D,VISC,BETA
COMMON/MISC/TP,PF,CPR0,HPO,ENK,DUMS(32)
COMMON/SPECIES/EN(25),ENLN(25),DELN(25),A(15,25)
COMMON/POINTS/MLVT,MLVP,GAMMA,F,W

ENTRY ECOUT
C EQUILIBRIUM COMBUSTION OUTPUT
WRITE(6,101)
101 FORMAT (1H1,50X,30H** EQUILIBRIUM COMBUSTION **)
     VI = 0.
     GO TO 2

ENTRY ESOUT
C EQUILIBRIUM SHOCK OUTPUT
WRITE(6,102)
102 FORMAT (1H1,47X,37H** EQUILIBRIUM SHOCK CALCULATION **)
     VI = V
     PI = P
     RHOI = RHO
     TI = T
     P21 = PF/PI
     T21 = TF/TI
     RHO21 = P21/T21*RHOI/MIXMW
     FROZ = .FALSE.
     GO TO 3

ENTRY FSOUT
C FROZEN SHOCK OUTPUT
WRITE(6,103)
103 FORMAT (1H1,49X,39H** FROZEN SHOCK CALCULATION **)
     PI = P
     VI = V
     RHOI = RHO
     TI = T
     P21 = PF/PI
     T21 = TF/TI
     RHO21 = P21/T21
     P = PF
     V = VI/RHO21
     RHO = RHOI*RHO21
     T = TI*T21
     GAMMAF = TCPR/(TCPR - 1./MIXMW)
     FROZ = .TRUE.

3 CALL THERM (TI,1.)
   PMLOG = ALOG(P/MIXMW)
   S = 0.
   DO 4 I = 1,LS
      IF (SIGMA(I) .EQ. 0.) GO TO 4
      S = S + SIGMA(I)*(SR(I) - ALOG(SIGMA(I)) - PMLOG)
   CONTINUE

4 CONTINUE
   S = S*.987165
   MACHI = SORT(M2)
   VF = VI/RHO21
   RHOF = RHO*RHO21
   CALL THERM (TF,1.)
   PMLOG = ALOG(PF/MIXMW)
   SF = 0.
   DO 5 I = 1,LS
      IF (FN(I) .EQ. 0.) GO TO 5
      SF = SF + FN(I)*(SR(I) - ALOG(FN(I)) - PMLOG)
   END
5 CONTINUE
SF = SF*1.987165
MACHF = SQRT(VF/R*VF/TF*WM/GAMMAF)
S21 = SF/S
G21 = GAMMAF/GAMMAI
IF (VI .EQ. 0.) GO TO 205
SVI = VI/MACHI
SVF = VF/MACHF
V21 = VF/VI
M21 = MACHF/MACHI
SV21 = SVF/SVI
GO TO 305

205 MACHI = 0.
SVI = 0.
SVF = 0.
V21 = 0.
SV21 = 0.
GO TO 305

305 IF (.NOT. FROZ .OR. ITPSZ .NE. 4) GO TO 405
C CALCULATE L(M) FOR KINETIC AREA FUNCTION
PST = 1.
ROSVST = (GAMMAI/SVI)*1.01325E+06
LSUBM = (1./PF)*(RH021/(RH021-1.))*(ROSVST/(PS**VISC)*MACHI)**((1.-ETA)/ETA)*((D*PI)/(4.*BETA))**(1./ETA)
WRITE (6,104)

104 FORMAT (11X,13HINITIAL STATE, 17X,11HFINAL STATE, 17X,19HFINAL/INIT
*IAL RATIO//)
C CONVERT FROM INTERNAL (CGS) UNITS TO FPS UNITS
PI = PI*1.0116.2
PF = PF*1.0116.2
VI = VI/30.6
VF = VF/30.6
RH0I = RH0I/62.43
RH0F = RH0F/62.43
TI = TI*1.8
TF = TF*1.8
SVI = SVI/30.6
SVF = SVF/30.6
WRITE(6,105) PI,PF,P21,VI,VF,V21,RHOI,RHOF,RHO21,TI,TF,T21,S,SF,
* S21,MACHI,MACHF,M21,GAMMAI,GAMMAF,G21,SVI,SVF,SV21
105 FORMAT (10X,8HPRESSURE,1PE35.5,E29.5,E32.5/11X,10H(LB/FT**2)/10X,
* 8HVELOCITY,E35.5,E29.5,E32.5/11X,7HDENSITY,E36.5,
* E29.5,E32.5/11X,10H(LB/FT**3)/10X,11HTEMPERATURE,E32.5,E29.5,
* E32.5/11X,7H(FT/SEC),E36.5,E29.5,E32.5/11X,14H(BTU/ L
* E/DEG R)/10X,11HMACH NUMBER,E32.5,F29.5,E32.5//10X,5HGREMLAMMA,E34.5,
* E29.5,E32.5//10X,14HSONIC VELOCITY,E29.5,E29.5,E32.5/11X,8H(FT/SEC
*C))
GO TO 8

6 IF (UNITO .NE. FPS) GO TO 7
C CONVERT FROM INTERNAL (CGS) UNITS TO SI UNITS
PI = PI*1.01325E+05
PF = PF*1.01325E+05
VI = VI*0.01

142
VF = VF*0.01
RHOI = RHOI*10000.
RHOF = RHOF*10000.
S = S*4.1840.
SF = SF*184.0
SVI = SVI*0.01
SVF = SVF*0.01
WRITE(6,106) PI,PF,P21,VI,VF,V21,RCII,ROII,TI,TF,T21,S,SF,
S21,MACHI,MACHF,M21,GAMMAI,GAMMAF,G21,SVI,SVF,SV21
106 FORMAT (10X,SHPRESSURE,1PE35.5,E29.5,E32.5/IIX, 8H(N/M**2)/10X,8HVE
LOCITY,E35.5,E29.5, E32.5/11X,7H(M/SEC)/10X,7H(1I28).DENSITY,E36.5,E29-5,
E32.5/11X,9H(KG/M**2)/10X,7HTEMPERATURE,E2.5,E_9.5,E32.5/11X,
7H(DEG K)/10X,7HENTROPY,F36.5,E29.5,E32.5/11X,16H(JOULE/KG/DEG K)
•/10X,11HMACH NUMBER,E32.5,E28.5,E32.5//10X,5HGAMMA,E38-5,E29-5,
E32.5//10X,16HSONIC VELOCITY,E29.5,E29.5,E32.5/11X,7H(M/SEC))
GO TO 8
PRINT OUTPUT IN INTERNAL (CGS) UNITS
7 WRITE(6,107) PI,PF,P21,VI,VF,V21,RCII,ROII,TI,TF,T21,S,SF,
S21,MACHI,MACHF,M21,GAMMAI,GAMMAF, G21,SVI,SVF,SV21
107 FORMAT (10X,SHPRESSURE,F35.4,F28.a,F32._/11X,5H (ATM)/10X,SHVELOCIT
Y,F33.2,F28.2,F34.4/11X,8H (CM/S_C)/10X,7HDENSITY,1PE36-5,E28-5,
0PF32.4/IIX,10H (GM/CM*_3)/IOX, 11HTEMFERATURE,F30.2,F28.2,F34.4/
11X,7H (DEG K)/10X,THENTROPY,F36.5,F28.2,F32._/1IX,16H(CAL/GM/DEG)
•/10X,11HMACH NUMBER,F32.4,F28.4,F32.4/*10X,5HGAMMA,F38.5,E28.5,
* F32.4/*10X,14HSONIC VELOCITY,E29.5,E29.5,E32.5*/11X,8H(CM/SEC))
8 WRITE
108 FORMAT (/67X,7HSPECIES,SX,13HMO/F FRACTION)
DO 9 I=I,LS
EN(I) = EN(I)*WM
WRITE(6,1095 (SPNM(K,I) ,K=I,2),EN(I)
109 FORMAT (68X,2A_,3X,1PE12.5)
9 CONTINUE
WRITE(6,110) WM,DLVTP,DLVPT
110 FORMAT (/10X,2HLOG VOLUME)/D(LOG V),F49.4/I_X,13HAT CONSTANT P//10X,22HD(LOG VOLUME)/D
*(LOG P),F49.4/14X,13HAT CONSTANT T)
RETURN
END
$IEFTC OUTPP DECK
SUBROUTINE OUTP
C OUTPUT CAN BE GIVEN IN (1) INTERNAL (CGS) UNITS, (2) FPS UNITS
C (3) SI UNITS
LOGICAL ALLM1,CONC,DBUGO,EXCHR,NEXT,RHCON,TCON
REAL MDOT,IVAR,N,M,MW,MIXMW,M2,MACH,LSUBM
DIMENSION SPNM(2,275),PRC(25),PRX(30),XXH(30),DLEEQ(30),MM(30),LP
COMMON/AFUN/CN(_),ITPSZ,LSURM,ETA,D,VISCI,BETAL
COMMON/SPEC/SNAM (2,305),MW (25),W (25),STOIC(25,30),OMEGA(25,30)

C ** TITLE PAGE
IF (VERS_.EQ. TIMEV) GO TO 98
I = 2
GO TO 99
98 I = 4
99 IF (VERSA_.EQ. AREA) I = I - 1
GO TO (100, 200, 300, 400), I
100 WRITE (6, 101)
101 FORMAT (1H1, 14X, 21HDISTANCE-AREA VERSION)
GO TO 3
200 WRITE (6, 201)
201 FORMAT (1H1, 12X, 25H DISTANCE-PRESSURE VERSION)
GO TO 3
300 WRITE (6, 301)
301 FORMAT (1H1, 16X, 17H TIME-AREA VERSION)
GO TO 3
400 WRITE (6, 401)
401 FORMAT (1H1, 14X, 21H TIME-PRESSURE VERSION)
3 WRITE (6, 102) (TITLE(I), I = I, 20)
102 FORMAT (1H1, 49X, 26HS NASA L
* EWS RESEARCH CENTER//26X, 20A4//9X, 8HREACTION, 31X, 6HREACTION,
* 38X, 23HREACTION RATE VARIABLES/10X, 6HNUMB, 7A4, 1HACTIVATION/I19X, 6HENERGY)
C PRINT REACTION INFORMATION
DO 6 J=1, L
N1 = LSR(1, J)
N2 = LSR(2, J)
N3 = LSR(3, J)
N4 = LSR(4, J)
WRITE (6, 103) J, (SPNM(I, N2), I = I, 2), (SPNM(I, N3), I = I, 2), A(J), N(J), * EACT(J)
103 FORMAT (12X, I2, 27X, 2A4, 2X, 1H+, 2X, 2A4, 23X, 1PE12.5, 5X, 0PF10.4, 5X, *
F10.2)
IF (N1 .GT. 0) GO TO 5
IF (N1 .LT. 0) GO TO 4
N1 = 26
GO TO 205
4 WRITE (6, 105) (SPNM(I, N4), I = I, 2)
105 FORMAT (1H+, 63X, 1H+, 2X, 2A4)
GO TO 5
5 IF (N4 .GT. 0) GO TO 205
IF (N4 .LT. 0) GO TO 204
N4 = 26
GO TO 205
204 WRITE (6, 1105) (SPNM(I, N1), I = I, 2)
1105 FORMAT (1H+, 27X, 2A4, 2X, 1H+)
GO TO 6
WRITE (6,104) (SPNM(I,N1),I=1,2), (SPNM(I,N4),I=1,2)
104 FORMAT (1H+,27X,2A4,2X,1H+,25X,1H+,2X,2A4)

C CONVERT ACTIVATION ENERGY TO B-FACTOR
6 B(J) = EACT(J)/1.987165

IF (.NOT. ALLM1) GO TO 7
WRITE (6,106)
106 FORMAT (///51X,2gHALL THIRD BODY RATIOS APE 1.0)
GO TO 13

7 WRITE (6,107)
107 FORMAT (///41X,50HALL THIRD BODY RATIOS APE 1.0 EXCEPT THE FOLLOWING)
K=0
DO 12 I=1,LS
DO 12 J=1,LB
IF (M(I,J) .EQ. I.) GO TO 12
K = K + 1
IF (K .EQ. 5) K = 1
GO TO (8,9,10,11),K
8 WRITE (6,108) (SPNM(K,I),K=1,2),J,M(I,J)
108 FORMAT (SX,2HM(,2A4,1H,,I2,3H) =,F10.5)
GO TO 12
9 WRITE (6,109) (SPNM(K,I),K=1,2),J,M(I,J)
109 FORMAT (1H+,36X,2HM(,2A4,1H,,I2,3H) =,F10.5)
GO TO 12
10 WRITE (6,110) (SPNM(K,I),K=1,2),J,M(I,J)
110 FORMAT (1H+,I00X,2HM(,2A4,1H,,I2,3H) =,F10.5)
GO TO 12
11 WRITE (6,111) (SPNM(K,I),K=1,2),J,M(I,J)
111 FORMAT (1H+,I00X,2HM(,2A4,1H,,I2,3H) =,F10.5)
GO TO 12
12 CONTINUE

13 IF (VERSI .EQ. TIMEV) GO TO 14
WRITE (6,112) HMIN,HMAX,HINT,EMAX
GO TO 15
14 WRITE (6,113) HMIN,HMAX,HINT,EMAX
GO TO 15

** SECOND PAGE
15 WRITE (6,114)
114 FORMAT (1H1,50X,31H ** ASSIGNED VARIABLE PROFILE /** //)
GO TO (16,18,19,20),ITPSZ

16 GO TO (116,216,316,416),IPRCOD
C ASSIGNED VARIABLE TABLE
116 WRITE (6,117) XU,AU
117 FORMAT (34X,64H THE AREA IS CALCULATED BY INTERPOLATION FROM THE FOLLOWING TABLE//36X,7HSATION,10X,17HAXIAL DISTANCE (,A2,1H),10X
* 7HAREA (,A4,A1,1H))
GO TO 516
216 WRITE (6,217) XU,AU
217 FORMAT (32X,68H THE PRESSURE IS CALCULATED BY INTERPOLATION FROM THE FOLLOWING TABLE//36X,7HSTATION,10X,17HAXIAL DISTANCE (,A2,1H),
* 9X,11HPRESSURE (,2A4,1H))
GO TO 516
WRITE (6,317) AU
317 FORMAT (34X,64HTHE AREA IS CALCULATED BY INTERPOLATION FROM THE PO AM144
HOLLOW TABLE//36X,7STATION,14X,11TIME (SEC),16X,7AREA ("A", AM145
* A1,1H)) AM146
GO TO 516 AM147
416 WRITE (6,417) AU AM148
417 FORMAT (32X,6HTHE PRESSURE IS CALCULATED BY INTERPOLATION FROM TH AM149
* FOLLOWING TABLE//36X,7STATION,14X,11TIME (SEC),15X,11PRESSUR AM150
* E (,2A4,1H)) AM151
516 DO 17 I=1,NTB AM152
17 WRITE (6,616) I,XTB(I),ATB(I) AM153
616 FORMAT (38X,I2,14X, IPEI2°5,15X,E12.5) AM154
GO TO 21 AM155
18 GO TO (218,318,418,518),IPRCOD AM156
C ASSIGNED VARIABLE POLYNOMIAL AM158
218 WRITE (6,219) AU,CX AM159
219 FORMAT (40X,52HTHE AREA IS CALCULATED FROM THE FOLLOWING POLYNOMIA AM160
*L//23X,6AREA (,A4,A1,5H) = (,1PE12.5,9H)X**3 + (,E12.5,9H)X**2 + AM161
*E(,E12.5,6H)X + (,E12.5,1H)) AM162
GO TO 21 AM163
318 WRITE (6,319) AU,CX AM164
319 FORMAT (38X,56HTHE PRESSURE IS CALCULATED FROM THE FOLLOWING POLYN AM165
*OMIAL//20X,10PRESSURE (,2A4,5H) = (,1PE12.5,9H)X**3 + (,E12.5,9H) AM166
*X**2 + (,E12.5,6H)X + (,E12.5,1H)) AM167
GO TO 21 AM168
418 WRITE (6,419) AU,CX AM169
419 FORMAT (40X,52HTHE AREA IS CALCULATED FROM THE FOLLOWING POLYNOMIA AM170
*L//23X,6AREA (,A4,A1,5H) = (,1PE12.5,9H)T**3 + (,E12.5,9H)T**2 + AM171
*E(,E12.5,6H)T + (,E12.5,1H)) AM172
GO TO 21 AM173
518 WRITE (6,519) AU,CX AM174
519 FORMAT (38X,56HTHE PRESSURE IS CALCULATED FROM THE FOLLOWING POLYN AM175
*OMIAL//20X,10PRESSURE (,2A4,5H) = (,1PE12.5,9H)T**3 + (,E12.5,9H) AM176
*T**2 + (,E12.5,6H)T + (,E12.5,1H)) AM177
GO TO 21 AM178
C SPECIAL AREA FUNCTION AM180
19 WRITE (6,118) LSUBM,ETA AM181
118 FORMAT (41X,50HTHE AREA IS CALCULATED FROM THE FOLLOWING FUNCTION/ AM182
';//46X,16H1/AREA = 1 - (X/,F10.3,4H)**((,F10.5,1H)) AM183
IF (ITPSZ .EQ. 4) WRITE (6,1118) D,VISC,BETAL AM184
1118 FORMAT (/6X,20HHYDRAULIC DIAMETER =,FR_4,3H CM,7X,23HVISCOSITY COE AM185
*EFFICIENT = ,E12.4,10H GM/CM-SEC,7X,6HRETA = ,F7.4) AM186
GO TO 21 AM187
C ZERO VELOCITY - ASSIGNED VARIABLE NOT REQUIRED AM189
20 WRITE (6,119) AM190
119 FORMAT (36X,60HTHIS IS A V=0 PROBLEM - AN ASSIGNED VARIABLE IS NOT AM191
* REQUIRED) AM192
C NEGLECTED SPECIES AM194
21 IF (I1 .NE. 0) GO TO 22 AM195
WRITE (6,120) AM196
120 FORMAT (///31X,70HO SPECIES WILL BE PERMANENTLY NEGLFCTED FROM AL AM197
*1 ERROR CONSIDERATIONS) AM198
GO TO 228 AM199
22 WRITE (6,121) AM200
121 FORMAT (///31X,69HTHE FOLLOWING SPECIES WILL BE NEGLFCTED FROM ALL AM201
* ERROR CONSIDERATIONS/)) AM202
K = 0 AM203
DO 28 II=1,II AM204

146
\[ I = \text{NEGL(II)} \]
\[ K = K + 1 \]
\[ \text{IF } (K \leq 6) K = 1 \]
\[ \text{GO TO } (23,24,25,26,27), K \]
\[ 23 \text{ WRITE } (5,122) (\text{SPNM}(J,I),J=1,2) \]
\[ 122 \text{ FORMAT (6IX,2A4) } \]
\[ 24 \text{ WRITE } (6,123) (\text{SPNM}(J,I),J=1,2) \]
\[ 123 \text{ FORMAT (11H+,76X,2A4) } \]
\[ 25 \text{ WRITE } (6,124) (\text{SPNM}(J,I),J=1,2) \]
\[ 124 \text{ FORMAT (11H+,44X,2A4) } \]
\[ 28 \text{ CONTINUE } \]
\[ 228 \text{ IF (RHOCON) WRITE (6,1126) } \]
\[ 1126 \text{ FORMAT (//3R,56HE, THE VOLUME (DENSITY) WILL BE HELD CONSTANT FOR THIS CASE) } \]
\[ \text{IF (TCON) WRITE (6,2126) } \]
\[ 2126 \text{ FORMAT (//40X,51HE, THE TEMPERATURE WILL BE HELD CONSTANT FOR THIS CASE) } \]
\[ \text{return} \]
\[ \text{ENTRY OUT2} \]
\[ \text{C INITIAL CONDITIONS} \]
\[ \text{WRITE (6,127)} \]
\[ 127 \text{ FORMAT (11H1,52X,26H** INITIAL CONDITIONS **/)} \]
\[ \text{GO TO 29} \]
\[ \text{ENTRY OUT3} \]
\[ \text{C GENERAL OUTPUT} \]
\[ \text{WRITE (6,128)} \]
\[ 128 \text{ FORMAT (11H1)} \]
\[ 29 \text{ MACH = SQRT(M2)} \]
\[ \text{MAX = MAX0(LS,LD)} \]
\[ \text{TENT = 0.} \]
\[ \text{CSUM = 0.} \]
\[ \text{PMLOG = ALOG(P*MIX*MW)} \]
\[ \text{C TOTAL ENTRPY AND MASS FRACTION SUM} \]
\[ \text{DO 30 I = 1,LS} \]
\[ \text{IF (SIGMA(I) \leq 0.) GO TO 30} \]
\[ \text{TENT = TENT + SIGMA(I)*(Sl(I) - ALOG(SIGMA(I)) - PMLOG)} \]
\[ 30 \text{ CSUM = CSUM + SIGMA(I)*MW(I)} \]
\[ \text{TENT = TENT*1.987165} \]
\[ \text{TXXH = 0.} \]
\[ \text{C ENERGY EXCHANGE RATES} \]
\[ \text{DO 31 J = 1,LD} \]
\[ \text{XXH(J) = XX(J)*DELH(J)} \]
\[ 31 \text{ TXXH = TXXH + XXH(J)} \]
\[ \text{IF (VERSI .EC. TIMEV) GO TO 32} \]
\[ \text{TIME = DVAR} \]
\[ X = IVAR \]
\[ \text{GO TO 33} \]
TIME = IVAR
X = DVAR

IF (UNITO .NE. FPS) GO TO 48

C CONV FROM INTERNAL (CGS) UNITS TO FPS UNITS
X = X/30.48
AREA = AREA/929.0304
DOTM = MDOT/453.59237
PP = P * 2116.2
VV = V / 30.48
RHO = RHO * 62.43
TT = T * 1.8

WRITE (6, 129) TIME, AREA, X, PP, NH, VV, AVH, RHO, (SNAM(I,JCV), I=1,2), * TT, DOTM, TENT, ERRN, MACH, COUNT, GAMMA

129 FORMAT (16X, 4HTIME, 1PE14.5, SH SEC, 14X, 4HAREA, EI4.5, 7H SQ FT, 14X, 14HAXIAL POSITION, E1_.5, 4H FT, //20X, 15HFLOW PROPERTIES, 45X, AM285
* 22HINTEGRATION INDICATORS //22X, RHPRESSURE, E22.5, 30X, 21HSTEPS FR AM287
* ON LAST PRINT, 9X, 24/23X, 10H (LB/FT**2) / 22X, 8HVELocity, E22.5, 30X, AM288
* 17H AVERAGE STEP SIZE, 0PE24.5/23X, 8H (FT/SEC) / 22X, 7HDENSITY, 1PE23.5 AM289
* 30X, 20H CONTROLLING VARIABLE, 11X, 2A4/23X, 10H (LB/FT**3) / 22X, 11HTEMP AM290
* SEC) / 22X, 7H TENTROPY, E23.5, 30X, 14H RELATIVE ERROR, 0PE27.5/23X, 14H (BTU AM292
* /LB/DEG R) /22X, 11H MACH NUMBER, 1PE19.5, 30X, 20H PREDICTOR ITERATIONS, AM293
* 11X, 22X, 5HGAMMA, E25.5) AM294

IF (I2 .EQ. 0) GO TO 34
IS = II + 1
DO 233 K = IS, IT
KK = NEGL(K)
ESP(1, K) = SPNM(1, KK)
ESP(2, K) = SPNM(2, KK)
WRITE (6, 130) ((ESP(I, K), I=1,2), K=IS, IT)

233 FORMAT (1H+, 81X, 18HELIMINATED SPECIES, 13X, 2A4, 2X, 2A4 / (II3X, 2A4, 2X, AM295
* 2A4)) AM296

34 WRITE (6, 131)

131 FORMAT (//56X, 19H CHEMICAL PROPERTIES//)

CONV = 0.02883
IF (CONC .OR. EXCHR) GO TO 36

C PRINT MASS FRACTIONS AND REACTION CONVERSION PATFS
WRITE (6, 132)

132 FORMAT (1X, 7HSPECIES, 4X, 13HM MASS FRACTION, 3X, 13H MOLE FRACTION, 3X, AM312
* 27H NET SPECIES PRODUCTION RATE, 5X, 8H REACTION, 3X, 28H NET REACTION C AM313
* ONVERSION RATE, 3X, 13HRATE CONSTANT)

WRITE (6, 133)

133 FORMAT (50X, 16H(MOLE/FT**3/SEC), 11X, 6H NUMBER, 7X, 22H(MOLE-FT**3/LP AM318
**2/SEC), 7X, 11H (CGS UNITS)) AM313

35 PRX(J) = XX(J)

CONV = 1.6243

GO TO 37

36 IF (CCNC .OR. (.NOT. EXCHR)) GO TO 39

C PRINT MASS FRACTIONS AND ENERGY EXCHANGE PATES
WRITE (6, 134)
134 FORMAT (1X,7HSPECIES,4X,13HMmass fraction,3X,13HMmole fraction,3X, AM329
* 27hnet species production rate,5X,8hreaction,5X,24hnet energy exc AM330
* hange rate,5X,13hrate constant) AM331
WRITE (6,135) AM332
135 FORMAT (50X,16H(MOLES/FT**3/SEC),11X,6HNUMBEP,17X,21H(BTU-FT**3/LB** AM333
*2/SEC),7X,11H(CG5 UNITS)) AM334
C AM335
COMPUTE MASS FRACTIONS AM336
37 DO 38 I=I,LS AM337
38 PRC(I) = SIGMA(I)*MW(I) AM338
GO TO 44 AM339
39 IF (.NOT. CONC) .OR. EXCHR) GO TO _I AM340
PRINT MOLAR CONCENTRATIONS AND REACTION CONVERSION PATES AM341
WRITE (6,136) AM342
136 FORMAT (1X,7HSPECIES,13HCONCENTRATION,3X,13HMmole fraction,3X, AM343
* 27hnet species production rate,5X,8hreaction,5X,24hnet reaction constant AM344
* mversion rate,3X,13hrate constant) AM345
WRITE (6,137) AM346
137 FORMAT (12X,13H(MOLES/FT**3),25X,16H(MOLE/FT**3/SEC),11X,6HNUMBE, AM347
* 7X,22H(MOLE-FT**3/LB**2/SEC),7X,11H(CG5 UNITS)) AM348
DO 40 J=I,LR AM349
40 PRX(J) = XX(J) AM350
CONV = I./62.43 AM351
GO TO 42 AM352
41 IF (.NOT. CONC) .OR. EXCHR) GO TO 43 AM353
PRINT MOLAR CONCENTRATIONS AND ENERGY EXCHANGE FATES AM354
WRITE (6,138) AM355
138 FORMAT (1X,7HSPECIES,4X,13HCOncentration,3X,13HMmole fraction,3X, AM356
* 27hnet species production rate,5X,8hreactio,5X,24hnet energy exc AM357
* hange rate,5X,13hrate constant) AM358
WRITE (6,139) AM359
139 FORMAT (12X,13H(MOLES/FT**3),25X,16H(MOLE/FT**3/SEC),11X,6HNUMBEP, AM360
* 8X,21H(BTU-FT**3/LB**2/SEC),7X,11H(CG5 UNITS)) AM361
DO 43 I=I,LS AM362
43 PRC(I) = SIGMA(I)*RHOO AM363
44 DO 47 IJ=I,MAX AM364
IF (IJ .GT. LS) GO TO 45 AM365
FMOL = SIGMA(IJ)*MIXMW AM366
WW = W(IJ)*62.43 AM367
XXX = PRX(IJ)*CONV AM368
WRITE (6,140) (SPN(I,IJ),I=I,2),P(IJ),FMOL,WW,XXX,IJ,GO TO 47 AM369
45 IF (IJ .GT. LS) GO TO 46 AM370
FMOL = SIGMA(IJ)*MIXMW AM371
WW = W(IJ)*62.43 AM372
WRITE (6,141) (SPN(I,IJ),I=I,2),P(IJ),FMOL,WW AM373
* E12.5) AM375
GO TO 47 AM376
46 XXX = PRX(IJ)*CONV AM377
WRITE (6,142) IJ,XXX,GO TO 47 AM378
142 FORMAT (79X,I2,14X,1PE12.5,11X,E12.5) AM379
47 CONTINUE AM380
TXXH = TXXH*0.02883 AM381
WRITE (6,143) MIXMW,TXXH,CSUM AM382
143
143 FORMAT (/X,24HMOLECULAR WEIGHT,FI3.5,5X,26HTOTAL ENERGY AM390
*EXCHANGE RATE,1PE15.5,7X,17HMASS FRACTION SUM,0PF14.8 AM391
WRITE (6,144) AM392
144 FORMAT (49X,21H(STU-FT**3/LB**2/SEC)) AM393
GO TO 78 AM394
48 IF (UNITO .NE. SI) GO TO 63 AM395
CONVERT FROM INTERNAL (CGS) UNITS TO SI UNITS AM396
X = X*.01 AM397
AREA = AREA*.0001 AM398
DOTM = MDOT*.0001 AM399
VV = V*.01 AM400
RHO = RHO*1000. AM401
TENT = TENT*4184.0 AM402
WRITE (6,145) TIME, AREA, X, PP, AV, AVH, RHO, (SNAM(I,JCV),I=I,2), AM403
* T, DOTM, TENT, ERRN, MACH, KOUNT, GAMMA AM404
145 FORMAT (16X,4HTIME, IPE1_.5, SH SEC, 14X, 4HAREA, E14.5, 7H SQ M, AM405
* 14X, 14AXIAL POSITION, E14.5, 4H M /// 20X, 15H FLOW PROPERTIES, 45X, AM406
* 22H INTEGRATION INDICATORS/22X, 8HPRESSURE, E22.5, 30X, 21H STEPS PR AM407
* ON LAST PRINT, 9X, I4/23X, 8H (N/M**2)/22X, 8H VELOCITY, E22.5, 30X, 17HAVE AM408
* RAGE STEP SIZE, 0PE24.5/23X, 7H (M/SEC)/22X, 7HDENSITY, 1PE23.5, 30X, AM409
* 20H CONTROLLING VARIABLE, 11X, 244/23X, 9H (KG/M**3)/22X, 11HTEMPERATURE AM410
* E, E19.5/23X, 7H (DEG K)/22X, 14HM ASS FLOW RATE, E16.5/23X, 8H (KG/SEC)/ AM411
* 22X, 14H ENTHALPY, E23.5, 30X, 14H RELATIVE ERROR, 0PE27.5/23X, 16H (JOULF/K AM412
* G/DEG K)/22X, 11HMACH NUMBER, 1PE19.5, 30X, 20H PREDICTOR ITERATIONS, AM413
* 11X, 13/22X, 5HGAMMA, E25.5) AM414
IF (I2 .EQ. 0) GO TO 49 AM415
IS = I1 + 1 AM416
DO 248 K=IS, IT AM417
KK = NEGL(K) AM418
ESP(I,K) = SPNM(1,KK) AM419
ESP(2,K) = SPNM(2,KK) AM420
WRITE (6,130) ((ESP(I,R),I=I,2),K=IS, IT) AM421
49 WRITE (6,131) AM422
CONV = 4.180 AM423
IF (CONC .OR. (.NOT. FXCHR)) GO TO 51 AM424
C PRINT MASS FRACTIONS AND REACTION CONVERSION RATES AM425
WRITE (6,132) AM426
WRITE (6,146) AM427
146 FORMAT (50X, 15H (MOLE/M**3/SEC), 12X, 6H NUMBER, 7X, 21H (MOLE-M**3/KG**2 AM428
*/SEC), 8X, 11H (CGS UNITS)) AM429
DO 50 J=1, LR AM430
50 PRX(J) = XX(J) AM431
CONV = 0.001 AM432
GO TO 52 AM433
51 IF (CONC .OR. (.NOT. FXCHR)) GO TO 54 AM434
C PRINT MASS FRACTIONS AND ENERGY EXCHANGE RATES AM435
WRITE (6,134) AM436
WRITE (6,147) AM437
147 FORMAT (50X,15H (MOLE/M**3/SEC), 12X, 6H NUMBER, 7X, 22H (JOULF-M**3/KG** AM438
*2/SEC), 7X, 11H (CGS UNITS)) AM439
. . . AM440
150
C COMPUTE MASS FRACIONS
52 DO 53 I=1,LS
53 PRC(I) = SIGMA(I)*MW(I)
   GO TO 59
54 IF ((.NOT. CONC) .OR. EXCHR) GO TO 56
C PRINT MOLAR CONCENTRATIONS AND REACTION CONVERSION RATES
WRITE (6,136)
WRITE (6,148)
148 FORMAT (12X,12H(MOLES/M**3),26X,15H(MOLE/M**3/SEC),12X,6HNUMBER,7X *
*21H(MOLE-M**3/KG**2/SEC),8X,11H(CGS UNITS))
   DO 55 J=I,LN
55 PRX(J) = XX(J)
   CONV = 0.001
   GO TO 57
PRINT MOLAR CONCENTRATIONS AND ENERGY EXCHANGE RATES
56 WRITE (6,138)
WRITE (6,19)
19 FORMAT (12X,12H(MOLES/M**3),26X,15H(MOLE/M**3/SEC),12X,6HNUMBER,7X *
*21H(JOULE-M**3/KG**2/SEC) ,7X,11H(CGS UNITS))
C COMPUTE MOLAR CONCENTRATIONS
57 DO 58 I=1,LS
58 PRC(I) = SIGMA(I)*RHOO
59 DO 62 IJ=1,MAX
   IF (IJ .GT. LS .OR. IJ .GT. LR) GO TO 60
   FMOL = SIGMA(IJ)*MIIXMW
   WW = W(IJ)*1000.
   XXX = PRX(IJ)*CONV
   WRITE (6,140) (SPNM(I,IJ),I=1,2),PRC(IJ),FMOL,WW,CONV,XXX,RATE(IJ)
   GO TO 62
60 IF (IJ .GT. LS) GO TO 61
   FMOL = SIGMA(IJ)*MIIXMW
   WW = W(IJ)*1000.
   WRITE (6,141) (SPNM(I,IJ),I=1,2),PRC(IJ),FMOL,WW
   GO TO 62
61 XXX = PRX(IJ)*CONV
   WRITE (6,142) IJ,XXX,RATE(IJ)
   CONTINUE
5XH = TXXH-18.0
   WRITE (6,150)
150 FORMAT (48X,22H(JOULE-M**3/KG**2/SEC))
   GO TO 78
C PRINT OUTPUT IN INTERNAL (CGS) UNITS
63 WRITE (6,151) (TIME,AREA,X,P,NH,V,AVH,PHO,(SNAM(I,JCV),I=1,2),
* T,MOT,TENT,EBRN,MACH,KGUNT,GAMMA
151 FORMAT (16X,4HTIME,1PE14.5,5H SEC,14X,4HAREA,1PE14.5,7H CM,/
*14X,14HAXIAL POSITION,1PE14.5,4H CM//20X,15HFLOW PROPERTIES,45X,2 AM500
*14X,14HINTTEGRATION INDICATORS//22X,8HREPRESSURE,OPF23.5,21X,21HSTEPS FROM AM503
* LAST PRINT,9X,14/23X,5H (ATM)/22X,8HVELOCITY,2F20.2,32X,17HAYFBAGE AM506
* STEP SIZE,E24.5/23X,8H(CM/SEC)/22X,7HDENSITY,1PE23.5,30X,20HCONTRO AM509
* LING VAPIABLE,11X,24/23X,10H (GM/CM**3)/22X,11HTEMPERATURE, AM507
* OPF17.2/23X,7H (DEG K)/22X,14HM ASS FLO RATE,1PE16.5/23X,8H (GM/SEC AM508
* )/22X,7HENTROFY,OPF23.4,30X,14HPREDICTOR ITERATIONS,11X, AM511
* I3//22X,8H(GAMMA,F25.4)
IF (I2 .EQ. 0) GO TO 64
IS = I1 + 1
DO 263 K=IS,IT
KK = NFG(K)
ESP(I,K) = SPNM(1,KK)
263 ESP(2,K) = SPNM(2,KK)
WRITE (6,130) ((ESP(I,K),I=1,2),K=IS,IT)
64 WRITE (6,131)
IF (CONC .OR. EXCHR) GO TO 66
C PRINT MASS FRACTIONS AND REACTION CONVERSION RATES
WRITE (6,132)
WRITE (6,152)
DO 65 J=1,LR
65 PX(J) = XX(J)
GO TO 67
66 IF (CONC .OR. (.NOT. EXCHR)) GO TO 69
C PRINT MASS FRACTIONS AND ENERGY EXCHANGE RATES
WRITE (6,134)
WRITE (6,153)
C COMPUTE MASS FRACTIONS
67 DO 68 I=1,LS
68 PRC(I) = SIGMA(I)*M(I)
GO TO 74
69 IF (.NOT CONC) .OR. EXCHR) GO TO 71
C PRINT MOLAR CONCENTRATIONS AND REACTION CONVERSION RATES
WRITE (6,136)
WRITE (6,154)
C COMPUTE MOLAR CONCENTRATIONS
67 DO 68 I=1,MAX
68 PRC(I) = SIGMA(I)*RHO
GO TO 75
C PRINT MOLAR CONCENTRATIONS AND ENERGY EXCHANGE RATES
71 WRITE (6,138)
WRITE (6,155)
C COMPUTE MOLAR CONCENTRATIONS
72 DO 73 I=1,LS
73 PRC(I) = SIGMA(I)*RHO
GO TO 77
75 IF (IJ .GT. LS) GO TO 76
FIII = SIGMA(IJ)_MIXMW
WRITE (6,141) (SPNM(I,IJ),I=1,2),PRC(IJ),FMOL,W(IJ)
GO TO 77
76 WRITE (6,142) IJ,PRX(IJ),RATE(IJ)
77 CONTINUE
WRITE (6,143) MIXMW,TXXH,CSUM
WRITE (6,156)
156 FORMAT (49X,21H(CAL-CM**3/GM_*2/SEC) )
78 WRITE (6,157)
157 FORMAT (//2(_X,8HVARIABLE,5X,10HDERIVATIVE,6X,9HINCREMENT,6X,14HRR
*LATIVE ERROR,4X))
1 = LSP3/2
LP = L
DO 79 I=1,L
LP = LP + 1
WRITE (6,158) (SNAM(K,I),K=1,2),F(I),RK(I),E(I),
* (SNAM(K,LP),K=1,2),F(LP),RK(LP),E(LP)
158 FORMAT (2(u,X,2AD,,2(_X, E12-5) ,5X,E12.5,SX))
79 CONTINUE
IF (2*L .EQ. LSP3) GO TO 80
WRITE (6,159) (SNAM(K,LSP3),T<=I,2),F(LSP3),RK(LSP3),E(LSP3)
159 FORMAT (70X,2A_,2(°,X,E 12-5} ,5X,E12.5)
IF {.NOT. DHUGO) GO TO 82
DEBUG OUTPUT (INTERNAL UNITS)
IF (V_RSA .NE. ARE_V_, GO TO 83
WRITE (6,160) AA,BB,DA,D2A,DTERM
160 FORMAT (IH1,12X,2HAA,18X,2HEB,13X,1HDD2(AREA) /D(IVAR),8X,1HDD2(AREA)
* )/D(IVAR) 2,8X,27H(1/AREA)*D(AREA)/D(IVAR) -AA/8X,E12.5,9X,E12.5,9X,
* E12.5,12X,E12.5,18X,E12.5)
80 IF (. NOT. DBGUGO) GO TO 82
C DEBUG OUTPUT (INTERNAL UNITS)
IF (VERSA .NE. AREAAN) GO TO 83
WRITE (6,160) AA,BB,DA,D2A,DTERM
160 FORMAT (IH1,12X,2HAA,18X,2HEB,13X,1HDD2(AREA) /D(IVAR),8X,1HDD2(AREA)
* )/D(IVAR) 2,8X,27H(1/AREA)*D(AREA)/D(IVAR) -AA/8X,E12.5,9X,E12.5,9X,
* E12.5,12X,E12.5,18X,E12.5)
83 WRITE (6,164) AA,BB,DA,D2A,DTERM
164 FORMAT (1H1,12X,2HAA,18X,2HEB,13X,1HDD2(AREA) /D(IVAR),8X,1HDD2(AREA)
* )/D(IVAR) 2,8X,27H(1/AREA)*D(AREA)/D(IVAR) -AA/8X,E12.5,9X,E12.5,9X,
* E12.5,12X,E12.5,18X,E12.5)
84 WRITE (6,161) (I,I=1,LR)
161 FORMAT (37X,58HOMEGA(I,J) RATE OF PRODUCTION OF SPECIES I BY RE
*ACTION J//1X,7HSPECIES,55X,8HREACTION/(18X,2,7HII15))
81 CONTINUE
DO 81 I=1,LS
WRITE (6,162) (SPNM(K,I),K=1,2),GMEGA(I,J),J=1,LP
162 FORMAT (/*,2X,2A4,2(4X,E12.5),5X,E12.5,5X))
82 IF (ABS(1.-CSUM) .LE. .001) RETURN
WRITE (6,163)
163 FORMAT (7H0(OUTP),5X,19HINVALID COMPOSITION
NEXT = .TRUE.
RETURN
END
$IEFTC PREDD DECK
SUBROUTINE PRED
C PERFORM ALL NECESSARY PRE-DERIVATIVE CALCULATIONS
DOUBLE PRECISION DP1,DP2

LOGICAL ALLM1,TCON,NEXT
REAL IVAR,MECT,LKEO,MM,N,_,MIXMW,M2
COMMON/CORE/VERSI,TIMEV,NEPSA,AVEAV,ELIM,TCON,PHOCON,IPRECCD
COMMON/COND/DVAR,AREA,MECT,P,IVAR,_,M2,_,SIGMA,LS,LSP3,NEXT
COMMON/SEP/SMAN(2,30),M(25),_,OMEGA(25,30)
COMMON/REAC/LSR(4,30),XX(10),FATE(30),LKEO(30),DLKEQ(30),M(30),LP
COMMON/BRAT/A(30),N(30),FACT(30),B(30),M(25,30),ALLM1
COMMON/SHSC/GRT(25),BRT(25),SP(25),CPP(25),DCPP(25)
COMMON/NECC/PR,MIXMW,M2,GAMMA,TCPP,P
COMMON/SABS/S1,AA,HB,S2,DA,D2A,DTMF

IF (TCON) GO TO 5
GO TO 1

ENTRY PRED1
MWARN = 0
1 THERMODYNAMIC PROPERTIES
CALL THRM (T,1.)
ALOGRT = ALCG (RR*T)
DO 4 J=1,LR
4 React_rate_CONSTANT
RATE(J) = A(J)*T**N(J)*EXP(-D(J)/T)
C IN KPC AND D(LN KEO)/DT
N1 = LSR(1, J)
N2 = LSR(2, J)
N3 = LSR(3, J)
N4 = LSR(4, J)
DELG = GRT(N3) - GRT(N2)
DELH = HRT(N3) - HRT(N2)
IF (N1 .eq. 0) GO TO 2
DELF = DELG + GRT(N4)
DELS = DELH + HRT(N4)
DELKEO(J) = -DELG - ALOGRT
DLKEQ(J) = (DELS - 1.) / T
GO TO 4
2 IF (N4 .eq. 0) GO TO 3
DELF = DELG - GRT(N1)
DELS = DELH - HRT(N1)
DELK(J) = -DELG + ALOGRT
DLKEO(J) = (DELS - 1.) / T
GO TO 4
3 DELG = DELG + GRT(N4) - GRT(N1)
DELH = DELH + HRT(N4) - HRT(N1)
DLKF(J) = -DELG
DLKEQ(J) = DELH / T
4 CONTINUE

C MIXTURE MOLECULAR WEIGHT
5 SSUM = 0.
DO 6 I=1,LS
6 SSUM = SSUM + SIGMA(I)
MIXMW = 1./SSUM
C ASSIGNED VARIABLE
IF (IPRECCD .gt. 2) GO TO 7
X = IVAR
IF (VERS - EO .eq. TIMEV) X = DVAR
CALL CINP (X,AVAR,DA,DD)
GO TO 4
7 TIME = DVAR
   IF (VERSI .EQ. TIMEV) TIME = IVAR
   CALL CINF (TIME,AVAR,DA,D2A)

C   CALCULATED VARIABLE
8 IF (VERSI .EQ. AREAV) GO TO 9
   P = AVAR
   IF (V .NE. 0.) AREA = MDOT/(RHO*V)
   GO TO 10

9 AREA = AVAR
   P = RHO*RT/MIXMW

C   MASS FLOW RATE
   MDOT = RHO*AREA*V

10 DO 20 J=1,LS
   N1 = LSR(1,J)
   N2 = LSR(2,J)
   N3 = LSR(3,J)
   N4 = LSR(4,J)

C   THIRD BODY FACTOR
   MM(J) = 0.
   IF (N1 .NE. 0. AND. N4 .NE. 0) GO TO 13
   IF (ALLI) GO TO 12
   DO 11 I=1,LS
   11 MM(J) = MM(J) + M(I,J)*SIGMA(I)
   GO TO 13

12 MM(J) = SSM

13 EXP1 = RATE(J)
   EXP2 = 1.
   IF (LKEQ(J) .GT. 0.) GO TO 14
   EXP2 = EXP(-LKEQ(J)/2.)
   GO TO 15

14 EXP1 = EXP(ALOG(RATE(J)) - LKEQ(J))

C   NET REACTION CONVERSION RATE
15 IF (N1 .GT. 0.) GO TO 17
   IF (N1 .LT. 0.) GO TO 16
   DP1 = RATE(J)*SIGMA(N2)
   DP2 = RHO*EXP1*SIGMA(N3)*EXP2*SIGMA(N4)*EXP2
   XX(J) = MM(J)*(DP1 - DP2)
   GO TO 20

16 DP1 = RATE(J)*SIGMA(N2)/RHO
   DP2 = EXP1*SIGMA(N3)*EXP2*SIGMA(N4)*EXP2
   XX(J) = DP1 - DP2
   GO TO 20

17 IF (N4 .GT. 0.) GO TO 19
   IF (N4 .LT. 0.) GO TO 18
   DP1 = RHO*SIGMA(N1)*RATE(J)*SIGMA(N2)
   DP2 = EXP1*EXP2*SIGMA(N3)*EXP2
   XX(J) = MM(J)*(DP1 - DP2)
   GO TO 20

18 DP1 = SIGMA(N1)*RATE(J)*SIGMA(N2)
   DP2 = EXP1*SIGMA(N3)*EXP2/RHO*EXP2
   XX(J) = DP1 - DP2
   GO TO 20

19 DP1 = SIGMA(N1)*RATE(J)*SIGMA(N2)
   DP2 = EXP2*SIGMA(N3)*EXP1*SIGMA(N4)*EXP2
   XX(J) = DP1 - DP2
20 CONTINUE
       RH02 = 3H0*RHO
       TCPR = 0.
       DO 22 I=1,LS

C TOTAL CP/R
       TCPR = TCPR + CPR(I)*SIGMA(I)
C NET SPECIES PRODUCTION RATE
       W(I) = 0.
       DO 21 J=1,LR
       OMEGA(I,J) = RH02*STOIC(I,J)*XX(J)
       21 W(I) = W(I) + OMEGA(I,J)
       22 CONTINUE

C GAMMA (FROZEN)
       GAMMA = TCPR/(TCPR - 1./MIXMW)
C MACH NUMBER SQUARED
       M2 = V/R*V/T*MIXMW/GAMMA
       IF (VERSA .NE. AREAV .OR. (M2 .LT. 0.9025 .OR. M2 .GT. 1.1025))
         * GO TO 23
       WMACH = SQRT(M2)
       WRITE (6,101) WMACH
       101 FORMAT (7H0 (PRED),5X,7HWARNING,3X,13HMACH NUMBER =,F8.4,19H IS APP
       *BOACHING 1.0)
       MWARN = MWARN + 1
       IF (MWARN .LT. 15) GO TO 23
       WRITE (6,102)
       102 FORMAT (7H0 (PRED),5X,25H15 WARNINGS HAVE OCCURED)
       NEXT = .TRUE.
       RETURN

23 CALL DERV
       RETURN
       END
$IEFTC DERVV DECK

SUBROUTINE DERV

C COMPUTE ALL DERIVATIVES WRT THE INDEPENDENT VARIABLE

DOUBLE PRECISION DPS1,DPS2
LOGICAL TCON,RHOCON
REAL IVAR,MIXMW,M2

COMMON/OPTS/VERSI,TIMEV,VERSA,AREA,AREAV,ELIM,TCON,RHOCON,IPRCOD
COMMON/COND/DVAR,AREA,MDOT,P,IVAR,V,RHO,T,SIGMA(25),LS,LSP3,NEXT
COMMON/SPEC/SNAM(2,30),MW(25),W(25),STOIC(25,30),SIGMA(25,30)
COMMON/GHSC/GBT(25),HRT(25),SP(25),CPR(25),OEP(25)
COMMON/BEAN/F(25),ALPHA(28),BETA(28,28)
COMMON/NECC/RT,MIXMW,M2,GAMMA,TCPR,P
COMMON/SABS/S1,AA,BB,S2,DA,D2A,DTEPM

EQUIVALENCE (DV,F(1))
\[ D2ADT2(D2) = V^2 * D2 + DV/V * DA \]
\[ D2ADX2(D2) = (D2/V - DV*DA)/V \]

\[ DPS1 = 0.0D0 \]
\[ DPS2 = 0.0D0 \]
\[ DO 1 I=1,3 \]
\[ F(I) = 0. \]
\[ 1 \text{ ALPHA}(I) = 0. \]

\[ \text{DENM} = \text{RHO} \]
\[ \text{IF (VERSI .NE. TIMEV) DENM} = \text{RHO} * V \]
\[ \text{DO 2 I=1,LS} \]
\[ \text{II} = I + 3 \]

\[ \text{C DSIGMA/DIVAR} \]
\[ \text{P(II)} = W(I)/\text{DENM} \]

\[ \text{C S1 FOR AA} \]
\[ \text{DPS1} = \text{DPS1} + P(II) \]

\[ \text{C S2 FOR BB} \]
\[ 2 \text{ DPS2} = \text{DPS2} + \text{HRT(I)}*F(II) \]

\[ S1 = \text{MIXMW} * \text{DPS1} \]
\[ S2 = \text{MIXMW} * \text{DPS2} \]

\[ \text{GAM1} = \text{GAMMA} - 1. \]

\[ \text{C BB FOR DERIVATIVES} \]
\[ \text{BB} = \text{GAM1}/(\text{GAMMA} * S2) \]

\[ \text{C AA FOR DERIVATIVES} \]
\[ \text{AA} = \text{S1} - \text{BB} \]

\[ \text{C DAVAR/DIVAR} \]
\[ \text{IF (VERSI .EQ. TIMEV) AND. IPRCOD .LE. 2) DA = V*DA} \]
\[ \text{IF (VERSI .NE. TIMEV) AND. IPRCOD .GE. 3) DA = DA/V} \]

\[ \text{IF (VERSA .NE. AREAV) GO TO 4} \]

\[ \text{C ASSIGNED AREA EQUATIONS} \]
\[ \text{DTERM} = \text{DA}/\text{AREA} - \text{AA} \]
\[ \text{T1} = 1. / (M2 - 1.) \]
\[ \text{T2} = M2 * T1 \]

\[ \text{C DV/DIVAR} \]
\[ \text{F(1)} = V*T1*DTERM \]

\[ \text{C DRHO/DIVAR} \]
\[ \text{IF (NOT. RHOCON) F(2) = -RHO*(T2*DTERM + AA)} \]

\[ \text{C DT/DIVAR} \]
\[ \text{IF (NOT. TCON) F(3) = -T*(GAM1*T2*DTERM + BB)} \]

\[ \text{C DAREA/DIVAR WRT IVAR} \]
\[ \text{IF (VERSI .EQ. TIMEV) AND. (IPRCOD .EQ. 1. AND. V .NE. 0.)) D2A =} \]
\[ \text{D2ADT2(D2A)} \]
\[ \text{IF (VERSI .NE. TIMEV AND. IPRCOD .EQ. 3) D2A = D2ADX2(D2A)} \]
\[ \text{T3} = (D2A - DA*DA/\text{AREA})/\text{AREA} \]
C DSIGMA/DIVAR WRT IVAR
  DO 3 I=4,LSP3
 3 ALPHA(I) = 0.
C DV/DIVAR WRT IVAR
   ALPHA(1) = V*T1*T3
C DRHO/DIVAR WRT IVAR
   IF (.NOT. RHOCON) ALPHA(2) = -RHO*T2*T3
C DT/DIVAR WRT IVAR
   IF (.NOT. TCON) ALPHA(3) = -T*DTEPM*T2*T3
   GO TO 6
C ASSIGNED PRESSURE EQUATIONS
4 DTERM = DA/P
   T2 = -1./GAMMA
C DV/DIVAR
   IF (V .NE. 0.) F(1) = -DA/(RHO*V)*1.01325E+06
C TRHO/DIVAR
   IF (.NOT. RHOCON) F(2) = -RHO*(T2^2 + T3)
C DT/DIVAR
   IF (.NOT. TCON) F(3) = -T*(GAMMA*T2^2 + BB)
C DP/DIVAR WRT IVAR
   IF (VFRSI .EQ. TIMEV AND IPRCOD .EQ. 2) D2A = D2ADF2(D2A)
   IF (VFRSI .NE. TIMEV AND IPRCOD .EQ. 4) D2A = D2ADX2(D2A)
   T3 = (D2A - DA*DA/P)/P
C DSIGMA/DIVAR WRT IVAR
  DO 5 I=4,LSP3
 5 ALPHA(I) = 0.
C DV/DIVAR WRT IVAR
   IF (V .NE. 0.) ALPHA(1) = -D2A/(RHO*V)*1.01325E+06
C DRHO/DIVAR WRT IVAR
   IF (.NOT. RHOCON) ALPHA(2) = -RHO*T2*T3
C DT/DIVAR WRT IVAR
   IF (.NOT. TCON) ALPHA(3) = -T*DTEPM*T2*T3
6 CALL PARD
RETURN
END
$IEFTC PARD DD DECK
SUBROUTINE PARD
C COMPUTE ALL MIXED PARTIAL DERIVATIVES
LOGICAL TCON,RHOCON
REAL LKEC,MM,N,M,MIXMW,M2
DIMENSION PXXRHO(30), PXXT(30), PXXSIG(30,25), PGSIG(25), PM2SIG(25)
* PS1SIG(25), PS2SIG(25), PAASIG(25), PBBSIG(25)

COMMON/opts/versi,tmev,versa,area,mdot,p,ivar,v,rho,t,sigma(25),ls,lsf3,next
COMMON/spec/sham(2,30),n(25),w(25),stoic(25,30),omega(25,30)
COMMON/neec/a(30),n(30),eact(30),b(30),m(25,30),allm1
COMHCN/iq(30),n(30),eact(30),b(30),m(25,30),allm1
COMMON/gs/ch(25),hrt(25),sp(25),cpp(25),dcmp(25)
COMMON/NECC/RR, RM2, GAMMA, TCPP, R
COMMON/SABS/SI,AA,BB,S2,DA,D2A,DEPE
COMMON/DERN/F(28),ALPHA(28),BETA(28,28)

DO 1 I=1,LSF3
DO 1 K=I,LSF3
1 BETA(I,K) = 0.

DO 2 J=1,LR
DO 2 I=I,LS
PXXSIG(J,I) = 0.

XX(J) WRT RHO,T,SIGMA(I)
DO 9 J=1,LR
N1 = LSR(1,J)
N2 = LSR(2,J)
N3 = LSR(3,J)
N4 = LSR(4,J)
EXP1 = RATE(J)
EXP2 = 1.

IF (LKEQ(J) .GT. 0.) GO TO 3
3 EXP1 = EXP(ALOG(RATE(J)) - LKEQ(J))
GO TO 4

4 IF (N1 .GT. 0.) GO TO 6
IF (N1 .LT. 0) GO TO 5
PXXRHO(J) = -MM(J)*EXP2*SIGMA(N3)*EXP1*SIGMA(N4)*EXP2
PXXT(J) = MM(J)*EXP1*RHO*SIGMA(N3)*EXP2*SIGMA(N4)*EXP2*DLKEQ(J)
PXXSIG(J,N2) = RATE(J)*MM(J) + XX(J)/MM(J)*M(N2,J)
PXXSIG(J,N3) = -MM(J)*EXP1*RHO*SIGMA(N3)*EXP2 + XX(J)/MM(J)*M(N3,J)
M(N3,J)
PXXSIG(J,N4) = -MM(J)*EXP1*RHO*EXP2*SIGMA(N3)*EXP2 + XX(J)/MM(J)*M(N4,J)
M(N4,J)
GO TO 9

5 PXXRHO(J) = -RATE(J)/RHO*SIGMA(N2)/RHO
PXXT(J) = EXP1*SIGMA(N3)*EXP2*SIGMA(N4)*EXP2*DLKEQ(J)
PXXSIG(J,N2) = RATE(J)/RHO
PXXSIG(J,N3) = -EXP2*(EXP1*SIGMA(N4))*EXP2
PXXSIG(J,N4) = -EXP2*(EXP1*SIGMA(N3))*EXP2
GO TO 9

6 IF (N4 .GT. 0.) GO TO 8
IF (N4 .LT. 0) GO TO 7
PXXRHO(J) = MM(J)*SIGMA(N1)*RATE(J)*SIGMA(N2)
PXXT(J) = EXP2*MM(J)*EXP1*SIGMA(N3)*EXP2*DLKEQ(J)
PXXSIG(J,N1) = MM(J)*RHO*RATE(J)*SIGMA(N2) + XX(J)/MM(J)*M(N1,J)
PXXSIG(J,N2) = MM(J)*RHO*SIGMA(N1) + XX(J)/MM(J)*M(N2,J)
PXXSIG(J,N3) = -EXP1*(EXP2*MM(J))*EXP2 + XX(J)/MM(J)*M(N3,J)
GO TO 9
7 PXXPHO(J) = EXP1*SIGMA(N3)*EXP2/RHO*EXP2/RHO
PXXT(J) = EXP1*SIGMA(N3)*EXP2/RHO*EXP2*DLKEQ(J)
PXXSIG(J,N1) = RATE(J)*SIGMA(N2)
PXXSIG(J,N2) = RATE(J)*SIGMA(N1)
PXXSIG(J,N3) = -EXP2*EXP1*(EXP2/RHO)
GO TO 9

8 PXXRHO(J) = 0.
PXXT(J) = EXP1*SIGMA(N3)*EXP2*SIGMA(N4)*EXP2*DLKEQ(J)
PXXSIG(J,N1) = RATE(J)*SIGMA(N2)
PXXSIG(J,N2) = RATE(J)*SIGMA(N1)
PXXSIG(J,N3) = -EXP2*(EXP1*SIGMA(N4))*EXP2
PXXSIG(J,N4) = -EXP2*(EXP1*SIGMA(N3))*EXP2

9 PXXT(J) = PXXT(J) + XX(J)*(N(J) + B(J)/T)/T

97 GTGM1 = GAMMA*(GAMMA - 1.)
PGAMT = 0.

C GAMMA WRT SIGMA(I) AND MACH NUMBER SQUARED WRT SIGMA(I)
DO 10 I=1,LS
PGSIG(I) = GTGM1*(MIXMW - CPR(I)/TCPR)
PM2SIG(I) = -M2*(MIXMW + PGSIG(I)/GAMMA)
10 PGAMT = PGAMT + SIGMA(I) -DCPH(I)

C GAMMA WRT T
PGAMT = -GTGM1/TCPR*PGAMT

C MACH NUMBER SQUARED WRT V
PM2V = 2.*V*MIXMW/(GAMMA*R*T)

C MACH NUMBER SQUARED WRT T
PM2T = -M2*(1./T + PGAMT/GAMMA)

TERM = RHO
IF (VERSI .EQ. TIMEV) GO TO 12
TERM = RHO/V

C DSIGMA/DIVAR WRT V
DO 11 II=4,LSP3
11 BETA(II,1) = -F(II)/V

C DSIGMA/DIVAR WRT T
DO 12 II=4,LSP3

C DSIGMA/I/DIVAR WRT SIGMA(K)
DO 16 II=4,LSP3

C S1 WRT V,PHO,T,SIGMA(I) AND S2 WRT V,PHO,T,SIGMA(I)
PS1V = 0.
PS1PHO = 0.
PS1T = 0.
PS2V = 0.
PS2RHO = 0.
PS2T = 0.
DO 18 II=4,LSP3
I = II - 3
PSIV = PSIV + ETA(I,1)
PSI_HO = PSI_HO + BETA(I,2)
PSIT = PSIT + BETA(I,3)
PS2V = PS2V + HRT(I)*BETA(I,1)
PS2RHO = PS2RHO - HRT(I)*BETA(I,2)
PS2T = PS2T + HRT(I)*BETA(I,3) + CPR(I)*F(I)/T
PSISIG(I) = 0.
PS2SIG(I) = 0.
DO 17 KK=1,LSP3
PSISIG(I) = PSISIG(I) + BETA(KK,II)
PS2SIG(I) = PS2SIG(I) + HWT(K)*BETA(KK,II)
PSISIG(I) = MIXMW*(PSISIG(I) - $1)
PS2SIG(I) = MIXMW*(PS2SIG(I) - S2)
PSIV = MIXMW*PSIV
PSI_HO = MIXMW*PSI_HO
PSIT = MIXMW*PSIT
PS2V = MIXMW*PS2V
PS2RHO = MIXMW*PS2RHO
PS2T = MIXMW*PS2T - S2/T
GM1DG = (GAMMA - 1.)/GAMMA
S2OG2 = S2/(GAMMA*GAMMA)

C BB WRT V
PBBV = GM1DG*PS2V
C BB WRT RHO
PBBRHO = GM1DG*PS2RHO
C BB WRT T
PBBT = GM1DG*PS2T + S2OG2*PGMT
C AA WRT V
PPAV = PSIV - PBBV
C AA WRT RHO
PAARHO = PS1RHO - PBBRHO
C AA WRT T
PAAT = PSIT - PBBT

C BB WRT SIGMA(I) AND AA WRT SIGMA(I)
DO 19 I=1,LS
PBBSIG(I) = GM1DG*PS2SIG(I) + S2OG2*PGSIG(I)
PAASIG(I) = PSISIG(I) - PBBSIG(I)

IP (VFRS_ANE, AREA_FWD) GO TO 24

C ASSIGN AREA EQUATIONS
T1 = 1./((M2 - 1.)
GAM1 = GAMMA - 1.

C DV/DIVAR WRT V
BETA(1,1) = T1*(DTERM - F(I)*PM2V - V*PAAV)
C DV/DIVAR WRT RHO
BETA(1,2) = -V*T1*PAARHO
C DV/DIVAR WRT T
BETA(1,3) = -T1*(V*PAAT + F(I)*PM2T)
C DV/DIVAR WRT SIGMA(I)
DO 20 II=4,LSP3
I = II - 3
BETA(1,II) = -T1*(V*PAASIG(I) + F(I)*PM2SIG(I))

IF (RHOCON) GO TO 22
C DRHO/DIVAR WRT V
   BETA(2,1) = RHO*T1*(PAAV + T1*DTERM*PM2V)
C DRHO/DIVAR WRT RHO
   BETA(2,2) = RHO*T1*PAARHO + F(2)/RHO
C DRHO/DIVAR WRT T
   BETA(2,3) = RHO*T1*(PAAT + T1*DTERM*PM2T)
C DRHO/DIVAR WRT SIGMA(I)
   DO 21 II=4,LSP3
      I = II - 3
   21 BETA(2,II) = RHO*T1*(PAASIG(I) + T1*DTERM*PM2SIG(I))

C DT/DIVAR WRT V
   BETA(3,1) = T*(GAMI*T1*(M2*PAAV + T1*DTERM*PM2V) - PBBV)
C DT/DIVAR WRT RHO
   BETA(3,2) = T*(GAMI*M2*PAARHO - PBBRHO)
C DT/DIVAR WRT T
   BETA(3,3) = T*(GAMI*(M2*PAAT + T1*DTERM*PM2T) - M2*DTERM*PGAMT
                  * ) - PBBT) + F(3)/T
C DT/DIVAR WRT SIGMA(I)
   DO 23 II=4,LSP3
      I = II - 3
   23 BETA(3,II) = T*(T1*(GAMI*(M2*PAASIG(I) + T1*DTERM*PM2SIG(I)) - M2*
                  * DTERM*PGSIG(I)) - PBBSIG(I))

RETURN

C ASSIGNED PRESSURE EQUATIONS
24 T1 = 1./(GAMMA*GAMMA)
C DV/DIVAR WRT V
   IF (V .NE. 0.) BETA(1,1) = -F(1)/V
C DV/DIVAR WRT RHO
   BETA(1,2) = -F(1)/RHO
C DV/DIVAR WRT T
   BETA(1,3) = 0.
C DV/DIVAR WRT SIGMA(I)
   DO 25 II=4,LSP3
      I = II - 3
   25 BETA(1,II) = 0.
   IF (RHOCON) GO TO 27
C DRHO/DIVAR WRT V
   BETA(2,1) = -RHO*PAAV
C DRHO/DIVAR WRT RHO
   BETA(2,2) = F(2)/RHO - RHO*PAARHO
C DRHO/DIVAR WRT T
   BETA(2,3) = -RHO*(PAAT + T1*DTERM*PGAMT)
C DRHO/DIVAR WRT SIGMA(I)
   DO 26 II=4,LSP3
      I = II - 3
   26 BETA(2,II) = -RHO*(PAASIG(I) + T1*DTERM*PGSIG(I))

27 IF (TCON) RETURN
C DT/DIVAR WRT V
   BETA(3,1) = -T*PBBV
C DT/DIVAR WRT RHO
   BETA(3,2) = -T*PBBRHO
C DT/DIVAR WRT T
   BETA(3,3) = BB - T*(PBBT - T1*DTERM*PGAMT) + F(3)/T
C DT/DIVAR WRT SIGMA(I)
   DO 28 II=4,LSP3
      I = II - 3

162
28 BET(3,II) = -T*(PBBSIG(I) - T1*DEPM*PGSIG(I))

RETURN
END

$IEFCC THRM DECK
SUBROUTINE THRM (T,HONLY)
C THIS ROUTINE CALCULATES (DIMENSIONLESS) THERMODYNAMIC PROPERTIES
C FROM POLYNOMIAL CURVE FITS

LOGICAL NEXT

COMMON/COND/DUM(33),LS,LSP3,NEXT
COMMON/GHSC/GPT(25),HAT(25),SR(25),CPR(25),DCPR(25)
COMMON/TCOF/C(7,2,25),TLOW,TMID,THI

F(T) = A1+T*(A2+T*(A3+T*(A4+T*A5)))

IF (T .EQ. TPREV) RETURN
IF (0.35*TLOW .LE. T .AND. T .LE. THI) GO TO 3
IF (T .LE. 1.20*THI) GO TO 2
WRITE (6,1005 T
100 FORMAT (7H0(THM) ,SX,5HERROR,3X,3HT =,Fg.2,16H IS OUT OF RANGE5
NEXT = .TRUE.
RETURN

2 WRITE (6,1015 T
101 FORMAT (TH0(THRM),5X,7HWARNING,3X,3HT :,F£.2,16H IS OUT OF RANGE,
_X,28HEXTRAPOLATED VALUES RFTURNED)

C LOCATE PROPER TEMPERATURE RANGE

3 K = 2
IF (T .GT. TMID) K = 1
DO 4 I=1,LS
C COMPUTE H/(R*T)
A1 = C(1,K,I) + C(6,K,I)/T
A2 = C(2,K,I)/2.
A3 = C(3,K,I)/3.
A4 = C(4,K,I)/4.
A5 = C(5,K,I)/5.
4 HRT(I) = F(T)
IF (HONLY .EQ. 0.) RETURN
TPREV = T
DO 5 I=1,LS
C COMPUTE G/(R*T)
A1 = C(1,K,I)*(1.-ALOG(T)) + C(6,K,I)/T - C(7,K,I)
A2 = -C(2,K,I)/2.
A3 = -C(3,K,I)/6.
A4 = -C(4,K,I)/12.
A5 = -C(5,K,I)/20.
GRT(I) = F(T)
C COMPUTE S/R
A1 = C(1,K,I)*ALOG(T) + C(7,K,I)
A2 = C(2,K,I)
A3 = C(3,K,I)/2.
A_ = c(_,K,I)/3.
A5 = c(5,K,I)/4.
SP(I) = F(T)
A1 = c(I,K,I)
A2 = c(2,K,I)
A3 = c(3,K,I)
A4 = c(4,K,I)
A5 = c(5,K,I)
CP(I) = F(T)
A1 = c(I,K,I)
A2 = c(2,K,I)
A3 = c(3,K,I)
A4 = c(4,K,I)
A5 = c(5,W,I)
CP(I) = F(T)
A1 = c(I,K,I)
A2 = c(2,K,I)
A3 = c(3,K,I)
A4 = c(4,K,I)
A5 = c(5,W,I)
RETURN
END
$IEFTC INTTEE DECK
SUBROUTINE INTTE
C SET UP AND CALL FOR INTEGRATION
C OBTAIN SUGGESTED STEP SIZE FOR NEXT INTEGRATION STEP
EXTERNAL PEBB
LOGICAL NEXT,ELIM
REAL IVAR
DIMENSION YN(33),Y(28),C(25)
COMMON/OPTS,YPSI,TIMEV,VEPSA,AFEA9,ELIM,TCON,PHOCON,IPRCOD
COMMON/COND/YP1(33),LS,LSP3,NEXT
COMMON/SINT/HMIN,HM1,HN,HNPI,HNX,AVH,EHMA,EFPN,JCVO,KOUI,EPFP
COMMON/EQRE/PK(28),OK(28),PK(28),E(28)
COMMON/SPEC/SKAM(2,25),KN(25),W(25),STIOIC(25,30),OMEGA(25,30)
EQUIVALENCE (IVAR,YNPI(5)),(Y,YNPI(6)),(C,YNPI(9)),(HN,HM1)
C INITIAL STEPS OR RESTART
ENTRY INTI
NREST = 0
E.MAX2 = EMAX/2.
EMAX56 = 5.*EMAX/6.
LSPR = LS + 8
HNPI = HINT
DO 3 T=1,LSP8
3 YN(I) = YNPI(I)
2 CALL CASI (HN,OK,HNPI,P)
HN = HNP1
CALL PRED
CALL CASI (HN,PK,HNPI,OK)
HN1 = HM
HN = HNP1
CALL PRED
DO 23 I=1,LS
IF (C(I) .GE. 0.) GO TO 23
WRITE (6,100)
100 FORMAT (7H0(INTE),5X,23HCOMPOSITION ERROR - NEGATIVE CONCENTRATION
*:5)
NEXT = .TRUE.
RETURN
23 CONTINUE
RETURN
C PREPARE TO CONTINUE INTEGRATION
ENTRY INTC
DO 4 I=1,LS
YNP1(I) = YN(I)
CALL PRED
RETURN
C GENERAL STEP
ENTRY INTC
CALL CASG (HN,OK,HNP1,RK)
C RELATIVE ERROR IN INTEGRATION STEP
ERRN = ERRN(Y,OK,E,JCV,HNP1)
C TEST FOR RESTART CONDITIONS
IF (ERRN .LE. EMAX .OR. HMIN .GT. HMAX) GO TO 7
WRITE (6,101) IVAR, {SNAM(J,JCV),J=1,2),HN,HN,HNP1
101 FORMAT (7H0(INTE),5X,25H10 PESTA_TS HAVE OCCURRED)
NEXT = .TRUE.
RETURN
4 YNP1(I) = YN(I)
CALL PRED
RETURN
STOP AFTER 10 RESTARTS
IF (NREST .LT. 10) GO TO 6
WRITE (6,103)
103 FORMAT (7H0(INTE),5X,25H10 PESTA_TS HAVE OCCURRED)
NEXT = .TRUE.
RETURN
6 NREST = NREST + 1
HMIN = HMIN/2.
HNP1 = HMIN
GO TO 2
7 HNM1 = HN
HN = HNP1
DO 8 I=1,LS
IF (I .GT. LSP3) GO TO 8
PK(I) = OK(I)
OK(I) = RK(I)
8 YN(I) = YNP1(I)
CALL PRED
C TEST FOR NEGATIVE CONCENTRATIONS
DO 9 I=1,LS
IF (C(I) .GE. 0.) GO TO 9
WRITE (6,100)
9 NEXT = .TRUE.
RETURN
C GENERAL STEP
ENTRY INTC
CALL CASG (HN,OK,HNP1,RK)
C RELATIVE ERROR IN INTEGRATION STEP
ERRN = ERRN(Y,OK,E,JCV,HNP1)
C TEST FOR RESTART CONDITIONS
IF (ERRN .LE. EMAX .OR. HMIN .GT. HMAX) GO TO 7
WRITE (6,101) IVAR, {SNAM(J,JCV),J=1,2),HN,HN,HNP1
101 FORMAT (7H0(INTE),5X,25H10 PESTA_TS HAVE OCCURRED)
NEXT = .TRUE.
RETURN
4 YNP1(I) = YN(I)
CALL PRED
RETURN
STOP AFTER 10 RESTARTS
IF (NREST .LT. 10) GO TO 6
WRITE (6,103)
103 FORMAT (7H0(INTE),5X,25H10 PESTA_TS HAVE OCCURRED)
NEXT = .TRUE.
RETURN
6 NREST = NREST + 1
HMIN = HMIN/2.
HNP1 = HMIN
GO TO 2
7 HNM1 = HN
HN = HNP1
DO 8 I=1,LS
IF (I .GT. LSP3) GO TO 8
PK(I) = OK(I)
OK(I) = RK(I)
8 YN(I) = YNP1(I)
CALL PRED
C TEST FOR NEGATIVE CONCENTRATIONS
DO 9 I=1,LS
IF (C(I) .GE. 0.) GO TO 9
WRITE (6,100)
9 NEXT = .TRUE.
RETURN
CONTINUE

OPTIONAL AUTOMATIC ELIMINATIONS
IF (ELIM) CALL AUTO

GET STEP SIZE FOR NEXT INTEGRATION STEP
KOUNT = 0
IF (E_RN .GE. EMAX2) GO TO 10
IF (HN .GE. HMAX) RETURN
CALL SEARCH (PERR,EMAX,HN,HNP1,HMAX) RETURN

10 IF (ERRN .LE. EMAX56) RETURN
IF (HN .LE. H_IN) RETURN
CALL SEARCH (PERR,EMAX,HMIN,HNPI,HN)
RETURN
END

$IEFTCASMM DECK
SUBROUTINE CASM

CHOOSE (1) INITIAL STEP (RESTAPT) FORMULA
(2) GENERAL STEP FORMULA

SET UP AUGMENTED MATRIX

COMPUTE INCREMENTS

DOUBLE PRECISION A
REAL IVAR

COMMON/OPTS/VERSI,TIMEV,VERS,AREA,ELIM,TCON,PHOCON,IPPCON
COMMON/COND/DVAR,AREA,MCCT,P,IVAR,Y(28),LS,LSEP,NEXT
COMMON/DERN/P(28),ALPHA(28),BETA(28,28)
COMMON/MATX/A(28,28)

EQUIVALENCE (VN1,Y(1))

DATA FPS/0.0001/

ENTRY CASI (HN,QK,HNI,RF)
ENTRY CASG (HN,QK,HNI,RF)

INITIAL STEP OR RESTART
INGEN = 1
JK = 0
10 F1 = 0.
F2 = HN1
F3 = HN1/2.
F4 = F3
GO TO 2

ENTRY CASG (HN,QK,HNI,RF)

GENERAL STEP
INGPN = 2
JK = 0
20 F1 = HN1*HN1/((2.*HN1 + HN)*HN)
F2 = HN1*(HN1 + HN)/((2.*HN1 + HN)
F3 = HN1
F4 = F2

2 LSP4 = LSP3 + 1

DO 4 I=1,LSP3
DO 3 J=1,LSP3
3 A(I,J) = -F4*BETA(I,J)
A(I,I) = 1.0 + A(I,I)
IF (DABS(A(I,I)) .GE. EPS) GO TO 4
IF (JK .GE. 3) GO TO 4
JK = JK + 1
HN1 = 2.0*(1.0 - EPS)/BETA(I,I)
GO TO (10,20), INGEN
4 A(I,LSP4) = F1*QK(I) + F2*(F(I) + ALPHA(I)*F3)

CALL LESV(RK)
VN = Y(1)
DO 5 I=1,LSP3
5 Y(I) = Y(I) + RK(I)
IVAR = IVAR + HN1

IF (VERS .EQ. TIME) GO TO 6
DVAR = DVAR + 2.*HN1/(VN + VN1)
RETURN
6 DVAR = DVAR + (VN + VN1)/2.*HN1
RETURN

END

$IBFTC LESV DECK
SUBROUTINE LESV (K)

C THIS ROUTINE IS A GENERAL DOUBLE PRECISION LINEAR EQUATION SOLVER
IN THIS PROGRAM IT IS USED TO COMPUTE THE INCREMENTS K(I)
DOUBLE PRECISION A, S, TS, B
LOGICAL NEXT
REAL K

DIMENSION S(28), K(28)
COMMON/COND/DUMMY(34), N, NEXT
COMMON/MATX/A(28,29)

NP = N+1
DO 5 I=1,N
5 GET SCALE FACTORS
TS = 0.0
DO 6 J=1,N
B = DABS(A(I,J))
IF (B .GT. TS) TS = B
6 CONTINUE
IF (TS .EQ. 0.0) GO TO 100

SCALE ROWS
DO 10 J=1,NP
10 A(I,J) = A(I,J)/TS
CONTINUE

BEGIN TRIANGULARIZATION
IF (N .EQ. 1) GO TO 25
NM = N-1
DO 15 J=1,NM
C FIND MAXIMUM ELEMENT IN COLUMN J BELOW DIAGONAL
II = J
JP = J+1
DO 16 I=JP,N
IF (DABS(A(I,J)) .GT. DABS(A(II,J))) II = I
16 CONTINUE
IF (II .EQ. J) GO TO 20
C INTERCHANGE ROWS II AND J
DO 17 L=J,Np
TS = A(II,L)
A(II,L) = A(J,L)
A(J,L) = TS
17 CONTINUE
C ZERO COLUMN J BELOW DIAGONAL
20 DO 18 I=JP,N
TS = A(I,J)/A(J,J)
IF (TS .EQ. 0.D0) GO TO 18
DO 19 L=JP,NP
Ig A
135 A(I,L) = A(I,L) - TS*A(J,L)
18 CONTINUE
15 CONTINUE
C BACK SUBSTITUTE
25 TS = A(N,N)
IF (DABS(TS) .LT. 1.D-10) WRITE (6,102)
102 FORMAT (7HO(LESV),5X,11HSINGULARITY)
S(N) = A(N,NP)/TS
K(N) = S(N)
IF (N .EQ. 1) RETURN
DO 26 I=2,N
M = NP - I
TS = A(M,M)
IF (DABS(TS) .LT. 1.D-10) WRITE (6,102)
B = A(M,NP)
MP = M+1
DO 27 L=MP,N
27 B = B - A(M,L)*S(L)
S(M) = B/TS
26 K(M) = S(M)
30 CONTINUE
RETURN
100 WRITE (6,101) I
101 FORMAT (7HO(LESV),3X,3HROW,14,39H OF THE COEFFICIENT MATRIX IS ALL
1 ZEROS)
DO 50 I=1,N
50 WRITE (6,103) (A(I,J), J=1,NP)
103 FORMAT (1H1,8F16.6/(1X,8E16.6))
NEXT = .TRUE.
RETURN
END
WRITE ERROR DECK
FUNCTION ERROR (Y,FK,E,JC,H)
C COMPUTE THE RELATIVE ERROR IN AN INTEGRATION STEP OF SIZE H
C DETERMINE THE CONTROLLING VARIABLE
DOUBLE PRECISION DNP1,DF,DEM1,C,ABSY
168
C = (H + HN)/(2.*H + HN)  
FAC1 = ABS((H + 2*H + HN)/(H + HN + HN1))  
ERROR = -1.  
DO 4 I = 1, LSP3  
   E(I) = 0.  
   IF (ABS(RK(I)) .EQ. 0.) GO TO 4  
   ABSY = ABS(Y(I))  
   IF (ABSY .EQ. 0.) GO TO 4  
   DNP1 = RK(I)/H  
   DN = QK(I)/HN  
   DNMI = PK(I)/HNM1  
   FAC2 = DABS((DNP1 - DN) - C*(DN - DNMI))  
C CHECK FOR CATASTROPHIC SUBTRACTION  
   IF (FAC2 .LE. ABS(DNP1)*1.0E-04) GO TO 5  
   E(I) = FAC1*(FAC2/ABSB1)  
5 IF (I .LE. 3 .OR. IT .EQ. 0) GO TO 3  
   IT = I - 3  
C SKIP NEGLECTED SPECIES  
   DO 2 J = 1, IT  
      IF (NEGL(J) .EQ. 0) GO TO 4  
   CONTINUE  
2 CONTINUE  
3 IF (E(I) .LE. ERROR) GO TO 4  
   ERROR = E(I)  
   JC = I  
   CONTINUE  
4 CONTINUE
RETURN  
END
$IFTPC PERRR DECK  
FUNCTION PERRR(H)  
C THIS ROUTINE PREDICTS THE ERROR WHICH CAN BE EXPECTED FROM A  
C STEP OF SIZE H  
C DOUBLE PRECISION SUM  
DIMENSION Y(28),RK(28),E(28)  
COMMON/COND/DUM(33),LS,LSP3,NEXT  
COMMON/SINT/HMIN,HNM1,HN,HNP1,HMAX,NH,AVH,EMAX,ERRN,JCV,KOUNT,ERRF  
COMMON/PQRE/PK(28),QK(28),DUM2(56)  
COMMON/SKIP/NEGL(25),I1,I2,IT  
C = H/(2.*H + HN)  
C0 = H/2.  
C1 = F/HN  
C2 = H + HN  
PERR = 0.  
DO 2 I = 1, LSP3  
   RK(I) = C0*(QK(I)/HN + F(I))  
2 CONTINUE
$IEFTC AUTOO DECK$  
*SUBROUTINE AUTO*

C AUTOMATIC ELIMINATION FROM ERROR CONSIDERATIONS OF SPECIES WITH
C NON-REPRESENTATIVE ERRORS

REAL MEDIAN

DIMENSION ERROR(25), EE(25)

COMMON/COND/DUMI(33), LS, LSP3, NEXT
COMMON/PQRE/DUM2(88), E(28)
COMMON/SKIP/NEGL(25), I1, I2, IT

EQUIVALENCE (EE(1), E(4))

I2 = 0
M = LS - I1
IF (M .LE. 3) RETURN

K = 0
DO 3 I = 1, LS
IF (I1 .EQ. 0) GO TO 2
DO 1 J = 1, I1
IF (I .EQ. NEGL(J)) GO TO 3
1 CONTINUE
2 K = K + 1
ERROR(K) = EE(I)
3 CONTINUE

N = M/2 + 1

DO 5 NN = 1, N
EMX = ERROR(NN)
I = NN
NI = NN + 1
DO 4 II = Ni, M
IF (ERROR(II) .LE. EMX) GO TO 4
FMX = ERROR(II)
I = II
4 CONTINUE

AV023
AV024
AV025
AV026
AV027
AV028
AV029
AV030
AV031
AV032
AV033
AV034
AV035
AV036
AV037
AV038
AV039
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AV041
AV042
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AV022
AV023
AV024
AV025
AV026
AV027
AV028
AV029
AV030
AV031
AV032
AV033
AV034
AV035
AV036
AV037
AV038
AV039
CONTINUE
ERROR(I) = FPPOR(NN)
ERROR(NN) = EMX
CONTINUE
MIDIAN = ERROR(N)
CUTOFF = 15.*MIDIAN
DO 8 I=1,LS
IF (11 .EQ. 0) GO TO 7
DO 6 J=I,I1
IF (I .EQ. NEG(J)) GO TO 8
6 CONTINUE
7 IF (EE(I) .LE. CUTOFF) GO TO 8
I2 = I2 + 1
K = I1 + I2
NEG(K) = I
8 CONTINUE
IT = 11 + I2
RETURN
END
$IPFTC CUBSS DECK
SUBROUTINE CUBS (X,Y,N)

DIMENSION X(N),Y(N)
DIMENSION A(40),B(40),C(40)
DIMENSION S(40),T(40),U(40)
COMMON/AFUN/C1,C2,C3,C,,ITPSZ,ELM,ETA,DIA,,VISC,BFTA
EQUIVALENCE (A(1),U(1)),(B(1),T(1)),(C(1),S(1))

F(X) = ((A1*X + A2)*X + A3)*X + A4
DF(X) = (3.*A1*X + 2.*A2)*X + A3
D2F(X) = 6.*A1*X + 2.*A2
G(A) = 1./(1. - A**ETA)
DG(B) = ETA/ELM**TERM**(ETA-1.)*B**3
D2G(C,D,E) = C*(ETA - 1. + 2.*ETA*TERM**ETA*D)/E

FROM INPUT TABLE COMPUTE COEFFICIENTS FOR CUBIC SPLINE INTERPOLATION

AND DIFFERENTIATION
CON1 = .3333333
CON2 = .16666667
DXI = X(2) - X(1)
DYI = Y(2) - Y(1)
DI = DYI/DXI
S(1) = CON1*DXI
T(1) = CON2*DXI
U(1) = DI - (((Y(3)-Y(1))/(X(3)-X(1))) + DI)/2.
WM = N-1
DO 2 I=2,NM
DXIM = DXI
DYIM = DIY
DTIM = DI
DXI = X(I+1) - X(I)
DYI = Y(I+1) - Y(I)
DI = DYI/DXI
S(I) = CON1*(DXIM + DXI)
T(I) = CON2*DXI

171
2 \( U(I) = \frac{D(I) - D(I+1)}{S(N)} \)
\( S(N) = \text{CON1} \times DXI \)
\( U(N) = \frac{(D(I) + (D(I+1) + D(I+2)) / (DXI + DXIM) / 2) - D(I)}{S(N)} \)

DO 3 I = 1, NM
TT = T(I)
T(I) = T(I) / S(I)
U(I) = U(I) / S(I)
S(I+1) = S(I+1) - TT * T(I)
3 U(I+1) = U(I+1) - TT * U(I)
U(N) = U(N) / S(N)
A(N) = U(N)
DO 4 J = 1, NM
I = N - J
4 A(I) = U(I) - T(I) * A(I+1)

DO 5 I = 1, NM
DXI = X(I+1) - X(I)
DYI = Y(I+1) - Y(I)
B(I) = DYI / DXI - CON2 * (A(I+1) - A(I)) / DXI
5 C(I) = Y(I+1) - CON2 * A(I+1) * DXI / DXI - B(I) * X(I+1)
RETURN

ENTRY CINP (XI, YI, DY, D2Y)
GO TO (66, 10, 11, 11, 13, 17, 100)

C COMPUTE Y, DY/DX, D2Y/DX2 FROM CUBIC SPLINE COEFFICIENTS

66 DO 6 I = 1, NM
IF (X(I) .GT. XI .AND. XI .LE. X(I+1)) GO TO 7
6 CONTINUE
WRITE (6, 100) XI, X(I), X(N)
100 FORMAT (7H0(CINP), 5X, XI =, F13.5, 17H, X(N) =, F13.5)
7 DXI = X(I+1) - X(I)
A1 = (A(I+1) - A(I)) / DXI / 6.
AIX = A(I) * X(I+1)
AXI = A(I+1) * X(I)
A2 = (AIX - AXI) / DXI / 2.
AIX = AIX / X(I+1)
AXI = AXI / X(I)
A3 = (AXI - AIX) / DXI / 2. + B(I)
AIX = AIX / X(I+1)
AXI = AXI / X(I)
A4 = (AIX - AXI) / DXI / 6. + C(I)

YI = F(XI)
DY = DF(XI)
D2Y = D2F(XI)
RETURN

C COMPUTE Y, DY/DX, D2Y/DX2 FROM INPUT POLYNOMIAL

10 A1 = C1
A2 = C2
A3 = C3
A4 = C4

YI = F(XI)
DY = DF(XI)
D2Y = D2F(XI)
RETURN
COMPUTE Y, DY/DX, D2Y/DX2 FROM INPUT SPECIAL FUNCTION

EXCEPTIONAL CASE AT X=0

11 IF (XI .LE. 0.) GO TO 12
   TERM = XI/ELM
   YI = G(TERM)
   DY = DG(YI)
   D2Y = D2G(DY,YI,XI)
RETURN

12 YI = 1.

FIT A CUBIC THROUGH THE POINTS (0.,Y1), (.05,Y2'), (.05,Y2''), AND (.10,Y3'') IN ORDER TO FIND Y1' AND Y1''

TERM = .05/ELM
   Y2 = G(TERM)
   Y2P = DG(Y2)
   Y2PP = D2G(Y2P,Y2,.05)
TERM = .10/ELM
   Y3 = G(TERM)
   Y3P = DG(Y3)
   Y3PP = D2G(Y3P,Y3,.10)

   DY = (.05*(Y3PP-Y2PP)/(.10-.05)/2 - Y2PP)*.05 + Y2P
   D2Y = Y2PP - .05*(Y3PP-Y2PP)/(-10-05)
RETURN

V=0 CASE - ASSIGNED AREA IS NOT REQUIRED

13 YI = 1.
   DY = 0.
   D2Y = 0.
RETURN

$IBFTC SEARCH DECK
SUBROUTINE SEARCH (F,FOFX,A,X,B)

THIS ROUTINE USES AN OPTIMAL SEQUENTIAL SEARCH TECHNIQUE TO FIND X IN (A,B) SUCH THAT F(X) = FOFX

ASSUMPTIONS
(1) F(X) CONTINUOUS ON THE CLOSED INTERVAL (A,B)
(2) FOFX IS NOT EQUAL TO ZERO

COMMON/SINT/DUM(10),KOUNT,FX

X1 = (2.*A + B)/3.
   KOUNT = 1
   F1 = F(X1)
IF (ABS(1.-F1/FOFX) .GT. 0.0001) GO TO 2
   X = X1
   FX = F1
RETURN

2 X2 = (A + 2.*B)/3.
   KOUNT = KOUNT + 1
   F2 = F(X2)
IF (ABS(1.-F2/FOFX) .GT. 0.0001) GO TO 3
   X = X2
   FX = F2
RETURN
3 DI = F1 - FOFX
   IF (DI*(FOFX-F2) .GT. 0.) GO TO 5
   IF (DI .LT. 0.) GO TO 4
   X2 = A
   KOUNT = KOUNT + 1
   F2 = F(X2)
   IF (F2 .LT. FOFX .AND. ABS(1.-F2/FOFX) .GT. 0.0001) GO TO 5
   X = A
   FX = F2
   RETURN

4 X1 = B
   KOUNT = KOUNT + 1
   F1 = F(X1)
   TP (F1 .GT. FOFX .AND. ABS(1.-F1/FOFY) .GT. 0.0001) GO TO 5
   X = B
   FX = F1
   RETURN

5 X = (X1 + X2)/2.
   KOUNT = KOUNT + 1
   FX = F(X)
   TP (ABS(1.-FX/FOFX) .LE. 0.0001) RETURN
   TP (KOUNT .EQ. 11) RETURN
   TP ((FX-FOFX)*(FOFX-F2) .LT. 0.) GO TO 6
   X1 = X
   GO TO 5
6 X2 = X
   F2 = FX
   GO TO 5
END

$IEPTC MATCO DECK
SUBROUTINE MATRIX
DOUBLE PRECISION G,X
DOUBLE PRECISION EN,ENLN,DELN
LOGICAL TP, HP, CONVG, TV, UV
COMMON/MISCF/P,CPRO,HSUB0,ENN,ENNL,LLMT (15) ,R0 (15)
COMMON/INDEX/TP,HP,EN,NS,I01,CONVG,KMAT,IMAT
COMMON/MATX/G(28,28),X(28)
COMMON/NECC/DUM (8) ,CPSUM,DUM2
EQUIVALENCF (NLN,L),(TP,TV),(HP,UV)
I02 = I01 + 1
I03 = I02 + 1
KMAT = IC3
IF (.NOT. CONVG .AND. TP) KMAT = I02
IMAT = KMAT - 1
C CLEAR MATRIX STORAGES TO ZERO
DO 211 I=1,IMAT
DO 211 K=1,KMAT
G(I,K)= 0.00D0
211 CONTINUE
SSS = 0.
HSUM = 0.
BEGIN SET UP OF ITERATION MATRIX

KK = L
TM = ALOG(PF/ENN)
DO 65 J=1,NS
H = HRT(J)*ENN(J)
F = (HRT(J) - SR(J) + ENLN(J) + TM)*ENN(J)
SS = H-F
TERM1 = H
IF (KMAT .EQ. IQ2) TERM1 = F
DO 55 I = 1, L

CALCULATE THE ELEMENTS R(I,K)

IF (A(I,J) .EQ. 0.) GO TO 55
TERM = A(I,J)*ENN(J)
DO 15 K=I, L
G(I,K) = G(I,K) + A(K,J)*TERM
15 CONTINUE

G(I,IQ1) = G(I,IQ1) + TERM
G(I,IQ2) = G(I,IQ2) + A(I,J)*TERM
IF (CONVG .OR. TP) GO TO 55
G(I,IQ3) = G(I,IQ3) + A(I,J)*F
55 CONTINUE

IF (KMAT .EQ. IQ2) GO TO 64
IF (CONVG .OR. HP) GO TO 59
G(IQ2,IQ1) = G(IQ2,IQ1) + SS
G(IQ2,IQ2) = G(IQ2,IQ2) + HRT(J)*SS
G(IQ2,IQ3) = G(IQ2,IQ3) + (SR(J) - ENLN(J) - TM)*F
GO TO 62
64 G(IQ1,IQ2) = G(IQ1,IQ2) + TERM1
65 CONTINUE

SSS = SSS + G(IQ2,IQ1)
HSUM = HSUM + G(IQ1,IQ2)
G(IQ1,IQ1) = SUMN - ENN

REFLECT SYMMETRIC PORTIONS OF THE MATRIX

ISYM = IQ1
IF (HP .OR. CONVG) ISYM=IQ2
DO 102 I=1,ISYM
DO 102 J=I,ISYM
G(J,I) = G(I,J)
102 CONTINUE

COMPLETE THE RIGHT HAND SIDE

IF (CONVG) GO TO 175
DO 145 I=1, L
G(I,KMAT) = G(I,KMAT) + BO(I) - G(I,IQ1)
G(IQ1,KMAT) = G(IQ1,KMAT) + ENN-SUMN
145 CONTINUE

COMPLETE ENERGY ROW AND TEMPERATURE COLUMN

IF (KMAT .EQ. IQ2) RETURN
IF (HP) ENERGY = HSUB0/TT - HSUM
G(IQ2,IQ3) = G(IQ2,IQ3) + ENERGY
SUBROUTINE GAUSS
SOLVE ANY LINEAR SET OF UP TO 20 EQUATIONS
DOUBLE PRECISION G,X,COEFX(20),SUM,Z
COMMON/MATX/G(28,28),X(28)
COMMON/INDEX/IP,HP,NLM,NS,I01,CONVG,DMAT,IMAT
EQUIVALENCE (IUSE,IMAT)
DATA BIGNO/I.E+38/
C BEGIN ELIMINATION OF NNTH VARIABLE
IUSE1=IUSE+1
6 DO 45 NN=I,IUSE
IF (NN-IUSE) 8,83,8
83 IF(G(NN,NN))31,23,31
C SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW
8 DO 18 I=NN,IUSE
COEFX(I) = BIGNO
IF(G(I,NN).EQ.0.) GO TO 18
COEFX(I) = 0.
DO 10 J=NN,IUSE
SUM = G(I,J)
IF(SUM.LT.0.) SUM=-SUM
IF(J.NE.NN) GO TO 9
Z = SUM
GO TO 10
9 IF(SUM.GT.COEFX(I)) COEFX(I)=SUM
10 CONTINUE
COEFX(I) = COEFX(I)/Z
18 CONTINUE
TEMP = BIGNO
I=0
20 DO 22 J=NN,IUSE
IF (COEFX(J)-TEMP) 87,22,22
87 TEMP=COEFX(J)
I=J
22 CONTINUE
IF(I) 28,23,28
C INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NNTH
C VARIABLE FROM THE REMAINING EQUATIONS
C INTERCHANGE EQUATIONS I AND NN
28 IF(NN-I) 29,31,29
29 DO 30 J=NN,IUSE
Z=G(I,J)
G(I,J)=G(NN,J)
G(NN,J)=Z
RETURN
END
30 CONTINUE

C DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH VARIABLE FROM THE REMAINING EQUATIONS

31 K = NN + 1
   DO 36 J = K, IUSE
      IF(G(NN,NN).EQ.0.) GO TO 23
      G(NN,J) = G(NN,J)/G(NN,NN)
   CONTINUE
   IF(K-IUSE) 88,45,88
88 DO 44 I = K, IUSE
   DO 44 J = K, IUSE
      S(I,J) = G(I,J) - G(I,NN)*G(NN,J)
   CONTINUE
45 CONTINUE

C BACKSOLVE FOR THE VARIABLES

47 J = K + 1
   X(K) = 0.0D0
   SUM = 0.0
   IF(IUSE - J) 51,48,48
48 DO 50 I = J, IUSE
      SUM = SUM + G(K,I)*X(I)
   CONTINUE
51 X(K) = G(K,IUSE) - SUM
   K = K - 1
   IF (K) 47,151,47
23 IUSE = IUSE-1
151 RETURN
END
Figure 1. - Main program (GCKP).
Figure 2. - Subroutine KINP.
Figure 3. - Subroutine PRED.
Calculate $f_i$, the derivative of species $i$ concentration with respect to the integration variable.

Calculate the first derivative of the assigned variable with respect to the integration variable.

Call for partial derivative calculations.

A

Start

Calculate $f_1$, $f_2$, $f_3$ - derivatives of velocity, density, temperature with respect to the integration variable, using assigned area equations.

Calculate $f_1$.

Set $f_2 = 0$.

Constant density case?

Yes

Calculate $f_2$.

Constant temperature case?

Yes

Set $f_3 = 0$.

No

Calculate $f_3$.

Calculate second derivative of area with respect to the integration variable.

Calculate second derivative of pressure with respect to integration variable.

B

Calculate $f_1$, $f_2$, $f_3$ - derivatives of velocity, density, temperature with respect to integration variable, using assigned pressure equations.

Calculate $f_1$.

Set $f_2 = 0$.

Constant density case?

Yes

Calculate $f_2$.

Constant temperature case?

Yes

Set $f_3 = 0$.

No

Calculate $f_3$.

Figure 4. - Subroutine DERV.
Calculate \( a +3 \), the partial derivative of \( f +3 \), with respect to integration variable.

Calculate \( a_2, a_3 \) - partial derivatives of \( f_1, f_2, f_3 \) with respect to the integration variable - using assigned area equations.

Calculate \( a_1, a_2, a_3 \) - partial derivatives of \( f_1, f_2, f_3 \) with respect to the integration variable - using assigned pressure equations.

Set \( \alpha_2 = 0 \).

Figure 4. - Concluded.
Calculate partial derivatives of net reaction conversion rate, gamma, and Mach number squared with respect to velocity, density, temperature, and species concentration.

Calculate \( \beta_{1+3,j} \) - partial derivatives of \( f_1 \) with respect to velocity, density, temperature, and species concentration.

Set \( \beta_{2,j} = 0 \)

Yes

Constant density case?

No

Calculate \( \beta_{2,j} \) - partial derivatives of \( f_2 \) with respect to velocity, density, temperature, and species concentration.

Set \( \beta_{3,j} = 0 \)

Yes

Constant temperature case?

No

Calculate \( \beta_{3,j} \) - partial derivatives of \( f_3 \) with respect to velocity, density, temperature, and species concentration.

Return

Figure 5. - Subroutine PARD.
Figure 6. - Subroutine INTG.
REFERENCES


