COMBUSTION OF HYDROGEN-AIR JETS
IN LOCAL CHEMICAL EQUILIBRIUM

(A Guide to the CHARNAL Computer Program)

by D. B. Spalding, B. E. Launder, A. P. Morse, and G. Maples

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Describes and gives listing in FORTRAN IV for a finite-difference computer program to predict flow properties for turbulent mixing with combustion of a circular jet of hydrogen into a co-flowing stream of air. The program, which is based upon the Imperial College group's PASSA series, solves differential equations for diffusion and dissipation of turbulent kinetic energy and also of the R.M.S. fluctuation of hydrogen concentration. The effective turbulent viscosity for use in the shear stress equation is computed from the equation \( \mu_t = C \rho k^2 / \varepsilon \), where \( C \) is a constant, \( \rho \) is density, \( k \) is turbulent kinetic energy, and \( \varepsilon \) is the dissipation rate. Chemical equilibrium is assumed throughout the flow.
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1. Introduction

The computer program CHARNAL (Calculator of Hydrogen-Air Reactions for NASA Langley) generates finite-difference predictions of turbulent, coaxial hydrogen-air jets undergoing combustion. The jets may be free, as indicated in Figure 1a (in which case the external stream is assumed to extend to arbitrarily large radius from the symmetry axis) or enclosed as in Figure 1b. At any point in the flow the mass fraction of the constituents of combustion is found on the assumption that chemical equilibrium prevails, the constituents being \( \text{H}_2, \text{O}_2, \text{H}_2\text{O}, \text{O}, \text{H}, \text{OH} \) and \( \text{N}_2 \).

The present report details the mathematical and physical basis of CHARNAL, discusses some sample predictions and provides a guide to the computer program itself. Section 2 is concerned with the first of these aspects: the basic conservation equations of momentum, stagnation enthalpy and chemical species are presented first and these are followed by a description of the turbulence and combustion models employed. A user's guide to the computer program appears in Section 3 while definitions of FORTRAN symbols and a listing of the program itself are contained in the Appendices. Thereafter, Section 4 presents and discusses the outcome of some test cases and, finally, Section 5 suggests some directions that further developments to the CHARNAL program might take.
2. The Mathematical and Physical Model

2.1 The Mean Flow Conservation Equations

CHARNAL calculates the steady state distributions within the jet of mean streamwise velocity, temperature and mass fraction of elemental hydrogen by reference to the conservation laws of momentum, energy and chemical species. These laws are expressed in terms of the following set of parabolic partial differential equations expressing respectively the transport of streamwise momentum, stagnation enthalpy and hydrogen mass fraction.

\[
\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial r} - \frac{1}{r} \frac{\partial}{\partial r} \left( \mu r \frac{\partial u}{\partial r} \right) = - \frac{dp}{dr} \quad (2.1-1)
\]

\[
\rho u \frac{\partial \hat{h}}{\partial x} + \rho v \frac{\partial \hat{h}}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left( \mu r \frac{\partial \hat{h}}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left\{ r \left[ (\mu_T - \Gamma_h) \frac{\partial}{\partial r} + \left( \Gamma_k - \Gamma_h \right) \frac{dt}{dr} + \Gamma_j \left( \Gamma_j - \Gamma_h \right) \ h_j \frac{\partial m_j}{\partial r} \right] \right\} \quad (2.1-2)
\]

\[
\rho u \frac{\partial f}{\partial x} + \rho v \frac{\partial f}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left( \Gamma_m r \frac{\partial f}{\partial r} \right) \quad (2.1-3)
\]

The mass fraction of elemental hydrogen, \( f \), is used as a variable for the reason that, unlike \( \text{H}_2 \), even during chemical reaction it remains a conserved property. The method of determining the individual chemical constituents of the flow is described in Section 2.3.

The set of partial differential equations is completed by the continuity equation in which the streamwise and radial velocities are connected by:

\[
\frac{\partial}{\partial x} (\rho u) + \frac{1}{r} \frac{\partial}{\partial r} (\rho vr) = 0 \quad (2.1-4)
\]
In fact CHARNAL solves the parabolic transport equations cast in a Von Mises system of coordinates (i.e., x and stream function as independent variables). This transformation has the effect of eliminating the radial velocity \( v \) from the equations, and, hence no explicit recourse needs to be made to equation (2.1-4).

The temperature of the mixture, \( T \), is obtained from known values of \( h, u \) and the mass fractions of the chemical constituents of the mixture from the expression:

\[
T = \frac{h - u^2/2 - k - \sum_j m_j \left( \Delta h_f - \Delta h_j \right)}{\sum_j m_j C_{pj}}
\]  
(2.1-5)

and \( C_{pj} = \frac{1}{T} \int_0^T C_{pj} dT \)  
(2.1-6)

2.2 The Turbulence Model

The effective turbulent transport coefficients \( \mu_t, \Gamma_h, \Gamma_u \) and \( \Gamma_k \) are determined by means of the \( k-\varepsilon \) model of turbulence which has been presented and applied to numerous turbulent free shear flows in Reference [2]. According to this model the magnitude of the viscosity depends only on the local values of the turbulence kinetic energy, \( k \) the dissipation rate of turbulence energy, \( \varepsilon \) and the fluid density. They are connected by the formula:

\[
\mu_t = C_\mu \rho k^2/\varepsilon
\]  
(2.2-1)

The quantities \( k \) and \( \varepsilon \) are found by way of the following pair of transport equations which are both similar to (and solved simultaneously with) those governing the mean flow:

\[
\rho u \frac{\partial k}{\partial x} + \rho v \frac{\partial k}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left[ \frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial r} \right] + \mu_t \left( \frac{\partial u}{\partial r} \right)^2 - \rho \varepsilon
\]  
(2.2-2)

\[
\rho u \frac{\partial \varepsilon}{\partial x} + \rho v \frac{\partial \varepsilon}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{\mu_t}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial r} \right) + \frac{C_1}{k} \varepsilon \mu_t \left( \frac{\partial u}{\partial r} \right)^2 - \frac{C_2 \rho \varepsilon^2}{k}
\]  
(2.2-3)
The quantities $C_\mu$, $C_1$, $C_2$, $\sigma_k$ and $\sigma_\varepsilon$ are dimensionless and are given the constant values below:

<table>
<thead>
<tr>
<th>$C_\mu$</th>
<th>$C_1$</th>
<th>$C_2$</th>
<th>$\sigma_k$</th>
<th>$\sigma_\varepsilon$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.09</td>
<td>1.43</td>
<td>1.92</td>
<td>1.0</td>
<td>1.3</td>
</tr>
</tbody>
</table>

These values are the same as those recommended in [2]. Equations (2.2-2) and (2.2-3) do not provide a physically exact prescription for finding $k$ and $\varepsilon$. Such a prescription is not possible because the exact equations for $k$ and $\varepsilon$ contain correlations whose magnitude is not directly ascertainable. These correlations are therefore approximated in terms of $k, \varepsilon$ and the mean velocity field; the approximated terms in (2.2-2) and (2.2-3) are the ones with the empirically determined coefficients. Models of the above kind, while being sufficiently simple not to affect computer costs significantly, have been found (see for example, references [2] and [3]) to possess considerable width of applicability, precisely the same model predicting features of both wall and free turbulence. It is probably the best model available at present for the kind of shear flows that CHARNAI is designed to compute.

The transport coefficients in the hydrogen-element and stagnation-enthalpy equations are given by

\[
\Gamma_h = \mu_t/\sigma_h ; \quad \Gamma_m = \mu_t/\sigma_m
\]

In the free jets and in the confined jets (provided the jet has not spread to the pipe wall)

\[
\sigma_h = \sigma_m = 0.7
\]

Once the jet has filled the pipe the effective Prandtl/Schmidt number is obtained from the formula:

\[
\sigma_h = \sigma_m = 0.95 - 0.45 \,(y/R)^2
\]
where \( y \) is distance in the radial direction measured from the pipe wall. The above variation, proposed by Rotta [4] and used by several workers since, is generally in accord with experimental data of the turbulent Prandtl number in fully-developed pipe flow. Note that because the same numerical values are assigned to \( \Gamma_n \) and \( \Gamma_m \), one of the source terms in equation (2.1-2) vanishes.

2.3 The Combustion Model

The equilibrium composition of the hydrogen air mixture can be calculated by reference to the set of reversible reactions:

\[
\begin{align*}
H_2 & \rightleftharpoons H + H \\
O_2 & \rightleftharpoons O + O \\
OH & \rightleftharpoons O + H \\
H_2O & \rightleftharpoons OH + H
\end{align*}
\]

The relative mass fractions of the above constituents are found by presuming that chemical equilibrium prevails at each point in the flow. Thus:

\[
\begin{align*}
m_{H_2}/m_H & = K_1 \\
m_{O_2}/m_O & = K_2 \\
m_{OH}/m_{O2}m_H & = K_3 \\
m_{H_2O}/m_{H2}m_{OH} & = K_4
\end{align*}
\]

where the \( K \)'s are functions of temperature and pressure. In addition we have by definition

\[
x = m_{O_2} + m_O + \frac{H_2}{H_2O} \left(m_{H_2O} \right) + \frac{H_0}{OH} \left(m_{OH} \right)
\]

and

\[
f = m_{H_2} + \frac{H_2}{H_2O} \left(m_{H_2O} \right) + \frac{H}{OH} \left(m_{OH} \right)
\]
In the above equation set, the quantities \( f \) and \( X \) are to be considered known: \( f \) is found from the conservation equation for total hydrogen (equation 2.1-3) and \( X \) is simply OFAC \( 1-f \) where OFAC is the mass fraction of oxygen in the external stream. The equilibrium "constants" \( K_1 \ldots K_4 \) are functions of temperature and pressure. CHARMAL incorporates the dependencies proposed by McBride [5].

Equations (2.3-5) - (2.3-10) thus provide a set of six equations in the six unknowns \( m_{H_2}, m_H, m_{H_2O}, m_{OH}, m_O, m_{O_2} \). The equations are non-linear (indeed, highly non-linear for regions of flow where the fuel/air ratio is nearly stoichiometric); their solution must therefore proceed iteratively. The solution technique adopted is described in Section 3-4.

The mass fraction of \( N_2 \) (which is considered to be entirely inert) is simply \( 1-X-f \).

Because the flow is turbulent, the level of hydrogen and of other variables will be continuously fluctuating about their mean values. The magnitude of the mean square hydrogen fluctuations, \( g \), is found from the following transport equation developed and tested by Spalding [6]

\[
\rho u \frac{\partial g}{\partial x} + \rho v \frac{\partial g}{\partial y} = \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{\mu_r}{\sigma_g} \frac{\partial g}{\partial r} \right) + C_{g1} \mu_t \left( \frac{\partial f}{\partial r} \right)^2 - C_{g2} \rho g \quad (2.3-11)
\]

where the constants \( \sigma_g, C_{g1}, \) and \( C_{g2} \) are assigned the values of 0.7, 2.8 and 2.0 respectively. Solution of the \( g \) equation enables the region of the flame over which stoichiometric conditions occur to be calculated. The inner boundary to this region occurs at a radius from the axis where \( f-g^2 = f_{\text{stoich}} \) and the outer boundary where \( f+g^2 = f_{\text{stoich}} \). The predicted path of these two surfaces for a hydrogen jet burning in an air stream is shown in Figure 10.

3.0 Details of the CHARMAL Computer Program

CHARMAL is a custom-developed version of the Patankar-Spalding PASSA program which, in turn, is a newer, more economical and flexible version of GEMMIX published in Reference [1].

Section 3.1 below gives a brief summary of the general Patankar and Spalding method of solving the boundary layer equations. Section 3.2 lists the major differences between CHARMAL and the original GEMMIX program, while Section 3.3 discusses in detail the listing of the present program (which is to be found in Appendix 2). Section 3.4 is devoted to
a discussion of subroutine LAi'iGLEY, which has been developed exclusively for the current work. Finally Section 3.4 gives overall instructions for the running of the program, in particular the input information that the user must provide.

3.1 The Patankar-Spalding Boundary Layer Procedure

The main features of the computational method are as follows:

(i) The primary differential equations (i.e., the transport equations for \( u, \hat{u}, f, g, k \) and \( \epsilon \)) are transformed so that the independent variables are the longitudinal distance, \( x \) and the dimensionless stream function, \( \psi \) defined as:

\[
\omega = (\psi - \psi_I) / (\psi_E - \psi_I) \tag{3.1-1}
\]

where \( \psi \) itself is obtained from the relation,

\[
\frac{\partial \psi}{\partial y} = \rho u r \tag{3.1-2}
\]

Subscripts I and E refer respectively to the "inner" and "outer" boundaries of the flow; for axisymmetric flows the inner surface is always the one nearer the symmetry axis. The resulting differential equations are all of the basic form,

\[
\frac{\partial \phi}{\partial x} + (a+b\omega) \frac{\partial \phi}{\partial \omega} = \frac{a}{\partial \omega} \left( c \frac{\partial \phi}{\partial \omega} \right) + d, \tag{3.1-3}
\]

where the terms on the left-hand side represent convection by the mean flow and those on the right-hand-side express respectively the diffusion and source of the entity \( \phi \). The coefficients, \( a \) and \( b \) are functions of the entrainment rates, whilst \( c \) involves the effective diffusion coefficient.

(ii) The differential equations are expressed as finite-difference equations, connecting the values of the dependent variables which prevail at the intersection points of a grid defined by lines of constant \( x \) and \( \omega \). These finite-difference equations are formed by integrating the differential equations over small control volumes associated with each grid node.
(iii) The integration proceeds by "marching" downstream, the values of the variables at grid points at the next downstream station being calculated from those at the upstream station and placed into the array locations occupied by the latter. At each forward step, new values are ascribed to \( \psi_E \) and \( \psi_I \), the stream functions at the grid boundaries. These values, together with the continuity equation, determine the geometrical location of the boundaries; and this determination is so arranged that the boundaries enclose all the fluid having a significant value of the shear stress (or other flux) without enclosing appreciably more than this. This feature allows the method to achieve good numerical accuracy without employing an excessively fine grid.

(iv) The finite-difference equations are formulated in an implicit manner, and solved by means of the well-known algorithm for tri-diagonal matrices. This allows large forward steps to be made without instability. The equations are linearized, upstream values of the transport properties being supposed to prevail over the whole of the forward step.

(v) The source terms are usually (but not necessarily) expressed as linear functions of the upstream and downstream values of the dependent variables. For example in the turbulent kinetic equation,

\[
\text{Source of } (k) = \left[ u_t \left( \frac{\partial u}{\partial y} \right) \right]^2 \left( \frac{\partial \varepsilon}{k} \right) U \quad \left[ \frac{T}{k} \right] \quad k_D
\]

where the subscripts \( U \) and \( D \) denote upstream and downstream values. This practice allows large forward step sizes to be used without the onset of inaccuracy or instability.

For further information on the general structure of the solution procedure the reader is referred to Reference [1].

3.2 New and Improved Features of the PASSA family of programs

PASSA programs retain the general width of applicability of the basic procedure, but are arranged to be more economical in terms of both execution time and storage capacity. The principal differences between the new method and its predecessor may be summarized:

(i) In PASSA, the finite-difference equations are solved sequentially. That is, for any variable, the coefficients of finite-difference equations are formed and the equations solved before moving on to the next differential equation. This contrasts with the former procedure where the coefficient for all the differential equations were stored simultaneously and then the matrix was inverted for each equation in turn.
(ii) The PASSA program does not make use of "slip nodes" in the formulation of the difference equations at the boundaries. In the earlier program, these nodes were employed to obtain the correct gradients of the dependent variables at the edge regions. PASSA treats the nodes near each flow boundary in exactly the same way as the interior nodes.

(iii) In PASSA all diffusivities and gradients of the dependent variables, such as the viscosity and the velocity gradient are evaluated at the actual grid nodes, whereas in the earlier program these quantities were evaluated at the edges of the control volumes (which by definition were midway between individual nodes in terms of \( \omega \)). PASSA also contains the option of using castellated profiles instead of linear variations of \( \phi \) between the grid nodes.

3.3 Details of the CHARNAI Program

A flow diagram for CHARNAI is provided in Table 1. The program consists of a MAIN program and a number of subroutines of which the most important are AUX, STRIDE, OUTPUT and LANGLEY.

3.3-1 The MAIN Program

MAIN contains the starting and stopping points of the computation and communicates directly or indirectly with all the other subroutines. It comprises twelve "chapters", each performing a specific function in the computational procedure. The most important of the operations are mentioned below:

Chapter 1. Values are assigned to various indices which control aspects of the computation throughout the program. The main categories are:

(i) the specification of the number of grid nodes and differential equations to be solved.

(ii) the nature of the flow boundaries (wall, free boundary or axis of symmetry)

(iii) the control of input, and

(iv) the designation of the flow type (number of chemical species, nature of initial conditions, etc.). This topic is discussed in more detail in Section 3.4.

Chapter 2. This chapter selects the primary dependent variables and auxiliary quantities to be calculated in the program. Comment cards have been included here for the user's benefit.

Chapter 3. Material constants such as molecular weights and the universal gas constant, turbulence parameters and Prandtl/Schmidt numbers are assigned values. The S.I. system of unit is used throughout the program. Subroutine LANGLEY
is called to provide data for the enthalpies of the chemical species and the equilibrium reaction constants.

Chapter 4. Specified here are the flow geometry (plane or axisymmetric), inclination of the streamlines to the axis of symmetry and the cross-stream distances for the initial profiles.

Chapter 5. The initial profiles are read in from data cards. Values are assigned to the axial velocity, absolute temperature and species concentrations at the grid nodes. All the data input are in dimensionless form, having been normalized with the largest value of each dependent variable at the initial station. In developing CHARMAH, fifteen test cases (specified by NASA Langley) have been run which required two different types of initial-profile specification.

(i) Continuous profiles (Test Case nos. 1-10, 13)

Figure 2a shows the initial-velocity-profile typical of these test cases. The two streams are separated by a wake region caused by the interaction of the boundary layers on the dividing wall. Since the velocity is uniform near the jet centreline, the computation starts from a mixing-layer region with entrainment at the inner flow boundary until this boundary grows to the axis of the jet (i.e., the end of the potential core).

(ii) Step profiles (Test Case nos. 11-12, 14-15)

In these four test cases, the boundary layers on the dividing wall are ignored and a step-change in the velocity profile is assumed (see Figure 2b). In these cases, the computation starts from a very thin mixing layer (with an assumed linear velocity profile) in the immediate vicinity of the step-change.

The initial profiles of turbulent kinetic energy are then evaluated by assuming a constant ratio with the shear stress (as expressed by the mixing length hypothesis), whence

\[ k = 3.33 \left( \frac{h_m}{y} \right)^2 \]  \hspace{1cm} (3.3-1)

The dissipation rates are then given by the Prandtl-Kolmogorov relationship

\[ \epsilon = \frac{k^{3/2}}{\sqrt{\epsilon}} \]  \hspace{1cm} (3.3-2)
Both the mixing length and dissipation length scale are assumed to be proportional to a typical width of the shear region. The scheme adopted is shown in Figure 2.

The free-stream turbulent kinetic energy is taken as $4 \times 10^{-4}$ of the square of the free-stream velocity. The same constant is used to determine the initial profile of concentration fluctuations from the local concentrations of hydrogen element, i.e., $g/f^2 = 4 \times 10^{-4}$.

A variable of major importance in the computational procedure is OFAC, which is the ratio of oxygen element to nitrogen in the outer stream, since this ratio is assumed to be constant across the flow.

Chapter 5 also calls subroutine LANGL2 to evaluate the initial enthalpy profile.

Chapter 6. The dimensionless stream function array is filled by integration of the profiles of density and velocity according to equations (3.1-1) and (3.1-2). The density is obtainable from the ideal gas relationship,

$$\rho = \frac{pM}{RT} \quad (3.3-3)$$

where the mean molecular weight of the mixture, $M$ is given by,

$$\frac{1}{M} = \sum \frac{m_j}{W_j} \quad (3.3-4)$$

Subroutine STRID1 is called to evaluate useful quantities relating the individual $M$'s.

Chapter 7. This marks the starting point of the main computation; it is the point to which control is returned after the execution of each forward step. The most important functions of this chapter are,

(i) to call LANGL3, which employs the chemical reaction constants relevant to the upstream conditions (i.e., pressure and temperature) to determine the local mass fractions,

(ii) to call LANGL4 to calculate the temperatures corresponding to these concentrations (by way of the upstream specific heats) and
(iii) to evaluate the density profile from the local temperatures and mass concentrations

Chapter 8. This chapter performs two main tasks. First it fixes the size of the forward step and secondly it calls subroutine STRID2 to calculate transverse distances. The forward step is usually made proportional to the width of the flow, with the constant of proportionality small in the initial region to avoid instabilities at the start of the calculation. For confined flows, the streamwise pressure gradient, which is a source term in the axial momentum equation, is not known a priori. CHARNAL adopts the same non-iterative practice employed in CERNIX, (see reference [1]). An estimate of the pressure change to be experienced over a forward step is obtained by reference to a 1-dimensional analysis. This usually results in the area of the flow differing from the pipe cross sectional area at the end of the forward step. However by adjusting the level of dp/dx over the next step the difference in area can be kept negligible (typically 0.01% of the pipe area).

Chapter 9. This chapter fixes the conditions at the flow boundaries. Only when a boundary is a wall must information (either the value of \( \phi \) or its diffusional flux) be specified at this point. (In the case of a free boundary, the relevant information is provided in STRID3 (based on the free-stream source terms) while at an axis of symmetry, the zero gradient condition usually applies).

Chapter 10. The first chapter of AUX is called to determine the effective viscosity (regarded as the sum of the turbulent and \( \mu \)oninar viscosities) at each node and to formulate the source term based on the axial pressure gradient. For a free boundary the entrainment rate is calculated via the degenerate form of the conservation equation for whichever of the dependent variables shows the largest changes near the edge of the flow. The entrainment is subject to certain controls to prevent the formation of 'tails' to the profiles and to prevent the onset of instability.

Chapter 11. This chapter deals with the output of information. At the first step, subroutine OUTP 1 is called to print-out information regarding the initial conditions. At certain axial positions (designated in Chapter 1) OUTP 2 is called to print-out such quantities as the entrainment rates, jet spreading rate, centreline values of the velocity, temperature and species concentrations and the fluxes of the dependent variables. Also OUTP 3 may be called (not necessarily at the same stations) to print-out the profiles of quantities of interest (velocity, temperature, concentrations, etc.).
Chapter 12. The last chapter terminates the execution after a specific axial distance has been covered. Otherwise, control is returned to Chapter 7.

3.3-2 AUX, STRIDE and \&IF

Only brief description is provided of these general-purpose subroutines as they are similar in structure and function to the correspondingly named subroutines in GENMIX (reference [1]). Subroutine AUX is called initially from Chapter 10 of \&AIN to provide the effective viscosities at the grid nodes. Chapter 2 is subdivided into five parts, one for each of the dependent variables other than the velocity. Each section evaluates the appropriate effective diffusivity and formulates the source arrays and is called in turn from STRID 3 as the finite difference equations are solved sequentially. The source terms for turbulent kinetic energy, dissipation rate and mean square concentration fluctuations are linearized according to equation (3.1-4), while that for stagnation enthalpy is loaded entirely into the upstream array.

Subroutine STRIDE is divided into four parts, of which the first two are largely preparatory, while the latter two contain the core of the numerical method of the program. STRID 0 merely sets to zero arrays such as those for the dependent variables and auxiliary quantities. It is here that the decision is made as to whether to employ linear (\(KAST(j) = 0\)) or castellated (\(KAST(j) = 1\)) profiles between the grid nodes. STRID 1 evaluates useful relationships between the values of \(\omega\) at neighboring nodes, these of course remaining constant for the whole of the calculation as the grid is always constrained to lie between limits of \(\omega=0\) and \(\omega=1\). STRID2 calculates the cross-stream distances at each axial station with but minor differences from the original program [1]. STRID3 contains the basic finite-difference formulation and technique of solution of the differential equations. Although different in appearance from the version published in reference [1], the differences are largely only ones of arrangement. It is not proposed to dwell on points of detail here, but suffice it to say that STRIDE is a subroutine which the user has very seldom any need to change. STRID3 terminates by determining conditions at the flow boundaries and by initiating the forward step.

Subroutine HF provides wall-function relationships to relate the fluxes (diffusional and convective) through the wall with the values of the dependent variables at the near-wall nodes. As appropriate to the high-Reynolds-number form of the turbulence model employed in this work, the wall functions are based on the assumption of a log-law velocity profile in the fully turbulent region of the flow.

3.3-3 OUTPUT and related Subroutines

Subroutine OUTPUT is divided into three parts, concerned respectively with the print-out of initial values of interest and station and profile variables. It communicates with PROFIL and thence with subroutine
PLOTS, which together may be used to provide non-dimensional plots of the profiles. OUTP1 reads alphanumeric information from data cards to provide the headings for the print-out. The meaning of the quantities printed from OUTP2 and CUTP3 is given in Appendix 1. Subroutine OUTP2 performs the useful function of checking for the overall conservation of fluxes of the dependent variables; in this analysis the concentration of hydrogen element is a conserved property as are the axial momentum and stagnation enthalpy (but for free flows only).

There is a large number of comment cards in OUTPUT, PROFIL and PLOTS to assist the reader in understanding the interlinkage between these subroutines. PROFIL is used to normalize the profiles and communicates with PLOTS which scales both the abscissa (transverse distance) and ordinate ($\phi$ values) of the dimensionless plots into the range 0 to 1, (with negative values printed as zero). Either the normalized (IPROF = 1) or the full dimensional (IPROF = 2) values of the dependent and auxiliary variables may be printed out in OUTP3. If the former approach is adopted, the full dimensional values are still printed at the first and last nodes (designated 1 and NPI respectively). The cross-stream distances $Y(I)$ are treated in this way, the first quantity printed being the radius of the internal flow boundary and the last the distance between the internal and external boundaries. Subroutine YINT may be called at any point in the program and is merely an interpolation subroutine. It is useful in the determination of such quantities as the half-width of the jet or locating the exact position where the value of an entity $\phi$ is a linear combination of the values of $\phi$ at the inner and outer boundaries of the flow.

3.3-4 Subroutine LANGLEY

Subroutine LANGLEY has been developed exclusively for the present work and is subdivided into four parts, whose purposes are respectively

(i) the loading of the individual species and the chemical equilibrium constants for the stipulated reactions.

(ii) the evaluation of the initial enthalpies by simple interpolation amongst the input data.

(iii) the calculation of the species mass fractions by solution of six simultaneous equations.

(iv) the evaluation of the cross-stream temperatures from the enthalpies and the upstream specific heats.

Data for enthalpies and chemical-reaction constants are those proposed by McBride [5]. The enthalpy of each species may be written in the form
where \( \Delta h_f, T \) denotes the heat of formation of the species at the reference temperature. It is usual to take the datum of enthalpy as zero at a reference temperature of 298.15°K, whence

\[
h = \int_{298.15^\circ K}^{T} C_p \, dT + \Delta h_f, 298.15^\circ K \nonumber
\]

\[
= \int_{0^\circ K}^{T} C_p \, dT + \left[ \Delta h_f, 298.15^\circ K - (h_{298.15^\circ K} - h_{0^\circ K}) \right] \nonumber
\]

\[
\equiv \overline{C_p} \, T + H_0 \quad (3.3-7)
\]

where \( \overline{C_p} (\equiv 1/ \int_{0^\circ K}^{T} C_p \, dT) \) denotes a mean specific heat and \( H_0 \) is the composite of the remaining terms. Values of \( h \) are read in at intervals of 100°K for temperatures of up to 6000°K, together with the value of \( H_0 \) for each species. The mean specific heats are then evaluated from equation (3.3-7) and stored (see Appendix 1 for array locations).

LANGL2 is called to obtain the initial enthalpy profile by linear interpolation of the \( h/T \) data. The enthalpy of the mixture is then given by

\[
h = \sum m_j h_j
\]

\[
= \sum m_j C_{p,j} T + \sum m_j H_{0,j} \quad (3.3-8)
\]
LANGL1 is also used to store data for the chemical equilibrium for the four reactions involved in the combustion process. These are again taken from McBride [5] and are in the form of constants relating the partial pressures of the individual species, i.e., for the reaction

\[ aX + bY = Z \]

(implies the formation of 1 unit of substance Z from (a) units of X and (b) units of Y), the partial pressures of the species are linked by a constant, \( K_p \) given by the relation

\[ K_p = \frac{p_z}{p_x^a p_y^b} \]  \hspace{1cm} (3.3-10)

[Because \( K_p \) (which is a function of temperature) varies markedly, numbers on the data cards refer to \( \log_{10} K_p \). \( K_p \)'s may be transformed into constants relating the species mass fractions by use of the ideal gas law, whence

\[ K_m = \frac{m_z}{m_x^a m_y^b} = K_p (pW)^{a+b-1} W_z / \left( \frac{W_x^a W_y^b}{W} \right) \]  \hspace{1cm} (3.3-11)

where \( W_j \) denotes the individual molecular weights and \( W \) is the mean molecular weight of the mixture. Values of \( (K_p W_z/W_x^a W_y^b) \) are stored for each reaction involved. In using Equation (3.3-11), it is to be remembered that the total pressure, \( p \) must always be expressed in atmospheres.

LANGL3 evaluates the concentrations of the individual species by six simultaneous algebraic equations, viz.

\[ K_{m,1} = \frac{m_O^2}{m_H^2} \]  \hspace{1cm} (3.3-12)

\[ K_{m,2} = \frac{m_H^2}{m_O} \]  \hspace{1cm} (3.3-13)

\[ K_{m,3} = \frac{m_O^m}{m_H^m} \]  \hspace{1cm} (3.3-14)
\[ K_{m,4} = \frac{m_{H_2O}}{m_{H}^2} \]  

\[ x = m_{O_2} + m_0 + \frac{w_{O}}{w_{H_2O}} m_{H_2O} + \frac{w_{O}}{w_{OH}} m_{OH} \]  

\[ f = m_{H_2} + m_H + \frac{w_{H}}{w_{H_2O}} m_{H_2O} + \frac{w_{H}}{w_{OH}} m_{OH} \]  

in which the equilibrium constants (which are functions of pressure, temperature and concentrations) are based on the upstream conditions, since the temperatures can only be calculated once the mass fractions have been found.

The first function performed by LAMGL3 is to evaluate the reaction constants and mean specific heats by linear interpolation amongst the input data. Equations (3.3-12) to (3.3-17) are then solved iteratively until convergence to within 1% is obtained for all species present to an extent of more than 10^-6, or until the number of iterations exceeds a certain limit. The actual iterative scheme is of necessity rather elaborate since the relative concentrations of the species can vary markedly. The following practices are adopted

(i) The concentration of nitrogen is easily calculable as \((1-GFAC)(1-f)\).

(ii) The concentrations of the remaining species at the previous axial position are used as a first estimate of the downstream values.

(iii) The equations for \(f\) and \(X[=OFAC(1-f)]\) are examined to determine the largest term on the right-hand side of each. For example, suppose that \(\frac{w_{O}}{w_{H_2O}} \cdot m_{H_2O}\) and \(m_{H_2}\) are the largest quantities.
(iv) Using the values of \( m_{H_2O} \) and \( m_{H_2} \), equations (3.3-12) to (3.3-15) can then be solved to determine the concentrations of the remaining four species.

(v) \( m_{H_2O} \) and \( m_{H_2} \) can then be re-evaluated from Equations (3.3-16) and (3.3-17).

(vi) The right-hand sides of the \( X \) and \( f \) equations are then re-examined and the next iteration cycle made to operate on the two largest quantities.

(vii) Iteration is repeated until the convergence criteria are satisfied or the number of iterations becomes excessive.

Convergence is usually rapid (2 iterations), but instability occurs whenever two of the terms in either of the additive equations [(3.3-16) and (3.3-17)] become of approximately equal magnitude. This happens (a) at high temperatures (> 3000°K) where the concentration of atoms approaches that of the molecules and (b) in the region of the stoichiometric point where the concentration of combustion products becomes large. In the flows under investigation, the maximum predicted temperature was approximately 2600°K; (b) was therefore the main source of instability. It often happened that on successive iterations different constituents were the largest terms in Equations (3.3-16) and (3.3-17). Oscillatory rather than convergent behavior would then result. However, under-relaxation of the species concentrations between successive iteration cycles generally achieved the required degree of convergence within 12 iterations. A warning message is printed out whenever the iteration process fails to converge within this limit.

When the species concentrations have been found, LANGL4 is called to evaluate the cross-stream temperatures. These are obtained from enthalpy profile via the relationship,

\[
T = \left( h - \sum j m_j H_{0,j} \right) / \sum j m_j C_p j, \tag{3.3-18}
\]

for which the mean specific heats are evaluated in LANGL3 on the basis of the upstream temperatures. One could regard this value of temperature as a first estimate of the actual value, since a more accurate estimate could be obtained by re-evaluating the \( K_m \)'s to obtain new values of the constituent mass fractions, a new mean specific heat, and from (3.3-18) a new \( T \). LANGLEY does not incorporate such an iteration cycle (though it would not be difficult for a user to add). Instead, under-relaxation of the temperature between upstream and downstream stations damps out any
temperature spikes which would otherwise appear at positions close to the stoichiometric point.

3.4 Use of the Present Program

CHARNAL solves 6 simultaneous partial differential equations and employs typically 25 nodes (although the storage blocks have been dimensioned to allow for as many as 40). The program is written in basic CDC Fortran language and requires approximately 12 seconds compilation time on a CDC 6600 machine (FUN compiler). Linear profiles are assumed for the variation of the dependent variables between the grid nodes and a typical forward step size of 0.1 times the local shear layer width is employed. Approximately 15 axial steps can be executed per second. Conservation of the individual fluxes is generally good to within +0.1%. In the present work, the profiles have been printed out in full dimensional form and are plotted at only one axial position (corresponding to the end of the potential core region). The program has a modest storage requirement, needing only approximately 24000 decimal storage locations.

The remainder of this section is concerned with the information that the user has to provide via data cards in subroutines MAIN and LANGLEY. In Chapter 1 of MAIN, control indices which have to be set are:

(i) Details of the grid and nature of the flow

KASENO : Test case number

NEQ : number of differential equations

N : number of grid nodes

KASE : type of flow; = 1 (free jet), = 2 (confined flow)

KIN : specification of internal flow boundary
   = 1 (wall)
   = 2 (free)

KEX : specification of external flow boundary
   = 3 (axis of symmetry)

KONFIN : denotes presence of confining duct wall;
   = 1 (wall present), = 2 (no wall)

IN, IO, IH : denote presence of individual species;
   = 0 (not present), = 1 (present)

WR : number of reactions

NS : number of chemical species
INUF : nature of initial profiles = 0 (continuous) = 1 (step-change)

XI : initial axial distance (in nozzle diameters)

XULAST : last axial distance (in nozzle diameters)

YIN : radius of internal flow boundary (in nozzle diameters)

YOUT : diameter of jet nozzle

RDUCT : radius of confining duct

PRESS : static pressure (in atmospheres)

TA : maximum temperature at initial station

uin : maximum velocity at initial station

YW1 : extent of inner shear region (in nozzle diameters) i.e., distance from axis of symmetry to minimum in velocity profile

uW1 : velocity at position denoted by YW1

I'll : grid node corresponding to YW1 and uW1

TDUCT : temperature of duct wall (for confined flows only)

(ii) Output parameters

XSTAT, NPROF, NPLOT : number of axial stations between print-out of (i) station variables, (ii) profile variables and (iii) non-dimensional plots

XSTAT, XPROF, XPLOT : the corresponding axial distances (in nozzle diameters)

The next data cards are read in from LAMGCL and refer to the chemical equilibrium constants for the 4 (NR) reactions and the enthalpies for the 7 (NS) species; these must be in the same order as the auxiliary variables are data-typed in Chapter 2 of MAIN. The data are read in at intervals of 100°K for temperatures up to 6000°K, so that for example, HT (2.35) refers to the enthalpy of species 2 (oxygen) at 3500°K.

Further data cards provide the initial profiles in Chapters 4 and 5 of MAIN. For those test cases involving step profiles, only the cross-
stream distances are required together with the values of velocity, temperature and species concentrations in each free stream. Appropriate profiles for the thin mixing layer under consideration are then generated internally. For cases with continuous profiles, the cross stream distances, velocities, temperatures and the concentrations (of those species whose presence has been previously indicated) are read in and converted to full dimensional form.

The remaining data cards contain alphanumeric data which are used to provide headings for the print-out. These are read in from LANGL1 and supply information on

(i) the test case number and description (2 cards)
(ii) the dependent variables of the calculation (10 cards)
(iii) the chemical reactions assumed (NR cards)
(iv) the species present (NS cards) and
(v) their chemical symbols (1 card).

4. Discussion of Sample Predictions

To examine the general capabilities of CHARIMAL, fifteen test cases, prescribed by NASA Langley, involving the mixing and combustion of a hydrogen jet with various coaxial gas streams have been computed. The computer outputs of these runs have been forwarded separately to the contracting agency. In this section we examine various features of the numerical predictions, the main attention being given to test cases 1 and 4, for which the prescribed initial profiles of velocity and temperature are given in Table 2.

Jet velocity and temperature profiles for Case 1 at four downstream stations are shown in Figures 3 and 4. The wake region of the profile arises from the wall boundary layers that are present on wall of the hydrogen pipe. As the shear flow develops downstream the jet spreads and the velocity level falls. Notice that the jet region is still present at X/D = 50*. From the temperature profiles shown in Figure 4 the region of

* In this case there is a slight momentum deficit in the shear flow so, far enough downstream, the velocity within the shear flow would be everywhere less than the free stream velocity.
combustion is clearly evident through the sharp peak in the temperature level. It is seen that the maximum temperature remains virtually constant as the shear flow develops downstream.

The decay of mass fraction $m_{H_2}$ is shown in Figure 5. Comparison is drawn between predictions for Case 1 and Case 3 in which initial conditions are similar to Case 1 except that the surrounding gas is nitrogen (which is non-reacting) rather than air. Also shown is a prediction from reference [2] obtained, with the same model of turbulence as that used here, for a non-reacting hydrogen air jet with velocity ratio similar to Case 1 but where the total temperature of the external stream was only 300°C; the density of the air is thus approximately 3 times that for Case 1. (The prediction from [2] was in satisfactory agreement with the experimental data of Eggers [7], which for clarity are omitted from Figure 5). Clearly, because of the smaller density of the external stream, the rate of dilution of the hydrogen jet is appreciably slower for the present test cases than in the reference [2] computation. The decay rate is seen to be faster for the hydrogen/nitrogen mixing than for the hydrogen/air jet. This behavior is attributable to the fact that combustion does not take place in Case 3, hence temperatures within the jet are lower and density correspondingly higher (if reaction is suppressed in test Case 1 the rate of decay of $m_{H_2}$ is nearly identical with that of Case 3).

Distributions of some of the important dependent variables affecting the flow development are shown in Figures 6-9. The station selected is 20 jet diameters downstream from the exit (through the profile shapes vary only slightly with streamwise position). It is seen from Figure 6 that the turbulence energy $k$ reaches its maximum value at the axis. This is generally a feature of axisymmetric jets and is in contrast with the behavior of plane jets where the peak energy level occurs near the position of maximum shear stress. (The different behavior is attributable to the more rapid axial decay that occurs in the round jet). Profiles of mean and mean-square-fluctuation levels of hydrogen element are shown in Figure 7. It is noted that the rapid decrease in the level of fluctuations in the outer part of the jet is the reason that the $f_+$ line in Figure 10 lies much closer than does $f_1$ to the stoichiometric line.

The calculated distributions of radicals and atomic species are shown in Figure 9. Their level is very sensitive to temperature and this is why a logarithmic scale is adopted for the ordinate. The peak calculated concentration of OH is approximately 1% by mass, about ten times as large as the maximum mass fractions of O and H. The corresponding distributions of molecular concentrations ($H_2$, $N_2$, $O_2$ and $H_2O$) are shown in Figure 10. The figure includes predictions for "case 8" as well as Case 1. Initial conditions for the former differ from Case 1 principally through the presence of appreciable water vapor in the external stream. It is seen that, as a result, the level of $H_2O$ is higher throughout the jet than in Case 1 and
the level of \( H_2 \) and \( O_2 \) correspondingly lower. The hydrogen profiles for the two cases are virtually identical.

Turning now to the confined flows, it must be said at the outset that, for the conditions prescribed in the test cases, the rate of spread of the jet was so slow that in no case do the predictions show the jet having reached the pipe wall by the downstream end of the field of computation. There are, nevertheless some effects of the flow confinement through these are mainly seen in the velocity development (Figure 5 shows that the centreline mass fraction of \( H_2 \) is only slightly diminished by the presence of the pipe wall). Because the flow is supersonic, the exothermic reaction leads to a rise in static pressure with distance along the duct. This adverse pressure gradient causes a reduction in the level of velocity as the jet develops along the duct; velocity profiles at three stations are shown in Figure 3. The variation of centreline velocity with \( x \) is shown in Figure 11 for four test cases. Note that, for Case 6 in which confined streams of hydrogen and nitrogen mix without chemical reaction, the variation of \( U \) is virtually identical with the corresponding unconfined flow, Case 3.

To convey an impression of the capabilities of CHARNAL for predicting both free and wall flows, Figure 12 shows predictions obtained for the mixing of subsonic \( H_2/air \) streams. In order to achieve a faster rate of spread than in any of the prescribed test cases the initial core jet velocity is set to five times that of the surrounding stream; moreover the diameter of the confining pipe has been reduced to 49 mm. Figure 12 shows the development of the velocity and temperature profiles along the duct. The jet reaches the pipe wall about 33 jet diameters from the start and by 40 diameters downstream the velocity profile looks generally like that found in pipe flow. By 75 diameters combustion is virtually complete and the temperature is uniform except in the vicinity of the wall.

5. Suggestions for Further Extensions and Refinements of CHARNAL

CHARNAL provides numerical predictions of how combustion will proceed in reacting hydrogen jets. It ought to be emphasized, however, that this behavior will not necessarily coincide - nor, sometimes, even approximate to - the actual development of the flow. Validation and comparison of the predicted behavior with available experimental data ought therefore to precede any use of the program for detailed design calculations. Without in any way preempting the outcome of such a series of comparisons, it may be helpful to indicate briefly some areas where improvements to the present version could be made. These are outlined briefly below.

(i) Combustion model

While the equilibrium combustion model embodied in CHARNAL may be adequate in high temperature flows, it evidently leads to unrealistically fast rates of combustion at low temperatures. The argument in favor of
assuming chemical equilibrium is that the chemical constituents may then be determined from solution of algebraic rather than differential equations with corresponding savings in computer time. The savings however are relatively modest because the algebraic set of equations are significantly non-linear and require iteration at each node to solve.

A further important point is that only with a differential reaction scheme can one take proper account of the role of species fluctuations on the progress of the chemical reaction. It is thus recommended that in the future CHARNAL be extended to include a finite-rate reaction model. At the same time consideration should be given to the inclusion of a more elaborate reaction model than that implied by equations (2.3-1 - 2.3-4).

Turning now to the turbulence-model, it must be said that there are a number of areas of uncertainty. The Proceedings of the Langley Conference on Free Shear Flows (of which reference [2] forms a small part) suggests that the Mach number of the fluid may exert an influence on the shear flow development at any rate for flows, such as the mixing layer, where turbulence levels are high. It is also known (see Reference [2]), that the quantity $C_u$, although assumed constant in the present work, increases appreciably when the average level of turbulence energy production at any station becomes small compared with the dissipation rate. Now it happens that in many of the test cases examined by CHARNAL the momentum excess due to the hydrogen jet moving faster than the external stream is just about balanced by the momentum deficient of the boundary layers on the nozzle walls. This situation leads to a rapid decrease in rate of energy production with $x$.

If these circumstances are the ones that prevail in the majority of tests to which CHARNAL is to be put it would therefore be desirable to replace the present constant $C_u$ by the elaborate dependency on energy production: dissipation rates presented in [2] (associated with the model designated $ke2$ in that reference). Such a change would produce a somewhat faster rate of spread of the jet than does the present model from about 15 diameters downstream of the jet exit to the point at which the jet reaches the pipe wall (if present). There is in addition the possibility that combustion will affect in some way the turbulence transport. There seems no conclusive evidence on this point yet but this perhaps mainly reflects the lack of sufficiently well documented experimental data.

A separate, albeit related, point to those discussed in the above paragraphs is the importance of accurate upstream profiles. An abiding feature of weak shear flows such as those tested by CHARNAL is their inability to 'forget' the nature of their origin. For example the far field behavior of axisymmetric wakes depends crucially on the shape of the wake-generating object. It follows, therefore, that in order to obtain reliable predictions of the present hydrogen/air jets it is necessary that the upstream values of the mean velocity and turbulence quantities be known accurately. However, no information was provided on the profiles of turbulence quantities and so "best estimates" had to be made estimates,
however, that may give the wrong levels of $k$ or $\varepsilon$ by a factor of two or three. It would certainly be helpful in clarifying the degree of realism provided by the present model of turbulence if a few more experiments could be performed for conditions similar to those examined by Eggers [7] in which especial attention was given to a full documentation of the upstream flow conditions.

6. References


7. Nomenclature

$C_\mu, C_1, C_2, C_{g1}, C_{g2}$ constant coefficients appearing in turbulence model.

$\overline{C}_{pj}$ mean specific heat of species $j$.

$D_j$ diameter of jet nozzle.

$f$ mass fraction of elemental hydrogen.

$g$ mean square fluctuations in $f$.

$h$ enthalpy.
\( \hat{h} \)  
sto\n stagnation enthalpy.

\( \Delta h \)

difference between enthalpy of species at 298.15\(^{\circ}\)K and 0\(^{\circ}\)K.

\( \Delta hf \)  
heat of formation of species \( j \).

\( k \)  
kinetic energy of turbulence.

\( \epsilon \)  
dissipation length scale \( k^{3/2}/\epsilon \).

\( l_m \)  
mixing length.

\( m_j \)  
mass fraction of species \( j \).

\( p \)  
static pressure.

\( r \)  
radius (measured from axis of jet).

\( R \)  
radius of pipe enclosing jets.

\( T \)  
temperature.

\( u \)  
local streamwise velocity.

\( \overline{uv} \)  
local turbulent shear stress.

\( v \)  
velocity normal to axis of jet.

\( W_j \)  
molecular weight of species \( j \).

\( x \)  
distance along center axis

\( X \)  
mass fraction of elemental oxygen.

\( Y_{wl1}, Y_{wl2} \)  
effective widths of shear flow, see Figure 2.

\( r \)  
effective turbulent flow transport coefficient (subscript denotes diffused quantity).

\( \epsilon \)  
rate of turbulence energy dissipation.

\( \mu_t \)  
turbulent viscosity.

\( \rho \)  
density of mixture.
σ effective Prandtl/Schmidt (subscript denotes diffused quantity).

Ψ any of the primary dependent variables.

ψ stream function defined by equations (3.1-2).

ω dimensionless stream function defined by equation (3.1-1).

**Subscripts**

E conditions on the jet axis.

D downstream.

E external edge of shear flow.

i value of quantity at initial station.

I internal edge of shear flow.

ref reference value of quantity.

U upstream.

∞ conditions prevailing beyond the outer edge of shear flow.
Table 1 Flow Chart of CIIUACAL Program.

**AUX**
1. Laminar and turbulent viscosities, axial pressure gradient source term
2. Diffusive and source terms for variables other than velocity

**LANGLEY**
1. Loading of thermodynamic data and chemical equilibrium constants, evaluation of mean specific heats
2. Initial entropy distribution
3. Evaluation of local equilibrium constants and mean specific heats, solution of six simultaneous equations for local mass fractions
4. Determination of local temperatures

**MAIN**
1. Parameters and control indices
2. Dependent and auxiliary variables
3. Material and turbulence constants
4. Flow geometry (transverse distances)
5. Initial conditions
6. Omega distribution
7. State of main integration loop (thermodynamic properties)
8. Spreading rate, axial pressure gradient, forward step
9. Boundary conditions
10. Transverse coefficients, entrainment
11. Output
12. Continuation/termination

**OUTPUT**
1. Initial conditions and headings for output
2. Station variables, calculation of fluxes of dependent variables
3. Profile variables

**PROFIL**
1. Output of individual profiles, assignment of arrays for plotting subroutine

**PLOTS**
1. Plotting of dimensionless profiles

**STRIDE**
0. Zeroing of important arrays
1. Omega relationships
2. Calculation of transverse distances
3. Setting up of finite difference coefficients, solution of matrices, adjustment of free boundary conditions, calculation of dependent variables or fluxes at flow boundaries, initiation of forward step

**YINT**
1. Interpolation subroutine

**W F**
1. Wall function relationships between near-wall values of $\phi$ and boundary fluxes
Table 2: Initial Profiles for Cases 1 and 4

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<th>Temp.</th>
<th>Velocity</th>
<th>Mass Fraction</th>
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Free Stream
a. Free

b. Confined

Wall Heat Fluxes and Friction Computed from Here Onwards

c. Finite Difference Grid

Figure 1. The Flow Geometry Treated by CHARNAL
At A, $U = 0.9 \ U_I + 0.1 \ U$
At B, $U = U$
At C, $U = 0.9 \ U_E + 0.1 \ U$

$y_{W1}$ = Characteristic Shear Width for Inner Region of Flow (Axis $\rightarrow$ B)
$y_{W2}$ = Characteristic Shear Width for Outer Region of Flow (B $\rightarrow$ Free Stream)

a. Continuous Velocity Profile

At A, $U = 0.9 \ U_I + 0.1 \ U_E$
At B, $U = 0.9 \ U_E + 0.1 \ U_I$

$y_{W1}$ = Characteristic Shear Width for Thin Mixing Layer

b. Step-Change Velocity Profile

Figure 2. Initial Velocity Profiles and Characteristic Flow Widths
Figure 3. Velocity Profiles
Figure 4. Temperature Profiles (Test Case No. 1)

- a, x/D_j = 6.13 (End of Potential Core)
- b, x/D_j = 10
- c, x/D_j = 20
- d, x/D_j = 50
Figure 5. Decay of Centreline Mass Fraction of Hydrogen

- a, Test Case No. 1 (H$_2$/air) Unconfined
- b, Test Case No. 3 (H$_2$/nitrogen) Unconfined
- c, Test Case No. 4 (H$_2$/air) Confined
- d, Ref [2] Computation of Non Reacting H$_2$/air Jets
Figure 6. Profiles of Velocity, Turbulent Kinetic Energy and Reynolds Shear Stress (Test Case No. 1)
Figure 7. Profiles of Temperature and Density and Hydrogen Element Concentration (Mean and Fluctuating) Test Case Number 1
Figure 8. Profiles of Radical and Atomic Concentrations (Test Case No. 1)
Figure 9. Mass Fractions of Molecular Species

(a) Case No. 1 \( x/D_j = 20 \)

(b) Case No. 8 (H\(_2\) Vitiating Air) \( x/D_j = 15 \)
Figure 10. Location of Flame Front and Jet Half-Width (Test Case Number 1)
a. Test Case No. 1 (H₂/air) Unconfined
b. Test Case No. 4 (H₂/air) Confined
c. Test Case No. 3 (H₂/nitrogen) Unconfined
d. Test Case No. 6 (H₂/nitrogen) Confined

Figure 11. Decay of Centreline Velocity Excess
Figure 12. Velocity and Temperature Profiles in Ducted Subsonic Jet. Initial Profiles
(a) \( x/D_j = 0 \), (b) \( x/D_j = 20 \), (c) \( x/D_j = 40 \), (d) \( x/D_j = 75 \)
Appendix 1: Listing of Fortran Variables
Appendix 1. Listing of Fortran Variables

Listed below are some of the most important Fortran variables used in the computer program. To prevent an excessive list, attention has been confined to those variables which are neither (a) self-evident in meaning, (b) indicated by comment cards in the program, (c) discussed in Section 3.5 or (d) connected solely with the finite difference formulation of the equations. Arrays are shown with the maximum numerical values of their subscripts.

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>AK</td>
<td>constant of proportionality in near-wall mixing length formulation, ( \varepsilon_m = \kappa y_G ).</td>
</tr>
<tr>
<td>ALMG</td>
<td>constant of proportionality in free shear layer mixing length formulation, ( \varepsilon_m = \lambda y_G ).</td>
</tr>
<tr>
<td>AMACH</td>
<td>Mach number, ( u/(\gamma RT)^{1/2} ).</td>
</tr>
<tr>
<td>CE1, CE2</td>
<td>constants in the dissipation rate equation</td>
</tr>
<tr>
<td>CFA</td>
<td>conversion factor from calories/gram, mole to joules/kg.</td>
</tr>
<tr>
<td>CFAC</td>
<td>pressure ( \times ) molecular weight of mixture</td>
</tr>
<tr>
<td>CG1, CG2</td>
<td>constants in mean square concentration fluctuations equation.</td>
</tr>
<tr>
<td>CLINE</td>
<td>local centreline mass fraction of molecular hydrogen ( \times ) initial value.</td>
</tr>
<tr>
<td>CHU</td>
<td>constant in Prandtl-Kolmogorov viscosity formulation, ( \nu_T = C_\mu \rho k^2/\varepsilon )</td>
</tr>
<tr>
<td>CONST</td>
<td>constant of proportionality, ( - \frac{UV}{k} = C_\mu^{1/2} )</td>
</tr>
<tr>
<td>CPBAR(7,60)</td>
<td>mean specific heats of chemical species at intervals of 100°K.</td>
</tr>
<tr>
<td>CPFIN(10)</td>
<td>mean specific heats of chemical species at upstream temperatures.</td>
</tr>
<tr>
<td>CSALFA</td>
<td>cosine of angle of inclination of streamlines to axis of symmetry.</td>
</tr>
<tr>
<td>Fortran Symbol</td>
<td>Significance</td>
</tr>
<tr>
<td>---------------</td>
<td>--------------</td>
</tr>
<tr>
<td>DPDX</td>
<td>axial pressure gradient, ( \frac{\partial p}{\partial x} )</td>
</tr>
<tr>
<td>DUDY (40)</td>
<td>mean velocity gradient, ( \frac{\partial u}{\partial y} )</td>
</tr>
<tr>
<td>DX</td>
<td>forward step size</td>
</tr>
<tr>
<td>DXLIM</td>
<td>limit of entrainment rates (bound to size of forward step)</td>
</tr>
<tr>
<td>DYHA</td>
<td>growth parameter of jet, ( \frac{dy}{dx} ) (see also YHA)</td>
</tr>
<tr>
<td>DDYHA</td>
<td>( \frac{d}{dx} (\frac{dy}{dx}) )</td>
</tr>
<tr>
<td>EHUL (40)</td>
<td>laminar viscosity, ( \mu )</td>
</tr>
<tr>
<td>EHUT (40)</td>
<td>turbulent viscosity, ( \mu_T )</td>
</tr>
<tr>
<td>ENTH (40)</td>
<td>static enthalpy, ( h )</td>
</tr>
<tr>
<td>F (10,40)</td>
<td>dependent variables (see Chapter 2 of MAIN)</td>
</tr>
<tr>
<td>FA1</td>
<td>constant for determination of free-stream turbulent kinetic energy and profile of mean square concentration fluctuations</td>
</tr>
<tr>
<td>FA2</td>
<td>constant of proportionality in a free shear layer dissipation length scale formulation, ( \ell_c = \lambda y_G )</td>
</tr>
<tr>
<td>FACI</td>
<td>location where ( f-g \frac{\partial}{\partial x} = f_{\text{stoich}} )</td>
</tr>
<tr>
<td>FACE</td>
<td>location where ( f+g \frac{\partial}{\partial x} = f_{\text{stoich}} )</td>
</tr>
<tr>
<td>FACH</td>
<td>location where ( f = f_{\text{stoich}} )</td>
</tr>
<tr>
<td>FRA</td>
<td>constant of proportionality between forward step size and width of shear layer</td>
</tr>
<tr>
<td>FS (10,40)</td>
<td>auxiliary variables (see Chapter 2 of MAIN)</td>
</tr>
<tr>
<td>FSTOICH</td>
<td>stoichiometric fuel composition</td>
</tr>
<tr>
<td>GAM (40)</td>
<td>effective diffusion coefficient</td>
</tr>
<tr>
<td>Fortran Symbols</td>
<td>Significance</td>
</tr>
<tr>
<td>----------------</td>
<td>-------------</td>
</tr>
<tr>
<td>GAMMA</td>
<td>ratio of principal specific heats, $C_p/C_v$</td>
</tr>
<tr>
<td>GASCON</td>
<td>universal gas constant</td>
</tr>
<tr>
<td>HO (10)</td>
<td>the quantities $\Delta h = h_{298.15^\circ K} - (h_{298.15^\circ K} - h_{0^\circ K})$ (see Section 3.3-4)</td>
</tr>
<tr>
<td>IAX</td>
<td>axial step number corresponding to end of potential core region</td>
</tr>
<tr>
<td>IEND</td>
<td>axial step corresponding to point where jet edge reaches duct wall</td>
</tr>
<tr>
<td>INDE (10)</td>
<td>indices denoting nature of boundary conditions</td>
</tr>
<tr>
<td>INDI (10)</td>
<td>= 1 ($\phi$ stated), = 2 (gradient $\phi$ stated)</td>
</tr>
<tr>
<td>IPD</td>
<td>turbulence model parameter; = 3 (use of plane flow constants), = 1 or 2 [see Launder et al (2)]</td>
</tr>
<tr>
<td>IPROF</td>
<td>profile index; = 1 (normalized values), = 2 (full dimensional values)</td>
</tr>
<tr>
<td>ISTAR (40)</td>
<td>number of iteration cycles allowed for convergence at each node</td>
</tr>
<tr>
<td>ISTEP</td>
<td>axial step number</td>
</tr>
<tr>
<td>J1</td>
<td>species with largest concentration in equation (3.3-16)</td>
</tr>
<tr>
<td>J2</td>
<td>species with largest concentration in equation (3.3-17)</td>
</tr>
<tr>
<td>KRAD</td>
<td>flow geometry index; = 1 (plane), = 2 (asixymmetric)</td>
</tr>
<tr>
<td>N</td>
<td>number of grid nodes, $n$</td>
</tr>
<tr>
<td>N+1</td>
<td>$n+1$</td>
</tr>
<tr>
<td>N-1</td>
<td>$n-1$</td>
</tr>
<tr>
<td>ORAC</td>
<td>ratio of oxygen element/nitrogen in outer stream</td>
</tr>
<tr>
<td>OH (40)</td>
<td>non-dimensional stream function</td>
</tr>
<tr>
<td>P (40)</td>
<td>static pressure</td>
</tr>
<tr>
<td>PEI</td>
<td>change in stream function across flow, $\psi_E - \psi_I$</td>
</tr>
<tr>
<td>Fortran Symbols</td>
<td>Significance</td>
</tr>
<tr>
<td>----------------</td>
<td>-------------</td>
</tr>
<tr>
<td>PR (10)</td>
<td>molecular Prandtl/Schmidt numbers</td>
</tr>
<tr>
<td>PRDRP</td>
<td>pressure drop, $p_i - p$</td>
</tr>
<tr>
<td>PRT (10)</td>
<td>turbulent Prandtl/Schmidt numbers</td>
</tr>
<tr>
<td>PSIE</td>
<td>value of stream function at external boundary $\psi_E$</td>
</tr>
<tr>
<td>PSII</td>
<td>value of stream function at internal boundary $\psi_I$</td>
</tr>
<tr>
<td>PSIR</td>
<td>value of stream function at duct wall $\psi_R$</td>
</tr>
<tr>
<td>QE</td>
<td>wall heat transfer rate</td>
</tr>
<tr>
<td>R (40)</td>
<td>distance from axis of symmetry ($= r_i + y \cos \alpha$)</td>
</tr>
</tbody>
</table>
| RC (5,60)      | chemical equilibrium constants for each reaction at intervals of 100°CK  
[N.B. RC (5,1) contains constants for the global reaction, $H_2 + \frac{1}{2}O_2 = H_2O$] |
<p>| RCON (10)      | chemical equilibrium constants at upstream conditions |
| REXD           | dimensionless excess radius in pressure gradient formulation for confined flows |
| RFLOH          | flow radius (see REXD) |
| RJE (10)       | diffusive flux at external boundary |
| RJI (10)       | diffusive flux at internal boundary |
| RJTE (10)      | total flux (convective and diffusive) at external boundary |
| RJTI (10)      | total flux (convective &amp; diffusive) at internal boundary |
| RME            | mass entrainment rate (radius mass flow rate) |
| RMI            | mass entrainment rate (radius mass flow rate) at internal boundary |
| ROUBAR         | mass flux for confined flows ($= \text{mass flow rate/}\text{X-sectional area of duct}$) |
| RTW (40)       | turbulence frequency (dissipation rate/turbulent kinetic energy), $\varepsilon/k$ |</p>
<table>
<thead>
<tr>
<th>Fortran Symbols</th>
<th>Translation</th>
</tr>
</thead>
<tbody>
<tr>
<td>SCH (40)</td>
<td>Prandtl/Schmidt number array for near-wall flows</td>
</tr>
<tr>
<td>SD (40)</td>
<td>storage location for &quot;downstream&quot; source terms</td>
</tr>
<tr>
<td>SU (40)</td>
<td>storage location for &quot;upstream&quot; source terms</td>
</tr>
<tr>
<td>TAUE</td>
<td>shear stress at wall</td>
</tr>
<tr>
<td>TBAR</td>
<td>bulk temperature ($\int_{\text{duct}} r U T , dy / \int_{\text{duct}} r U , dy$)</td>
</tr>
<tr>
<td>TLINE</td>
<td>local centreline temperature/initial value</td>
</tr>
<tr>
<td>UBAR</td>
<td>bulk velocity ($= \int_{\text{duct}} r U^2 , dy / \int_{\text{duct}} r U , dy$)</td>
</tr>
<tr>
<td>UEIN</td>
<td>initial centreline velocity excess ($u_e - u_\infty$)</td>
</tr>
<tr>
<td>ULINE</td>
<td>limit on entrainment at external boundary (to prevent formation of profiles with 'long tails')</td>
</tr>
<tr>
<td>ULINEINITI</td>
<td>limit on entrainment at external boundary (to prevent formation of profiles with 'long tails')</td>
</tr>
<tr>
<td>VMIX</td>
<td>reciprocal of molecular weight</td>
</tr>
<tr>
<td>HM (10)</td>
<td>molecular weight</td>
</tr>
<tr>
<td>HX</td>
<td>concentration of oxygen element</td>
</tr>
<tr>
<td>XAX</td>
<td>length of potential core (in nozzle diameters)</td>
</tr>
<tr>
<td>XD</td>
<td>axial distance at downstream station</td>
</tr>
<tr>
<td>XU</td>
<td>axial distance at upstream station</td>
</tr>
<tr>
<td>XUD</td>
<td>upstream axial distance/jet nozzle diameter</td>
</tr>
<tr>
<td>Y (40)</td>
<td>transverse distance from internal flow boundary</td>
</tr>
<tr>
<td>YHA</td>
<td>jet half-width, $y_{0.5}$</td>
</tr>
</tbody>
</table>
C PROGRAM CHANNL (INPUT, OUTPUT: TAPES=INPUT, TAPE=OUTPUT)
C
C SPALDING AND PATANKAR PASSA PROGRAMME FOR BOUNDARY LAYER FLOWS
C MODIFIED BY A. MOHSE FOR PREDICTION OF CONFINED/FREE HYDROGEN-AIR
C MIXTURES FOR LANGLEY RESEARCH CENTER, U.S.A. JUNE 1973
C
C DIMENSION THETA (40)
COMMON/GENERAL/CSALFA, DPDX, DX, ENTH (40), F (10, 40), FS (10, 40), GI (30),
I GAMES, GAMS (40) I IF (IN, INDI (10), INDI (10) I ISTEP, IUTRIP, ITEST, KEA, K1,
2KRAD, NNEC, NPL, UNI (40), UND (40), BON (40), BOK (40), CAST (10), PHI (40), PSII
3P (40), R (40), RH0 (40), RHI (10), RJI (10), RPKRMI, SD (40), SU (40), VM (10),
4XD, XI, Y (40), YDF (40), YE, YJ, RJTE (10), RJTI (10)
COMMON/GRAD/RFL0, READ, KASE
COMMON/CJC/JU, JX, JY, JZ, JH, JG, JF, JLE, JGJ, JB
COMMON/CLUS/JH3, JH2, JH1, JH0, JH, JG, JF, JLE, JGJ, JB
COMMON/CT/JXY/HX, ALMG, CMU, CMUIN, CE1, CE2, CG1, CG2, CPI, PRXY (40),
1DOSY (40), EMUL (40), EMUT (40), IPD, PR (10), PRT (10), RHO, RT (40)
COMMON/OUTP/IX, IEND, YIN, YOUT, YHA, YYYA, YYYRA, RPKRMI, KP, KS, KT,
1KASEPO, KSTAT (20), XPROF (20), XPLOR (20), PRESS
COMMON/CWRF/Y (2), IINF (2), EWall, H
COMMON/TPLOT/XSTAT (20), XSTAT (20), YTAPE (10), YPLOT (10), YPLOT (10), YPLOT (10),
1YPM (10), YPMR (10), YOUT (40), IPROF
COMMON/CPTRF/IO2, IN2, IH2O, IFA, NS, AG, AGO, WSU, AST, GASCON, GAM1
C
C CHAPTER 1
C
C PARAMETERS AND CONTROL INDICES
READ (5, 1150) KASEPO, NPNO, KASE, INSTAT, NPROF, NPLUT, IH1, KIN, KEA, KWIN
1, INP, IP2, IH2O, NR4, NS, IUNF
READ (5, 1150) XI, XULAST, YIN, YOUT, RPKRMI, PRESS, TA, UN
IF (INF .EQ. 0) READ (5, 501) YW1, UW1, IW1
IF (KASE .EQ. 2) READ (5, 500) TDKCT
PRESS = PRESS * 1. * 15
XI = XI * YOUT
XULAST = XULAST * YOUT
YIN = YIN * YOUT
DPDX = 0
READ (5, 1152) (XSTAT (1), I = 1, NSTAT)
READ (5, 1152) (XPROF (1), I = 1, NPROF)
READ (5, 1152) (XPLOR (1), I = 1, NPLUT)
XPROF (NPROF + 1) = XSTAT (NSTAT + 1) = XPLOR (NPLUT + 1) = 1. E + 30
CALL STR100
LAX = 10000
IF (FN0 = 100000) IEN0 = 0
LASTD = 20000
IPROF = 2
KP = 1
KS = 1
KT = 1
ULIMI = 10
ULIMR = 10
DXXR = 0.05
FA = 0.9
FAI = 0.85
C ***LARGER FORWARD STEP FOR TEST CASE NO. 16 TO COVER LONGER DISTANCE
IF (KASEPO .EQ. 16) FAI = 0.125

C
Do 14 J=1,NEW
14 IXDE(J)=1
IXDE(JA)=2
IRUF(1)=IRUF(2)=0
IVCF=2

******************************************************************************

CHAPTER 2

******SELECTION OF DEPENDENT VARIABLES

DATA JU,JK,JU,JHS,JA,JG,UTE,JLE,JUV,JB/1,2,3,4,5,6,7,8,9,10/

C
C F(JU,i) KINEMATIC ENERGY OF TURBULENCE
C F(JK,i) DISSIPATION RATE
C F(JHS,i) STAGNATION ENTHALPY
C F(JA,i) MASS FRACTION OF HYDROGEN SPECIES (H2,H,H2O,OH)
C F(JG,i) MEAN SQUARE CONCENTRATION FLUCTUATIONS (OF H ELEMENT)
C F(UTE,i) ABSOLUTE TEMPERATURE
C F(JLE,i) DISSIPATION LENGTH SCALE
C F(JUV,i) REYNOLDS STRESS CORRELATION (UV)
C F(JB,i) MASS FRACTION OF SPECIES B

C

******AUXILIARY VARIABLES

C
C FS(JH2,i) CONCENTRATION OF H2
C FS(JH,i) CONCENTRATION OF H
C FS(JOH,i) CONCENTRATION OF OH
C FS(JH2O,i) CONCENTRATION OF H2O
C FS(JO,i) CONCENTRATION OF O
C FS(JN2,i) CONCENTRATION OF N2

DATA JH2,JH,JOH,JH2O,JH,JO,JN2/1,2,3,4,5,6,7/

C

******MOLECULAR WEIGHTS (AND THEIR RATIOS)

DATA (WM(J),J=1,7)/2.016,32.0,17.008,18.016,1.008,16.0,28.016/
WM0=WM(J0)/WM(JOH)
WMH20=WM(JH2O)/WM(JOH)
WM0=1.*WMH20

******************************************************************************

CHAPTER 3

******CONSTANTS

C ********MATERIAL CONSTANTS (S.I. UNITS)

RAS=9314.
GAMMA=1.4

C

******CHEMICAL EQUILIBRIUM CONSTANTS AND ENTHALPIES

CALL LANGLE1

C

******TURBULENCE CONSTANTS

AK=4.
ALMG=1.1
CMUIN=0.09
CONST1=SQRT(CMUIN)
CMU=CMUIN
CF=1.43
CF2=1.42
CF=7.8
CF2=7.0

C

******SPECIFICATION OF PRANDTL/SCHMIDT NUMBERS

PRT(JU)=1.0

50
PRT(JK)=1.0
PRT(JN)=1.3
PRT(JHS)=.7
PRT(JA)=.7
PRT(JG)=.7
DO 40 J=1,NEQ
40 PR(J)=1.0
FA1=4.0E-04
FA2=875
FALL=9.
H=9

CHAPTER 4

SPECIFICATION OF GEOMETRY

KRAU=2
CSALFA=1.
R(I)=YIN
NFAO(5*500) (Y(I),I=1,NP1)
DO 40 I=1,NP1
IF(INF.EQ.1) Y(I)=.1*Y(I).
40 Y(I)=Y(I)+YOUT-YIN
IF(KFAU.EQ.2) GO TO 183
DO 182 I=1,NP1
182 R(I)=1.
GO TO 181
181 DO 200 I=1,NP1
200 R(I)=R(I)+Y(I)*CSALFA

CHAPTER 5

INITIAL CONDITIONS

181 DO 450 I=1,NP1
450 PI=EXPRESS
IF(INF.EQ.1) GO TO 723

CONTINUOUS PROFILES

YJ=YJ+YOUT
YJ=YJ-YIN
YJ=YJ+YJ
READ(5*500) (F(JU,I),I=1,NP1)
READ(5*500) (F(JTE,I),I=1,NP1)
READ(5*500) (FS(JH2,I),I=1,NP1)
IF(INP.EQ.1) READ(5*500) (FS(JH20,I),I=1,NP1)
IF(INP.EQ.1) READ(5*500) (FS(JH20,I),I=1,NP1)

MASS FRACTION OF HYDROGEN ELEMENT

DO 105 I=1,NP1
105 F(JA,I)=FS(JH2,I)+FS(JH,I)+W00*FS(JH20,I)+W00*FS(JOH,I)

RATIO OF OXYGEN ELEMENT TO NITROGEN IN OUTER STREAM

OFAC=FS(JN2,NP1)+W00*FS(JH20,NP1)
OFAC=OFAC/(OFAC+FS(JN2,NP1))

CONVERSION OF INITIAL PROFILES

DO 45 I=1,NP1
45 F(JA,I)=F(JU,I)*WIN

TURBULENT KINETIC ENERGIES BY MIXING LENGTH HYPOTHESIS

DO 108 I=2,N

51
C DEFINE CHARACTERISTIC SHEAR LAYER WIDTHS
    UREF=F(JU,I)+F(JU,I-1)
    DO 1062 I=1,NP1
    IF(F(JU,I).LT.UREF) GO TO 1063
1062 CONTINUE
    YW2=Y(I-1)-(Y(I)-Y(I-1)) * (UREF-F(JU,I-1))/(F(JU,I)-F(JU,I-1))
    YW2=ALMG*YW2
    IF(KASENO.EQ.16) GO TO 8702
    UREF=F(JU,I)+F(JU,NP1)
    DO 1064 I=IW1,NP1
    IF(F(JU,I).GT.UREF) GO TO 1065
1064 CONTINUE
    YW3=Y(I-1)-(Y(I)-Y(I-1)) * (UREF-F(JU,I-1))/(F(JU,I)-F(JU,I-1))
    YW3=ALMG*YW3
8702 IF(KASENO.EQ.16) YW3=YW2
    DO 1066 I=1,1
1066 F(JK,I)=CONST*YW2*YW2*DY(I)
    DO 1067 I=1,NP1
1067 F(JK,I)=CONST*YW3*YW3*DY(I)
    DO 1068 I=1,NP1
    AKMIN=FA1*F(JU,I)*F(JU,I)
1068 F(JK,I)=MAX1(F(JK,I),AKMIN)
C DISSIPATION RATES
    YW2=YW2/ALMG*FA2
    YW3=YW3/ALMG*FA2
    DO 1069 I=1,1
1069 F(JD,I)=F(JK,I)*SQRT(F(JK,I))/YW2
    DO 1070 I=IW2,NP1
1070 F(JD,I)=F(JK,I)*SQRT(F(JK,I))/YW3
    GO TO 417
723 CONTINUE
C STEP PROFILES
    READ(5,500) UI,UE,TE,02E,AN2E,H20E
    NP1=NP1/2
C CONSTRUCT LINEAR VELOCITY PROFILE
    DO 11 I=1,NP1
    YHAT=Y(I)/Y(NP1)
    F(JU,I)=UT+YHAT*(UE-UI)
    IF(I.GT.NP1/2) GO TO 454
    F(JT,I)=TI
    FS(JH2,I)=1.
    FS(JH2,I-1)=0.
    FS(JH2,I-2)=0.
    FS(JH2,I+1)=0.
    FS(JH2,I+2)=0.
    GO TO 11
454 F(JTE,I)=TE
    FS(JH2,I)=0.
    FS(JH2,I-1)=02E
    FS(JH2,I-2)=AN2E
    FS(JH2,I-3)=H20E
    11 F(JA2,I)=FS(JH2,I)+FS(JH2,I-1)+20E*FS(JH2,I)+T0*FS(JOH,I)
    OFAC=FS(JN2,NP1)+W00*FS(JH2,NP1)
    OFAC=OFAC/(OFAC+FS(JN2,NP1))
C ***TURBULENT KINETIC ENERGIES
DO 472 I=2,N
472 F(JK,I)=UGRAD
DO 473 I=1,NP1
AKMIN=FA1*F(JU,I)+F(JK,I)
473 IF(F(JK,I).LT.AKMIN) F(JK,I)=AKMIN
ALNTH=FA2*ALNTH
C ***DISSIPATION RATES
DO 474 I=1,NP1
474 F(JD,I)=F(JK,I)*SORT(F(JK,I))/ALNTH
C ***STAGNATION ENTHALPIES
DO 417 I=1,NP1
CALL LANGLE2
417 F(JH5,I)=ALNTH(I)+1.5*F(JU,I)+2*F(JK,I)
C ***MEAN SQUARE CONCENTRATION FLUCTUATIONS (OF H ELEMENT)
DO 12 I=1,NP1
12 F(JO,I)=FA1*F(JA,I)+F(JA,I)
C************************************************************
CHAPTER 6
C*****************OMEGA DISTRIBUTION
DO 50 I=1,NP1
VMIX=0.
DO 107 J=1,NS
107 VMIX=VMIX+FS(J,I)/H(J)
RHO(I)=P(I)/GASCON/VMIX/F(JT,I)
50 THEETA(I)=RHO(I)*F(JU,I)*R(I)
DO 50S I=2,NP1
ZETA(I)=THEETA(I)*THEETA(I-1)*(Y(I)-Y(I-1))
505 OM(I)=OM(I-1)+ZETA
PSII=PHTO(I)*F(JU,I)*YIN
IF(KRAD.EQ.2) PSII=S*PSII*YIN
PSIE=OM(NP1)+PSII
PEI=OM(NP1)
DO 50A I=2,NP1
50A OM(I)=OM(I)/PEI
CALL STRID1
C******************************************************************************
CHAPTER 7
C**********THERMODYNAMIC AND TURBULENCE PROPERTIES (START OF MAIN LOOP)
106 CONTINUE
IF(ISLTP.GE.IAX) KIN=3
IF(ISLTP.GE.IEND) KEX=1
C ***LIMITS ON SPECIES MASS FRACTION
FAMIN=1.E-30
FAMAX=1.
DO 455 I=1,NP1
455 F(JA,I)=AMIN(F(JA,I),FAMAX)
C ***LIMITS ON TURBULENCE PROPERTIES
FGMIN=1.E-30
FKMIN=1.E-30
DO 600 I=1,NP1
600 F(JG,I)=AMAX(F(JG,I),FGMIN)
FKMAX=F(JU,I)*F(JU,I)
C *** LOCAL MASS FRACTIONS
CALL LANGL3
C *** LOCAL PRECUES AND TEMPERATURES
DO 601 I=1,NP1
P(I)=EP(I)+DP
601 F(JHS(I))=F(JHS(I))-5*F(JU(I))**2-F(JK(I))
CALL LANGL4
DO 602 I=1,NP1
TF(DBG(I))=F(DBG(I))
602 CONTINUE
C*** SPREADING RATE
C*** STREAM FUNCTION AT DUCT WALL
IF (ISTEP.EQ.0) GO TO 239
DYHA=(YHA-YHALS)/(XU-PXU)
DDYHA=(OUHA-DYHAV)/DYHA
239 CONTINUE
C*** STREAM FUNCTION AT DUCT WALL
CALL STRIN2
IF (ISTEP.EQ.0) GO TO 1370
IF (KASE.EQ.2) GO TO 1370
C*** STREAM FUNCTION AT DUCT WALL
PSI=PSIE**2*PHQ(NP1)*P(JU,NP1)*(RDUCT**2-R(NP1)**2)
ROUHAR=2.*PSI/RDUCT**2
1370 IF (KEX.EQ.1) KONFIN=1
GO TO (71,72)*KONFIN
71 IF (ISTEP.EQ.0) RDUCT=R(NP1)
IF (IVCF.EQ.2) GO TO 1338
C*** PASSA VERSION OF PRESSURE GRADIENT FOR CONFINED FLOWS
C*** CALCULATION OF PRESSURE ADJUSTMENT
C *** VISION WITH GRID FILLING THE DUCT
IF (ISTEP.EQ.0) GO TO 72
ADUCT=5*(RDUCT*RDUCT-R(1)**2)
AFLOW=5*PN(NP1)*P(NP1)-4*(1)**2
PSINIF=PFI
54
ROUHAR=PSI*DIFF/ADUCT
HRAH=0.
DO 73 I=2,N
73 HRAH=HRAH*5**HOM(I)*F(JU,I)
ROBAR=ROURAH/UBAR
UDP=1./((ROBAR*F(JU,I)-RJI(JU))*DX/ADUCT/UBAR)
UDRODP=ROHBAR/GAMMA/PRESS
DROU=ROU*URBAR*(AFLO*ADUCT-1.)
DP=DRU/(ROBAR*UDP*UDRODP)
IFAC=IFAC*DP/UBAR+.1.
C ***ADJUSTMENT OF VELOCITY, PRESSURE AND DENSITY
DO 74 I=1,NP1
F(JU,I)=F(JU,I)*IFAC
P(I)=P(I)*DP
74 RH0(I)=RH0(I)*((1.+GAMMA*DP/P(I))
DPX=DPX*DP/DX
C ***RECALCULATION OF DISTANCES
CALL STRID2
GO TO 72
C ***GENMIX VERSION OF PRESSURE GRADIENT FOR CONFINED FLOWS
133a STORE=-TBAR
TRAN=0.
UBAH=0.
DO 1340 I=2,N
TRAR=TRAR*5**HOM(I)*F(JTE,I)
1340 TRAR=TRAR*5**HOM(I)*F(JU,I)
IF(ISTEP.GE.IEND) RFLOW=IR(NP1)
IF(ISTEP.GE.IEND) GO TO 9719
TBAR=(PSI*F(JTE,I)*PEI*TBAR*(PSIR-PSIE)*F(JTE,NP1))/PSIR
UBAR=(PSI*F(JU,I)*PEI*UBAR*(PSIR-PSIE)*F(JU,NP1))/PSIR
IF(ISTEP.GE.IEND) GO TO 72
DP=ROUHAR+UBAR*(1.-STORE/TBAR)
RFLOW=SQRT((R(NP1)**2+2.*(PSIR-PSIE)/(RHO(NP1)*F(JU,NP1))))
9719 CONTINUE
IF(ISTEP.GE.IEND) DP=-ROUHAR*UBAR*(1.-STORE/TBAR)
REXD=(HFLOW-ROU*CT)/ROU*T
DP=DP-FA*ROUHAR*UBAR*REX
IF(ISTEP.GE.IEND) DP=DP-2.*RJE(JU)/R(NP1)**2*DX
DP=DP/(1.-ROUHAR*UBAR/P(I))
DPX=DPX/DP/DX
C ***FORWARD STEP
73 DX=FA*DY(NP1)
IF(INF.EQ.1) DX=FA*DY(NP1)
IF(INF.EQ.1) DX=DX*FLOAT(ISTEP+1)/50.
IF(INF.EQ.1) DX=DX*FLOAT(ISTEP-IEND+9)
IF(INF.EQ.1) DX=DX*FLOAT(ISTEP-IEND+9)
IF(ARS(REXD).GT.0.05) DX=DX*0.05/ABS(REXD)
DX=AMX1(DX*XULAST-XU)
XD=XU+DX
C***************************************************************
CHAPTER 9
C CHECKS ADJUSTMENT OF BOUNDARY CONDITIONS
C FREE BOUNDARY VALUES ADJUSTED IN STRIDE (3)
IF(KIN.EQ.2) GO TO 95
RMI=0.
IF(KMTEU.EQ.2) R(I)=0.
YIN=0.
PSII=0.
95 IF(KFX.EQ.1) GO TO 106
F(JU,NP1) = 0.
RJF(JA) = 0.
F(JK,NP1) = 0.
F(JD,NP1) = 0.
F(JG,NP1) = 0.
F(JTE,NP1) = TDUC
T = NP1
CALL LANGI2
F(JHS,NP1) = ENTH(NP1)

CHAPTER 10

TRANSPORT AND ENTRAINMENT PROPERTIES

CALL AUX(JU)

ENTRAINMENT CONTROL

ENTRAINMENT ATTENTION TO VELOCITY AND TEMPERATURE CHANGES

IF(KIN*NE,*2) GO TO 94
RME=RE/PRT(JA)
RAT=ABS((F(JU,2)-F(JU,1))/(F(JU,NP1)-F(JU,1)+1.E-30))
AMNI=ABS((F(JU,N)-F(JU,NP1))/(F(JU,NP1)-F(JU,1)+1.E-30))
RAT=AMAX(RAT,AMNI)

IF(RAT<LT,ULIM) RME=RMI*RAT/ULIM

94 IF(KEX*NE,*2) GO TO 97
RME=RE/NP1+Y(NP1)-Y(NM1))
RME=RME/PRT(JA)
RAT=ABS((F(JU,N)-F(JU,NP1))/(F(JU,NP1)-F(JU,1)+1.E-30))
AMNI=ABS((F(JTE,N)-F(JTE,NP1))/(F(JTE,NP1)-F(JTE,1)+1.E-30))
RAT=AMAX(RAT,AMNI)

IF(RAT<LT,ULIM) RME=RME*RAT/ULIM

97 IF((CH1-RME)*DX,LT,PEI*DXLIM) GO TO 96
DX=DXLIM*PEI/(RMI*RME)
XD=X+DX

CONTINUE

96 CONTINUE

IF(KASE<EN,1) GO TO 960
IF(ISTEP<EN,END) GO TO 960
IEND=ISTEP+1
XEND=X+YOUT

WHITE(0,508) IEND, XEND

960 CONTINUE

ADJUSTMENT OF FORWARD STEP FOR JET TO REACH DUCT WALL

IF(K(NP1),LT,999*RDUC) GO TO 960

95 CONTINUE

ADJUSTMENT OF FORWARD STEP TO REACH AXIS OF SYMMETRY

IF(KIN*NE,*2) GO TO 195
IF(PSI1,GT,RMI*DX) GO TO 195
DX=PSI1/RMI
XD=X+DX
IAX=ISTEP+1
XAX=X+YOUT

WHITE(6,507) IAX, XAX

CHAPTER 11

OUTPUT

195 IF(ISTEP<NE,*4) GO TO 193
193 XUD=XU/YOUT
   IF (XUD.LT.XSTAT(KS)) GO TO 111
   KS=KS+1
   CALL OUTP2
321 IF (XUD.LT.XPROF(KP)) GO TO 112
   KP=KP+1
   CALL OUTP3
113 IF (ISTEP.NE.IAX.AND.ISTEP.NE.IEND) GO TO 113
117 CALL OUTP3
   CALL OUTP3
   IF (IFIN.EQ.1) GO TO 1001

C*********************************************************
C ***FORMAT STATEMENTS
507 FORMAT(7F10.3)
501 FORMAT(2F10.3,I4)
507 FORMAT(/IH0.9---MIXING LAYER REGION ENDS AT ISTEP=",I5,3X,*LENGTH O
1F POTENTIAL CORE =",F7.2,* DIAMETERS*/)
507 FORMAT(/IH0.9---JET REACHES DUCT WALL AT ISTEP=",I5,3X,*DOWNSTREAM
1DISTANCE =",F7.2,* DIAMETERS*/)
1156 FORMAT(1H4)
1152 FORMAT(1P7E11.3)
2703 FORMAT(/IH0.9--- NEGATIVE TEMPERATURE OF",1PE11.3,* CALCULATED AT
1NODE",13,* AT ISTEP=",I5)
C*********************************************************

CHAPTER 12
C********CONTINUATION/TERMINATION
113 IF (ISTEP.GE.LASTP.OR.XU.GE.XULAST) GO TO 1001
   CALL STRIP3
   GO TO 100
1001 CONTINUE
   STOP
   END

COMPILER SPACE
C=============================================================================
C********** AXIAL VELOCITY
C **** LAMINAR VISCOUSITY (APPROXIMATE POWER LAW RELATIONSHIPS)
C --- IgNEAT ATOMIC AND RADICAL CONCENTRATIONS
DO 66 I=1,NP1
SUM=FS(JH2,I)+FS(J02,I)+FS(JN2,I)+FS(JH2O,I)
EMUL(I)=0.
C --- HYDROGEN (H2)
EMUL(I)=EMUL(I)+FS(JH2,I)*8.42E-06*(F(JTE,I)/273.)***0.675
C --- OXYGEN (O2)
EMUL(I)=EMUL(I)+FS(J02,I)*1.92E-05*(F(JTE,I)/273.)***0.735
C --- NITROGEN (N2)
EMUL(I)=EMUL(I)+FS(JN2,I)*1.66E-05*(F(JTE,I)/273.)***0.690
C --- METER VAPOR
EMUL(I)=EMUL(I)+FS(JH2O,I)*1.71E-05*(F(JTE,I)/500.)***1.050
69 FMLU(I)=EMUL(I)/SUM
C *** DETERMINATION OF ACCELERATION PARAMETER
ACC=ARS(ACC-AHS(ACC))
CALL YINT(Y,X,YRS,JU)
ACC=5*YRS*ACC-AHS(F(JU+1)-F(JU+NP1))
ACC=ACC**2.
IF(ISTEP,Eq.0) GO TO 74
C *** EVALUATION OF INTEGRATED PRODUCTION/DISSPATION RATIO
IF(IPD.NE.2) GO TO 73
IF(ISTEP.LT.5) GO TO 74
IF(ISTEP.EQ.5) GO TO 152
IF(MOD(ISTEP,10).NE.0) GO TO 123
153 TPER=TPERI=TR=TRI=0.
DO 5A I=2,NP1
TRP=TR
TR=EMUL(I)*DUDY(I)*R(I)
TRI=TRI*5*(TR+TRP)*(Y(I)-Y(I-1))
TPER=TPER+TPERI=TR=TRI=0.
5A TPERI=TPERI*5*(TPER+TPERP)*(Y(I)-Y(I-1))
PUMP=PDE
PDE=TPERI/TR
IF(ISTEP.NE.5) PDE=.5*(PDE+PUMP)
W=2.8
ALPHA=.55
AH=2*sin(13.14159*(PDE-.5))-.1
IF(PDE.LE.1.) ALPH.A=.55+.213*AH
G=1.*(1.-ALPHA*PDE)/W
G=G/(1.+(PDE-1.)/W)**2
G=7.407*G*(1.-ALPHA)/W
C ***AXIAL VELOCITY GRADIENTS

DUDY(1) = 0.
DUDY(NP1) = 0.
DUDY50(1) = 0.
DUDY50(NP1) = 0.

YDIFP = Y(3) - Y(2)
DUDYP = ARS((F(JU,3) - F(JU,2)) / YDIFP + 1. * E=30)

GO To (1,2,2), KIN

1 DUDY(P) = (0.5 * YDIFP + YI) / YI * DUDYP

GO To 3

2 DUDY(P) = YI / (0.5 * YDIFP + YI) * DUDYP

GO To 3

DUDY50(2) = DUDY(2) * Y2

DO 9 I = 3, NMI

YDIFM = YDIFP

YDIFP = Y(I+1) - Y(I)
DUDYM = DUDYP

DUDY(P) = ABS((F(JU,1+1) - F(JU,1)) / YDIFP + 1. * E=30)

9 DUDY(I) = (Y(I+1) - Y(I-1)) / (YDIFP / DUDYM + YDIFM / DUDYP)

GO To (4,5,5), KEX

4 DUDY(N) = (0.5 * YDIFP + YE) / YE * DUDYP

GO To 17

5 DUDY(N) = YE / (0.5 * YDIFP + YE) * DUDYP

GO To 3

17 DUDY50(N) = DUDY(N) * Y2

GO To 9

C ***TURBULENT VISCOSITY FORMULATION

DO 1030 I = 2, N

EMUT(I) = CMU * RHO(I) * F(JU,1) / HT4(I)

1030 F(JU,1) = -EMUT(I) * DUDY(I) / RHO(I)

DO 1033 I = 2, NP1

1033 IF(F(JU,1)) LT, F(JU,1-1)) F(JUV,1) = = F(JUV,1)

C ***ADD LAMINAR AND TURBULENT COMPONENTS

IF(CHIT) 1050, 1050, 1052

1050 DO 1051 I = 2, N

1051 GAM(I) = EMUL(I) * EMUT(I)

GO To 1052

1052 DO 1053 I = 2, N

1053 IF(EMUT(I)) LT, EMUL(I) * CHIT) 1060, 1060, 1061

1060 GAM(I) = EMUL(I)

EMUT(1) = 0.

GO To 106.

1061 GAM(I) = EMUL(I) * EMUT(I)

GO To 1052

1062 EMUT(1) = 0.

EMUT(NP1) = 0.

C ***AXIAL PRESSURE GRADIENT (SOURCE TERM)

GAM3 = GAM(3)

GAMPI = GAM(NP1)
DO 111 I=1,NP1
SU(I)=NPDX
111 SD(I)=0.
RETURN

C******************************************************************************
C TURBULENT KINETIC ENERGY
C 299 IF(J,NE.,JK) GO TO 399
DO 201 I=3,N
201 GAM(I)=EMIL(I)/PR(JK)*EMUT(I)/PRT(JK)
DO 212 I=1,NP1
SU(I)=EMUT(I)*DUDESA(I)
212 SD(I)=RTH(I)*RHO(I)
IF(KIN,NE.,1) GO TO 215
FJK2=NRJ(JU)/R(1)*RHO(1)*RTCMU
SU(2)=1.E30*FJK2
SD(2)=1.E30
215 IF(KFX,NE.,1) RETURN
FJKN=JE(JU)/(R(NP1)*RHO(NP1)*RTCMU)
SU(N)=1.E30*FJKN
SD(N)=-1.E30
RETURN

C******************************************************************************
C DISSIPATION RATE
C 399 IF(J,NE.,JD) GO TO 499
DO A01 I=3,N
A01 GAM(I)=EMIL(I)/PR(JD)*EMUT(I)/PRT(JD)
DO A10 I=1,NP1
SU(I)=CE1*EMUT(I)*RTH(I)*DUDESA(I)
CE2=1.92-.0667*ACC
IF(IPN,LE,2) CE2=1.92-.1336*ACC
IF(IPN,LE,3) CE2=1.92
A10 SD(I)=CE2*RHO(I)*RTH(I)
IF(KIN,NE.,1) GO TO 812
SU(2)=FJK2*1.5/ACKDO/Y(2)*1.E30
SD(2)=-1.E30
A15 IF(KFX,NE.,1) RETURN
SU(N)=FJKN*1.5/ACKDO/Y(NP1)/Y(N)*1.E30
SD(N)=-1.E30
RETURN

C******************************************************************************
C STAGNATION ENTHALPY
C 499 IF(J,NE.,JHS) GO TO 599
C PRANDTL/SCHMITT NUMBERS FOR NEAR-WALL REGION (ROTIA)
C AXISYMMETRIC FLOWS ONLY
C ---N.H. SAME RELATIONSHIP FOR SPECIES DIFFUSION
C 330 IF(KRAD,LE,1) GO TO 331
IF(KFX,NE.,1) GO TO 331
DO 330 I=1,NP1
Y=1.*R(I)/K(NP1)
330 SCH(I)=.95+.45*Y*W
GO TO 332
331 DO 333 I=1,NP1
333 SCH(I)=PRT(JHS)
332 DO 301 I=2,N
301 GAM(I)=EMIL(I)/PR(JHS)*EMUT(I)/SCH(I)
DO 302 I=1,NP1
302 SD(I)=F(JU+I)**2
DO 303 I=2,NM1

60
FAc1=(SCH(I)*1) *(GAM(I)*GAM(I+1))/(YDIF(I)+1,E-30)
303 S D(I)=FAc1* (S D(I+1)-S D(I)) *0.5
DO 307 I=2,NM1
FAc2=(SCH(I)/PRT(JK)-1) *(GAM(I)*GAM(I+1))/(YUIF(I)+1,E-30)
307 S D(I)=S D(I+1)+FAc2*(F(JK,I+1)-F(JK,I))
SD(1)=0.
SD(N)=0.
DO 304 I=2,N
304 SD(I)=(SD(I)-SD(I-1)) *2/ TDA(I)
DO 305 I=1,NP1
305 SD(I)=0.
SU(1)=0.
SU(NP1)=0.
RETURN
C**********************************************************************
C#MASS FRACTION OF HYDROGEN ELEMENT
599 IF(J,NE.JA) GO TO 699
DO 901 I=2,N
901 GAM(I)=EMIL(I)/PR(JA)*EMUT(I)/SCH(I)
DO 902 I=1,NP1
902 SU(I)=SD(I)=0.
RETURN
C**********************************************************************
C#SQUARE CONCENTRATION FLUCTUATIONS (OF H ELEMENT)
699 IF(J,NE.JA) GO TO 799
YDIFP=Y(3)-Y(2)
DCDY=ABS((F(JA,3)-F(JA,2))/YDIFP+1,E-30)
IF(KIN.EQ.1) GO TO 711
DCDY=Y(IF)/(5*YDIFP*YI)*DCDY
DCDY=DCDY**2
SU(2)=CG1*DCDY*EMUT(2)
SD(2)=CG2*HTW(2)*RHO(2)
SU(1)=0.
SD(1)=CG2*HTW(1)*RHO(1)
GO TO 712
711 G2=(PJE(J)/R(2)/RHO(2))**2*CG1/CG2/FJK2
SU(2)=G2**1,E+30
SD(2)=1.F+30
715 DO 710 I=3,NM1
YDIFP=YDIFP
YDIFP=Y(I+1)-Y(I)
DCDY=DCDY
DCDY=ABS((F(JA,I+1)-F(JA,I))/YDIFP+1,E-30)
DCDY=DCDY/(Y(I+1)-Y(I-1))/(YUIFP/DCDY*YDIFM/DCDY)*0.2
SU(I)=CG1*DCDY*EMUT(2)
710 SD(I)=CG2*HTW(I)*RHO(I)
IF(KFX.EQ.1) GO TO 713
DCDY=Y(I)/(5*YDIFP*YI)*DCDY
DCDY=DCDY**2
SU(N)=CG1*DCDY*EMUT(N)
SD(N)=CG2*HTW(N)*RHO(N)
SU(NP1)=0.
SD(NP1)=CG2*HTW(NP1)*RHO(NP1)
RETURN
713 G3=(PJE(J)/R(N)/RHO(N))**2*CG1/CG2/FJKN
SU(N)=G3**1,E+30
SD(N)=-1.F+30
799 CONTINUE
SUBROUTINE STRIDE
DIMENSION AHL(40), HOMT3(40), OMS(40), PHOM(40), PGOM(40), THL(40)
DIMENSION A(40), H(40), C(40), D(40)
COMMON/GENERAL/ACC, CSALFA, DDX, ENTH(40), F(10,40), FS(10,40), GAM3,
1, GAM4, GAM(40), I1, IFIN, INDE(10), INDI(10), ISTEP, IUTRAP, ITEST, KEA,
2, KRAI, NNEQ, NP1, NN1, OM(40), OMD(40), ROM(40), KAST(10), PEI,
3, PSIE, PSI, P3(40), R(J)(40), RHQ(40), RJ(10), RJT(10), RJE(10), RJE(10),
4, SD(40), SU(40), THL(40), XN, YN, (40), YNIF(40), YE, YI, RJTE(10), RJTE(10)
COMMON/CJEC/JU, JN, JN2, JH, JH20, JH20, JH20, JH20, JH20, JH20
COMMON/AUXST/THA(40), U1P
COMMON/NIET/FDIFS(20,2), TS(20,2), BP(2)
COMMON/CPROP/102, IN2, IN20, OFACT, MFT, NS, QNO, WRO, WSO, WSO, GASCON, GAMMA

C *** CONTROL INDICES
ENTRY STRID0
NP1 = N + 1
NII = N - 1
OM(1,1) = 0.
OM(NP1,1) = 1.
GAM3 = 0.
GAMN = 0.
ISTEP = 0.
IFIN = 0.
IUTRAP = 2.

C *** ZEROING OF IMPORTANT ARRAYS
DO 353 J = 1, NEQ
    KAST(J) = 0.
353 HJE(J) = RJT(J) = 0.
DO 354 I = 1, NP1
    DO 354 J = 1, NS
354 FS(I,J) = 0.
    DO 355 I = 1, NP1
        DO 355 J = 1, 10
355 F(J) = 0.
    DO 356 I = 1, NP1
356 ENTH(I) = 0.
RETURN

C *** STRIDE (1)
C *** OMEGA RELATIONSHIPS
ENTRY STRID1
DO 100 I = 1, N
    OMD(1) = OM(I+1) - OM(I)
100 OMS(I) = OM(I+1) + OM(I)
DO 101 I = 1, N
    BOM(I) = OM(I+1) - OM(I-1)
    HOMT3(I1) = BOM(I) * 3.
101 CONTINUE
    BOM(2) = OM(3) + OM(2)
    BOM(N) = 2. - OM(N) - OM(NM1)
    OM2 = OM(3) / OMD(2)
    OM3 = 1. - OM2
    OMS2 = OM3 * 2
    OMS3 = OM(2) * 2
    OMS2 = OMS2/(OMS2 - OMS3)
    OMS3 = 1. - OMS2
**OMN** = (OMD(N) + OMD(NM1))**2
OMN1 = OMD(N)**2
OMN = OMN/(OMN - OMNM1)
OMNM1 = 1. - OMN
Y(1) = 0.
BP(1) = 1.
BP(2) = 1.
TND(E(JU)) = 1
IND(E(JU)) = 1
RETURN

C * *** STRIDE (2)
ENTRY STRID2
C ** TEST FOR NEGATIVE VELOCITIES
1010 IF(IUTRAP,GT,0) GO TO 1011
DO 1012 I = 2, N
IF(F(JU,I),GT,0.) GO TO 1012
1700 FORMAT(/1HO,=-- NEGATIVE VELOCITY DF*, IPE11.3,* CALCULATED AT NOO
1F*,13.,* AT ISTEP=*,15)
F(JU,J) = F-30
IF(IUTRAP,GT,1) IFIN=1
1015 IF(IUTRAP,GT,2) ITEST=1
C ** CROSS-STREAM DISTANCES (Y*S AND R*S)
C ** EDGE REGIONS
1011 RUP = RHO(2) * F(JU,2)
RU1=RHO(1) * F(JU,1)
RURAT = RU1/RUP
GO TO (1013*1014,1014), KIN
1017 GO TO (1017*1019), KRAD
1016 BP(1) = 0.333333 + 0.666667*RURAT
GO TO 1013
1013 YI = PE1 * OMD(1)/(NP(1) * RUP)
RUNP1 = RHO(NP1) * F(JU,NP1)
RUN = RHO(N) * F(JU,N)
RURAT = RUNP1/RUN
GO TO (1020*1021,1021), KEA
1021 GO TO (1024*1025), KRAD
1024 BP(2) = 0.333333 + 0.666667*RURAT
GO TO 1026
1026 YE = PE1*OMD(N)/(BP(2) * RUN)
C ** Y*S, R*S, T*U*A*S AND YDIF*S
C ** YDIF (I)=2.* (Y(I+1)-Y(I))/R(I+1.5)
Y(2) = YI
YDIF(1) = 2.* YI
DO 1017 I = 2, N-1
TDA(I) = PE1*BOH(I)/RUP
RUM=RUP
RUP = RHO(I+1) * F(JU,I+1)
YDIF(I) = PE1*OMD(I)/(1./RUM+1./RUP)
1017 Y(I+1) = Y(I)*YDIF(I-1)*5
TDA(I) = PE1*BOH(N)/RUP
Y(NP1) = Y(N) + YE
YDIF(N) = 2.* YE
IF(KRAD,F0,2) RETURN
C ** MODIFICATIONS FOR AXIAL SYMMETRY

64
IF(CALFA.NF.0.) GO TO 1110
C **C.0.0.0.0.0.0.
C COSD2=5*CALFA
CIF(R(I).NF.0.) GO TO 1105
C **R(I).0.0.0.0.0.
DO 1106 I = 2, NP1
Y(I)=SQRT(ABS(Y(I)/COSD2))
1104 R(I)=Y(I)*CALFA
GO TO 1107
C **R(I).0.0.0.0.0.
1105 R1D2=.5*R(I)
R1D2SQR=R1D2*R1D2
DO 1104 I = 2, NP1
Y(I)=Y(I)/(R1D2+SQR(ABS(R1D2SQR+COSD2*Y(I)))))
1104 R(I)=R(I)+Y(I)*CALFA
1107 DO 1106 I = 1, N
1106 YDIF(I)=YDIF(I)*(1./(R(I)+R(I+1)))*2
GO TO 1112
C. **C.0.0.0.0.0.0.
1112 DO 1111 I = 2, NP1
Y(I)=Y(I)/R(I)
1111 R(I)=P(I)
R1SQR=P(I)*2
DO 1109 I = 2, N
1109 YDIF(I)=YDIF(I)/R1SQR
1112 Y(N)=Y(2)
YF=Y(NP1)-Y(N)
RFTUPM
C******************************
C^ STRIDE (3)
C **MAIN NUMERICAL METHOD
C INTEGRATION STRIDE
IF (KIN .EQ. 1) CALL WF(1)
IF (KFA .EQ. 1) CALL WF(2)
C **MINIMUMS
3000 G=RMS=1ME
PX=PF1/I(D)
PD4=0.25*PX
GD4=0.25*G
PGD4=0.25*GD4
RMIDJ=0.25*RMI
PG0M(I)=0.
C-----------------------THL, AHL, PGOM AND PBOM
THL(I) = 0.
DO 3010 I = 2, N
HL=HMTD2-6D4*Atn(I)
THL(I) = 2.*HL
AHL(I) = ABS(HL)
PGBM(I)=PGD4*Atn(I)
3010 PBDM(I)=PX*@1M4(I)
C **START OF J LOOP
DO 3320 J=1,NEQ
IF(J.NE.JH) CALL AUX(J)
TTP=0.
PG0MP = 0.
C ALL (NP1) = 0.
C **SETTING UP COEFFICIENTS
AKAST = FLOAT(1-KAST(J))
\[ \text{KAST1} = \text{KAST}(I) + 1 \]
\[ \text{INDEX}=\text{IND}(J) \]
\[ \text{INDEXF}=\text{IND}(J) \]
\[ \text{DO 3004} I=2+N \]
\[ \text{SU}(I) = \text{SU}(I) \times \text{TDA}(I) \]
\[ \text{SD}(I) = \text{SD}(I) \times \text{TDA}(I) \]
\[ \text{PGOMM} = \text{PGOMP} \]
\[ \text{PGOMP} = \text{PGOM}(I) \times \text{AKAST} \]
\[ \text{TH} = \text{THP} \]
\[ \text{TP} = \frac{\text{GAM}(I) + \text{GAM}(I+1)}{\text{YU}} \]
\[ \text{TPP} = \text{TP} \times \text{AHL}(I) \times \text{ABS}(\text{TP}-\text{AHL}(I)) \]
\[ \text{A}(I) = \text{TPP} - \text{THL}(I) - \text{PGOMP} \]
\[ \text{B}(I) = \text{TPP} - \text{THL}(I-1) - \text{PGOMP} \]
\[ \text{IND1}=2/I \]
\[ \text{IND2}=1/(\text{NP1}-I) \]
\[ \text{INDEX}=1+\text{IND1}+\text{IND2} \]
\[ \text{GO TO} (303,305),\text{KAST1} \]
\[ \text{304} \]
\[ \text{C}(I) = \text{PU0} \times \text{BOMT3}(I) \times \text{F}(J,I) \times \text{OMD}(I) \times \text{F}(J,I+1) \times \text{OMD}(I-1) \times \text{F}(J,I-1) \times \text{SU}(I) \]
\[ \text{GO TO } 306 \]
\[ \text{305} \]
\[ \text{C}(I) = \text{PGOM}(I) \times \text{F}(J,I) \times \text{SU}(I) \]
\[ \text{304} \]
\[ \text{D}(I) = \text{PU0} \times \text{SD}(I) \]
\[ \text{C} \quad \text{**MODIFICATIONS FOR BOUNDARIES} \]
\[ \text{INDEX}=1+\text{IND1}+2+\text{IND2} \]
\[ \text{GO TO} (3004,3005,3006), \text{INDEX} \]
\[ \text{3004} \]
\[ \text{A}(I) = \text{A}(I) \times \text{PGOM}(2) \times \text{AKAST} \]
\[ \text{B}(I) = 2 \times \text{RVI} \]
\[ \text{GO TO} (3009,3004,3005), \text{KIN} \]
\[ \text{3009} \]
\[ \text{GO TO} (3011,3003), \text{INDEX} \]
\[ \text{3011} \]
\[ \text{TT} = 2 \times \text{TS}(J,1) \]
\[ \text{B}(I) = \text{AMAX1}(\text{TT} \times \text{B}(I),0) \]
\[ \text{C}(I) = \text{C}(I) - \text{TT} \times \text{FDIFS}(J,1) \]
\[ \text{GO TO } 3004 \]
\[ \text{3005} \]
\[ \text{B}(I) = 0 \]
\[ \text{D}(I) = \text{D}(I) \times 2 \times \text{HME} \]
\[ \text{C}(I) = \text{C}(I) \times 2 \times \text{HMT}(E) \]
\[ \text{GO TO } 3004 \]
\[ \text{3006} \]
\[ \text{A}(I) = 2 \times \text{RME} \]
\[ \text{GO TO} (3012,3004), \text{KEX} \]
\[ \text{3015} \]
\[ \text{GO TO} (3013,3005), \text{INDEX} \]
\[ \text{3013} \]
\[ \text{TT} = 2 \times \text{TS}(J,2) \]
\[ \text{A}(I) = \text{AMAX1}(\text{TT} \times \text{A}(I),0) \]
\[ \text{C}(I) = \text{C}(I) - \text{TT} \times \text{FDIFS}(J,2) \]
\[ \text{GO TO } 3004 \]
\[ \text{3005} \]
\[ \text{A}(I) = 0 \]
\[ \text{D}(I) = \text{D}(I) \times 2 \times \text{HME} \]
\[ \text{C}(I) = \text{C}(I) \times 2 \times \text{HMT}(F) \]
\[ \text{GO TO } 3004 \]
\[ \text{C} \quad \text{***ADJUST FREE-BOUNDARY VALUES} \]
\[ \text{RUI} = \text{RHO}(1) \times \text{F}(J,1) \]
\[ \text{IF} (\text{INT}(J),2 \times \text{RUI}, \text{RU1}, \text{EQ}, 0, ) \text{ GO TO } 3006 \]
\[ \text{F}(J,1) = (\text{F}(J,1) \times \text{SU}(1) \times \text{DX}/\text{RU1})/(1. - \text{SD}(1) \times \text{DX}/\text{RU1}) \]
\[ \text{3006} \]
\[ \text{RUIP1} = \text{RHO}(\text{NP1}) \times \text{F}(J,\text{NP1}) \]
\[ \text{IF} (\text{KEX}(J),2 \times \text{RUIP1}, \text{RU1P1}, \text{EQ}, 0, ) \text{ GO TO } 3007 \]
\[ \text{F}(J,\text{NP1}) = (\text{F}(J,\text{NP1}) \times \text{SU}(\text{NP1}) \times \text{DX}/\text{RU1P1})/(1. - \text{SD}(\text{NP1}) \times \text{DX}/\text{RU1P1}) \]
\[ \text{C} \quad \text{***SOLVF FOR DOWNSTREAM F#S} \]
\[ \text{3007} \]
\[ \text{A}(2) = (\text{A}(2) \times \text{F}(J,1) \times \text{C}(2)) / \text{N}(2) \]
A(2) = A(2) / U(2)
DO 3N21 I = 3, N
T = D(I) - B(I) * A(I - 1)
A(I) = A(I) / T
3N21 B(I) = (B(I) * R(I - 1) + C(I)) / T
DO 3N22 IDASH = 1, NM1
T = NP1 - IDASH
3N22 F(J+I) = A(I) * F(J, I+1) + B(I)
C ** ADJUST BOUNDARY VALUES
3N21 GO TO (3210, 3220, 3230), KIN
3N20 GO TO (30N, 3211) * INDEX1
3N11 RMT = RMT + TS(J, 1)
RJTI(J) = RJTI(J) - RMI * F(J, 1)
IF (PMT, pT, 0.) GO TO 307
F(J, 1) = F(J, 2)
GO TO 3220
3N07 F(J, 1) = (RJTI(J) + TS(J, 1) * (F(J, 2) + FDIFS(J, 1))) / RMT
GO TO 3220
3N06 RJTI(J) = TS(J, 1) * (F(J, 1) - F(J, 2) - FDIFS(J, 1))
RJTI(J) = RJTI(J) + RMI * F(J, 1)
GO TO 3220
3N23 IF (R(1) * En, 0.) GO TO 309
F(J, 1) = F(J, 2) * OM2 + F(J, 3) * OM3
GO TO 3220
3N09 F(J, 1) = F(J, 2) * OM2 + F(J, 3) * OM3
3N25 GO TO (3310, 3320, 3330), * EX
3N10 GO TO (31N, 3311), * INDEXE
3N11 RMT = RMT + TS(J, 2)
RJE(J) = RJE(J) - RME * F(J, NP1)
IF (RMT, pT, 0.) GO TO 317
F(J, NP1) = F(J, N)
GO TO 3320
3N17 F(J, NP1) = (-RJTE(J) + TS(J, 2) * (F(J, N) + FDIFS(J, 2))) / RMT
GO TO 3320
3N16 RJTE(J) = -TS(J, 2) * (F(J, NP1) - F(J, N) - FDIFS(J, 2))
RJTE(J) = RJTE(J) + RME * F(J, NP1)
GO TO 3320
3N33 F(J, NP1) = F(J, N) * OMN + F(J, NM1) * OMNM1
3N32 CONTINUE
XU = XN
ACC = F(JU, 1) - H1P / DX
PSII = PSII - RMI * DX
PSIE = PSIE - RME * DX
PEI = PSIE + PSII
ISTEP = ISTEP + 1
RETURN
END

COMPILER SPACE
SUBROUTINE WF(K)
COMMON/GENRAL/ACC,CSALFA,DPDX,DX,ENTH(40),F(10,40),FS(10,40),GAM(3,
GAMN,GAM(40),IFIN,INDE(10),INDI(10),ISTEP,IUTRAP,TEST,KEK,KEK,
PKRAQ,N,NFQ,NP1,N1,0:1(40),UMD(40),BOM(40),KAST(10),PEI,PSIE,PSIL,
3P(40),R(40),RMO(40),RJF(10),RJI(10),RME,RMI,SD(40),SU(40),WMM(10),
4X0,XU,Y(40),YDF(40),YF,RJ(R),RJTE(10),RJTI(10)
COMMON/CFJ/MA,JK,JO,JS,JA,JG,JTE,JLE,JUV,JB
COMMON/CJJK/RH,AK,ALMG,CMUIN,CE1,CE2,CG1,CG2,CRT,DUXY(40),
1DUDYSQ(40),EHUL(40),EMUT(40),IPD,PR(10),PRT(10),RTW(40)
COMMON/CWRF/YH(2),XRIF(2),EWALL,H
COMMON/WFST/FDIFS(20,2),TS(20,2),BP(2)
COMMON/CJJK/SCH(40)

DATA SHALF/0.04/
GO TO (10,11),K
10 IN=1
IN=2
GO TO 12
11 IWF=NWF1
IN=N
CONTINUE
C *REFERENCE QUANTITIES
1RREFABS(F(JU,IN))=F(JU,IN)
RRHORF=0.5*(RHO(40)+RHO(40))
RUREF=RHMREF*URRF
RREF=R(N)
RRRF=RREF*URRF
VREF=FMUL(IW)
YREF=ABS(Y(IN))=Y(IN)
E=RUREF*YREF/VREF
AM=(RME-RMI)*CMM(IW))/RRREF
FF=-SU(IW)*YREF/RUREF/VREF
12 IF(RELAT>132.25) GO TO 110
C ***LOG LAW ASSUMPTION
121 CONTINUE
LAM=0
NIT=N
101 SHALF1=SHALF
YRP=RYR*SHALF
C ***CALCULATION OF E FOR ROUGHNESS
E=E=WALL
IF(IPHF(K),EQ.0) GO TO 16
C ***SAND-GRAIN ROUGHNESS
IF(YRP.GT.3.333333) E=30./YRP
16 FR=REF*E
S=SHALF**S
SLOC<<AM*EF
TF(SL<,GT,0.1) GO TO 104
SLOC=1.E-30
SHALF=SRT(ABS(AM*EF))
104 BEE=SOR1(SLOC/AY)
ARG=FR*S(40)+AM*(1.*BEE+.5*E)/SHALF)
IF(ARG>GT,11.**E) GO TO 106
GO TO 110
104 SHALF=AK/ALGF(ARG)
IF(A=1,SHALF=SHALF1).LT..0001.OK.NIT,GT,10) GO TO 102
NIT=NIT+1

68
GO TO 101

101 S=SHALF*1.
BP(K)=(1./BP)/1.*BEE)
GO TO 103

C LAMINAR FLOW

111 L=1
AMRE=AMRE
FRE=EFF*HE
IF(ABS(AMRE) .LT. 0.1) GO TO 111
EXPFR=EXP(AMRE)
STORE=EXPFR-1.*AMRE
AMRESQ=AMRE*AMRE
SRE=AMRE*1.*STORE/FRE/AMRESQ)/(EXPFR-1.*)
OUT1=SRE*STORE/AMRESQ+FRE*STORE/5.*AMRESQ)/(AMRESQ*AMRE)
GO TO 112

112 SRE=(?*FRE*(1.*AMRE/3.))/(2.*AMRE)
OUT1=SRE*(5.*AMRE/6.)*FRE*(16667*AMRE/24.
GO TO 113

113 S=SH/PK
AP(K)=OUT1

103 DO 500 J=1,NEQ
   FDFJS(J,K)=0.
   IF(J,F,E,JMS) FDFJS(J,K)=(H=1.*)*5*UREF
   IF(J,F,E,JOI) GO TO 200
   TS(J,K)=S+AMREF
   GO TO 500

C STAGNATION ENTHALPY AND MASS FRACTION

200 CONTINUE
   IF(RF.LT.132.25) GO TO 210
   IF(LAM.EQ,1.) GO TO 210

201 CONTINUE
   PPRAT=PH(J)/PHT(J)
   IF(KPAU.EQ.2) PPRAT=PR(J)/SCH(N)
   PJAY=9.*1.*P=1.)/PPRAT*1.25
   SF=S/(PHT(J)*(1.+PJAY*SHAF)
   IF(KPAU.EQ.2) SF=S/(SCH(N)*(1.+PJAY*SHAF)
   GO TO 213

C LAMINAR FLOW

210 IF(ABS(AMRE) .LT. 0.1) GO TO 211
   SF=AM*/EXP(PH(J)*AMRE)=1.0
   GO TO 212

211 SF=1.*PH(J)/RE/(1.+5*PR(J)*AMRE
212 CONTINUE
   TS(J,K)=SF*HRUHF
   500 CONTINUE
RETURN
END

COMPLMR SPACE
**CHAPTER 1**

**LOADING OF EQUILIBRIUM CONSTANTS, ENTHALPIES AND SPECIFIC HEATS**

ENTRY LANLEY

**REFERENCE ENTHALPIES**

```
DATA (HO(J), J=1,7) /-2023.8, -2074.7, 7205.6, -50616.5, 57949.1, -1872.3/
```

**CHEMICAL EQUILIBRIUM CONSTANTS**

```
DO 20 J=1,7
   READ(5,1000) (RC(J, I), I=1,60)
20   RC(J, I)=AM(N1(RC(J, I)), 100.)
```

**CONSTANTS FOR GLOBAL REACTION**

```
DO 15 I=1,60
   15 RC(5, I)=RC(4, I)*RC(3, J)/RC(1, I)*SORT(RC(2, I))
```

**CONVERSION INTO CONSTANTS FOR CONCENTRATION RATIOS**

```
A10=WM(JH2)/WM(JH)
A20=WM(JO2)/WM(JO)
A30=WM(JOH)/WM(JO)/WM(JH)
A40=WM(JH2O)/WM(JOH)/WM(JH)
A50=WM(JH2)/WM(JH2)/SORT(WM(JO2))
DO 571 I=1,60
   RC(1, I)=RO(1, I)*A10
   RC(2, I)=RO(2, I)*A20
   RC(3, I)=RO(3, I)*A30
   RC(4, I)=RO(4, I)*A40
   571 RC(5, I)=RO(5, I)*A50
```

**ENTHALPIES AND MEAN SPECIFIC HEATS**

```
DO 30 J=1,NS
   CFA=1.87*WM(J)
   HO(J)=HO(J)*CFA
   READ(5,2000) (HT(J, I), I=1,60)
30   HT(J, I)=HT(J, I)*CFA
```

**ITERATION PARAMETERS**

```
IHEGIN=3
ITMAX=12
CC=.01
RPC=.5
RPD=1.-RPC
```
**Chapter 2**

**Initial Enthalpies**

```
ENTRY LANAL2
ENTH(I)=0.
IFACX=FACX
FACS=FACX-FLOAT(IFACX)
DO 115 J=1,NP1
ENTH(J)=HT(J,IFACX)+FACS*(HT(J,IFACX+1)-HT(J,IFACX))
115 CONTINUE
```

**Return**

---

**Chapter 3**

**Local Mass Fractions**

```
ENTRY LANAL3
C *** LOCATE POSITION WHERE HYDROGEN CONCENTRATION IS STOICHIOMETRIC
X=1.-F(JA,I)
X=X*FAC
IF(F(JA,I)/(X+1.E-10).LT.FSTOICH) GO TO 625
DO 621 I=1,NP1
X=1.-F(JA,I)
X=X*FAC
PARA=RAT=1.E-10
RAT=F(JA,I)/(X+1.E-10)
IF(HAT.LT.T*.FSTOICH) GO TO 1060
621 CONTINUE
625 ILCH=I=1
ILCP=I
FACM=Y(I-1)*(Y(I)-Y(I-1))/(F(JA,I))
GO TO 626
626 DO 20A IDM=1,NP1
1=NP1+1-IDM
IF(I,LT.ILCP) GO TO 740
GO TO 742
740 I=ILCP=I
742 TSM=MAX1(F(JF,I),250.)
C *** CONCENTRATIONS OF OXYGEN ELEMENT AND NITROGEN
XN2PO=1.-F(JA,I)
X=0FAC*XN2PO
FS(JN2PO,I)=XN2PO-X
RAT=F(JA,I)/(X+1.E-10)
DO 304 L=1,NP1
304 TSM=TSM-0.25
C *** EQUILIBRIUM CONSTANTS AND MEAN SPECIFIC HEATS FOR UPSTREAM STATE
FACX=.01*TSM
IFACX=FACX
FACS=FACX-FLOAT(IFACX)
DO 1055 L=1,NRP
1055 RCON(L)=RF(L,IFACX)+FACS*(RC(L,IFACX+1)-RC(L,IFACX))
CFAC=RHU(I)+RASCON(RF(JF,I),1.E-05)
DO 1056 L=1,NRP
1056 RCON(L)=RCON(L)*CFAC
```
**Equation for Hydrogen-Nitrogen Mixtures**

**START OF ITERATION CYCLE**

**DETERMINE LARGEST TERM IN EACH GROUP**

--- **EQUATION FOR OXYGEN ELEMENT**

\[ J_1 = J_{O2} \]
\[ F_{M1} = F(S(J_{O2}, I)) \]
\[ \text{IF} (F(S(J_{O1}, I)) \cdot LT. F(S(J_{O2}, I))) \text{GO TO} 210 \]
\[ J_1 = J_{O1} \]
\[ F_{M1} = F(S(J_{O1}, I)) \]

--- **EQUATION FOR HYDROGEN ELEMENT**

\[ J_2 = J_{H2} \]
\[ F_{M2} = F(S(J_{H2}, I)) \]
\[ \text{IF} (F(S(J_{H1}, I)) \cdot LT. F(S(J_{H2}, I))) \text{GO TO} 212 \]
\[ J_2 = J_{H1} \]
\[ F_{M2} = F(S(J_{H1}, I)) \]

--- **PRECAUTION IF H20 IS LARGEST OF BOTH GROUPS**

\[ \text{IF} \left( \text{NOT} \left( \text{J}_1 \cdot \text{EQ.} \cdot \text{J}_{H20} \text{AND} \cdot \text{J}_2 \cdot \text{EQ.} \cdot \text{J}_{H20} \right) \right) \text{GO TO} 279 \]
\[ \text{IF} (F(S(J_{H1}, I)) \cdot LT. F(S(J_{H2}, I))) \text{GO TO} 622 \]
\[ J_1 = J_{H2} \]
\[ F_{M1} = F(S(J_{H2}, I)) \]

**CONTINUE**

--- **EQUATION FOR QUADRATIC EQUATION FOR HYDROGEN-NITROGEN MIXTURES**

\[ F(S(J_{H1}, I)) = \text{SQRT} \left( 1 \cdot 4 \cdot F(J_{A1}) \cdot R\text{CON}(1) \right) \]
\[ F(S(J_{H1}, I)) = \frac{5 \cdot F(S(J_{H1}, I))}{R\text{CON}(1)} \]
\[ F(S(J_{H2}, I)) = F(J_{A1}) - F(S(J_{H1}, I)) \text{GO TO 208} \]

**CONTINUE**

--- **DETERMINE LARGEST TERM IN EACH GROUP**

--- **EQUATION FOR OXYGEN ELEMENT**

\[ J_1 = J_{O2} \]
\[ F_{M1} = F(S(J_{O2}, I)) \]
\[ \text{IF} (F(S(J_{O1}, I)) \cdot LT. F(S(J_{O2}, I))) \text{GO TO} 210 \]
\[ J_1 = J_{O1} \]
\[ F_{M1} = F(S(J_{O1}, I)) \]

--- **EQUATION FOR HYDROGEN ELEMENT**

\[ J_2 = J_{H2} \]
\[ F_{M2} = F(S(J_{H2}, I)) \]
\[ \text{IF} (F(S(J_{H1}, I)) \cdot LT. F(S(J_{H2}, I))) \text{GO TO} 212 \]
\[ J_2 = J_{H1} \]
\[ F_{M2} = F(S(J_{H1}, I)) \]

--- **PRECAUTION IF H20 IS LARGEST OF BOTH GROUPS**

\[ \text{IF} \left( \text{NOT} \left( \text{J}_1 \cdot \text{EQ.} \cdot \text{J}_{H20} \text{AND} \cdot \text{J}_2 \cdot \text{EQ.} \cdot \text{J}_{H20} \right) \right) \text{GO TO} 279 \]
\[ \text{IF} (F(S(J_{H1}, I)) \cdot LT. F(S(J_{H2}, I))) \text{GO TO} 622 \]
\[ J_1 = J_{H2} \]
\[ F_{M1} = F(S(J_{H2}, I)) \]

**CONTINUE**

--- **EQUATION FOR OXYGEN ELEMENT**

\[ J_1 = J_{O2} \]
\[ F_{M1} = F(S(J_{O2}, I)) \]
\[ \text{IF} (F(S(J_{O1}, I)) \cdot LT. F(S(J_{O2}, I))) \text{GO TO} 210 \]
\[ J_1 = J_{O1} \]
\[ F_{M1} = F(S(J_{O1}, I)) \]

--- **EQUATION FOR HYDROGEN ELEMENT**

\[ J_2 = J_{H2} \]
\[ F_{M2} = F(S(J_{H2}, I)) \]
\[ \text{IF} (F(S(J_{H1}, I)) \cdot LT. F(S(J_{H2}, I))) \text{GO TO} 212 \]
\[ J_2 = J_{H1} \]
\[ F_{M2} = F(S(J_{H1}, I)) \]

--- **PRECAUTION IF H20 IS LARGEST OF BOTH GROUPS**

\[ \text{IF} \left( \text{NOT} \left( \text{J}_1 \cdot \text{EQ.} \cdot \text{J}_{H20} \text{AND} \cdot \text{J}_2 \cdot \text{EQ.} \cdot \text{J}_{H20} \right) \right) \text{GO TO} 279 \]
\[ \text{IF} (F(S(J_{H1}, I)) \cdot LT. F(S(J_{H2}, I))) \text{GO TO} 622 \]
\[ J_1 = J_{H2} \]
\[ F_{M1} = F(S(J_{H2}, I)) \]

**CONTINUE**

--- **EQUATION FOR OXYGEN ELEMENT**

\[ J_1 = J_{O2} \]
\[ F_{M1} = F(S(J_{O2}, I)) \]
\[ \text{IF} (F(S(J_{O1}, I)) \cdot LT. F(S(J_{O2}, I))) \text{GO TO} 210 \]
\[ J_1 = J_{O1} \]
\[ F_{M1} = F(S(J_{O1}, I)) \]

--- **EQUATION FOR HYDROGEN ELEMENT**

\[ J_2 = J_{H2} \]
\[ F_{M2} = F(S(J_{H2}, I)) \]
\[ \text{IF} (F(S(J_{H1}, I)) \cdot LT. F(S(J_{H2}, I))) \text{GO TO} 212 \]
\[ J_2 = J_{H1} \]
\[ F_{M2} = F(S(J_{H1}, I)) \]

--- **PRECAUTION IF H20 IS LARGEST OF BOTH GROUPS**

\[ \text{IF} \left( \text{NOT} \left( \text{J}_1 \cdot \text{EQ.} \cdot \text{J}_{H20} \text{AND} \cdot \text{J}_2 \cdot \text{EQ.} \cdot \text{J}_{H20} \right) \right) \text{GO TO} 279 \]
\[ \text{IF} (F(S(J_{H1}, I)) \cdot LT. F(S(J_{H2}, I))) \text{GO TO} 622 \]
\[ J_1 = J_{H2} \]
\[ F_{M1} = F(S(J_{H2}, I)) \]

**CONTINUE**

--- **EQUATION FOR OXYGEN ELEMENT**

\[ J_1 = J_{O2} \]
\[ F_{M1} = F(S(J_{O2}, I)) \]
\[ \text{IF} (F(S(J_{O1}, I)) \cdot LT. F(S(J_{O2}, I))) \text{GO TO} 210 \]
\[ J_1 = J_{O1} \]
\[ F_{M1} = F(S(J_{O1}, I)) \]

--- **EQUATION FOR HYDROGEN ELEMENT**

\[ J_2 = J_{H2} \]
\[ F_{M2} = F(S(J_{H2}, I)) \]
\[ \text{IF} (F(S(J_{H1}, I)) \cdot LT. F(S(J_{H2}, I))) \text{GO TO} 212 \]
\[ J_2 = J_{H1} \]
\[ F_{M2} = F(S(J_{H1}, I)) \]

--- **PRECAUTION IF H20 IS LARGEST OF BOTH GROUPS**

\[ \text{IF} \left( \text{NOT} \left( \text{J}_1 \cdot \text{EQ.} \cdot \text{J}_{H20} \text{AND} \cdot \text{J}_2 \cdot \text{EQ.} \cdot \text{J}_{H20} \right) \right) \text{GO TO} 279 \]
\[ \text{IF} (F(S(J_{H1}, I)) \cdot LT. F(S(J_{H2}, I))) \text{GO TO} 622 \]
\[ J_1 = J_{H2} \]
\[ F_{M1} = F(S(J_{H2}, I)) \]

**CONTINUE**

--- **EQUATION FOR OXYGEN ELEMENT**

\[ J_1 = J_{O2} \]
\[ F_{M1} = F(S(J_{O2}, I)) \]
\[ \text{IF} (F(S(J_{O1}, I)) \cdot LT. F(S(J_{O2}, I))) \text{GO TO} 210 \]
\[ J_1 = J_{O1} \]
\[ F_{M1} = F(S(J_{O1}, I)) \]

--- **EQUATION FOR HYDROGEN ELEMENT**

\[ J_2 = J_{H2} \]
\[ F_{M2} = F(S(J_{H2}, I)) \]
\[ \text{IF} (F(S(J_{H1}, I)) \cdot LT. F(S(J_{H2}, I))) \text{GO TO} 212 \]
\[ J_2 = J_{H1} \]
\[ F_{M2} = F(S(J_{H1}, I)) \]

--- **PRECAUTION IF H20 IS LARGEST OF BOTH GROUPS**

\[ \text{IF} \left( \text{NOT} \left( \text{J}_1 \cdot \text{EQ.} \cdot \text{J}_{H20} \text{AND} \cdot \text{J}_2 \cdot \text{EQ.} \cdot \text{J}_{H20} \right) \right) \text{GO TO} 279 \]
\[ \text{IF} (F(S(J_{H1}, I)) \cdot LT. F(S(J_{H2}, I))) \text{GO TO} 622 \]
\[ J_1 = J_{H2} \]
\[ F_{M1} = F(S(J_{H2}, I)) \]
FM2 = FS(JOH, I) * WTO
GO TO 379

279 CONTINUE

C** PRECAUTION IF OH IS LARGEST OF BOTH GROUPS
IF ( NOT ( (J1 . EQ. JOH . AND. J2 . EQ. JH20) ) ) GO TO 379
IF ( RAT * GE . FSTOICH ) GO TO 367
J1 = JN2
FM1 = FS(JO2, I)
IF ( FS(JO2, I) . LT . FS(JO2, I) ) GO TO 358
J1 = JN
FM1 = FS(JO1, I)
358 IF ( FS(JH20, I) . NE . LT . FM1 ) GO TO 379
J1 = JH20
FM1 = FS(JH20, I) * WSO
GO TO 379

367 J2 = JH2
FM2 = FS(JH2, I)
IF ( FS(JH2, I) . LT . FS(JH2, I) ) GO TO 381
J2 = JH
FM2 = FS(JH2, I)
381 IF ( FS(JH20, I) . NE . LT . FM2 ) GO TO 379
J2 = JH20
FM2 = FS(JH20, I) * WSO
GO TO 379

379 CONTINUE

C** VERIFICATION PRECAUTION
IF ( F(JA, I) . LT . 3999 ) J1 = JH20
IF ( F(JA, I) . LT . 0001 ) J2 = JH20

GO TO 240

C--------------------------- H2 OR H AS J2
IF ( J2 . NE . JH2 . AND. J2 . NE . JH ) GO TO 240
IF ( J2 . EQ . JH2 ) FS(JH2, I) = SQRT ( FS(JH2, I) ) / RCON ( 1 )
IF ( J2 . EQ . JH2 ) FS(JH2, I) = FS(JH, I) * W2 * RCON ( 1 )
IF ( J1 . EQ . JH20 ) GO TO 233
IF ( J1 . EQ . JH20 ) GO TO 427
IF ( J1 . EQ . JH20 ) FS(JH2, I) = SQRT ( FS(JH2, I) ) / RCON ( 2 )
IF ( J1 . EQ . JH20 ) FS(JO1, I) = SQRT ( FS(JO1, I) ) / RCON ( 1 )
FS(JH20, I) = FS(JH20, I) * SQRT ( FS(JH20, I) ) / RCON ( 5 )
FS(JH20, I) = FS(JH20, I) * RCON ( 1 )
FS(JH20, I) = FS(JH20, I) * FS(JH, I) / RCON ( 3 )
FS(JH20, I) = FS(JH20, I) / RCON ( 3 )
FS(JH20, I) = FS(JH20, I) * RCON ( 3 )
GO TO 290

333 FS(JO1, I) = FS(JH20, I) / FS(JH20, I) / RCON ( 5 ) * W2
FS(JO1, I) = FS(JH20, I) / RCON ( 2 )
FS(JO1, I) = FS(JO1, I) / RCON ( 3 )
GO TO 290

427 FS(JO1, I) = SQRT ( FS(JO1, I) ) / RCON ( 3 )
FS(JO1, I) = FS(JO1, I) * W2 * RCON ( 2 )
FS(JH20, I) = FS(JH20, I) * FS(JH, I) * RCON ( 4 )
FS(JH20, I) = FS(JH20, I) / RCON ( 4 )
GO TO 290

249 IF ( J2 . NE . JH20 ) GO TO 250

C---------------------------------------- H20 AS J2
IF ( J1 . EQ . JH20 ) FS(JH20, I) = FS(JH20, I) * W2 * RCON ( 2 )
IF ( J1 . EQ . JH20 ) FS(JH20, I) = SQRT ( FS(JH20, I) ) / RCON ( 2 )
IF ( J1 . EQ . JH20 ) GO TO 430
FS(JH, I) = FS(JH, I) * W2 * FS(JH, I) / RCON ( 4 ) / RCON ( 3 )
FS(JH, I) = FS(JH, I) * W2 * RCON ( 2 )
FS(JH, I) = FS(JH, I) / RCON ( 3 )
FS(JH, I) = FS(JH, I) / RCON ( 3 )
GO TO 430

C CONTINUE

FS(JH20, I) = FS(JH20, I) / SQRT ( FS(JH20, I) ) / RCON ( 5 )
FS(JH20, I) = FS(JH20, I) / RCON ( 1 )
IF ( J1 . EQ . JH20 ) GO TO 290
FS(JH, I) = FS(JH, I) * FS(JH, I) / RCON ( 3 )

73
GO TO 290

259 CONTINUE
   IF (J1.EQ.J0) FS(J02,I)=FS(J0,I)*RCON(2)
   IF (J1.EQ.J02) FS(J02,I)=SQRT(FS(J02,I)/RCON(2))
   IF (J1.EQ.JH2O) GO TO 501
   FS(JH,I)=FS(J0H,I)/FS(J0,I)/RCON(3)
   FS(JH20,I)=FS(JH,I)**2/RCON(1)
   FS(JH20,I)=FS(JH,I)*FS(J0H,I)*RCON(4)
GO TO 240

501 FS(JH,I)=FS(JH2O,I)/FS(J0H,I)/RCON(4)
   FS(JH2I,I)=FS(JH,I)**2/RCON(1)
504 FS(J0,I)=FS(J0H,I)/FS(JH,I)/RCON(3)
   FS(J0,I)=FS(J0,I)**2/RCON(2)

299 CONTINUE

C ***RE-EVALUATE LARGEST TERMS FROM ADDITIVE EQUATIONS
   IF (MAT.LE.FSTOICH) GO TO 810

A39 CONTINUE
   FM1=FM1
   IF (J1.EQ.J0H) FM1=FM1=FS(J0H,I)*WRO
   IF (J1.EQ.J02) FM1=FM1=FS(J02,I)
   IF (J1.EQ.JH2O) FM1=FM1=FS(J0H,I)
   IF (J1.EQ.JH2O) FM1=FM1=FS(JH20,I)*WSO
   FS(J1,I)=FM1
   IF (J1.EQ.JH2O) FS(J1,I)=FS(J1,I)/WSO
   IF (J1.EQ.J0H) FS(J1,I)=FM1/WRO
   IF (MAT.LE.FSTOICH) GO TO 820

A19 CONTINUE
   FM2=FS(J1,I)
   IF (J2.EQ.J0H) FM2=FM2=FS(J0H,I)*WTO
   IF (J2.EQ.JH2O) FM2=FM2=FS(JH2O,I)*WQO
   FS(J2,I)=FM2
   IF (J2.EQ.J0H) FS(J2,I)=FM2/WTO
   IF (MAT.LE.FSTOICH) GO TO 830

A29 CONTINUE
   ITER=ITER+1
   ISATP(I)=ITER
   IF (ITER.LT.IHFIN) GO TO 6A9

C ****UNDER-RELAXATION OF MASS FRACTIONS
   DO 6A8 L=1,NS
   AAA FS(L,I)=RPC*FS(L,I)+HPD*STORE(L)

6A9 CONTINUE
   DO 325 L=1,NS
   RFM(L)=(FS(L,I)-STORE(L))/(FS(L,I)+1.E-40)

C ****LIMITS ON MASS FRACTIONS
   DO 339 L=1,NS
   FS(L,I)=AMAX1(FS(L,I)+1.0)
339 FS(L,I)=AMAX1(FS(L,I)+0.0)
   DO 326 L=1,NS
326 STORE(L)=FS(L,I)
   RMAX=0.0
   DO 327 L=1,NS
   IF (FS(L,I)>L.LT.1.0.LT.0.0E-06) GO TO 327
   RMAX=AMAX1(RMAX,ABS(REM(L)))
327 CONTINUE
C ***CONVERGENCE CRITERION
  IF (ITER.GT.ITMAX .OR. ABS(RMAX) .GT. CC) GO TO 208
  GO TO 175

208 CONTINUE
  DO 345 J=1,NS
  DO 345 I=1,NP1
  345 FS(J,I)=MAX1(FS(J,I),0.0)
C ***TEST FOR POOR CONVERGENCE
  DO 8227 I=1,NP1
  8227 IF (ISTAR(I).GT.ITMAX) WRITE (6,8228) ISTAR(I),I,ISTEP
  8228 FORMAT(10X,6H--- POOR CONVERGENCE (12,14 ITERATIONS) AT NODE*,I3,*'
  1 AND STEP NO.*14)
  RETURN

C********************

CHAPTER 4
C***LOCAL TEMPERATURES
ENTRY LANAL4

9613 PTEMP(I)=F(JTE,I)
  DO 405 I=1,NP1
  SMC=0.
  DO 466 J=1,NS
  FNTH(I)=EINTH(I)-FS(J,I)*HO(J)
  466 SMC=SMC+FS(J,I)*CPMN(J,I)
  405 F(JTE,I)=FNTH(I)/SMC
C ***UNDER-RELAXATION OF TEMPERATURES IN REACTION ZONE
  ILM=ILUCM-3
  ILP=ILUCP+3
  DO 149 I=1,NP1
  IF (.NOT. (ITE.GE.ILM .AND. I.LE.ILP)) GO TO 149
  F(JTE,I)=5.*F(JTE,I)+PTEMP(I)
  149 CONTINUE
C ***FORMAT STATEMENTS
  100N FORMAT(7F10.4)
  200N FORMAT(7F10.1)
  RETURN
END

COMPILER SPACE
**STATION VARIABLES**
ENTRY OUTP2
XUD=XU/YOUT

**MEAN SQUARE FLUCTUATIONS (OF H ELEMENT)**
IF IN? EQ O AND, I,H2O, EQ O GO TO 165

**LOCATE POSITION OF FLAME FRONT**
ASSUMING #BATTLEMENT# VARIATION OF SPECIES CONCENTRATION
DO 161 I=1,NP1
RAT=FSTOICH*(1.-FS(JN2,I))
PARA=SFH2-1.E-10
SFH2=(F(JA,I)+SORT(F(JG,I)))/RAT
IF(SFH2.LT.1.) GO TO 162
161 CONTINUE

162 FACI=F(I-1)*Y(I)-Y(I-1)*(1.-PARA)/(SFH2-PARA)
DO 163 I=1,NP1
RAT=FSTOICH*(1.-FS(JN2,I))
PARA=SFH2-1.E-10
SFH2=(F(JA,I)+SORT(F(JG,I)))/RAT
IF(SFH2.LT.1.) GO TO 164
163 CONTINUE

164 FACE=F(I-1)*Y(I)-Y(I-1)*(1.-PARA)/(SFH2-PARA)
165 CONTINUE

PRDRP=PRESS1-P(1)
ULINE=(F(JU+1)-F(JU,NP1))/UEin
CLINE=FS(JH2,1)/(CIN+1,E=30)
TLINE=F(JTE+1)/TIN
WRITE(6,101) ISTEP,XX,XUD,DX,YHA,YOH,DDYHA,YDX
WRITE(6,102) KEX,YIN,Y(NP1),PDE,ACC,CFU,CE2
WRITE(6,103) PSII,PSIE,PEI,REME,FACI,FACE,FACM
WRITE(6,109) F(JU,1),F(JA,1),F(JTE,1),ULINE,CLINE,TLINE,PRDRP

**CHECK FOR FLUX CONSERVATION**
DO 1027 J=1,NEQ
FLUX(J)=(F(J+2)*OM(2)+F(J)*OM(N))*2.
DO 1027 I=2,NEQ
1027 FLUX(J)=FLUX(J)+(F(J,I)+F(J+1)*OM(I))
DO 1028 J=1,NEQ
IF(KAST(J)) 1029,1029,1028
1029 FLUX(J)=FLUX(J)-25*(F(J,N)-F(J-2)*OM(3)-OM(2))+
1*(F(J,N-1)-F(J,N))*OM(N)-OM(N+1))
1028 FLUX(J)=5*FLUX(J)*PRF*PSII*PSIF(J,N1)-PSIE*F(J,NP1)
WRITE(6,103) J,FLUX(J),J,NEQ
IF(KASE.EQ.2) WRITE(6,1155) RFLOW,RDUCT,REXD,P(1),DPDX
IF(KFX.NE.1) RETURN
OF=RJF(JH2)/X(NP1)
TAUE=REJ(JU)/X(NP1)
WRITE(6,110) INDE(JHS),F(JTE,NP1),OF,TAUE
RETURN

**PROFILE VARIABLES**
ENTRY OUTP3

**INFORMATION (TEMPORARY) ON NEW OUTPUT ROUTINE.**
**PROFILE** ASSIGNING VALUES FOR PLOT. AND ALSO WRITES **PROFILES.** IT IS CALLED BY ...
**CALL PROFILE** (JPROF,TITLE,FIRST,ADD,DIV,FINAL,KPLOT,SYM)
**WHERE JPROF#J# REFERS TO THE F(J,I) ARRAY**
**JPROF#AT#0# MEANS USE F(JPROF#I#) ARRAY AND WRITE PROFILE.**
**JPROF#AT#0# MEANS USE OUT(1)+ARRAY AND WRITE PROFILE.**

77
C/ JPROF=0 MEANS NO ACTION UNLESS KPLOT.LT.0
C/ N*0 OUT(I) ARRAY IS OVERWRITTEN BY PROFIL.
C/ TITLE IS THE NAME OF THE PROFILE, PLOTTED BY SYMBOL.
C/ FIRST AND FINAL ARE FIRST AND LAST VARIABLES WRITTEN IN PROFILE
C/ AND DIV MODIFY PROFILES FROM I=2 TO I=N
C/ KPLOT>0 MEANS ASSIGN YTPROFILE(KPLOT,I) ARRAY.
C/ KPLOT=0 MEANS NO PLOT ASSIGNMENTS.
C/ KPROFILE.LT.0 MEANS ASSIGN THE Y(I) ARRAY TO THE XPROFILE(I) ARRAY.
C/ SYMBOL IS THE CHARACTER USED IN PLOT.

C --- ZERO YTPROFILE ARRAYS

IF (ISTEP,GT,1) GO TO 401
   DO 402 I=1,NP1
   402 OUT(I)=0.
   DO 403 K=1,10
   403 CALL PROFIL(0,1,0,0,0,0,1,0, K,1,0)
   401 CONTINUE

C --- DISTANCES (Y)

   CALL PROFIL(0,6,HY/Y(NP1),Y(NP1),1,0)

C --- AXIAL VELOCITIES (JU)

   DIV=F(JU,1)-F(JU,NP1)+1.E-30
   CALL PROFIL(JU,6,HU VELO,F(JU,1),E,F(JU,NP1),DIV,F(JU,NP1),1,1HU)

C --- STAGMATION ENTHALPIES (JHS)

   DIV=F(JHS,1)-F(JHS,NP1)
   CALL PROFIL(JHS,6,H H STAG,F(JHS,1),E,F(JHS,NP1),DIV,F(JHS,NP1),0,0)

C --- TURBULENT KINETIC ENERGIES (JK)

   DIV=F(JK,1)-F(JK,NP1)+1.E-30
   CALL PROFIL(JK,6,HK,E,TI,F(JK,1),E,F(JK,NP1),5,1HK)

C --- DISSIPATION RATES (JD)

   CALL PROFIL(JD,6,HDISS,F(JD,1),E,F(JD,NP1),6,1HD)

C --- DISSIPATION LENGTH SCALES (JLE)

   DO 1201 I=1,N
   1201 F(JLE,I)=0
   F(JLE,NP1)=0.
   DIV=Y(NP1)
   CALL PROFIL(JLE,6,HLENGTH,F(JLE,1),E,F(JLE,NP1),10,1HL)

C --- TURBULENT VISCOSITIES (EMUT)

   WRITE(9,63A) (EMUT(I),I=1,NP1)

C --- DENSITIES

   WRITE(9,65A) (RHOM(I),I=1,NP1)

C --- REYNOLDS STRESS CORRELATION (JUV)

   DIV=F(JUV,1)-F(JUV,NP1)+1.E-30
   CALL PROFIL(JUV,6,HEUV,F(JUV,1),E,F(JUV,NP1),2,1HS)

C --- SPECIES MASS FRACTIONS (JA)

   DIV=F(JA,1)-F(JA,NP1)+1.E-30
   CALL PROFIL(JA,7,HF(JA),F(JA,1),E,F(JA,NP1),3,1HA)

C --- CONCENTRATION FLUCTUATIONS (OF H ELEMENT)

   DIV=F(JG,1)-F(JG,NP1)+1.E-30
   CALL PROFIL(JG,7,HF(JG),F(JG,1),E,F(JG,NP1),9,1HG)

C --- ABSOLUTE TEMPERATURES (JTE)

   DIV=F(JTE,1)-F(JTE,NP1)+1.E-30
   CALL PROFIL(JTE,4,TEMP,F(JTE,1),E,F(JTE,NP1),H,1HT)

C --- OUTPUT OF INDIVIDUAL SPECIES CONCENTRATIONS

   DO 625 I=1,NS
   625 WRITE(9,626) ASYMFL(J),F(S(J,I),I=1,NP1)

C --- PLOTTING OF PROFILES

78
605 IF (ISTEP.EQ.0) RETURN
IF (ISTEP.EQ.90.INX.OR.ISTEP.EQ.IEND) GO TO 435
IF (XID.LT.XPLOT(1)) RETURN
KT=KT+1
435 WRITE(6,1691) XU,ISTEP
CALL PLOT(KT)
GO TO 435

C **********************************************************************

C DATA STATEMENTS

C **********************************************************************

END

COMPILED SPACE

79
SUBROUTINE PROFIL (JPROF, TITLE, FIRST, ADD, DIV, FIN, KPL, SYM)

COMM/GEN/ACC/CSLAM/DPARX, DX, ETH, F(10,40), F(10,40), GAM, 
ICAM, GAM(70), I, IF IN, INDE(10), IND, ISTEP, IUTR, ITEST, KEX, 
KN, L, NLH, NPL, NPI, NPL, OM(40), OMD(40), OMD(40), OMD(40), KAST(10), PEI, PSIE, PSII, 
3P(40), 3P(40), RH(40), RJE(10), RJI(10), RME, RMII, SD(40), SU(40), VM(10), 
4XT, XI, Y(40), Y(40), Y(40), Y(40), Y(40), Y(40), Y(40), Y(40), Y(40), Y(40), Y(40), 
COMMON/CLS/JU, JK, JD, JH5, JA, JG, JF, MO, JU, JB 
COMMON/TPLOT/XTAXIS, XTPLOT(40), YAXS(10), YTPLOT(10,40), 
YMAX, YMAX, YMAX, YMAX, YMAX, YMAX, YMAX, YMAX, YMAX, YMAX, YMAX, 
100 IF (KPL) 500, 700, 700
700 IF (JPROF) 200, 200, 100
100 UO 101 I = 1, NPI
101 OUT(I) = F(JPROF, I)
200 YMAX = I, E-30
DO 201 I = 1, NPI
      YMAX = YMAX(YMAX, OUT(I))
201 OUT(I) = (OUT(I) + ADD) / DIV
      IF (JPROF, 30, ADD, 1) WRITE (6, 900) TITLE, FIRST, (OUT(I), I = 1, N)
      IF (JPROF, 30, ADD, 2) WRITE (6, 900) TITLE, (F(JPROF, I), I = 1, N)
      IF (KPL) 500, 600, 400
400 DO 401 I = 1, NPI
401 YTPLOT(KPL, I) = OUT(I)
      YAXS(KPL) = TITLE
      YSYM(KPL) = SYM
      YMAX(KPL) = YMAX
      RETURN
500 DO 501 I = 1, NPI
501 XTPLOT(I) = (Y(I) + ADD) / DIV
      XTPLOT = TITLE
      WHITE (9, 900) TITLE, FIRST, (XTPLOT(I), I = 2, N ), FINAL
600 RETURN
900 FORMAT (1H, A6, 1P11E11.3 / (7X, 1P11E11.3)))
END

COMPILER SPACE
SUBROUTINE PLOTS(x, idim, imax, xaxis, y, ymax, jdim, jmax, yaxes, symbol)
C SUBROUTINE FOR PLOTTING J CURVES OF Y(J,I) AGAINST X(I)
C
X AND Y ARE ASSUMED TO BE IN ANY RANGE EXCEPT THAT NEGATIVE VALUES
ARE PLOTTED AS ZERO.
X AND Y ARE SCAL ARED TO THE RANGE 0 TO 1 BY DIVISION BY THE MAXIMA
WHICH ARE ALSO PRINTED
IDIM IS THE VARIABLE DIMENSION FOR X.
IMAX IS THE NUMBER OF X VALUES
XAXIS STORES THE NAME OF THE X-AXIS.
JDIM IS THE VARIABLE DIMENSION FOR Y.
JMAX IS THE NUMBER OF CURVES TO BE PLOTTED (UP TO 10).
THE ARRAY YAXES(J) STORES THE NAME OF THE CURVES.
THE ARRAY SYMBOL(J) STORES THE SINGLE CHARACTERS USED FOR PLOTTING.

DIMENSION X(IDIM), Y(JDIM, IDIM), YMAX(JDIM), YAXES(JDIM), SYMBOL(JDIM)

1, (I=1,11)
DATA DOT, CROSS, BLANK/1H, 1H, 1H /

SCALING X ARRAY TO THE RANGE 0 TO 50
XMAX=1.E-30 DO 1 I=1, IMAX
1 IF(X(I) .GT. XMAX) XMAX=X(I)
DO 2 I=1, IMAX
X(I)=X(I)/XMAX*50.
2 IF(X(I) .LT. 0.) X(I)=0.

SCALING Y ARRAY TO THE RANGE 0 TO 100
DO 3 J=1, JMAX
AYMAX=1.E-30 DO 4 I=1, IMAX
4 AYMAX=AYMAXL(Y(J,I)/AYMAX)*100., 0.)
3 Y(J,I)=AYMAXL((Y(J,I)/AYMAX)*100., 0.)

IDENTIFYING THE VARIOUS CURVES TO BE PLOTTED
WRITE(6,163) XAXIS, XMAX
WRITE(6,160) (YAXES(I), I=1, JMAX)
WRITE(6,166) (SYMBOL(I), I=1, JMAX)
WRITE(6,162) (YMAX(I), I=1, JMAX)
DO 5 I=1, 11
5 A(I)=0.1*FLOAT(I-1)
WRITE(6,161) (A(I), I=1, 11)

MAIN LOOP. EACH PASS PRODUCES AN X-CONSTANT LINE
DO 40 I=1, 51
IF(I.EQ.1.0R.1.I.EQ.51) GO TO 32
GO TO 33

ALLOCATE . OR + AS MARKER ON THE Y-AXIS
32 DO 30 K=1, 101
30 A(K)=DOT
DO 31 K=11, 101, 10
31 A(K)=CROSS

ALLOCATE . OR + MARK ON THE X-AXIS, ALSO THE APPROPRIATE X VALUE
33 A(I)=DOT
34 K=K+5
IF(K) 44, 7, 46
A(1) = CROS$ 
A(101) = CROS$ 
XL = 0.0, A2 = FLOAT(I-1)

CHECK IF ANY Y( X(I) ) VALUE LIES ON THIS X-CONSTANT LINE
IF YES GO TO 41, OTHERWISE GO TO 42
   DO 43 K = 1, IMAX
     IF( IFIX(X(K) + 1.5) - I ) 43 + 41 + 43
   CONTINUE

LOCATE Y( X(I) )
   DO 44 J = 1, JMAX
     NY = Y(J) * 1.5
     A(NY) = SYMBOL(J)
   CONTINUE

PRINT X-CONSTANT LINE
   WRITE (6,155) XL, (A(K): K = 1, 101) * XL

PUTTING BLANKS INTO X-CONSTANT LINE
   DO 49 I = 1, 101
     A(I) = BLANK
   CONTINUE

RETURN

FORMAT (11H Y-AXES ARE 5X, 10 (1X, A10))
FORMAT (11H MAXIMUM VALUES, 1PE10.3)
FORMAT (11H X-AXIS IS 1AXIS IS 1AXIS IS MAXIMUM VALUE = 1PE10.3)
FORMAT (11H SYMBOL, 11X, 10 (1X, A10))
END
SUBROUTINE YINT(FRAC,YFRAC,JJ)
COMMON/GENERAL/ACC,CSALFA,DMDX,DM,ENTH(40),F(10,40),FS(10,40),GAM3,
GM,GMAN,GAN(40),I,IFIN,INDE(10),INDI(10),ISTEP,ITRAP,ITEST,KEX,KIH,
KMD,KNO,KODE(40),KOM(40),KOMD(40),KOMD(40),KON(40),KONT(10),KOST(10),KPE,
PSIE,PSII,RS(40),RH(40),RHO(40),RJE(10),RJI(10),RME,ROI,SO(40),SU(40),WM(10),
XJ,XJ,XJ,Y(46),YDF(40),YF,YI,YJETE(10),YJTI(10)
COMMON/CJ,JU,JK,JD,JHS,JA,JG,JE,JLE,JUV,JB
COMMON/CFJ/C1,02,102,102
C**************************INTERPOLATION SUBROUTINE
C***********************************************************************

REFDIF=FRAC-AHS(F(JJ,NP1)-F(JJ,1))
IF(REFDIF,NE.0) GO TO 10
YFRAC=FRAC*Y(NP1)
WRITE(6,1) YFRAC
1 FORMAT(7H ISTEP=,14,4H XU=,1PE10.3,52H IN SUBROUTINE YINT, REFDIF=
1.0, SO YFRAC=FRAC*Y(NP1)=,E10.3)
WRITE(6,2) FRAC, JJ, NP1, F(JJ,NP1), F(JJ,1)
2 FORMAT(6H FRAC=,1PE10.3,4H JJ=,13,5H NP1=,14,
11H F(JJ,NP1)=,E10.3,9H F(JJ,1)=,E10.3)
RETURN
10 IF(FRAC.HT) GO TO 30
DO 20 I=2,N
20 T=AHS(F(JJ,I)-F(JJ,1))
IF(T.REFDIF) 20,21,21
21 T=AHS(F(JJ,1)-F(JJ,I-1))
IF(T.22.33,22
22 CONTINUE
RETURN
25 DO 44 IDACH=2,N
44 T=AHS(F(JJ,I)-F(JJ,1))
IF(T.41,44,40
41 T=AHS(F(JJ,1)-F(JJ,I-1))
IF(T.42,44,42
42 CONTINUE
RETURN
43 YFRAC=Y(I)-T*(Y(I+1)-Y(I))
RETURN
44 CONTINUE
RETURN
END

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