

**NASA CONTRACTOR
REPORT**



NASA CR-2407

NASA CR-2407

**COMBUSTION OF HYDROGEN-AIR JETS
IN LOCAL CHEMICAL EQUILIBRIUM
(A Guide to the CHARNAI Computer Program)**

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NATIONAL AERONAUTICS AND SPACE ADMINISTRATION • WASHINGTON, D. C. • JUNE 1974

1. Report No. NASA CR-2407		2. Government Accession No.		3. Recipient's Catalog No.	
4. Title and Subtitle COMBUSTION OF HYDROGEN-AIR JETS IN LOCAL CHEMICAL EQUILIBRIUM (A GUIDE TO THE CHARNAI COMPUTER PROGRAM)				5. Report Date June 1974	
				6. Performing Organization Code	
7. Author(s) D. B. Spalding, B. E. Launder, A. P. Morse, and G. Maples				8. Performing Organization Report No. 73-1	
9. Performing Organization Name and Address Fluid Mechanics and Thermal Systems, Inc. Route 2, Box 11, Waverly, Alabama 36879				10. Work Unit No. 501-04-03-02	
				11. Contract or Grant No. NAS 1-12167	
				13. Type of Report and Period Covered Contractor Report	
12. Sponsoring Agency Name and Address National Aeronautics and Space Administration Washington, D.C. 20546				14. Sponsoring Agency Code	
15. Supplementary Notes Final report.					
16. Abstract 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 $\mu_t = C\rho k^2/\epsilon$, where C is a constant, ρ is density, k is turbulent kinetic energy, and ϵ is the dissipation rate. Chemical equilibrium is assumed throughout the flow.					
17. Key Words (Suggested by Author(s)) Supersonic combustion Turbulent mixing Hydrogen-air Coaxial jet			18. Distribution Statement Unclassified - Unlimited STAR Category 12		
19. Security Classif. (of this report) Unclassified		20. Security Classif. (of this page) Unclassified		21. No. of Pages 85	22. Price* \$4.00

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1. Introduction

The computer program CHAR^NAL (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 H_2 , O_2 , H_2O , O , H , OH and N_2 .

The present report details the mathematical and physical basis of CHAR^NAL, 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 CHAR^NAL 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.

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

$$\rho u \frac{\partial \hat{h}}{\partial x} + \rho v \frac{\partial \hat{h}}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left(\mu_t r \frac{\partial \hat{h}}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left\{ r \left[\left(\mu_t - \Gamma_h \right) \frac{\partial}{\partial r} \left(u^2/2 \right) + \left(\Gamma_k - \Gamma_h \right) \frac{dk}{dr} + \sum_j \left(\Gamma_j - \Gamma_h \right) h_j \frac{\partial m_j}{\partial r} \right] \right\} \quad (2.1-2)$$

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

The mass fraction of elemental hydrogen, f , is used as a variable for the reason that, unlike 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:

$$\frac{\partial}{\partial x} \rho u + \frac{1}{r} \frac{\partial}{\partial r} (\rho v r) = 0 \quad (2.1-4)$$

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:

$$T = \frac{\left[\hat{h} - u^2/2 - k - \sum_j m_j \left\{ \Delta h_f - \Delta h \right\} \right]}{\sum_j m_j \bar{c}_{pj}} \quad (2.1-5)$$

$$\text{and } \bar{c}_{pj} = \frac{1}{T} \int_{0^\circ \text{K}}^T c_{pj} dT \quad (2.1-6)$$

2.2 The Turbulence Model

The effective turbulent transport coefficients μ_t , Γ_h , Γ_m and Γ_k are determined by means of the $k\epsilon$ 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, ϵ and the fluid density. They are connected by the formula:

$$\mu_t = C_\mu \rho k^2 / \epsilon \quad (2.2-1)$$

The quantities k and ϵ 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:

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

$$\rho u \frac{\partial \epsilon}{\partial x} + \rho v \frac{\partial \epsilon}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{\mu_t}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial r} \right) + \frac{C_1}{k} \epsilon \mu_t \left(\frac{\partial u}{\partial r} \right)^2 - \frac{C_2 \rho \epsilon^2}{k} \quad (2.2-3)$$

The quantities C_μ , C_1 , C_2 , σ_k and σ_ϵ are dimensionless and are given the constant values below

C_μ	C_1	C_2	σ_k	σ_ϵ
.09	1.43	1.92	1.0	1.3

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 ϵ . Such a prescription is not possible because the exact equations for k and ϵ contain correlations whose magnitude is not directly ascertainable. These correlations are therefore approximated in terms of k, ϵ 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 CHARNAL is designed to compute.

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

$$\Gamma_h \equiv \mu_t / \sigma_h \quad ; \quad \Gamma_m \equiv \mu_t / \sigma_m \quad (2.2-4)$$

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

$$\sigma_h = \sigma_m = 0.7 \quad (2.2-5)$$

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

$$\sigma_h = \sigma_m = 0.95 - .45 (y/R)^2 \quad (2.2-6)$$

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 Γ_h and Γ_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:



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

$$m_{\text{H}_2}/m_{\text{H}}^2 = K_1 \quad (2.3-5)$$

$$m_{\text{O}_2}/m_{\text{O}}^2 = K_2 \quad (2.3-6)$$

$$m_{\text{OH}}/m_{\text{O}}m_{\text{H}} = K_3 \quad (2.3-7)$$

$$m_{\text{H}_2\text{O}}/m_{\text{H}}m_{\text{OH}} = K_4 \quad (2.3-8)$$

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

$$X \equiv m_{\text{O}_2} + m_{\text{O}} + \frac{W_{\text{O}}}{W_{\text{H}_2\text{O}}} (m_{\text{H}_2\text{O}}) + \frac{W_{\text{O}}}{W_{\text{OH}}} (m_{\text{OH}}) \quad (2.3-9)$$

and

$$f \equiv m_{\text{H}_2} + \frac{W_{\text{H}_2}}{W_{\text{H}_2\text{O}}} (m_{\text{H}_2\text{O}}) + \frac{W_{\text{H}}}{W_{\text{OH}}} (m_{\text{OH}}) \quad (2.3-10)$$

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" $K_1 \dots K_4$ are functions of temperature and pressure. CHARVAL 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]

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

where the constants σ_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 $f-g^{1/2} = f_{stoich}$ and the outer boundary where $f+g^{1/2} = f_{stoich}$. 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 CHARVAL Computer Program

CHARVAL is a custom-developed version of the Patankar-Spalding PASSA program which, in turn, is a newer, more economical and flexible version of GENMIX 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 CHARVAL and the original GENMIX 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 LANGLEY, 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 , h , f , g , k and ϵ) are transformed so that the independent variables are the longitudinal distance, x and the dimensionless stream function, ω defined as:

$$\omega \equiv (\psi - \psi_I) / (\psi_E - \psi_I) \quad (3.1-1)$$

where ψ itself is obtained from the relation,

$$\frac{\partial \psi}{\partial y} = \rho u r \quad (3.1-2)$$

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,

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

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 ϕ . 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 ω . 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 ψ_E and ψ_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,

$$\text{Source of } (k) = \left[\mu_t \left(\frac{\partial u}{\partial y} \right) \right]_U^2 - \left[(\rho \epsilon / k) \right]_U k_D \quad (3.1-4)$$

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 ω). PASSA also contains the option of using castellated profiles instead of linear variations of ϕ between the grid nodes.

3.3 Details of the CHARNAL Program

A flow diagram for CHARNAL 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 CHARVAL, 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

$$k = 3.33 \left[\ell_m \left(\frac{\partial u}{\partial y} \right) \right]^2 \quad (3.3-1)$$

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

$$\epsilon = k^{3/2} / \ell_e \quad (3.3-2)$$

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 4×10^{-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,

$$\rho = pW/RT \quad (3.3-3)$$

where the mean molecular weight of the mixture, W is given by,

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

Subroutine STRID1 is called to evaluate useful quantities relating the individual W '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 GENIIX, (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 ϕ 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 laminar 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 GENIIX (reference [1]). Subroutine AUX is called initially from Chapter 10 of MAIN 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 ω 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 !IF 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 sub-routines. PROFIL is used to normalize the profiles and communicates with PLOTS which scales both the abscissa (transverse distance) and ordinate (ϕ 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 NP1 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 ϕ is a linear combination of the values of ϕ 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

$$h - h_{\text{ref}} = \int_{T_{\text{ref}}}^T C_p dT + \Delta h_{f, T_{\text{ref}}} \quad (3.3-5)$$

where $\Delta h_{f, T_{\text{ref}}}$ 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

$$h = \int_{298.15^\circ\text{K}}^T C_p dT + \Delta h_{f, 298.15^\circ\text{K}} \quad (3.3-6)$$

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

$$\equiv \bar{C}_p T + H_0 \quad (3.3-7)$$

where \bar{C}_p ($\equiv 1/T \int_{0^\circ\text{K}}^T C_p dT$) denotes a mean specific heat and H_0 is the

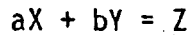
composite of the remaining terms. Values of h are read in at intervals of 100°K for temperatures of up to 6000°K, together with the value of H_0 for each species. The mean specific heats are then evaluated from equation (3.3-7) and stored (see Appendix 1 for array locations).

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



(implying 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

$$K_p = p_Z / p_X^a p_Y^b \quad (3.3-10)$$

[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

$$K_m = m_Z / m_X^a m_Y^b = K_p (pW)^{a+b-1} W_Z / (W_X^a W_Y^b) \quad (3.3-11)$$

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.

$$K_{m,1} = m_{O_2} / m_H^2 \quad (3.3-12)$$

$$K_{m,2} = m_{H_2} / m_{O_2}^2 \quad (3.3-13)$$

$$K_{m,3} = m_{OH} / m_{O_2} m_H \quad (3.3-14)$$

$$K_{m,4} = m_{H_2O} / m_{H^+} m_{OH} \quad (3.3-15)$$

$$X = m_{O_2} + m_O + \frac{W_O}{W_{H_2O}} m_{H_2O} + \frac{W_O}{W_{OH}} m_{OH} \quad (3.3-16)$$

$$f = m_{H_2} + m_H + \frac{W_{H_2}}{W_{H_2O}} m_{H_2O} + \frac{W_H}{W_{OH}} m_{OH} \quad (3.3-17)$$

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 LANGL3 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 $(1-OFAC)(1-f)$.
- (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 ($> 3000^\circ K$) 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 $2600^\circ K$; (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, LANGLE4 is called to evaluate the cross-stream temperatures. These are obtained from enthalpy profile via the relationship,

$$T = (h - \sum m_j H_{0,j}) / m_j \bar{C}_{p,j} \quad (3.3-18)$$

for which the mean specific heats are evaluated in LANGLE3 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 stoichometric 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)
- IN2, IO2, IH2O : denote presence of individual species;
= 0 (not present), = 1 (present)
- NR : number of reactions
- NS : number of chemical species

INUF : nature of initial profiles = 0 (continuous)
 = 1 (step-change)
 XU : 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
 IW1 : grid node corresponding to YW1 and UW1
 TDUCT : temperature of duct wall (for confined
 flows only)

(ii) Output parameters

ISTAT, 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 LANGL1 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 CHARVAL, fifteen test cases, prescribed by IASA 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°K; 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_- 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 though 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 centre line 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. ⁴

To convey an impression of the capabilities of CHARVAL 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 49mm. 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 CHARVAL

CHARVAL 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 CHARVAL 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 CHARVAL 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_μ , 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 CHARVAL 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 CHARVAL is to be put it would therefore be desirable to replace the present constant c_μ by the elaborate dependency on energy production: dissipation rates presented in [2] (associated with the model designated $k\epsilon^2$ 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 CHARVAL 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 ϵ 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

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2. B. E. Launder, A. Morse, D. B. Spalding and W. Rodi, 'Prediction of Free Shear Flows - A comparison of the performance of six turbulence models' Proceedings of Free Shear Flows Conference, 1972 NASA SP 321.
3. B. E. Launder and D. B. Spalding, 'Turbulence models and their application to the prediction of internal flow' Heat and Fluid Flow 2, 1972.
4. J. C. Rotta, 'Turbulent boundary layers in incompressible flow' in Progress in Aeronautical Sciences, Vol. 2, (ed A. Ferri, D. Kuchemann and L. H. G. Sterne) Macmillan, 1962.
5. B. McBride, 'Thermodynamic properties to 6000°K for 210 substances involving the first 18-elements' NASA SP-3001, 1963.
6. D. B. Spalding, 'Concentration fluctuations in a round jet', J. Chem. Eng. Sci. 26, 95, 1971.
7. J. H. Eggers, 'Turbulence mixing of coaxial compressible hydrogen-air jets, NASA TN D-6487, 1971.

7. Nomenclature

$C_u, C_1, C_2, C_{g1}, C_{g2}$	constant coefficients appearing in turbulence model.
\bar{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}	stagnation enthalpy.
Δh	difference between enthalpy of species at 298.15°K and 0°K.
Δh_f	heat of formation of species j.
k	kinetic energy of turbulence.
l_ϵ	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_{w1}, Y_{w2}	effective widths of shear flow, see Figure 2.
Γ	effective turbulent flow transport coefficient (subscript denotes diffused quantity).
ϵ	rate of turbulence energy dissipation.
μ_t	turbulent viscosity.
ρ	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 CEMINAL Program.

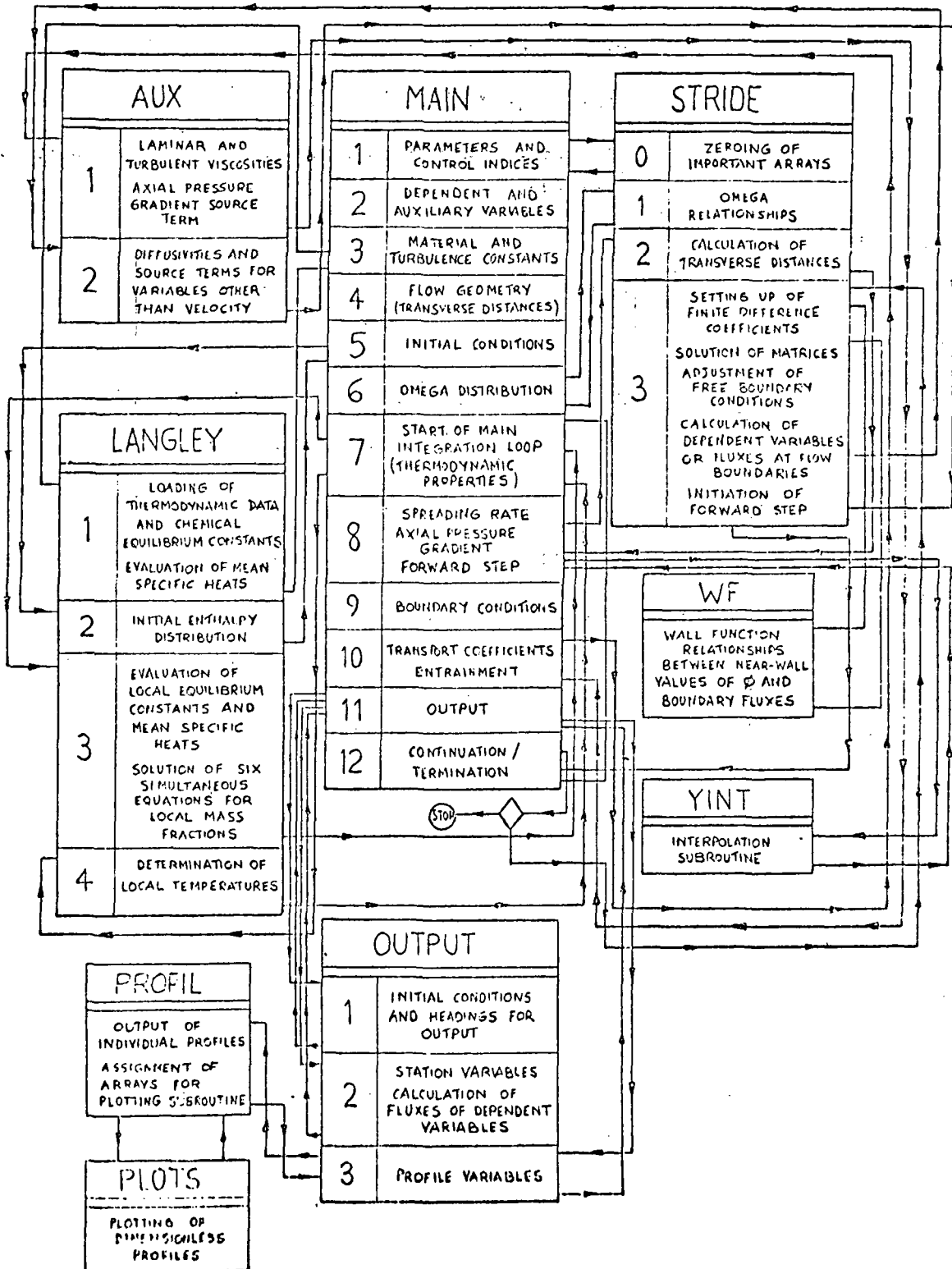
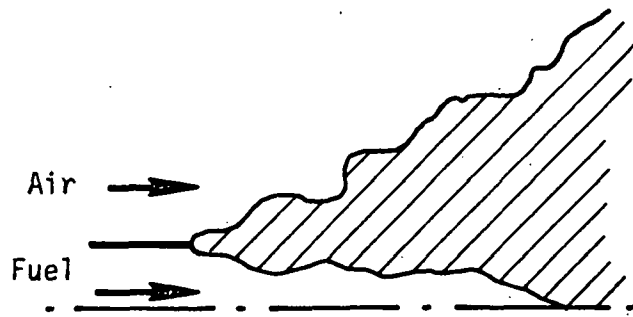
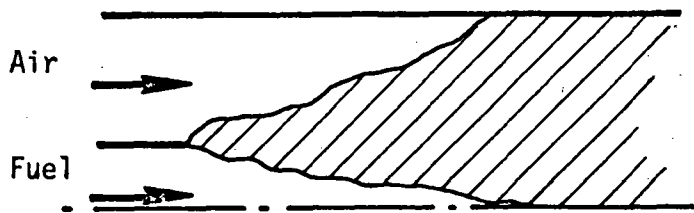


Table 2 Initial Profiles for Cases 1 and 4

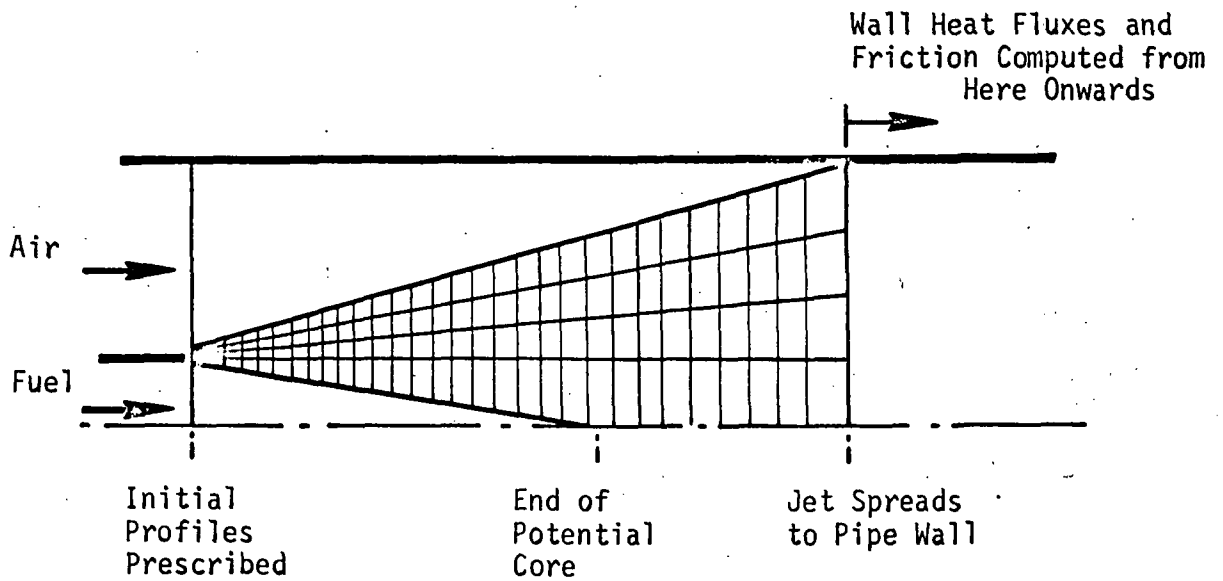
R/D _j	Temp.	Velocity	Mass Fraction						
	(K)	(m sec ⁻¹)	H ₂	H	OH	H ₂ O	O ₂	O	N ₂
0	193	2111	1						
.046	193	2111	1						
.137	193	2111	1						
.227	202	2108	1						
.273	240	2037	1						
.318	502	1209	1						
.363	694	198	1						
.409	1058	660					.232		.768
.454	1163	1001					.232		.768
.500	1173	1138					.232		.768
.590	1178	1220					.232		.768
.726	1176	1245					.232		.768
.950	1171	1283					.232		.768
1.05	1171	1283					.232		.768
↓ Free Stream									



a. Free

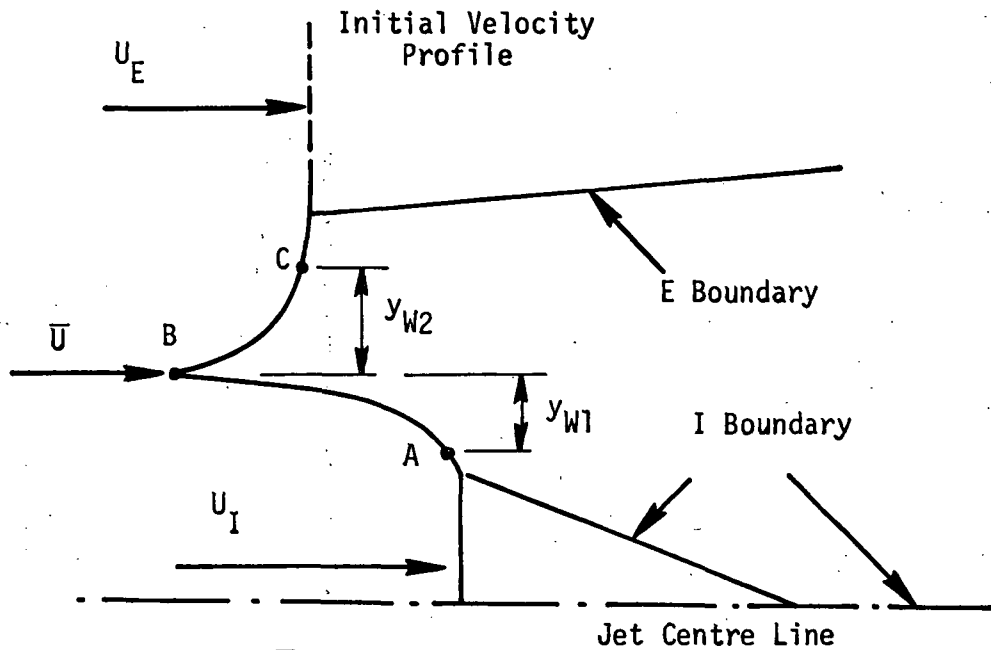


b. Confined



c. Finite Difference Grid

Figure 1. The Flow Geometry Treated by CHARNAI



At A, $U = 0.9 U_I + 0.1 \bar{U}$

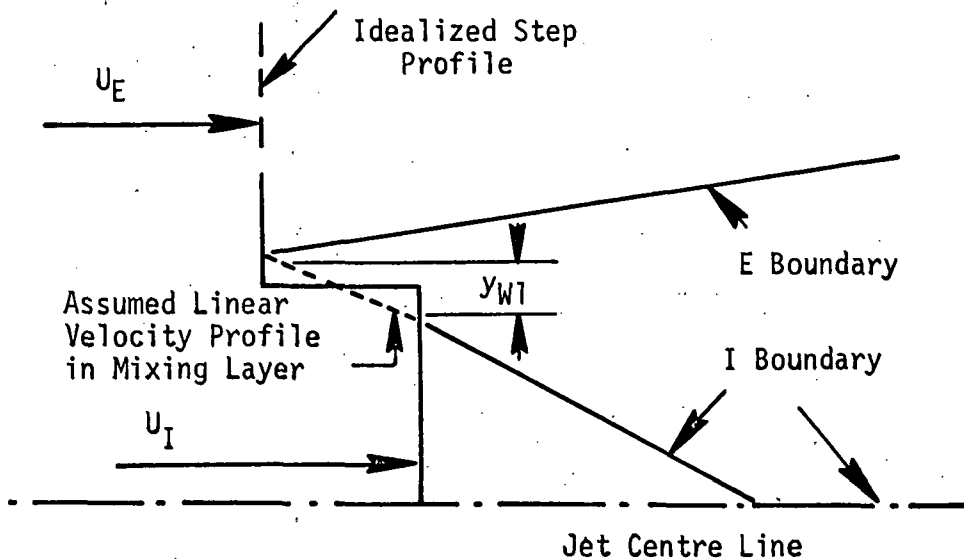
At B, $U = \bar{U}$

At C, $U = 0.9 U_E + 0.1 \bar{U}$

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

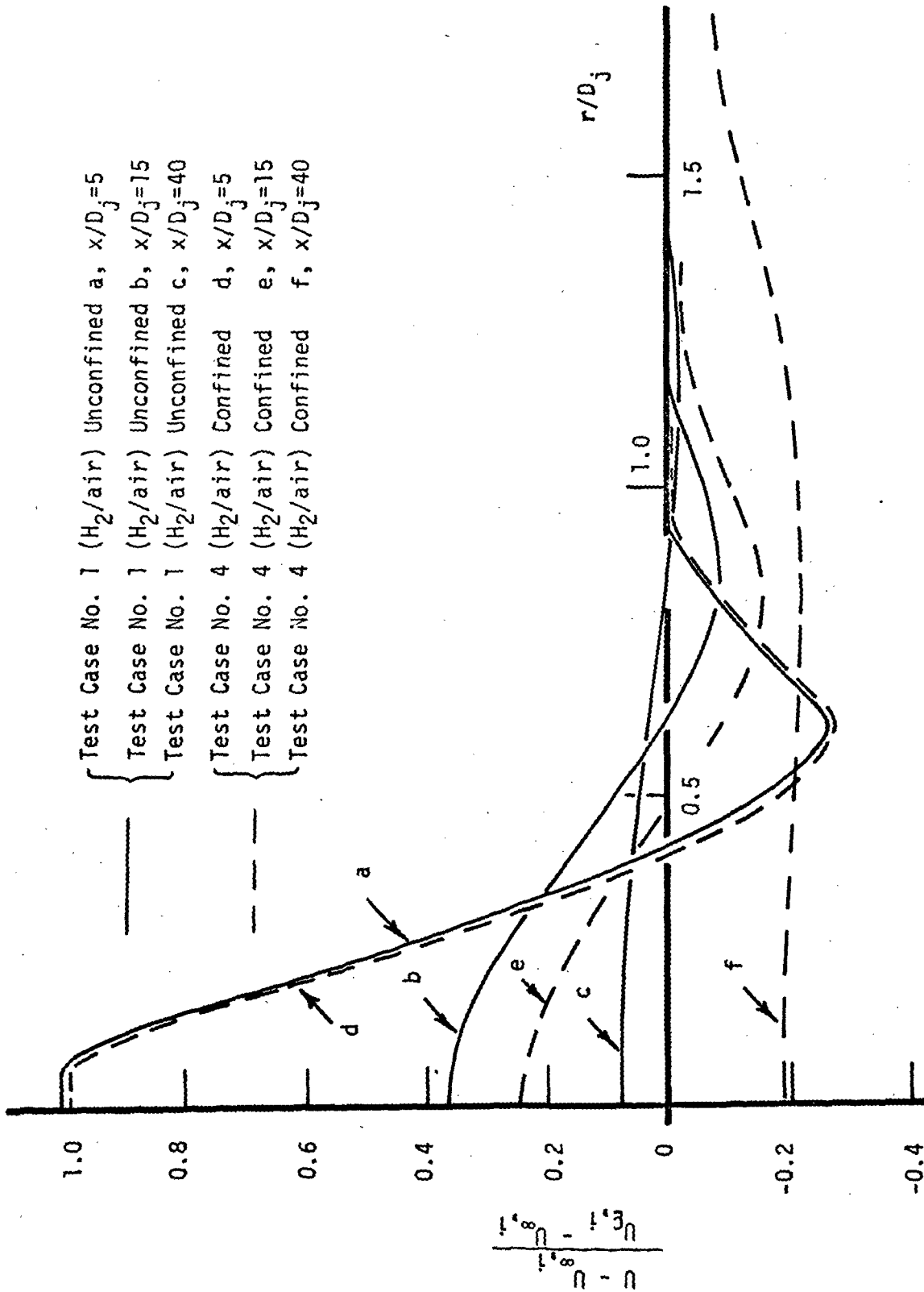


Figure 3. Velocity Profiles

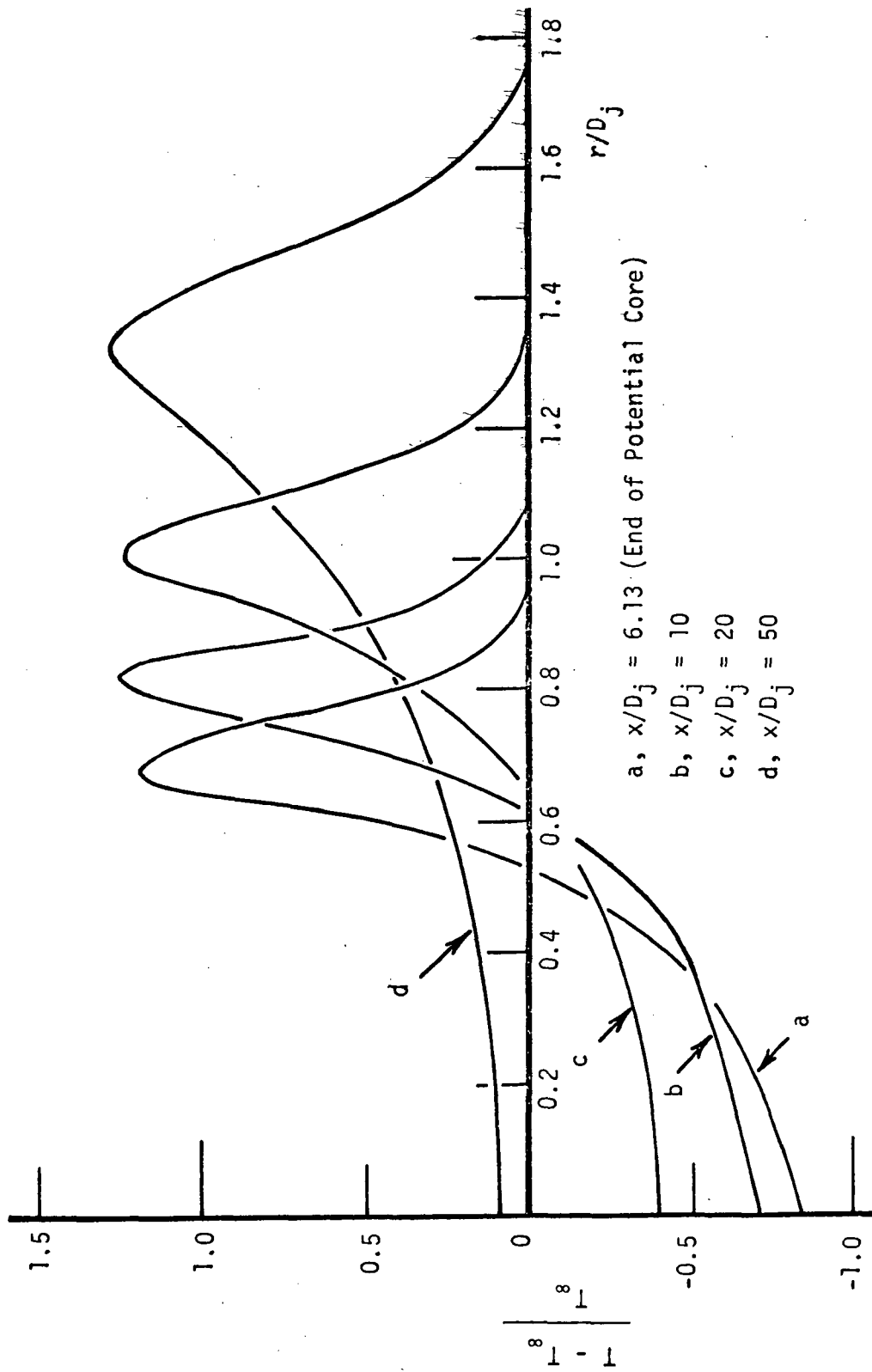


Figure 4. Temperature Profiles (Test Case No. 1)

- a, Test Case No. 1 (H₂/air) Unconfined
- b, Test Case No. 3 (H₂/nitrogen) Unconfined
- c, Test Case No. 4 (H₂/air) Confined
- d, Ref [2] Computation of Non Reacting H₂/air Jets

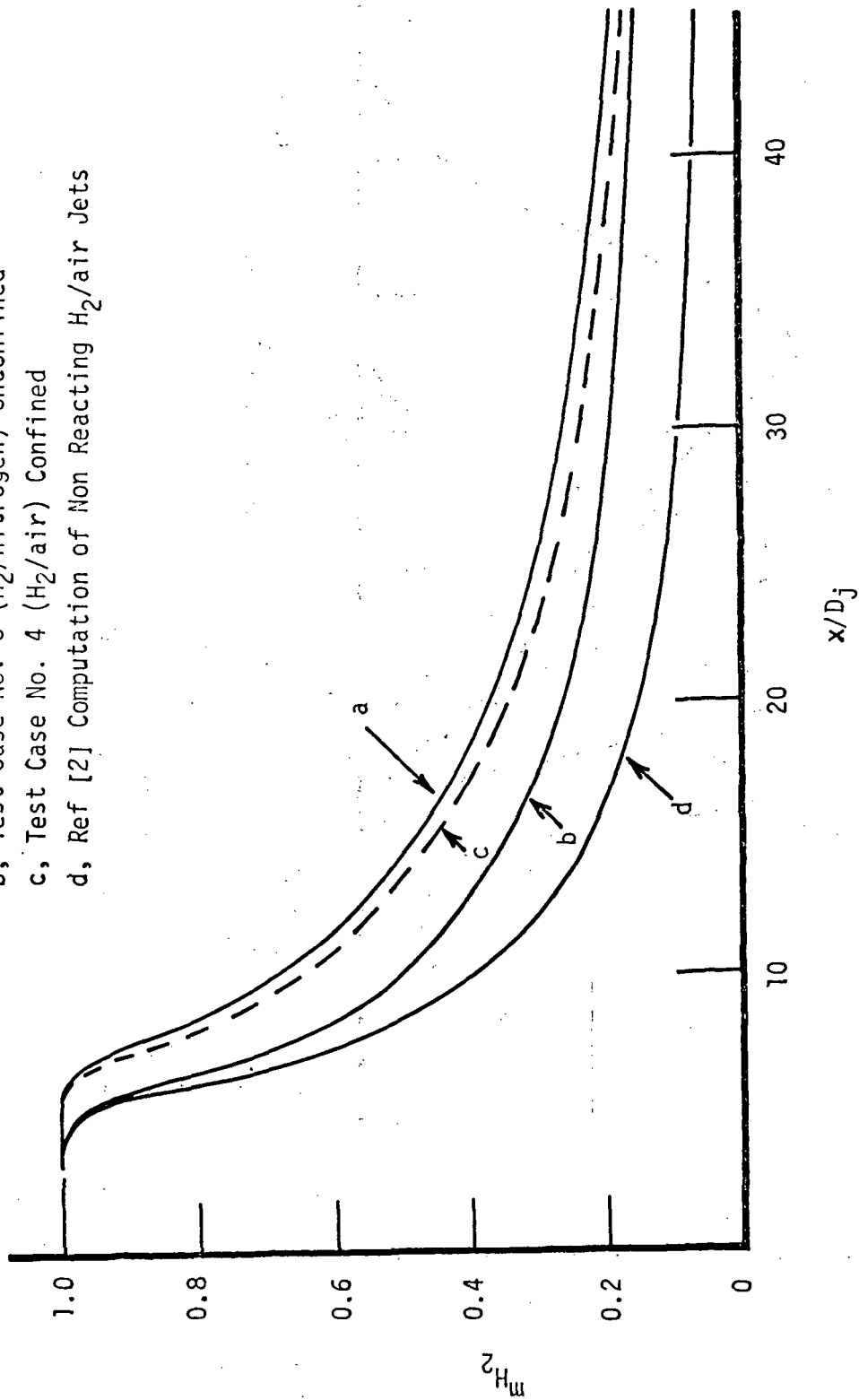


Figure 5. Decay of Centreline Mass Fraction of Hydrogen

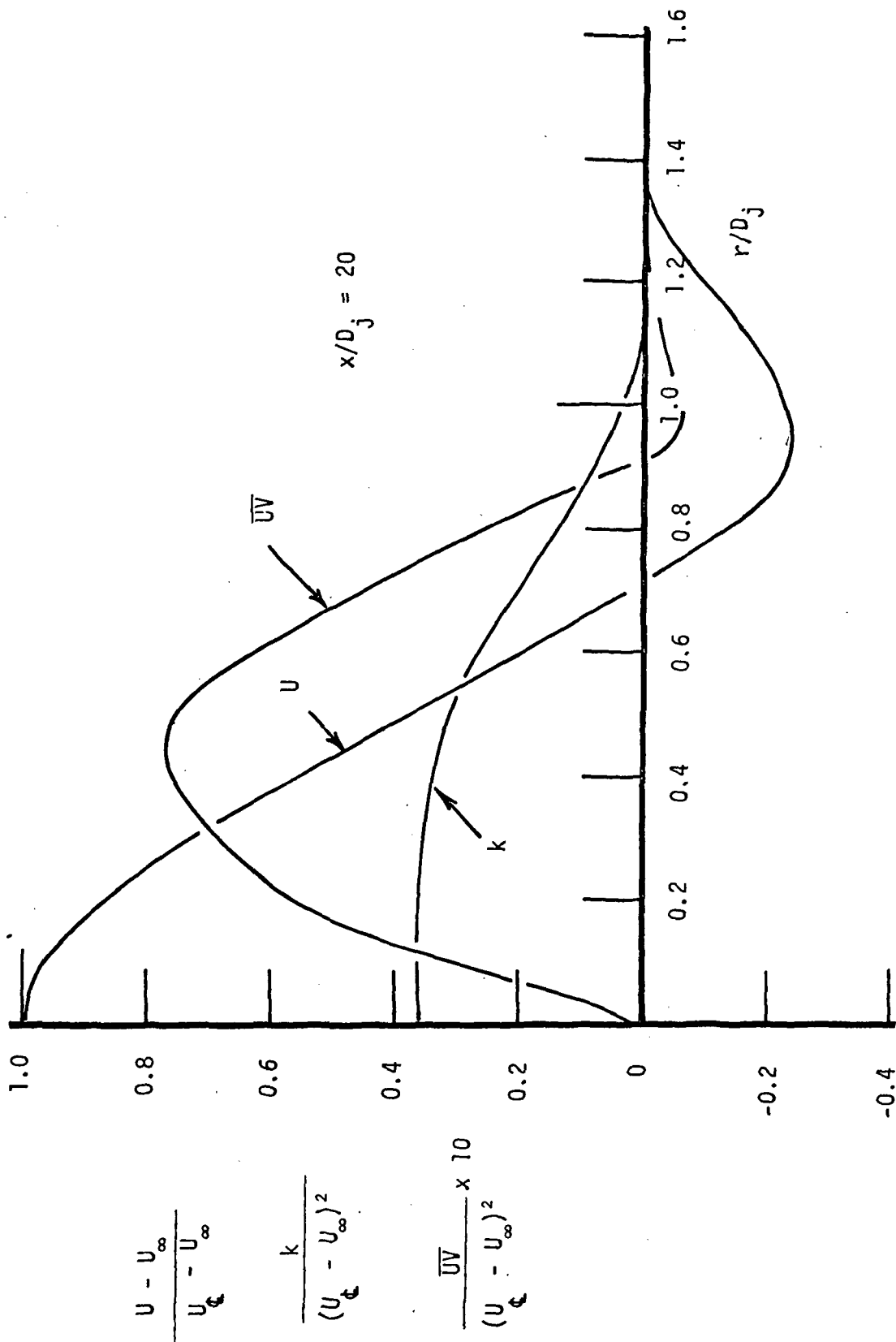
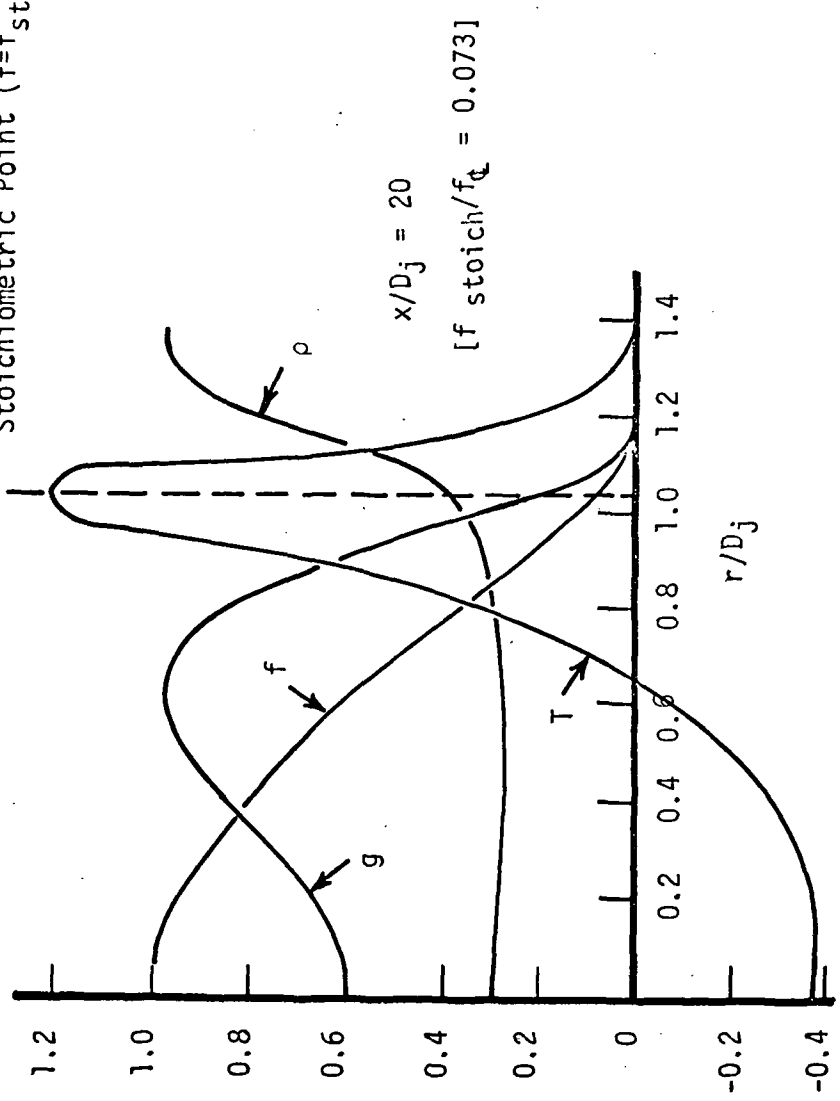


Figure 6. Profiles of Velocity, Turbulent Kinetic Energy and Reynolds Shear Stress (Test Case No. 1)

Stoichiometric Point ($f=f_{\text{stoich}}$)



$\frac{T - T_\infty}{T_\infty}$
 ρ/ρ_∞
 f/f_c
 $g/f_c^2 \times 10$

Figure 7. Profiles of Temperature and Density and Hydrogen Element Concentration (Mean and Fluctuating) Test Case Number 1

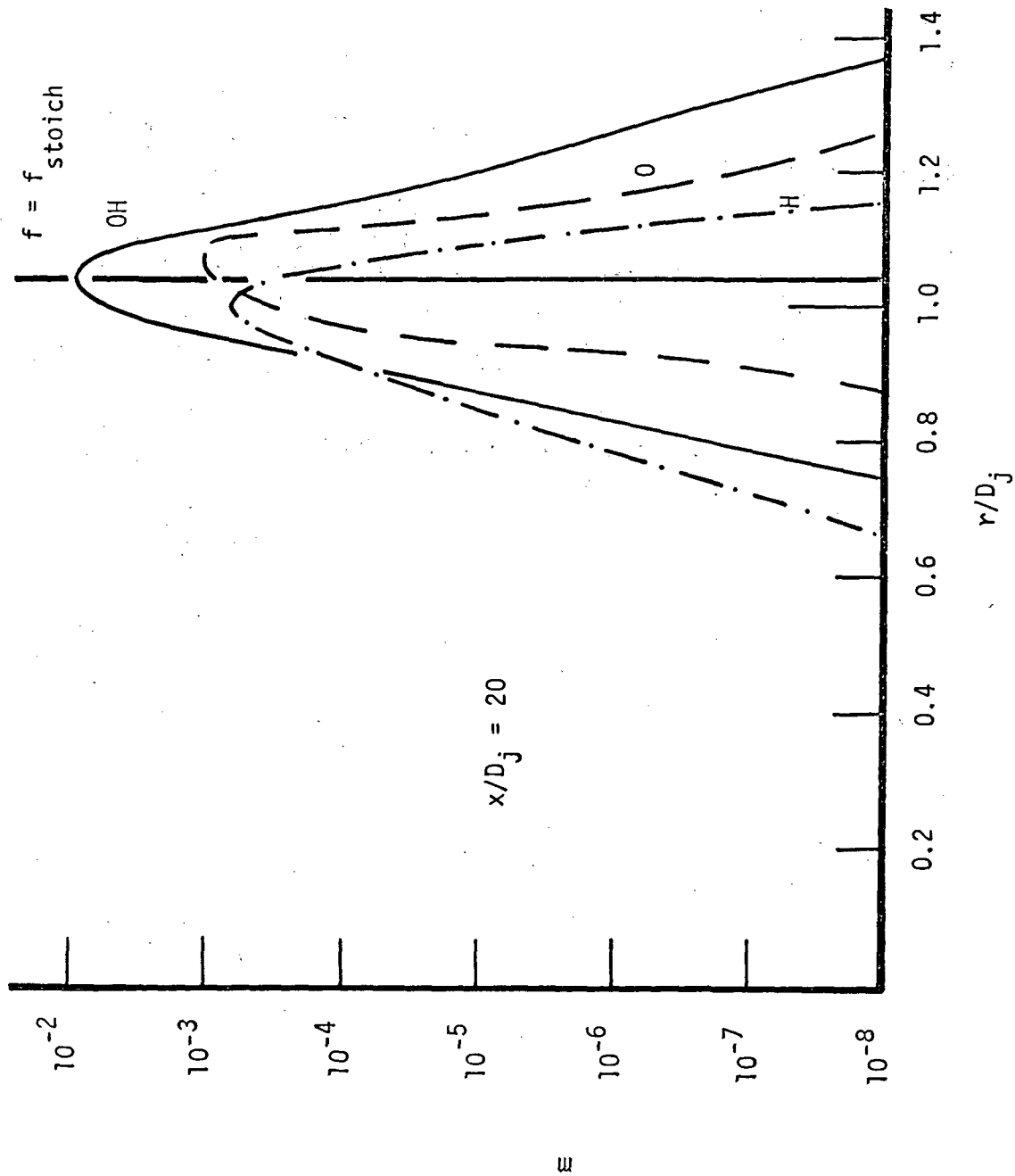
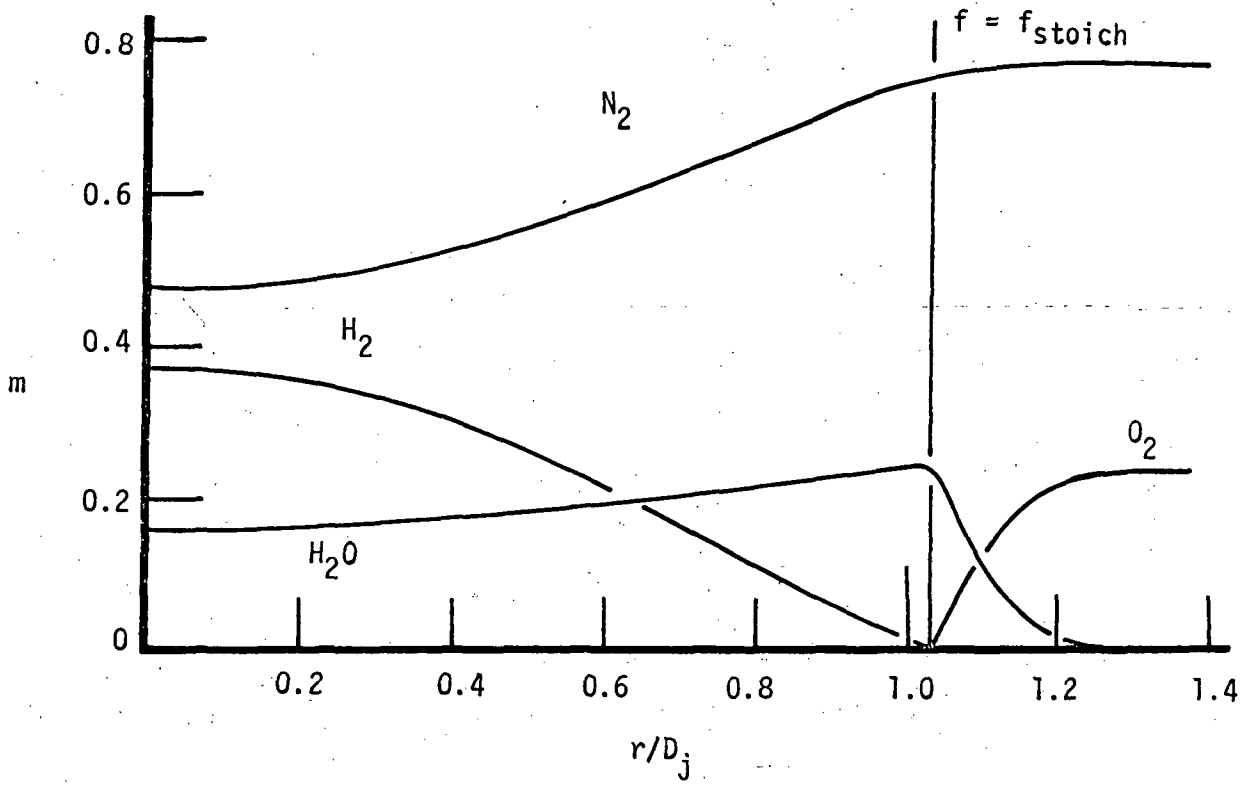
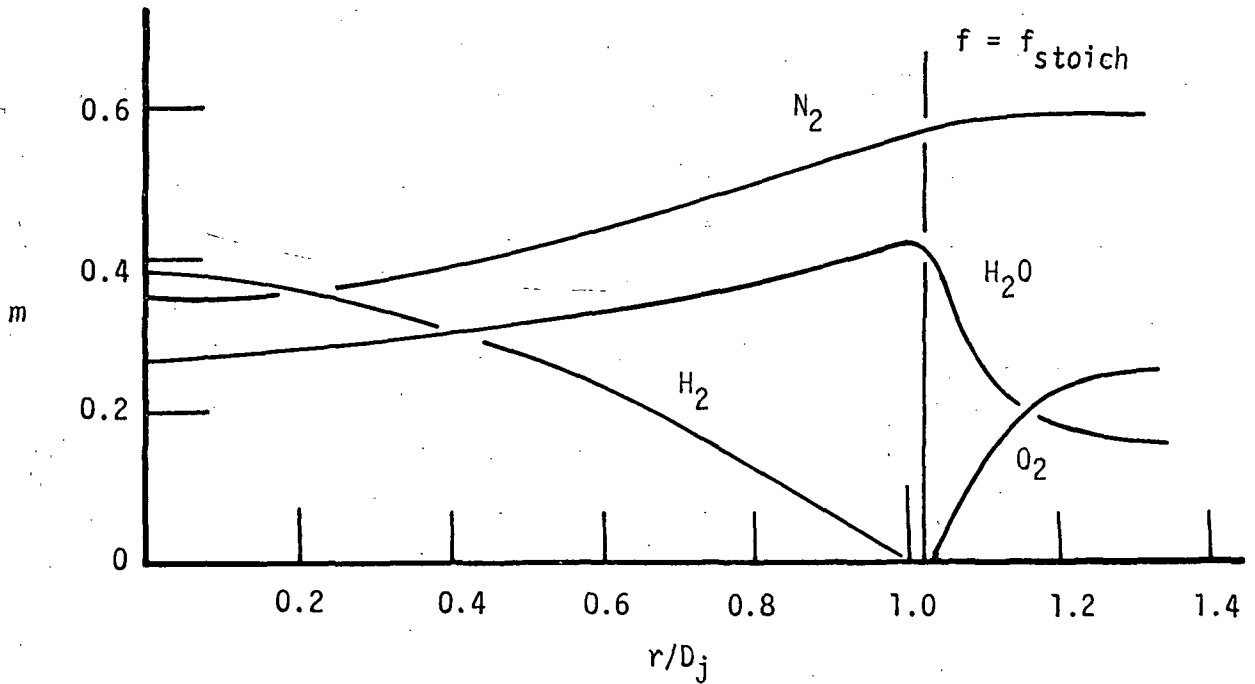


Figure 8. Profiles of Radical and Atomic Concentrations (Test Case No. 1)



a. Case No. 1 $x/D_j = 20$



b. Case No. 8 (H_2 Vitiated Air) $x/D_j = 15$
 Figure 9. Mass Fractions of Molecular Species

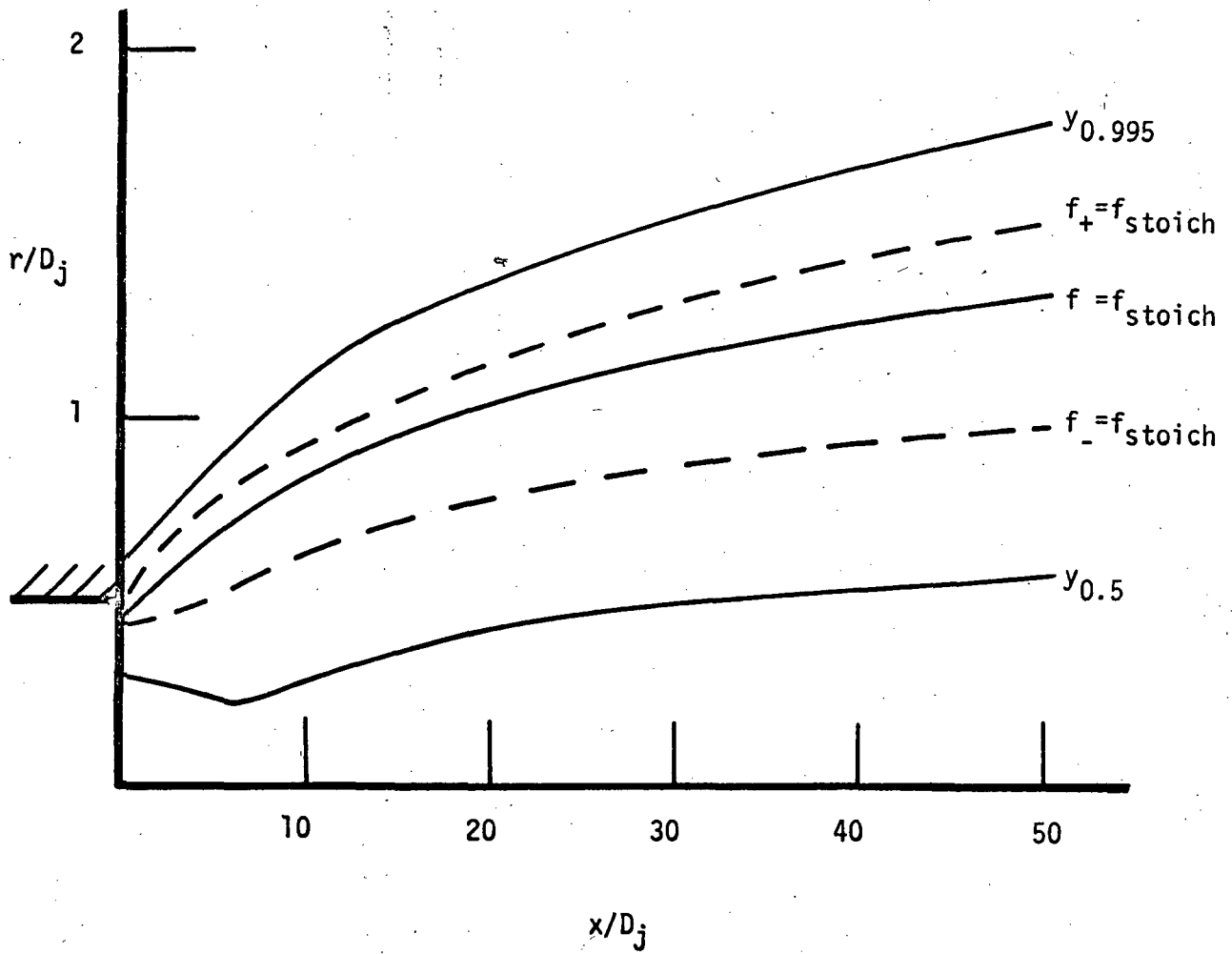
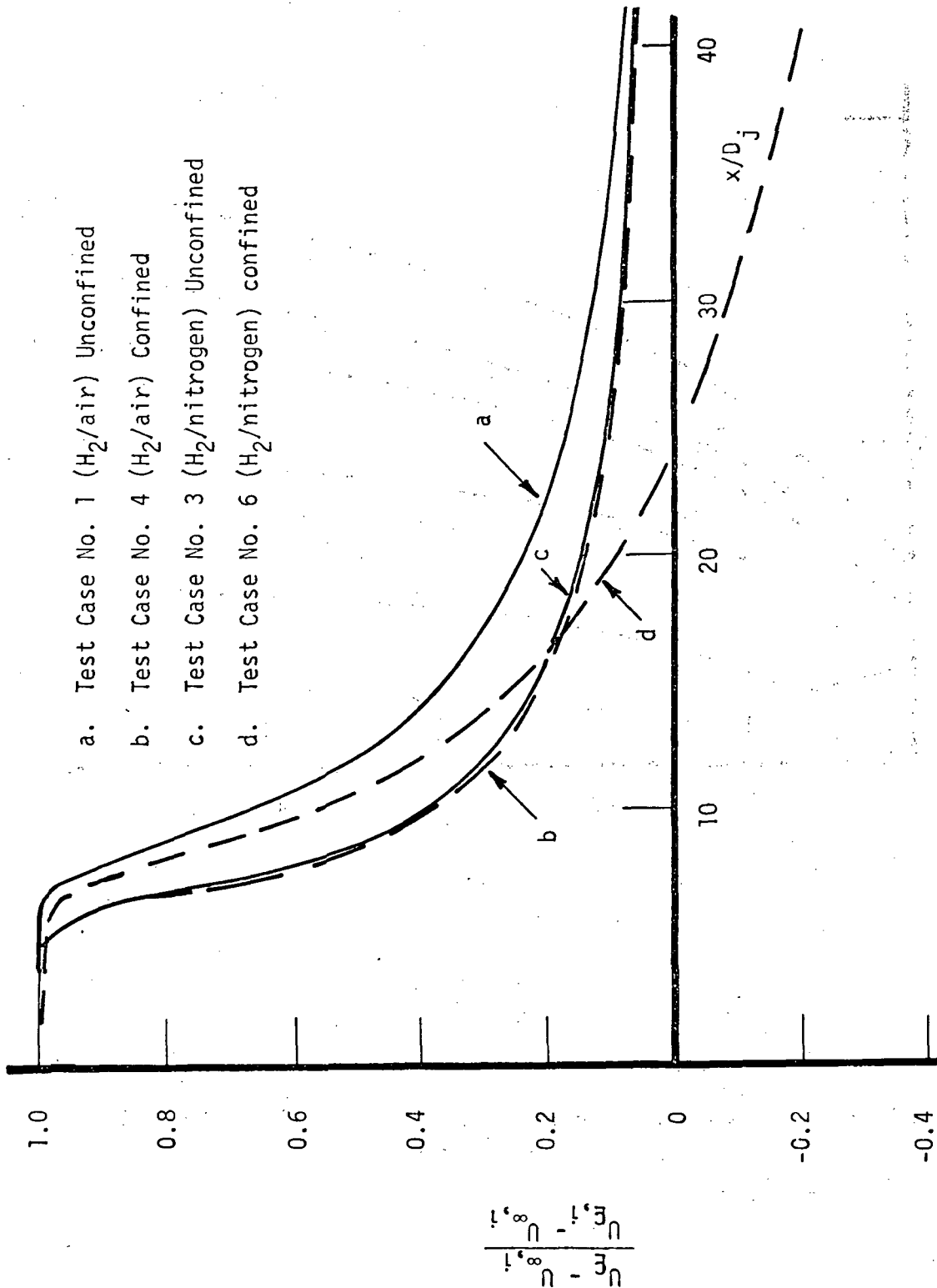


Figure 10. Location of Flame Front and Jet Half-Width (Test Case Number 1)



- 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

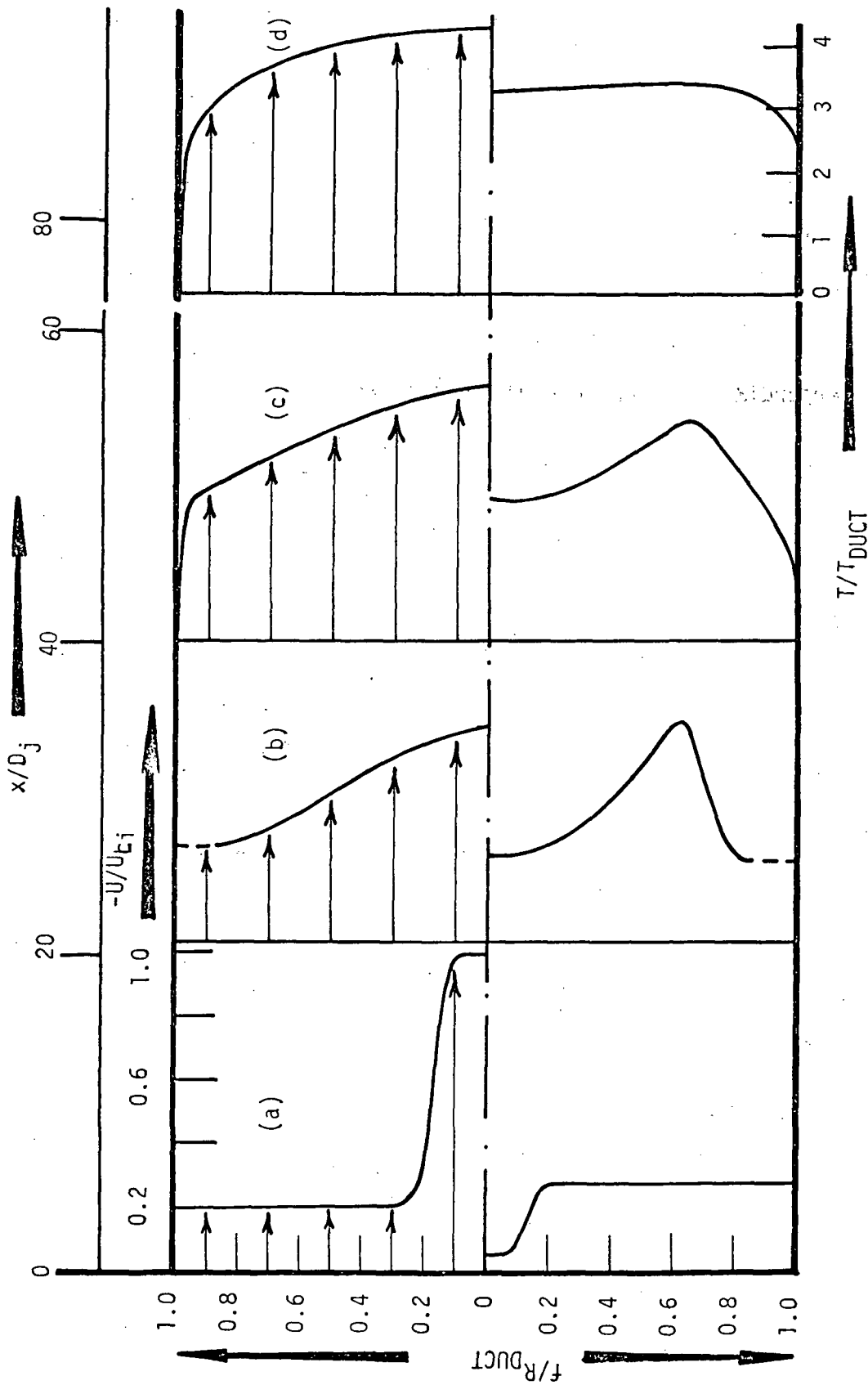


Figure 12. Velocity and Temperature Profiles in Ducted Subsonic Jet. Initial Profiles. (a) $x/D_j = 0$, (b) $x/D_j = 20$, (c) $x/D_j = 40$, (d) $x/D_j = 75$

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.

<u>Fortran Symbol</u>	<u>Significance</u>
AK	: constant of proportionality in near-wall mixing length formulation, $l_m = \kappa y_G$.
ALMG	: constant of proportionality in free shear layer mixing length formulation, $l_m = \lambda y_G$.
AMACH	: Mach number, $u/(\gamma RT)^{1/2}$.
CE1	} : constants in the dissipation rate equation
CE2	
CFA	: conversion factor from calories/gram. mole to joules/kg.
CFAC	: pressure x molecular weight of mixture
CG1	} : constants in mean square concentration fluctuations equation.
CG2	
CLINE	: local centreline mass fraction of molecular hydrogen ÷ initial value.
CMU	: constant in Prandtl-Kolmogorov viscosity formulation $\mu_T = C_\mu \rho k^2 / \epsilon$
CONST	: constant of proportionality, $-\frac{\overline{uv}}{k} (= C_\mu^{1/2})$
CPBAR (7,60)	: mean specific heats of chemical species at intervals of 100°K.
CPMN (10)	: mean specific heats of chemical species at upstream temperatures.
CSALFA	: cosine of angle of inclination of streamlines to axis of symmetry.

<u>Fortran Symbol</u>	<u>Significance</u>
DPDX	: axial pressure gradient, $\partial p / \partial x$
DUDY (40)	: mean velocity gradient, $\partial u / \partial y$
DX	: forward step size
DXLIM	: limit of entrainment rates (bound to size of forward step).
DYHA	: growth parameter of jet, $dy_{0.5} / dx$ (see also YHA)
DDYHA	: $\frac{d}{dx} (dy_{0.5} / dx)$
EMUL (40)	: laminar viscosity, μ
EMUT (40)	: turbulent viscosity, μ_T
ENTH (40)	: static enthalpy, h
F (10,40)	: dependent variables (see Chapter 2 of MAIN)
FA1	: constant for determination of free-stream turbulent kinetic energy and profile of mean square concentration fluctuations
FA2	: constant of proportionality in a free shear layer dissipation length scale formulation, $\lambda_\epsilon = \lambda Y_G$
FACI	: location where $f - g^{1/2} = f_{stoich}$
FACE	: location where $f + g^{1/2} = f_{stoich}$
FACM	: location where $f = f_{stoich}$
FRA	: constant of proportionality between forward step size and width of shear layer
FS (10,40)	: auxiliary variables (see Chapter 2 of MAIN)
FSTOICH	: stoichiometric fuel composition
GAM (40)	: effective diffusion coefficient

<u>Fortran Symbols</u>	<u>Significance</u>
GAMMA	: ratio of principal specific heats, C_p/C_v
GASCON	: universal gas constant
HO (10)	: the quantities $\Delta h_{f,298.15^\circ K} - (h_{298.15^\circ K} - h_{0^\circ K})$ (see Section 3.3-4)
IAX	: axial step number corresponding to end of potential core region
IEND	: axial step corresponding to point where jet edge reaches duct wall
INDE (10)	: indices denoting nature of boundary conditions
INDI (10)	= 1 (ϕ stated), = 2 (gradient ϕ stated)
IPD	: turbulence model parameter; = 3 (use of plane flow constants), = 1 or 2 [see Launder et al (2)]
IPROF	: profile index; = 1 (normalized values), = 2 (full dimensional values)
ISTAR (40)	: number of iteration cycles allowed for convergence at each node
ISTEP	: axial step number
J1	: species with largest concentration in equation (3.3-16)
J2	: species with largest concentration in equation (3.3-17)
KRAD	: flow geometry index; = 1 (plane), = 2 (asixymmetric)
N	: number of grid nodes, n
NP1	: n-1
NP1	: n+1
OFAC	: ratio of oxygen element/nitrogen in outer stream
OM (40)	: non-dimensional stream function
P (40)	: static pressure
PEI	: change in stream function across flow, $\psi_E - \psi_I$

<u>Fortran Symbols</u>	<u>Significance</u>
PR (10)	: molecular Prandtl/Schmidt numbers
PRDRP	: pressure drop, $p_j - p$
PRT (10)	: turbulent Prandtl/Schmidt numbers
PSIE	: value of stream function at external boundary ψ_E
PSII	: value of stream function at internal boundary ψ_I
PSIR	: value of stream function at duct wall ψ_R
QE	: wall heat transfer rate
R (40)	: distance from axis of symmetry ($= r_I + y \cos \alpha$)
RC (5,60)	: chemical equilibrium constants for each reaction at intervals of 100°K [N.B. RC (5,1) contains constants for the global reaction, $H_2 + \frac{1}{2}O_2 = H_2O$]
RCOW (10)	: chemical equilibrium constants at upstream conditions
REXD	: dimensionless excess radius in pressure gradient formulation for confined flows
RFLOW	: 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 & 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 ($=$ mass flow rate/ X-sectional area of duct)
RTW (40)	: turbulence frequency (dissipation rate/turbulent kinetic energy), ϵ/k

<u>Fortran Symbols</u>	<u>Translation</u>
SCH (40)	: Prandtl/Schmidt number array for near-wall flows
SD (40)	: storage location for "downstream" source terms
SU (40)	: storage location for "upstream" source terms
TAUE	: shear stress at wall
TBAR	: bulk temperature ($\int_{\text{duct}} r UTdy / \int_{\text{duct}} r Udy$)
TLINE	: local centreline temperature/initial value
UBAR	: bulk velocity ($= \int_{\text{duct}} r U^2dy / \int_{\text{duct}} r Udy$)
UEIN	: initial centreline velocity excess ($u_{\xi} - u_{\infty}$) _i
ULINE	: limit on entrainment at external boundary (to prevent formation of profiles with 'long tails')
ULIMI	: limit on entrainment at external boundary (to prevent formation of profiles with 'long tails')
ULINE	: local centreline velocity excess ($(u_{\xi} - u_{\infty}) / (u_{\xi} - u_{\infty})$) _i
VMIX	: reciprocal of molecular weight
WFi (10)	: molecular weight
X	: concentration of oxygen element
XAX	: length of potential core (in nozzle diameters)
XD	: axial distance at downstream station
XU	: axial distance at upstream station
XUD	: upstream axial distance/jet nozzle diameter
Y (40)	: transverse distance from internal flow boundary
YHA	: jet half-width, $y_{0.5}$

```

PROGRAM CHARNAL (INPUT,OUTPUT,TAPES=INPUT,TAPE6=OUTPUT)
C*****
C
C SPALDING AND PATANKAR PASSA PROGRAMME FOR BOUNDARY LAYER FLOWS
C MODIFIED BY A. MORSE 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/ACC,CSALFA,DPDX,DX,ENTH(40),F(10,40),FS(10,40),GAMB,
1GAMU,GAM(ZO)*I,IFIN,INDF(10),INDI(10),ISTEP,IUTRAP,ITEST,KEA,KIN,
2KRAD,N,NEQ,NP1,NP1,OP(40),OMD(40),BOM(40),KAST(10),PEI,PSIE,PSII,
3P(40),R(40),RHO(40),RJE(10),RJI(10),RME,RMI,SD(40),SU(40),WH(10),
4XD,XU,Y(40),YDIF(40),YE,YI,RJTE(10),RJTI(10)
COMMON/CRAD/RFLOW,REXD,KASE
COMMON/CJS/JU,JK,JD,JHS,JA,JG,JTF,JLF,JUV,JB
COMMON/CF5/JH2,J02,J0H,JH20,JH,JO,JN2
COMMON/CTIRB/AK,ALMG,CMU,CMUIN,CE1,CE2,CG1,CG2,CPIT,DDDY(40),
1DDYSO(40),EMUL(40),EMUT(40),IPD,PR(10),PRT(10),RTW(40)
COMMON/OUTPT/IAX,IEND,YIN,YOUT,YHA,UYHA,DDYHA,RDUCT,KP,KS,KT,
1KASENO,XSTAT(20),XPROF(20),XPLOT(20),PRESS
COMMON/CWVF/YR(2),IRUF(2),EWALL,H
COMMON/TPLT/XTAXIS,XTPLOT(40),YTAXES(10),YTPLOT(10,40),
1YTMAX(10),YTSYMB(10),OUT(40),IPROF
COMMON/CPROP/I02,IN2,IH2O,OFAC,NR,NS,#GO,WRO,WSO,WTO,GASCON,GAMMA
C*****
CHAPTER 1
C*****PARAMETERS AND CONTROL INDICES
READ(5,1150) KASENO,N,NEQ,KASE,NSTAT,NPROF,NPLOT,IPD,KIN,KEA,KONFI
1N,I02,IN2,IH2O,NR,NS,IUNF
READ(5,1152) XU,XULAST,YIN,YOUT,RDUCT,PRESS,TA,UIIN
IF(IUNF.EQ.0) READ(5,501) YW1,UW1,IW1
IF(KASE.EQ.2) READ(5,500) TDUCT
PRESS=PRESS*1.E+05
XU=XU+YOUT
XULAST=XULAST+YOUT
YIN=YIN+YOUT
DPDX=0.
READ(5,1152) (XSTAT(I),I=1,NSTAT)
READ(5,1152) (XPROF(I),I=1,NPROF)
READ(5,1152) (XPLOT(I),I=1,NPLOT)
XPROF(NPROF+1)=XSTAT(NSTAT+1)=XPLOT(NPLOT+1)=1.E+30
CALL STRIDO
IAX=100000
IEND=100000
IF(KEA.EQ.1) IEND=0
LASTPR=2000
IPROF=2
KP=1
KS=1
KT=)
ULIMI=.01
ULIME=.01
DXLIM=.05
FRA=.09
AFA=.25
C ***LARGER FORWARD STEP FOR TEST CASE NO.16 TO COVER LONGER DISTANCE
IF(KASENO.EQ.16) FRA=.125

```

```

DO 14 J=1,NEQ
.14 INDE(J)=1
INDE(JA)=2
IRUF(1)=IRUF(2)=0
IVCF=2

```

C*****

CHAPTER 2

C*****SELECTION OF DEPENDENT VARIABLES

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

- C F(JU,I)...AXIAL VELOCITY
- C F(JK,I)...KINETIC ENERGY OF TURBULENCE
- C F(JD,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(JTE,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

***AUXILIARY VARIABLES

- 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(JO2,I)...CONCENTRATION OF O2
- C FS(JO,I)...CONCENTRATION OF O
- C FS(JN2,I)...CONCENTRATION OF N2

DATA JH2,JO2,JOH,JH2O,JH,JO,JN2/1,2,3,4,5,6,7/

***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/
WRO=WM(JO)/WM(JOH)
WTO=1.-WRO
WSO=WM(JO)/WM(JH2O)
WCO=1.-WSO

C*****

CHAPTER 3

C*****CONSTANTS

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

GASCON=8314.
GAMMA=1.4

***CHEMICAL EQUILIBRIUM CONSTANTS AND ENTHALPIES

CALL LANGL1

***TURBULENCE CONSTANTS

AK=.4
ALMG=.11
CMUIN=.09
CONST=1./SQRT(CMUIN)
CMUJ=CMUIN
CF1=1.43
CF2=1.92
CG1=2.8
CG2=2.0

***SPECIFICATION OF PRANDTL/SCHMIDT NUMBERS

PRT(JU)=1.0

```

PRT(JK)=1.0
PRT(JD)=1.3
PRT(JHS)=.7
PRT(JA)=.7
PRT(JR)=.7
PRT(JG)=.7
DO 401 J=1,NEQ
401 PR(J)=1.0
FA1=4.E-04
FA2=.875
FWALL=9.
H=.9
CRIT=0.
C*****
CHAPTER 4
C****SPECIFICATION OF GEOMETRY
KRAU=2
CSALFA=1.
R(1)=YIN
READ(5,500) (Y(I),I=1,NP1)
DO 40 I=1,NP1
IF(IUNF.EQ.1) Y(I)=.1*Y(I)
40 Y(I)=Y(I)*YOUT-YIN
IF(KRAU.EQ.2) GO TO 183
DO 182 I=1,NP1
182 R(I)=1.
GO TO 181
183 DO 200 I=1,NP1
200 R(I)=R(1)+Y(I)*CSALFA
C*****
CHAPTER 5
C****INITIAL CONDITIONS
181 DO 450 I=1,NP1
450 P(I)=PRESS
IF(IUNF.EQ.1) GO TO 723
C ***CONTINUOUS PROFILES
YW1=YW1*YOUT
Yw1=Yw1-YIN
UW1=(UW1+UIN
IW2=IW1+1
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(IQ2.EQ.1) READ(5,500) (FS(JO2,I),I=1,NP1)
IF(IN2.EQ.1) READ(5,500) (FS(JN2,I),I=1,NP1)
IF(IH20.EQ.1) READ(5,500) (FS(JH20,I),I=1,NP1)
C ***MASS FRACTION OF HYDROGEN ELEMENT
DO 105 I=1,NP1
105 F(JA,I)=FS(JH2,I)+FS(JH,I)+WQO*FS(JH20,I)+WTO*FS(JOH,I)
C ***RATIO OF OXYGEN ELEMENT TO NITROGEN IN OUTER STREAM
OFAC=FS(JO2,NP1)+WQO*FS(JH20,NP1)
OFAC=OFAC/(OFAC+FS(JN2,NP1))
C ***CONVERSION OF INITIAL PROFILES
DO 45 I=1,NP1
F(JU,I)=F(JU,I)*UIN
45 F(JTE,I)=F(JTE,I)*TA
C ***TURBULENT KINETIC ENERGIES BY MIXING LENGTH HYPOTHESIS
DO 108 I=2,N

```

```

DUDY(I)=(F(JU,I+1)-F(JU,I-1))/(Y(I+1)-Y(I-1))
1062 DUDY(I)=DUDY(I)*DUDY(I)
DUDY(1)=DUDY(NP1)=0.
C ***DEFINE CHARACTERISTIC SHEAR LAYER WIDTHS
UREF=.9*F(JU,1)+.1*UW1
DO 1062 I=1,NP1
IF(F(JU,I).LT.UREF) GO TO 1063
1062 CONTINUE
1063 YW2=Y(I-1)+(Y(I)-Y(I-1))*(UREF-F(JU,I-1))/(F(JU,I)-F(JU,I-1))
YW2=YW1-YW2
YW2=ALMG*YW2
IF(KASENO.EQ.16) GO TO 8702
UREF=.1*UW1+.9*F(JU,NP1)
DO 1064 I=IW1,NP1
IF(F(JU,I).GT.UREF) GO TO 1065
1064 CONTINUE
1065 YW3=Y(I-1)+(Y(I)-Y(I-1))*(UREF-F(JU,I-1))/(F(JU,I)-F(JU,I-1))
YW3=YW3-YW1
YW3=ALMG*YW3
8702 IF(KASENO.EQ.16) YW3=YW2
DO 1066 I=1,IW1
1066 F(JK,I)=CONST*YW2*YW2*DUDY(I)
DO 1067 I=IW2,NP1
1067 F(JK,I)=CONST*YW3*YW3*DUDY(I)
DO 1068 I=1,NP1
AKMIN=FA1*F(JU,I)*F(JU,I)
1068 F(JK,I)=AMAX1(F(JK,I),AKMIN)
C ***DISSIPATION RATES
YW2=YW2/ALMG*FA2
YW3=YW3/ALMG*FA2
DO 1069 I=1,IW1
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,TI,TE,O2E,AN2E,H2OE
NPID2=NP1/2
C ***CONSTRUCT LINEAR VELOCITY PROFILE
DO 11 I=1,NP1
YRAT=Y(I)/Y(NP1)
F(JU,I)=UI+YRAT*(UE-UI)
IF(I.GT.NPID2) GO TO 454
F(JTE,I)=TI
FS(JH2,I)=1.
FS(JO2,I)=0.
FS(JN2,I)=0.
FS(JH20,I)=0.
GO TO 11
454 F(JTE,I)=TE
FS(JH2,I)=0.
FS(JO2,I)=O2E
FS(JN2,I)=AN2E
FS(JH20,I)=H2OE
11 F(JA,I)=FS(JH2,I)+FS(JH,I)+WQO*FS(JH20,I)+WTO*FS(JOH,I)
OFAC=FS(JO2,NP1)+W50*FS(JH20,NP1)
OFAC=OFAC/(OFAC+FS(JN2,NP1))

```

```

ALNTH=.8*Y(NP1)
UGRAD=(UE-UI)/Y(NP1)
UGRAD=UGRAD*ALMG*ALNTH
UGRAD=CONST*UGRAD*UGRAD
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(JU,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)*SQRT(F(JK,I))/ALNTH
C ***STAGNATION ENTHALPIES
417 DO 49 I=1,NP1
CALL LANGL2
49 F(JHS,I)=FNTH(I)+.5*F(JU,I)**2+F(JK,I)
C ***MEAN SQUARE CONCENTRATION FLUCTUATIONS (OF H ELEMENT)
DO 12 I=1,NP1
12 F(JG,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)/WN(J)
RHO(I)=P(I)/GASCON/VMIX/F(JTE,I)
50 THETA(I)=RHO(I)*F(JU,I)*R(I)
DO 505 I=2,NP1
ZETA=.5*(THETA(I)+THETA(I-1))*(Y(I)-Y(I-1))
505 OM(I)=OM(I-1)+ZETA
PSII=RHO(I)*F(JU,I)*YIN
JF(KRAD.EC.2) PSII=.5*PSII*YIN
PSIE=OM(NP1)+PSII
PEI=OM(NP1)
DO 506 I=2,NP1
506 OM(I)=OM(I)/PEI
CALL STRID1
C*****
CHAPTER 7
C*****THERMODYNAMIC AND TURBULENCE PROPERTIES (START OF MAIN LOOP)
100 CONTINUE
IF(ISTEP.GE.IAX) KIN=3
IF(ISTEP.GE.IEND) KEX=1
C ***LIMITS ON SPECIES MASS FRACTION
FAMIN=1.E-30
FAMAX=1.
DO 455 I=1,NP1
F(JA,I)=AMIN1(F(JA,I),FAMAX)
455 F(JA,I)=AMAX1(F(JA,I),FAMIN)
C ***LIMITS ON TURBULENCE PROPERTIES
FGMIN=1.E-30
FKMIN=1.E-30
DO 600 I=1,NP1
F(JG,I)=AMAX1(F(JG,I),FGMIN)
FKMAX=F(JG,I)*F(JU,I)

```

```

      F(JK,I)=AMIN1(F(JK,I),FKMAX)
      F(JK,I)=AMAX1(F(JK,I),FKMIN)
      FDMIN=F(JK,I)*SQRT(F(JK,I))/Y(NP1)
600  F(JD,I)=AMAX1(F(JD,I),FDMIN)
      DP=DPDX*DX
      IF(ISTEP.EQ.0) GO TO 425
C   ***LOCAL MASS FRACTIONS
      CALL LANGL3
C   ***LOCAL PRESSURES AND TEMPERATURES
      DO 601 I=1,NP1
        P(I)=P(I)+DP
601  F(NTH,I)=F(JHS,I)-.5*F(JU,I)**2-F(JK,I)
      CALL LANGL4
      DO 602 I=1,NP1
        IF(F(JTE,I).GT.0.) GO TO 1083
        WRITE(6,2702) F(JTE,I),I,ISTEP
        IFIN=1
1083  VMIX=0.
      DO 109 J=1,NS
        109  VMIX=VMIX+FS(J,I)/WM(J)
602  RHO(I)=P(I)/GASCON/VMIX/F(JTE,I)
425  CONTINUE
      IF(IFIN.EQ.1) GO TO 117
C*****
CHAPTER 8
C*****TRANSPORT PROPERTIES, PRESSURE GRADIENT AND FORWARD STEP
      IF(KIN.NE.2) GO TO 522
      IF(KRAD.EQ.2) GO TO 521
      YIN=PSII/(RHO(1)*F(JU,1))
      GO TO 522
521  YIN=SQRT(ABS(2.*PSII/(RHO(1)*F(JU,1))))
      R(1)=YIN
C   ***SPREADING RATE
522  CONTINUE
      CALL YINT(.5,YHA,JU)
      IF(ISTEP.EQ.0) GO TO 239
      DYHA=(YHA-YHALS)/(XU-PXU)
      DDYHA=(DYHA-DYHAV)/DYHA
239  YHALS=YHA
      DYHAV=DYHA
      PXU=XU
238  CALL STRID2
      IF(ISTEP.NE.0) GO TO 1370
      IF(KASE.NE.2) GO TO 1370
C   ***STREAM FUNCTION AT DUCT WALL
      PSIR=PSIE+.5*RHO(NP1)*F(JU,NP1)*(RDUCT**2-R(NP1)**2)
      ROUBAR=2.*PSIR/RDUCT**2
1370  IF(KEX.EQ.1) KONFIN=1
      GO TO (71,72),KONFIN
71  IF(ISTEP.EQ.IEND) 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   ---VERSION WITH GRID FILLING THE DUCT
      IF(ISTEP.EQ.0) GO TO 72
      ADUCT=.5*(RDUCT*RDUCT-R(1)*R(1))
      AFLOW=.5*(R(NP1)*R(NP1)-R(1)*R(1))
      PSIDIF=PEI

```



```

ROUBAR=PSIDIF/ADUCT
UBAR=0.
DO 73 I=2,N
73  UBAR=UBAR+.5*BOM(I)*F(JU,I)
    ROUBAR=ROUBAR/UBAR
    DUDP=-1./(ROUBAR+(RJE(JU)-RJI(JU))*DX/ADUCT/UBAR)
    UDRODP=ROUBAR/GAMMA/PRESS
    DROU=ROUBAR*(AFLOW/ADUCT-1.)
    DP=DROU/(ROUBAR*DUDP+UDRODP)
    UFAC=DP*DUDP/UBAR+1.
C   ***ADJUSTMENT OF VELOCITY, PRESSURE AND DENSITY
    DO 74 I=1,NP1
    F(JU,I)=F(JU,I)*UFAC
    P(I)=P(I)+DP
74  RHO(I)=RHO(I)*(1.+GAMMA*DP/P(I))
    DPDX=DPDX+DP/DX
C   ***RECALCULATION OF DISTANCES
    CALL STRID2
    GO TO 72
C   ***GENMIX VERSION OF PRESSURE GRADIENT FOR CONFINED FLOWS
133A STORE=TBAR
    TBAR=0.
    UBAR=0.
    DO 1340 I=2,N
1340 TBAR=TBAR+.5*BOM(I)*F(JTE,I)
    UBAR=UBAR+.5*BOM(I)*F(JU,I)
    IF(ISTEP.GE.IEND) RFLOW=R(NP1)
    IF(ISTEP.GE.IEND) GO TO 9719
    TBAR=(PSIT*F(JTE,1)+PEI*TBAR+(PSIR-PSIE)*F(JTE,NP1))/PSIR
    UBAR=(PSJI*F(JU,1)+PEI*UBAR+(PSIR-PSIE)*F(JU,NP1))/PSIR
    IF(ISTEP.EQ.0) GO TO 72
    DP=-ROUBAR*UBAR*(1.-STORE/TBAR)
    RFLOW=SQRT(R(NP1)**2+2.*(PSIR-PSIE)/(RHO(NP1)*F(JU,NP1)))
9719 CONTINUE
    IF(ISTEP.GE.IEND) DP=-ROUBAR*UBAR*(1.-STORE/TBAR)
    REXD=(RFLOW-RDUCT)/RDUCT
    DP=DP-AFA*ROUBAR*UBAR*REXD
    IF(ISTEP.GT.IEND) DP=DP-2.*RJE(JU)/R(NP1)**2*DX
    DP=DP/(1.-ROUBAR*UBAR/P(1))
    DPDX=DP/DX
C   ***FORWARD STEP
72  DX=FPA*Y(NP1)
    IF(IUNF.EQ.1) DX=FRA*R(NP1)
    IF(ISTEP.LT.50) DX=DX*FLOAT(ISTEP+1)/50.
    IF(ISTEP.GE.IEND.AND.ISTEP.LE.IEND+9) DX=.1*DX*FLOAT(ISTEP-IEND+1)
    IF(ABS(REXD).GT..005) DX=DX*.005/ABS(REXD)
    DX=AMIN1(DX,XULAST-XU)
    XD=XU+DX
C*****
CHAPTER 9
C*****ADJUSTMENT OF BOUNDARY CONDITIONS
C   ***FREE BOUNDARY VALUES ADJUSTED IN STRIDE (3)
    IF(KJN.EQ.2) GO TO 95
    RHI=0.
    IF(KPAU.EQ.2) R(1)=0.
    YIN=0.
    PSII=0.
95  IF(KEX.NE.1) GO TO 196

```

```

F(JU,NP1)=0.
RJE(JA)=0.
F(JK,NP1)=0.
F(JD,NP1)=0.
F(JG,NP1)=0.
F(JTE,NP1)=TDUCT
I=NP1
CALL LANGL2
F(JHS,NP1)=ENTH(NP1)

```

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C*****
CHAPTER 10

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C****TRANSPORT AND ENTRAINMENT PROPERTIES
196 CALL AUX(JU)

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IF(ISTEP.EE.IEND) RME=0.
C ***ENTRAINMENT CONTROL
C ***RESTRICT ATTENTION TO VELOCITY AND TEMPERATURE CHANGES
IF(KIN.NE.2) GO TO 94
RMI=R(3)*GAMB/Y(3)
RMI=RMI/PRT(JA)
RAT=ARS((F(JU,2)-F(JU,1))/(F(JU,NP1)-F(JU,1)+1.E-30))
AMGN=ABS((F(JTE,2)-F(JTE,1))/(F(JTE,NP1)-F(JTE,1)+1.E-30))
RAT=AMAX1(RAT,AMGN)
IF(RAT.LT.ULIMI) RMI=RMI*RAT/ULIMI
94 IF(KEX.NE.2) GO TO 97
RME=-R(NM1)*GAMN/(Y(NP1)-Y(NM1))
RME=RME/PRT(JA)
RAT=ARS((F(JU,N)-F(JU,NP1))/(F(JU,NP1)-F(JU,1)+1.E-30))
AMGN=ABS((F(JTE,N)-F(JTE,NP1))/(F(JTE,NP1)-F(JTE,1)+1.E-30))
RAT=AMAX1(RAT,AMGN)
IF(RAT.LT.ULIME) RME=RME*RAT/ULIME
97 IF((RMI-RME)*DX.LT.PEI*DXLIM) GO TO 96
DX=DXLIM*PEI/(RMI-RME)
XD=XI+DX
94 CONTINUE
IF(KASE.EQ.1) GO TO 960
IF(ISTEP.EE.IEND) GO TO 960
C ***ADJUSTMENT OF FORWARD STEP FOR JET TO REACH DUCT WALL
IF(R(NP1).LT..999*RDUCT) GO TO 960
IEND=ISTEP+1
XEND=XD/YOUT
WRITE(6,508) IEND,XEND
960 CONTINUE
C ***ADJUSTMENT OF FORWARD STEP TO REACH AXIS OF SYMMETRY
IF(KIN.NE.2) GO TO 195
IF(PSII.GT.RMI*DX) GO TO 195
DX=PSII/RMI
XD=XI+DX
IAX=ISTEP+1
XAX=XD/YOUT
WRITE(6,507) IAX,XAX

```

```

C*****
CHAPTER 11

```

```

C****OUTPUT
195 IF(ISTEP.NE.0) GO TO 193
CALL OUTP1
CALL OUTP2
CALL OUTP3
GO TO 113

```

```

193 XUD=XII/YOIJT
    IF(XUD.LT.XSTAT(KS)) GO TO
    KS=KS+1
    CALL OUTP3
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
500 FORMAT(7F10.3)
501 FORMAT(2F10.3,I4)
507 FORMAT(/1H0,!--MIXING LAYER REGION ENDS AT ISTEP=*,I5,3X,*LENGTH 0
    IF POTENTIAL CORE =*,F7.2,* DIAMETERS*/)
508 FORMAT(/1H0,!--JET REACHES DUCT WALL AT ISTEP=*,I5,3X,*DOWNSTREAM
    IDISTANCE =*,F7.2,* DIAMETERS*/)
1150 FORMAT(18I4)
1152 FORMAT(1P7E11.3)
2703 FORMAT(/1H0,--- NEGATIVE TEMPERATURE OF*,1PE11.3,* CALCULATED AT
    INODE=*.I3,* AT ISTEP=*,I5)
C*****
CHAPTER 12
C*****CONTINUATION/TERMINATION
113 IF(ISTEP.GE.LASTEP.OR.XU.GE.XULAST) GO TO 1001
    CALL STRID3
    GO TO 100
1001 CONTINUE
    STOP
    END

```

COMPILER SPACE

```

SUBROUTINE AUX(J)
COMMON/GENERAL/ACC,CSALFA,DPDX,DX,ENTH(40),F(10,40),FS(10,40),GAM3,
1GAMN,GAM(40),I,IFIN,INDE(10),INDI(10),ISTEP,IUTRAP,ITEST,KEX,KIN,
2KRAD,N,NEQ,NP1,NP1,OM(40),OMD(40),DOM(40),KAST(10),PEI,PSIE,PSII,
3P(40),R(40),RHO(40),RJE(10),RJI(10),RME,RMI,SD(40),SU(40),WM(10),
4XD,XI,Y(40),YDIF(40),YE,YI,RJTE(10),RJTI(10)
COMMON/CJS/JU,JK,JD,JHS,JA,JG,JTE,JLE,JUV,JB
COMMON/CF5/JH2,J02,JOH,JH20,JH,JO,JN2
COMMON/CTJRB/AK,ALMG,CMU,CMUIN,CE1,CE2,CG1,CG2,CRIT,DUDY(40),
1DUDYSO(40),EMUL(40),EMUT(40),IPD,PR(10),PRT(10),RTW(40)
COMMON/AUXST/TDA(40),UIP
COMMON/CIGMA/SCH(40)

```

C*****

C*****AXIAL VELOCITY

IF(J.NE.JI) GO TO 299

C ***LAMINAR VISCOSITY (APPROXIMATE POWER LAW RELATIONSHIPS)

C ---IGNORE ATOMIC AND RADICAL CONCENTRATIONS

DO 69 I=1,NP1

SUM=FS(JH2,I)+FS(J02,I)+FS(JN2,I)+FS(JH20,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 ---WATER VAPOUR

EMUL(I)=EMUL(I)+FS(JH20,I)*1.71E-05*(F(JTE,I)/500.)**1.050

69 EMUL(I)=EMUL(I)/SUM

C ***DETERMINATION OF ACCELERATION PARAMETER

ACC=ABS(ACC-ABS(ACC))

CALL YINT(.99,YRS,JU)

ACC=.5*YRS*ACC/ABS(F(JU,1)-F(JU,NP1))

ACC=ACC**0.2

IF(ISTEP.EQ.0) GO TO 74

C ***EVALUATION OF INTEGRATED PRODUCTION/DISSIPATION 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

152 TPER=TPERT=TR=TRI=0.

DO 56 I=2,NP1

TRP=TR

TR=EMUT(I)*DUDY(I)*R(I)

TRI=TRI+.5*(TR+TRP)*(Y(I)-Y(I-1))

TPERP=TPER

TPER=RTW(I)*TR

56 TPERI=TPERI+.5*(TPER+TPERP)*(Y(I)-Y(I-1))

PUMP=PDE

PDE=TPERI/TRI
IF(ISTEP.NE.5) PDE=.5*(PDE+PUMP)

W=2.8

ALPHA=.55

AH=SIN(3.14159*(PDE-.5))-1.

IF(PDE.LE.1.) ALPHA=.55+.213*AH

G=1.-(1.-ALPHA*PDE)/W

G=G/(1.+(PDE-1.)/W)**2

G=7.407*G*(1.-ALPHA)/W

```

123 CMU=.09*G-.0534*ACC
    GO TO 121
73 CMU=.09-.04*ACC
    IF(IPD.EQ.3) CMU=.09
    GO TO 121
74 CMU=CMUIN
121 RTCMU=SQRT(CMU)
    AKCDQ=AK/CMU**0.75
    U1P=F(JU,1)
C ***AXIAL VELOCITY GRADIENTS
    DUDY(1) = 0.
    DUDY(NP1) = 0.
    DUDYSQ(1) = 0.
    DUDYSQ(NP1) = 0.
    YDIFP = Y(3) - Y(2)
    DUDYP = ABS((F(JU,3) - F(JU,2))/YDIFP + 1.E-30)
    GO TO (1,2,2), KIN
1 DUDY(2) = (0.5*YDIFP + YI)/YI * DUDYP
    GO TO 3
2 DUDY(2) = YI/(0.5*YDIFP + YI)*DUDYP
3 DUDYSQ(2) = DUDY(2)**2
    DO 9 I = 3, NP1
    YDIFM = YDIFP
    YDIFP = Y(I+1) - Y(I)
    DUDYM = DUDYP
    DUDYP = ABS((F(JU,I+1) - F(JU,I))/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
17 DUDYSQ(N) = DUDY(N)**2
    DO 13 I=1,NP1
    DUDYSQ(I) = DUDY(I)**2
13 RTW(I) = F(JD,I)/(F(JK,I)+1.E-30)
C ***TURBULENT VISCOSITY FORMULATION
    DO 1030 I=2,N
    EMUT(I) = CMU*RHO(I)*F(JK,I)/RTW(I)
1030 F(JUV,I) = -EMUT(I)*DUDY(I)/RHO(I)
    DO 1033 I=2,NP1
1033 TF(F(JU,I),LT,F(JU,I-1)) F(JUV,I) = -F(JUV,I)
C ***ADD LAMINAR AND TURBULENT COMPONENTS
    IF(CRIT) 1050,1050,1052
1050 DO 1051 I=2,N
1051 GAM(I) = EMUL(I) + EMUT(I)
    GO TO 1060
1052 DO 106 I=2,N
    IF(EMUT(I) - EMUL(I)*CRIT) 1060,1060,1061
1060 GAM(I) = EMUL(I)
    EMUT(I) = 0.
    GO TO 106
1061 GAM(I) = EMUL(I) + EMUT(I)
106 CONTINUE
1062 EMUT(1) = 0.
    EMUT(NP1) = 0.
C ***AXIAL PRESSURE GRADIENT (SOURCE TERM)
    GAM3 = GAM(3)
    GAMN = GAM(NP1)

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      DO 111 I=1,NP1
      SU(I)=-DPDX
111 SD(I)=0.
      RETURN
C*****
C****TURBULENT KINETIC ENERGY
209 IF (J.NE.JK) GO TO 399
      DO 201 I=2,N
201 GAM(I)=EMUL(I)/PR(JK)+EMUT(I)/PRT(JK)
      DO 212 I = 1,NP1
      SU(I) = EMUT(I)*DUDYSQ(I)
212 SD(I)=-RTW(I)*RHO(I)
      IF (KIN.NE.1) GO TO 215
      FJK2=-RJI(JU)/(R(1)*RHO(1)*RTCMU)
      SU(2)=1.E30*FJK2
      SD(2)=-1.F30
215 IF (KFX.NE.1) RETURN
      FJKN=REJE(JU)/(R(NP1)*RHO(NP1)*RTCMU)
      SU(N )=1.E30*FJKN
      SD(N )=-1.E30
      RETURN
C*****
C****DISSIPATION RATE
399 IF (J.NE.JD) GO TO 499
      DO 801 I=2,N
801 GAM(I)=EMUL(I)/PR(JD)+EMUT(I)/PRT(JD)
      DO 810 I=1,NP1
      SU(I)=CE1*EMUT(I)*RTW(I)*DUDYSQ(I)
      CE2=1.92-.0667*ACC
      IF (IPD.EQ.2) CE2=1.92-.1336*ACC
      IF (IPD.EQ.3) CE2=1.92
810 SD(I)=-CE2*RHO(I)*RTW(I)
      IF (KIN.NE.1) GO TO 812
      SU(2)=FJK2**1.5/AKCDQ/Y(2)*1.E+30
      SD(2) = -1.E30
812 IF (KFX.NE.1) RETURN
      SU(N )=FJKN **1.5/AKCDQ/(Y(NP1)-Y(N ))*1.E30
      SD(N) = -1.E30
      RETURN
C*****
C****STAGNATION ENTHALPY
499 IF (J.NE.JHS) GO TO 599
C ***PRANDTL/SCHMIDT NUMBERS FOR NEAR-WALL REGION (ROTTA)
C ---AXISYMMETRIC FLOWS ONLY
C ---N.B. SAME RELATIONSHIP FOR SPECIES DIFFUSION
      IF (KRAD.EQ.1) GO TO 331
      IF (KEY.NE.1) GO TO 331
      DO 330 I=1,NP1
      YW=1.-R(I)/R(NP1)
330 SCH(J)=.95-.45*YW*YW
      GO TO 332
331 DO 333 I=1,NP1
333 SCH(J)=PRT(JHS)
332 DO 301 I=2,N
301 GAM(I)=EMUL(I)/PR(JHS)+EMUT(I)/SCH(I)
      DO 302 I=1, NP1
302 S D(I)=F(JU,I)**2
      DO 303 I=2,NM1

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303 FAC1=(SCH(I)-1.)*(GAM(I)+GAM(I+1))/(YDIF(I)+1.E-30)
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))/(YDIF(I)+1.E-30)
307 S D(J)=S D(I)+FAC2*(F(JK,I+1)-F(JK,I))
SD(1)=0.
SD(N)=0.
DO 304 I=2,N
304 SU(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)=EMUL(I)/PR(JA)+EMUT(I)/SCH(I)
DO 902 I=1,NP1
902 SU(I)=SD(I)=0.
RETURN
C*****
C ***MEAN SQUARE CONCENTRATION FLUCTUATIONS (OF H ELEMENT)
699 IF(J.NE.JA) GO TO 799
YDIFP=Y(3)-Y(2)
DCDYP=ABS((F(JA,3)-F(JA,2))/YDIFP+1.E-30)
IF(KIN.EQ.1) GO TO 711
DCDY=YI/(.5*YDIFP+YI)*DCDYP
DCDYSQ=DCDY**2
SU(2)=CG1*DCDYSQ*EMUT(2)
SD(2)=-CG2*RTW(2)*RHO(2)
SU(1)=0.
SD(1)=-CG2*RTW(1)*RHO(1)
GO TO 712
711 G2=(PJI(J)/R(2)/RHO(2))*2*CG1/CG2/FJK2
SU(2)=G2*1.E+30
SD(2)=-1.F+30
712 DO 713 I=3,NM1
YDIFM=YDIFP
YDIF=Y(I+1)-Y(I)
DCDYM=DCDYP
DCDYP=ABS((F(JA,I+1)-F(JA,I))/YDIFP+1.E-30)
DCDYSQ=((Y(I+1)-Y(I-1))/(YDIFP/DCDYM+YDIFM/DCDYP))**2
SU(I)=CG1*DCDYSQ*EMUT(I)
713 SD(I)=-CG2*RTW(I)*RHO(I)
IF(KEX.EQ.1) GO TO 713
DCDY=YE/(.5*YDIFP+YE)*DCDYP
DCDYSQ=DCDY**2
SU(N)=CG1*DCDYSQ*EMUT(N)
SD(N)=-CG2*RTW(N)*RHO(N)
SU(NP1)=0.
SD(NP1)=-CG2*RTW(NP1)*RHO(NP1)
RETURN
713 GN=(PJI(J)/R(N)/RHO(N))*2*CG1/CG2/FJKN
SU(N)=GN*1.E+30
SD(N)=-1.F+30
799 CONTINUE

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SUBROUTINE STRIDE
DIMENSION AHL(40),BOMT3(40),OMS(40),PBOM(40),PGOM(40),THL(40)
DIMENSION A(40),P(40),C(40),D(40)
COMMON/GENERAL/ACC,CSALFA,DPDX,DX,ENTH(40),F(10,40),FS(10,40),GAM3,
1GAMN,GAM(40),I,IFIN,INDE(10),INDI(10),ISTEP,IUTRAP,ITEST,KEX,KIN,
2KRAD,N,NEO,NP1,NM1,OM(40),OMD(40),HOM(40),KAST(10),PEI,PSIE,PSII,
3P(40),R(40),RHO(40),RJE(10),RJI(10),RME,RMI,SD(40),SU(40),WM(10),
4XD,XII,Y(40),YDIF(40),YE,YI,RJTE(10),RJTI(10)
COMMON/CJS/JU,JK,JD,JHS,JA,JG,JTE,JLE,JUV,JB
COMMON/CFS/JH2,J02,JOH,JH20,JH,JO,JN2
COMMON/AUXST/TDA(40),UIP
COMMON/WFCT/FDIFS(20,2),TS(20,2),BP(2)
COMMON/CPROP/I02,IN2,IH20,OFAC,NR,NS,W00,WRO,WSO,WTO,GASCON,GAMMA
C*****
C**** STRIDE (0)
C ***CONTROL INDICES
ENTRY STRID0
NP1=N+1
NM1 = N-1
OM(1)=0.
OM(NP1) = 1.
GAM3 = 0.
GAMN=0.
ISTEP=0
IFIN=0
IUTRAP=2
C ***ZEROING OF IMPORTANT ARRAYS
DO 353 J=1,NEO
KAST(J)=0
353 RJE(J)=RJI(J)=0.
DO 354 I=1,NP1
DO 354 J=1,NS
354 FS(J,I)=0.
DO 355 I=1,NP1
DO 355 J=1,10
355 F(J,I)=0.
DO 356 I=1,NP1
356 ENTH(I)=0.
RETURN
C*****
C**** STRIDE (1)
C ***OMEGA RELATIONSHIPS
ENTRY STRID1
DO 100 I = 1, N
OMD(I)=OM(I+1)-OM(I)
100 OMS(I)=OM(I+1)+OM(I)
DO 101 I = 3, NM1
BOM(I)=OM(I+1)-OM(I-1)
BOMT3(I)=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 = OM(3)**2
OMS3 = OM(2)**2
OMS2 = OMS2/(OMS2-OMS3)
OMS3 = 1. - OMS2

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```

OMN = (OMD(N) + OMD(NM1))**2
OMNM1 = OMD(N)**2
OMN = OMN/(OMN - OMNM1)
OMNM1 = 1. - OMN
Y(1)=0.
BP(1)=1.
BP(2)=1.
INDE(JU)=1
INDI(JU)=1
RETURN
C*****
C**** STRIDE (2)
      ENTRY STRID2
C ***TEST FOR NEGATIVE VELOCITIES
1010 IF(IUTRAP.EQ.0) GO TO 1011
      DO 1012 I = 2, N
        IF(F(JU,I).GT.0.) GO TO 1012
        WRITE(6,1200) F(JU,I),I,ISTEP
1200  FORMAT(/1H0,*--- NEGATIVE VELOCITY OF*,1PE11.3,* CALCULATED AT NOD
      1E*,13.* AT ISTEP=*,15)
        F(JU,I)=1.E-30
        IF(IUTRAP.GT.1) IFIN=1
1012 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)
      RUI=RHO(1)*F(JU,1)
      RURAT = RUI/RUP
      GO TO (1013,1014,1014), KIN
1014 GO TO (1018,1019), KRAD
1018 BP(1) = 0.333333 + 0.666667*RURAT
      GO TO 1013
1019 BP(1) = (R(1)*(5.*RURAT+1.)+3.*R(2)*(RURAT+1.))/(R(1)+R(2))/6.
1013 YI = PEI * OMD(1)/(BP(1)*RUP)
      RUNP1 = RHO(NP1) * F(JU,NP1)
      RUN = RHO(N) * F(JU,N)
      RURAT = RUNP1/RUN
      GO TO (1020,1021,1021), KEX
1021 GO TO (1024,1025), KRAD
1024 BP(2) = 0.333333 + 0.666667*RURAT
      GO TO 1020
1025 BP(2) = (R(NP1)*(5.*RURAT+1.)+3.*R(N)*(RURAT+1.))/(R(NP1)+R(N))/6.
1020 YE = PEI*OMD(N)/(BP(2)*RUN)
C ***Y'S, R'S, TDA'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, NM1
        TDA(I)=PEI*BOM(I)/RUP
        RUM=RUP
        RUP=RHO(I+1)*F(JU,I+1)
        YDIF(I)=PEI*OMD(I)*(1./RUM+1./RUP)
1017 Y(I+1)=Y(I)+YDIF(I)*.5
        TDA(N)=PEI*BOM(N)/RUP
        Y(NP1) = Y(N) + YE
        YDIF(N) = 2. * YE
        IF(KRAD.EQ.1) RETURN
C ***MODIFICATIONS FOR AXIAL SYMMETRY

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```

1123 IF(CSALFA.EQ.0.) GO TO 1110
C ***CSALFA .NE. ZERO
  COSD2=.5*CSALFA
  IF(R(1).NE.0.) GO TO 1105
C ***R(1) .EQ. ZERO
  DO 1106 I = 2, NP1
    Y(I)=SQRT(ABS(Y(I)/COSD2))
1106 R(I)=Y(I)*CSALFA
  GO TO 1107
C ***R(1) .NE. ZERO
1105 R1D2=.5*R(1)
  R1D2SQ=R1D2*R1D2
  DO 1104 I = 2, NP1
    Y(I)=Y(I)/(R1D2+SQRT(ABS(R1D2SQ+COSD2*Y(I))))
1104 R(I)=R(1)+Y(I)*CSALFA
1107 DO 1108 I = 1, N
1108 YDIF(I)=YDIF(I)*4./(R(I)+R(I+1))*2
  GO TO 1112
C ***CSALFA .EQ. ZERO
1110 DO 1111 I = 2, NP1
  Y(I)=Y(I)/R(1)
1111 R(I)=R(1)
  R1SQ=R(1)**2
  DO 1109 I=2,N
1109 YDIF(I)=YDIF(I)/R1SQ
1112 YI = Y(2)
  YE = Y(NP1) - Y(N)
  RETURN
C*****
C**** STRIDE (3)
C ***MAIN NUMERICAL METHOD
  ENTRY STRID3
  IF (KIN .EQ. 1) CALL WF(1)
  IF (KEX .EQ. 1) CALL WF(2)
C ***PRELIMINARIES
3000 G=RMI-RME
  PX=PEI/DX
  PD4=.25*PX
  GD4=.25*G
  PGD4=PD4+GD4
  RMD2=.5*RMI
  PGOM(1)=0.
C-----THL, AHL, PGOM AND PBOM
  THL(J) = 0.
  DO 3010 I = 2, N
  HL=RMD2-GD4*OMS(I)
  THL(J) = 2.*HL
  AHL(I) = ABS(HL)
  PGOM(I)=PGD4*OMD(I)
3010 PBOM(I)=PX*HOM(I)
C ***START OF J LOOP
  DO 3320 J=1,NEQ
  IF(J.NE.JII) CALL AUX(J)
  TTP=0.
  PGOMP = 0.
  GAM(NP1) = 0.
C ***SETTING UP COEFFICIENTS
  AKAST = FLOAT(1 -KAST(J))

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```

KAST1 = KAST(J) + 1
INDEXI=INDI(J)
INDEXE=INDE(J)
DO 3004 I=2,N
SU(I) = SU(I) * TDA(I)
SD(I) = SD(I) * TDA(I)
PGOMM = PGOMP
PGOMP = PGOM(I) * AKAST
TTM=TTP
TP = (GAM(I) + GAM(I+1))/YDIF(I)
TTP = TP + AHL(I) + ABS(TP-AHL(I))
A(I)=TTP-THL(I)-PGOMP
B(I)=TTM+THL(I-1)-PGOMM
IND1=2/I
IND2=1/(NP1-I)
INDEX=1+IND1+IND2
GO TO (303,305),INDEX
303 GO TO (304,305), KAST1
304 C(I)=PD4*(BOMT3(I)*F(J,I)+OMD(I)*F(J,I+1)+OMD(I-1)*F(J,I-1))+SU(I)
GO TO 306
305 C(I)=PBOM(I)*F(J,I)+SU(I)
306 D(I)=PBOM(I)-SD(I)
C ***MODIFICATIONS FOR BOUNDARIES
INDEX=1+IND1+2*IND2
GO TO (3004,3008,3002), INDEX
3008 A(I)=A(I)+PGOM(2)*AKAST
B(I)=2.*RMI
GO TO (3009,3004,3004), KIN
3009 GO TO (3011,3003), INDEXI
3011 TT=2.*TS(J,1)
B(I)=AMAX1(TT+B(I),0.)
C(I)=C(I)-TT*FDIFS(J,1)
GO TO 3004
3003 B(I)=0.
D(I)=D(I)+2.*RMI
C(I)=C(I)+2.*RJTI(J)
GO TO 3004
3002 B(I)=R(I)+PGOM(NP1)*AKAST
A(I)=-2.*RME
GO TO (3012,3004), KEX
3012 GO TO (3013,3005), INDEXE
3013 TT=2.*TS(J,2)
A(I)=AMAX1(TT+A(I),0.)
C(I)=C(I)-TT*FDIFS(J,2)
GO TO 3004
3005 A(I)=0.
D(I)=D(I)-2.*RME
C(I)=C(I)-2.*RJTE(J)
3004 D(I)=D(I)+A(I)+B(I)
C ***ADJUST FREE-BOUNDARY VALUES
RUI = RHO(1) * F(JU,1)
IF(KIN.NE.2.OR.RUI.EQ.0.) GO TO 3006
F(J,1) = (F(J,1)+SU(1)*DX/RUI)/(1.-SD(1)*DX/RUI)
3006 RUNP1=RHO(NP1)*F(JU,NP1)
IF(KEX.NE.2.OR.RUNP1.EQ.0.) GO TO 3007
F(J,NP1) = (F(J,NP1)+SU(NP1)*DX/RUNP1)/(1.-SD(NP1)*DX/RUNP1)
C ***SOLVE FOR DOWNSTREAM F#S
3007 B(2)=(B(2)*F(J,1)+C(2))/D(2)

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      A(2)=A(2)/D(2)
      DO 3021 I = 3, N
      T=D(I)-B(I)*A(I-1)
      A(I)=A(I)/T
3021 B(I)=(B(I)*B(I-1)+C(I))/T
      DO 3022 IDASH=1,NMI
      I=NP1-IDASH
3022 F(J,I)=A(I)*F(J,I+1)+B(I)
C ***ADJUST BOUNDARY VALUES
      GO TO (3210,3220,3230), KIN
3210 GO TO (30A,3211), INDEXI
3211 RMT=RMI+TS(J,1)
      RJI(J) = RJTI(J) - RMI*F(J,1)
      IF (PMT .GT. 0.) GO TO 307
      F(J,1) = F(J,2)
      GO TO 3220
307 F(J,1) = (RJTI(J) + TS(J,1)*(F(J,2) + FDIFS(J,1)))/RMT
      GO TO 3220
30A RJI(J) = TS(J,1) * (F(J,1)-F(J,2)-FDIFS(J,1))
      RJTI(J) = RJI(J) + RMI*F(J,1)
      GO TO 3220
3230 IF(R(1).EQ.0.) GO TO 309
      F(J,1)=F(J,2)*OMS2+F(J,3)*OMS3
      GO TO 3220
309 F(J,1)=F(J,2)*OM2+F(J,3)*OM3
3220 GO TO (3310,3320,3330), KEX
3310 GO TO (31A,3311), INDEXE
3311 RMT=-RME+TS(J,2)
      RJE(J) = RJTE(J) - RME*F(J,NP1)
      IF (RMT .GT. 0.) GO TO 317
      F(J,NP1) = F(J,N)
      GO TO 3320
317 F(J,NP1) = (-RJTE(J) + TS(J,2)*(F(J,N)+FDIFS(J,2)))/RMT
      GO TO 3320
31A RJE(J) = -TS(J,2)*(F(J,NP1)-F(J,N)-FDIFS(J,2))
      RJTE(J) = RJE(J) + RME*F(J,NP1)
      GO TO 3320
3330 F(J,NP1)=F(J,N)*OMN+F(J,NM1)*OMNM1
3320 CONTINUE
      XU=XD
      ACC=(F(JU,1)-U1P)/DX
      PSII=PSII-RMI*DX
      PSIE=PSIE-RME*DX
      PEI=PSIE-PSII
      ISTEP=ISTEP+1
      RETURN
      END

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COMPTLER SPACE

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SUBROUTINE WF(K)
COMMON/GENERAL/ACC,CSALFA,DPDX,DX,ENTH(40),F(10,40),FS(10,40),GAM3,
1GAMN,GAM(40),I,IFIN,INDE(10),INDI(10),ISTEP,IUTRAP,ITEST,KEX,KIN,
2KRAD,N,NEQ,NP1,NP1,OH(40),OMD(40),BOM(40),KAST(10),PEI,PSIE,PSII,
3P(40),R(40),RHO(40),RJE(10),RJI(10),RME,RMI,SD(40),SU(40),WM(10),
4XD,XU,Y(40),YDIF(40),YE,YI,RJTE(10),RJTI(10)
COMMON/CJS/JU,JK,JD,JHS,JA,JG,JTE,JLE,JUV,JB
COMMON/CJS/JH2,J02,J0H,JH20,JH,JO,JN2
COMMON/CT/RR/AK,ALMG,CMU,CMUIN,CE1,CE2,CG1,CG2,CRIT,DUDY(40),
1DUDYSQ(40),EMUL(40),EMUT(40),IPD,PR(10),PRT(10),RTW(40)
COMMON/CWWF/YR(2),IRUF(2),EWALL,H
COMMON/WFST/FDIFS(20,2),TS(20,2),BP(2)
COMMON/CIRMA/SCH(40)

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C*****
DATA SHALF/.04/
GO TO (10,11),K
10 IW=1
   IN=2
   GO TO 12
11 IW=NP1
   IN=N
12 CONTINUE
C ***REFERENCE QUANTITIES
  UREF=ABS(F(JU,IW)-F(JU,IN))
  RHOREF=0.5*(RHO(IW)+RHO(IN))
  RUREF=RHOREF*UREF
  RREF=R(IN)
  RRUREF=RRFF*RUREF
  VREF=EMUL(IW)
  YREF=ABS(Y(IW)-Y(IN))
  RE=RUREF*YREF/VREF
  AM=(RMI-(RME-RMI)*OM(IW))/RRUREF
  EF=-SU(IW)*YREF/RUREF/UREF
122 IF(RE.LT.132.25) GO TO 110
C ***LOG LAW ASSUMPTION
121 CONTINUE
  LAM=0
  NIT=0
101 SHALF1=SHALF
  YRP=RYR*SHALF
C ***CALCULATION OF E FOR ROUGHNESS
  F=EWALL
  IF(IPUF(K).EQ.0) GO TO 16
C ***SAND-GRAIN ROUGHNESS
  IF(YRP.GT.3.3333) E=30./YRP
16 FR=RE*E
  S=SHALF**2
  SLOC=S+AM*EF
  IF(SLOC.GT.0.) GO TO 104
  SLOC=1.E-30
  SHALF=SQRT(ABS(AM+EF))
104 BEE=SQRT(SLOC/AK)
  ARG=FR*(SHALF+(AM/(1.+BEE)+.5*EF)/SHALF)
  IF(ARG.GT.11.*E) GO TO 106
  GO TO 110
106 SHALF=AK/ALOG(ARG)
  IF(ARS(SHALF-SHALF1).LT..0001.OR.NIT.GT.10) GO TO 102
  NIT=NIT+1

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GO TO 101
102 S=SHALF**5
    RP(K)=1./(1.+BEE)
    GO TO 103
C ***LAMINAR FLOW
110 LAM=1
    AMRE=AM*RE
    FRE=EF*RE
    IF(ABS(AMRE).LT..01) GO TO 111
    EXPMRE=EXP(AMRE)
    STORE=EXPMRE-1.-AMRE
    AMRESQ=AMRE*AMRE
    SRE=AMRE*(1.-STORE*FRE/AMRESQ)/(EXPMRE-1.)
    OUT1=SRE*STORE/AMRESQ+FRE*(STORE-.5*AMRESQ)/(AMRESQ*AMRE)
    GO TO 112
111 SRE=(2.-FRE*(1.+AMRE/3.))/(2.+AMRE)
    OUT1=SRE*(.5+AMRE/6.)+FRE*(.16667+AMRE/24.)
112 IF(SFE.GT.1.E-30) GO TO 113
    SRE=1.E-30
    OUT1=.33333
113 S=SRF/RE
    RP(K)=OUT1
103 DO 5000 J=1,NEQ
    FDIFS(J,K)=0.
    IF(J.EQ.JHS) FDIFS(J,K)=(H-1.)*.5*UREF**2
    IF(J.NE.JH) GO TO 200
    TS(J,K)=S*RRUREF
    GO TO 5000
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
    PRRAT=PR(J)/PHT(J)
    IF(KPAD.EQ.2) PRRAT=PR(J)/SCH(N)
    PJAY=9.*(PRRAT-1.)/PRRAT**2.25
    SF=S/(PRT(J)*(1.+PJAY*SHALF))
    IF(KPAD.EQ.2) SF=S/(SCH(N)*(1.+PJAY*SHALF))
    GO TO 213
C ***LAMINAR FLOW
210 IF(ABS(AMRE).LT..01) GO TO 211
    SF=AM/(EXP(PR(J)*AMRE)-1.)
    GO TO 212
211 SF=1./PR(J)/RE/(1.+5*PR(J)*AMRE)
212 CONTINUE
213 TS(J,K)=SF*RRUREF
5000 CONTINUE
    RETURN
    END

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COMPILER SPACE

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SUBROUTINE LANGLEY
C*****
  DIMENSION CPMN(7,60), PTEMP(40), RCON(10), STORE(10), REM(10)
  COMMON/GENERAL/ACC, CSALFA, DPDX, DX, ENTH(40), F(10,40), FS(10,40), GAM3,
  1GAMN, GAM(40), I, IFIN, INDE(10), INDI(10), ISTEP, IUTRAP, ITEST, KEX, KIN,
  2KRAD, N, NEQ, NP1, NM1, OR(40), OMD(40), ROM(40), KAST(10), PEI, PSIF, PSII,
  3P(40), R(40), RH0(40), RJE(10), RJI(10), RME, RMI, SU(40), WM(10),
  4XD, XU, Y(40), YDIF(40), YE, YI, RJTE(10), RJTI(10)
  COMMON/CJS/JU, JK, JD, JHS, JA, JG, JTE, JLE, JUV, JB
  COMMON/CFs/JH2, JO2, JOH, JH20, JH, JO, JN2
  COMMON/CSTAR/HO(7), CPBAR(7,60), HT(7,60), RC(5,60), ISTAR(40), FACN
  COMMON/CTURB/AK, ALMG, CMU, CMUIN, CE1, CE2, CG1, CG2, CRIT, DUDY(40),
  1DUDYSQ(40), EMUL(40), EMUT(40), IPD, PR(10), PRT(10), RTW(40)
  COMMON/CPROP/IO2, IN2, IH20, OFAC, NR, NS, WOO, WRO, WSO, WTO, GASCON, GAMMA
C*****
CHAPTER 1
C****LOADING OF EQUILIBRIUM CONSTANTS, ENTHALPIES AND SPECIFIC HEATS
  ENTRY LANGL1
C  ***REFERENCE ENTHALPIES
  DATA (HO(J), J=1,7)/-2023.8, -2074.7, 7205.6, -60164.7, 50616.5, 57949.1
  1, -2072.3/
C  ***CHEMICAL EQUILIBRIUM CONSTANTS
  DO 20 J=1, NR
  READ(5,1000) (RC(J,I), I=1,60)
  DO 20 I=1, 60
  RC(J,I)=AMIN1(RC(J,I), 100.)
  20 RC(J,I)=10.*RC(J,I)
C  ***CONSTANTS FOR GLOBAL REACTION
  DO 15 I=1, 60
  15 RC(5,I)=RC(4,I)*RC(3,I)/(RC(1,I)*SQRT(RC(2,I)))
C  ***CONVERSION INTO CONSTANTS FOR CONCENTRATION RATIOS
  A10=WM(JH2)/WM(JH)**2
  A20=WM(JO2)/WM(JO)**2
  A30=WM(JOH)/WM(JO)/WM(JH)
  A40=WM(JH20)/WM(JOH)/WM(JH)
  A50=WM(JH20)/WM(JH2)/SQRT(WM(JO2))
  DO 571 I=1, 60
  RC(1,I)=R0(1,I)*A10
  RC(2,I)=R0(2,I)*A20
  RC(3,I)=R0(3,I)*A30
  RC(4,I)=R0(4,I)*A40
  571 RC(5,I)=R0(5,I)*A50
C  ***ENTHALPIES AND MEAN SPECIFIC HEATS
  DO 30 J=1, NS
  CFA=4187./WM(J)
  HO(J)=HO(J)*CFA
  READ(5,2000) (HT(J,I), I=1,60)
  DO 30 I=1, 60
  HT(J,I)=HT(J,I)*CFA
  30 CPBAR(J,I)=.01*(HT(J,I)-HO(J))/FLOAT(I)
C
C  ***ITERATION PARAMETERS
  IBEGIN=3
  ITMAX=12
  CC=.01
  RPC=.5
  RPD=1.-RPC
C

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      FSTOICH=2.*WM(JH2)/WM(JO2)
      NRP=NR+1
      RETURN
C*****
CHAPTER 2
C*****INITIAL ENTHALPIES
      ENTRY LANGL2
      ENTH(I)=0.
      FACX=.01*F(JTE,I)
      IFACX=FACX
      FACS=FACX-FLOAT(IFACX)
      DO 115 J=1,NS
      ENTL=HT(J,IFACX)+FACS*(HT(J,IFACX+1)-HT(J,IFACX))
115 ENTH(I)=ENTH(I)+FS(J,I)*ENTL
      RETURN
C*****
CHAPTER 3
C*****LOCAL MASS FRACTIONS
      ENTRY LANGL3
C ***LOCATE POSITION WHERE HYDROGEN CONCENTRATION IS STOICHIOMETRIC
      X=1.-F(JA,1)
      X=X*OFAC
      IF(F(JA,1)/(X+1.E-10).LT.FSTOICH) GO TO 625
      DO 621 I=1,NP1
      X=1.-F(JA,I)
      X=X*OFAC
      PARA=RAT-1.E-10
      RAT=F(JA,I)/(X+1.E-10)
      IF(RAT.LT.FSTOICH) GO TO 1060
621 CONTINUE
1060 ILOCM=I-1
      ILOCP=I
      FACM=Y(I-1)+(Y(I)-Y(I-1))/(RAT-PARA)*(FSTOICH-PARA)
      GO TO 626
625 ILOCM=0
      ILOCP=1
626 DO 208 IDM=1,NP1
      I=NP1+1-IDM
      IF(I.LT.ILOCP) GO TO 740
      GO TO 742
740 I=ILOCP-I
742 TSM=AMAX1(F(JTE,I),250.)
C ***CONCENTRATIONS OF OXYGEN ELEMENT AND NITROGEN
      XN2PO=1.-F(JA,I)
      X=OFAC*XN2PO
      FS(JN2,I)=XN2PO-X
      RAT=F(JA,I)/(X+1.E-10)
      DO 304 L=1,NS
304 STORE(L)=0.
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)=RC(L,IFACX)+FACS*(RC(L,IFACX+1)-RC(L,IFACX))
      CFAC=RHU(I)*GASCON*F(JTE,I)*1.E-05
      DO 1056 L=1,NR
1056 RCON(L)=RCON(L)*CFAC

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RCON(NRP)=RCON(NRP)*SQRT(CFAC)
DO 317 L=1,NS
317 CPMN(L,I)=CPBAR(L,IFACX)+FACS*(CPBAR(L,IFACX+1)-CPBAR(L,IFACX))
ITER=0
IF(.NOT.(F02.EQ.0.AND.IH20.EQ.0)) GO TO 175
C ***SOLUTION OF QUADRATIC EQUATION FOR HYDROGEN-NITROGEN MIXTURES
FS(JH,I)=SQRT(1.+4.*F(JA,I)*RCON(1))
FS(JH,I)=.5*(FS(JH,I)-1.)/RCON(1)
FS(JH2,I)=F(JA,I)-FS(JH,I)
GO TO 208.
175 CONTINUE
C ***START OF ITERATION CYCLE
C ***DETERMINE LARGEST TERM IN EACH GROUP
C ---EQUATION FOR OXYGEN ELEMENT
J1=J02
FM1=FS(J02,I)
IF(FS(J0,I).LT.FS(J02,I)) GO TO 210
J1=J0
FM1=FS(J0,I)
210 IF(FS(JH20,I)*W50.LT.FM1) GO TO 211
J1=JH20
FM1=FS(JH20,I)*W50
211 IF(FS(JOH,I)*WRO.LE.FM1) GO TO 350
J1=JOH
FM1=FS(JOH,I)*WRO
350 CONTINUE
C ---EQUATION FOR HYDROGEN ELEMENT
J2=JH2
FM2=FS(JH2,I)
IF(FS(JH,I).LT.FS(JH2,I)) GO TO 212
J2=JH
FM2=FS(JH,I)
212 IF(FS(JH20,I)*W00.LT.FM2) GO TO 253
J2=JH20
FM2=FS(JH20,I)*W00
253 IF(FS(JOH,I)*WTO.LE.FM2) GO TO 353
J2=JOH
FM2=FS(JOH,I)*WTO
353 CONTINUE
C*** PRECAUTION IF H2O IS LARGEST OF BOTH GROUPS
IF(.NOT.(J1.EQ.JH20.AND.J2.EQ.JH20)) GO TO 279
IF(RAT.GE.FSTOICH) GO TO 356
J1=J02
FM1=FS(J02,I)
IF(FS(J0,I).LT.FS(J02,I)) GO TO 622
J1=J0
FM1=FS(J0,I)
622 IF(FS(JOH,I)*WRO.LT.FM1) GO TO 379
J1=JOH
FM1=FS(JOH,I)*WRO
GO TO 379
356 J2=JH2
FM2=FS(JH2,I)
IF(FS(JH,I).LT.FS(JH2,I)) GO TO 361
J2=JH
FM2=FS(JH,I)
361 IF(FS(JOH,I)*WTO.LT.FM2) GO TO 379
J2=JOH

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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=J02
FM1=FS(J02,I)
IF(FS(J0,I).LT.FS(J02,I)) GO TO 358
J1=J0
FM1=FS(J0,I)
358 IF(FS(JH20,I)*WSO.LT.FM1) GO TO 379
J1=JH20
FM1=FS(JH20,I)*WSO
GO TO 379
367 J2=JH2
FM2=FS(JH2,I)
IF(FS(JH,I).LT.FS(JH2,I)) GO TO 381
J2=JH
FM2=FS(JH,I)
381 IF(FS(JH20,I)*WQO.LT.FM2) GO TO 379
J2=JH20
FM2=FS(JH20,I)*WQO
379 CONTINUE
C ***OVER-RIDING PRECAUTION
IF(F(JA,I).GT..9999) J1=JH20
IF(F(JA,I).LT..0001) J2=JH20
C-----H2 GR H AS J2
IF(J2.NE.JH2.AND.J2.NE.JH) GO TO 240
IF(J2.EQ.JH2) FS(JH,I)=SQRT(FS(JH2,I)/RCON(1))
IF(J2.EQ.JH) FS(JH2,I)=FS(JH,I)**2*RCON(1)
IF(J1.EQ.JH20) GO TO 233
IF(J1.EQ.JOH) GO TO 427
IF(J1.EQ.J0) FS(J02,I)=FS(J0,I)**2*RCON(2)
IF(J1.EQ.J02) FS(J0,I)=SQRT(FS(J02,I)/RCON(2))
FS(JH20,I)=FS(JH2,I)*SQRT(FS(J02,I))*RCON(5)
FS(JOH,I)=FS(J0,I)*FS(JH,I)*RCON(3)
GO TO 290
233 FS(J02,I)=(FS(JH20,I)/FS(JH2,I)/RCON(5))**2
FS(J0,I)=SQRT(FS(J02,I)/RCON(2))
FS(JOH,I)=FS(J0,I)*FS(JH,I)*RCON(3)
GO TO 290
427 FS(J0,I)=FS(JOH,I)/FS(JH,I)/RCON(3)
FS(J02,I)=FS(J0,I)**2*RCON(2)
FS(JH20,I)=FS(JH,I)*FS(JOH,I)*RCON(4)
GO TO 290
240 IF(J2.NE.JH20) GO TO 250
C-----H20 AS J2
IF(J1.EQ.J0) FS(J02,I)=FS(J0,I)**2*RCON(2)
IF(J1.EQ.J02) FS(J0,I)=SQRT(FS(J02,I)/RCON(2))
IF(J1.NE.JOH) GO TO 430
FS(J0,I)=FS(JOH,I)**2/FS(JH20,I)*RCON(4)/RCON(3)
FS(J02,I)=FS(J0,I)**2*RCON(2)
430 CONTINUE
FS(JH2,I)=FS(JH20,I)/SQRT(FS(J02,I))/RCON(5)
FS(JH,I)=SQRT(FS(JH2,I)/RCON(1))
IF(J1.EQ.JOH) GO TO 290
FS(JOH,I)=FS(J0,I)*FS(JH,I)*RCON(3)

```

GO TO 290

C----- OH AS J2

250 CONTINUE
IF (J1.EQ.J0) FS(J02,I)=FS(J0,I)**2*RCON(2)
IF (J1.EQ.J02) FS(J0,I)=SQRT(FS(J02,I)/RCON(2))
IF (J1.EQ.JH20) GO TO 501
FS(JH,I)=FS(J0H,I)/FS(J0,I)/RCON(3)
FS(JH2,I)=FS(JH,I)**2*RCON(1)
FS(JH20,I)=FS(JH,I)*FS(J0H,I)*RCON(4)
GO TO 290

501 FS(JH,I)=FS(JH20,I)/FS(J0H,I)/RCON(4)

FS(JH2,I)=FS(JH,I)**2*RCON(1)

504 FS(J0,I)=FS(J0H,I)/FS(JH,I)/RCON(3)

FS(J02,I)=FS(J0,I)**2*RCON(2)

290 CONTINUE

C ***RE-EVALUATE LARGEST TERMS FROM ADDITIVE EQUATIONS

IF (RAT.LE.FSTOICH) GO TO 810

830 CONTINUE

FM1=X

IF (J1.NE.J0H) FM1=FM1-FS(J0H,I)*WRO

IF (J1.NE.J02) FM1=FM1-FS(J02,I)

IF (J1.NE.J0) FM1=FM1-FS(J0,I)

IF (J1.NE.JH20) FM1=FM1-FS(JH20,I)*WSO

FS(J,I)=FM1

IF (J1.EQ.JH20) FS(J1,I)=FS(J1,I)/WSO

IF (J1.EQ.J0H) FS(J1,I)=FM1/WRO

IF (RAT.LE.FSTOICH) GO TO 820

810 CONTINUE

FM2=F(JA,I)

IF (J2.NE.J0H) FM2=FM2-FS(J0H,I)*WTO

IF (J2.NE.JH2) FM2=FM2-FS(JH2,I)

IF (J2.NE.JH) FM2=FM2-FS(JH,I)

IF (J2.NE.JH20) FM2=FM2-FS(JH20,I)*WQO

FS(J2,I)=FM2

IF (J2.EQ.JH20) FS(J2,I)=FM2/WQO

IF (J2.EQ.J0H) FS(J2,I)=FM2/WTO

IF (RAT.LE.FSTOICH) GO TO 830

820 CONTINUE

ITER=ITER+1

ISTAR(I)=ITER

IF (ITER.LT.IHEGIN) GO TO 689

C ***UNDER-RELAXATION OF MASS FRACTIONS

DO 688 L=1,NS

688 FS(L,I)=RPC*FS(L,I)+RPD*STORE(L)

689 CONTINUE

DO 325 L=1,NS

325 REM(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)=AMIN1(FS(L,I),1.)

339 FS(L,I)=AMAX1(FS(L,I),0.)

DO 326 L=1,NS

326 STORE(L)=FS(L,I)

RMAX=0.

DO 327 L=1,NS

IF (FS(L,I).LT.1.E-06) GO TO 327

RMAX=AMAX1(RMAX,ABS(REM(L)))

327 CONTINUE

```

C ***CONVERGENCE CRITERION
  IF(ITER.GT.ITMAX.OR.ABS(RMAX)...(.CC) GO TO 208
  GO TO 175
208 CONTINUE
  DO 345 J=1,NS
  DO 345 I=1,NP1
  345 FS(J,I)=AMAX1(FS(J,I),0.)
C ***TEST FOR POOR CONVERGENCE
  DO 8227 I=1,NP1
  8227 IF(ISTAR(I).GT.ITMAX) WRITE(6,8828) ISTAR(I),I,ISTEP
  8828 FORMAT(10X,'--- POOR CONVERGENCE (*,I2,* ITERATIONS) AT NODE*,I3,*
  I AND STEP NO.*,I4)
  RETURN
C*****
CHAPTER 4
C****LOCAL TEMPERATURES
  ENTRY LANCL4
  DO 9613 I=1,NP1
  9613 PTEMP(I)=F(JTE,I)
  DO 405 I=1,NP1
  SMC=0.
  DO 406 J=1,NS
  ENTH(I)=ENTH(I)-FS(J,I)*HO(J)
  406 SMC=SMC+Fc(J,I)*CPMN(J,I)
  405 F(JTE,I)=ENTH(I)/SMC
C ***UNDER-RELAXATION OF TEMPERATURES IN REACTION ZONE
  ILM=ILOCM-3
  ILP=ILOCP+3
  DO 149 I=1,NP1
  IF(.NOT.(I.GE.ILM.AND.I.LE.ILP)) GO TO 149
  F(JTE,I)=.5*(F(JTE,I)+PTEMP(I))
  149 CONTINUE
C ***FORMAT STATEMENTS
  1000 FORMAT(7F10.4)
  2000 FORMAT(7F10.1)
  RETURN
  END

```

COMPILER SPACE

```

SUBROUTINE OUTPUT
C*****
DIMENSION FLUX(10), ATITL1(13), ATITL2(13), AVRBLE(6,10), ASYMBL(7)
COMMON/GENRAL/ACC, CSALFA, OPDX, CX, ENTH(40), F(10,40), FS(10,40), GAM3,
1GAMN, GAM(40), I, IFIN, INDE(10), INDI(10), ISTEP, IUTRAP, ITEST, KEX, KIN,
2KRAD, N, NEQ, NP1, NP1, OM(40), OMD(40), BOM(40), KAST(10), PEI, PSIE, PSII,
3P(40), K(40), RHO(40), RJF(10), RJI(10), FME, RMI, SD(40), SU(40), WM(10),
4XD, XU, Y(40), YDIF(40), YE, YI, RJTE(10), RJTI(10)
COMMON/CRAD/RFL0%, REXD, KASE
COMMON/CJS/JU, JK, JD, JHS, JA, JG, JTE, JLE, JUV, JB
COMMON/CFS/JH2, JO2, JOH, JH20, JH, JO, JN2
COMMON/CSTAR/HO(7), CPBAR(7,60), HT(7,60), RC(5,60), ISTAR(40), FACM
COMMON/CTHRU/AK, ALMG, CMU, CMUIN, CE1, CE2, CG1, CG2, CRIT, DUDY(40),
1DUDYSO(40), EMUL(40), FMUT(40), IPD, PR(10), PRT(10), RTW(40)
COMMON/OUTPT/IA, IEND, YIN, YOUT, YHA, DYHA, DDYHA, RDUCT, KP, KS, KT,
1KASENO, XSTAT(20), XPROF(20), XPLOTT(20), PRESS
COMMON/TPLOTB/XTAXIS, XTPLOT(40), YTAXES(10), YTPLOT(10,40),
1YTMAX(10), YTSYMB(10), OUT(40), IPROF
COMMON/CPROP/JO2, IN2, IH20, OFAC, NR, NS, WGO, WRO, WSO, WTO, GASCON, GAMMA
C*****
C ***INITIAL VALUES OF INTEREST
ENTRY OUTP1
FSTOICH=2.*WM(JH2)/WM(JO2)
FSTOICH=FSTOICH/(1.+FSTOICH)
READ(5,1153) (ATITL1(K),K=1,13)
READ(5,1153) (ATITL2(K),K=1,13)
READ(5,1154) ((AVRBLE(K,L),K=1,6),L=1,10)
REFY=RHO(1)*F(JU,1)*2.*Y(NP1)/EMUL(1)
VMIX=0.
DO 1016 J=1,NS
1016 VMIX=VMIX*FS(J,1)/WM(J)
AMACH=F(JH,1)/SQRT(GAMMA*GASCON*F(JTE,1)*VMIX)
PRESS1=PRESS
UIN=F(JU,1)
UFIN=F(JU,1)-F(JU,NP1)
CIN=FS(JH2,1)
TIN=F(JTE,1)
C ***OUTPUT OF ALPHANUMERIC DATA
WRITE(6,1021) (ATITL1(K),K=1,13), (ATITL2(K),K=1,13)
WRITE(6,1022) (L, (AVRBLE(K,L),K=1,6),L=1,NEQ)
WRITE(6,1023)
WRITE(6,1024) CMU,CE1,CE2,CG1,CG2,AK,ALMG,CRIT,IPD
WRITE(6,1032) (OM(I),I=1,NP1)
WRITE(6,1033) NR,NS
READ(5,1154) ((AVRBLE(K,L),K=1,6),L=1,NR)
WRITE(6,1034)
WRITE(6,1022) (L, (AVRBLE(K,L),K=1,6),L=1,NR)
READ(5,1154) ((AVRBLE(K,L),K=1,6),L=1,NS)
WRITE(6,1035)
WRITE(6,1022) (L, (AVRBLE(K,L),K=1,6),L=1,NS)
WRITE(6,1036)
WRITE(6,1025)
READ(5,1153) (ASYMBL(K),K=1,7)
DO 1017 J=1,NEQ
1017 WRITE(6,1020) J,PR(J),PRT(J),KAST(J)
WRITE(6,1037) REFY,AMACH,YIN,YOUT,RDUCT,PRESS1,UIN,CIN,TIN
RETURN
C*****

```

```

C ***STATION VARIABLES
  ENTRY OUTP2
  XUD=XII/YOUT
C ***MEAN SQUARE FLUCTUATIONS (OF H ELEMENT)
  IF (I02.EQ.0.AND.IH2O.EQ.0) GO TO 165
C ***LOCATE POSITION OF FLAME FRONT
C ---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)-SQRT(F(JG,I)))/RAT
    IF(SFH2.LT.1.) GO TO 162
161 CONTINUE
162 FACI=Y(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)+SQRT(F(JG,I)))/RAT
    IF(SFH2.LT.1.) GO TO 164
163 CONTINUE
164 FACE=Y(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(6,1006) ISTEP,XU,XUD,DX,YHA,DYHA,DDYHA,YDX
  WRITE(6,1007) KIN,KEX,YIN,Y(NP1),PDE,ACC,CMU,CE2
  WRITE(6,1008) PSII,PSIE,PEI,RMI,RME,FACI,FACE,FACM
  WRITE(6,1009) F(JU,1),F(JA,1),F(JTE,1),ULINE,CLINE,TLINE,PRDRP
C ***CHECK FOR FLUX CONSERVATION
  DO 1027 J=1,NEQ
    FLUX(J)=(F(J,2)*OM(2)+F(J,N)*(1.-OM(N)))*2.
    DO 1027 I=2,NM1
1027 FLUX(J)=FLUX(J)+(F(J,I)+F(J,I+1))*OMD(I)
    DO 1028 J=1,NEQ
      IF(KAST(J)) 1029,1029,1028
1029 FLUX(J)=FLUX(J)-.25*((F(J,3)-F(J,2))*(OM(3)-OM(2))+
  1 (F(J,NM1)-F(J,N))*(OM(N)-OM(NM1)))
102A FLUX(J)=.5*FLUX(J)*PEI+PSII*F(J,1)-PSIE*F(J,NP1)
  WRITE(6,1030) (J,FLUX(J),J=1,NEQ)
  IF(KASE.EQ.2) WRITE(6,1155) RFLOW,RDUCT,REXD,P(1),DPDX
  IF(KEX.NE.1) RETURN
  OF=RJE(JHE)/R(NP1)
  TAUE=RJE(JU)/R(NP1)
  WRITE(6,1010) INDE(JHS),F(JTE,NP1),QE,TAUE
  RETURN
C*****
  ENTRY OUTP3
C ***PROFILE VARIABLES
C-----
C/ INFORMATION (TEMPORARY) ON NEW OUTPUT ROUTINE.
C/ SUBROUTINE PROFIL ASSIGNS VALUES FOR PLOT, AND ALSO WRITES
C/ PROFILES. IT IS CALLED BY ...
C/ CALL PROFIL(JPROF,TITLE,FIRST,ADD,DIV,FINAL,KPLOT,SYMBOL)
C/ WHERE JPROF=J REFERS TO THE F(J,I) ARRAY
C/ JPROF.GT.0 MEANS USE F(JPROF,I) ARRAY AND WRITE PROFILE.
C/ JPROF.LT.0 MEANS USE OUT(I)+ARRAY AND WRITE PROFILE.

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C/ JPROF=0 MEANS NO ACTION UNLESS KPLOT.LT.0
C N=0. OUT(I) ARRAY IS OVERRITTEN 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/ ADD AND DIV MODIFY PROFILES FROM I=2 TO I=N
C/ KPLOT.GT.0 MEANS ASSIGN YTPLOT(KPLOT,I) ARRAY.
C/ KPLOT=0 MEANS NO PLOT ASSIGNMENTS.
C/ KPLOT.LT.0 MEANS ASSIGN THE Y(I) ARRAY TO THE XTPLOT(I) ARRAY.
C/ SYMBOL IS THE CHARACTER USED IN PLOT.
-----
C ***ZERO YTPLOT 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(0,1H*,0.,0.,1.,0., K,1H*)
401  CONTINUE
C ***DISTANCES (Y)
  CALL PROFIL( 0,6HY/Y(NP .R(1),0.,Y(NP1),Y(NP1),-1,0)
C ***AXIAL VELOCITIES (JU)
  DIV=(F(JU,1)-F(JU,NP1)+1.E-30
  CALL PROFIL(JU,6HU VELO,F(JU,1),-F(JU,NP1),DIV,F(JU,NP1),1,1HU)
C ***STAGNATION ENTHALPIES (JHS)
  DIV=(F(JHS,1)-F(JHS,NP1)
  CALL PROFIL(JHS,6HH STAG,F(JHS,1),-F(JHS,NP1),DIV,F(JHS,NP1),0,0)
C ***TURBULENT KINETIC ENERGIES (JK)
  DIV=(F(JU,1)-F(JU,NP1)+1.E-30)**2
  CALL PROFIL(JK,6HK.E.TI) ,F(JK,1),0.,DIV,F(JK,NP1), 5,1HK)
C ***DISSIPATION RATES (JD)
  CALL PROFIL(JD,6HD DISS,F(JD,1),0.,1.,F(JD,NP1),6,1HD)
C ***DISSIPATION LENGTH SCALES (JLE)
  DO 1201 I=2,N
1201 F(JLE,I)=SQRT(F(JK,I))/(RTW(I)+1.E-30)
  F(JLE,1)=0.
  F(JLE,NP1)=0.
  DIV=Y(NP1)
  CALL PROFIL(JLE,6HLENGTH,F(JLE,1),0.,DIV,F(JLE,NP1), 10,1HL)
C ***TURBULENT VISCOSITIES# (EMUT)
  WRITE(6,628) (EMUT(I),I=1,NP1)
C ***DENSITIES
  WRITE(6,659) (RHO(I),I=1,NP1)
C ***REYNOLDS STRESS CORRELATION (JUV)
  DIV=(F(JU,1)-F(JU,NP1)+1.E-30)**2
  CALL PROFIL(JUV,6HUV ,F(JUV,1),0.,DIV,F(JUV,NP1),2,1HS)
C ***SPECIES MASS FRACTIONS (JA)
  DIV=(F(JA,1)-F(JA,NP1)+1.E-30
  CALL PROFIL(JA,7HF(JA,I),F(JA,1),-F(JA,NP1),DIV,F(JA,NP1),3,1HA)
C****R.M.S. CONCENTRATION FLUCTUATIONS (OF H ELEMENT)
  DIV=(F(JA,1)-F(JA,NP1)+1.E-30
  CALL PROFIL(JG,7HF(JG,I),F(JG,1),-F(JG,NP1),DIV,F(JG,NP1),9,1HG)
C ***ABSOLUTE TEMPERATURES (JTE)
  DIV=(F(JTE,1)-F(JTE,NP1)+1.E-30
  CALL PROFIL(JTE,4HTEMP,F(JTE,1),-F(JTE,NP1),DIV,F(JTE,NP1),8,1HT)
C ***OUTPUT OF INDIVIDUAL SPECIES CONCENTRATIONS
  DO 625 J=1,NS
625  WRITE(6,626) ASYMBL(J),(FS(J,I),I=1,NP1)
  WRITE(6,627) (ISTAR(I),I=1,NP1)
C ***PLOTTING OF PROFILES

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```

605 IF (ISTEP.EQ.0) RETURN
IF (ISTEP.EQ.IAX.OR.ISTEP.EQ.IEND) GO TO 435
IF (XID.LT.XPLOT(KT)) RETURN
KT=KT+1
435 WRITE(6,1091) XU,ISTEP
CALL PLOTS(XTPLOT,35.NP1,XTAXIS,YTPLOT,YTMAX,10,10,YTAXES,YTSYMS)
C*****
C ***FORMAT STATEMENTS
626 FORMAT(1H ,A6,1P11E11.3/(7X,1P11E11.3))
627 FORMAT(1H ,6HITER ,11I11/(7X,11I11))
628 FORMAT(1H ,6HEMUT ,1P11E11.3/(7X,1P11E11.3))
629 FORMAT(1H ,6HRHO ,1P11E11.3/(7X,1P11E11.3))
1006 FORMAT(/1H0,*ISTEP=#,I5,1X,*XU=#,1PE11.3,1X,*XUD=#,1PE11.3,1X,*OX
1=#,1PE11.3,1X,*YHA=#,1PE11.3,1X,*DYHA=#,1PE11.3,1X,*DDYHA=#,1PE11.
23,1X,*YDX=#,1PE11.3)
1007 FORMAT(1X,*KIH=#,I2,1X,*KEX=#,I2,1X,*YIN=#,1PE11.3,1X,*Y(NP1)=#,1P
1E11.3,1X,*PDE=#,1PE11.3,1X,*ACC=#,1PE11.3,1X,*CMU=#,1PE11.3,1X,*CE
22=#,1PE11.3)
1008 FORMAT(1X,*PSII=#,1PE11.3,1X,*PSIE=#,1PE11.3,1X,*PEI=#,1PE11.3,1X,
1*PMI=#,1PE11.3,1X,*RME=#,1PE11.3,1X,*FACI=#,1PE11.3,1X,*FACE=#,1PE
211.3,1X,*FACM=#,1PE11.3)
1009 FORMAT(1X,*U1=#,1PE11.3,1X,*M1=#,1PE11.3,1X,*T1=#,1PE11.3,1X,*U1/
1I=#,1PE11.3,1X,*M1/MI=#,1PE11.3,1X,*T1/TI=#,1PE11.3,1X,*PRDRP=#,1P
2E11.3)
1010 FORMAT(1X,*INDE(JHS)=#,I2,1X,*TWALL=#,1PE11.3,1X,*HT.TRANSF.=#,1PE
111.3,1X,*cHEAR STRESS=#,1PE11.3)
1021 FORMAT(1H1,4X,13A6/5X,13A6//5X,*----- ORDER OF DEPENDENT VARIABLE
1S IS#/)
1022 FORMAT(6X,I2,*,*,6A6)
1023 FORMAT(/1H0,*-- CONSTANTS IN TURBULENCE MODEL*)
1024 FORMAT(/4X,*CMU=#,F8.3,3X,*CE1=#,F8.3,3X,*CE2=#,F8.3,3X,*CG1=#,F8.
13,3X,*CG2=#,F8.3,3X,*AK=#,F8.3,3X,*ALMG=#,F8.3,3X,*CRIT=#,F8.3,3X,
2*JPD=#,I2)
1025 FORMAT(/1H0,*-- PRANDTL SCHMIDT NUMBERS ARE#/)
1026 FORMAT(4X,*J=#,I2,3X,*PR(J)=#,F9.3,3X,*PRT(J)=#,F9.3,3X,*KAST(J)=#
1,J2)
1030 FORMAT(5H FLUX, 7(1H(,I2,2H)=,1PE10.3,2X))
1032 FORMAT(1H0,*-- OMEGA DISTRIBUTION --#/(4X,1P11E11.3))
1033 FORMAT(/1H0,*-- NUMBER OF REACTIONS =#,I3,10X,*-- NUMBER OF SPECIES
1=#,I3)
1034 FORMAT(/1H0,5X,*-- REACTIONS ARE*)
1035 FORMAT(/1H0,5X,*-- CHEMICAL SPECIES ARE*)
1036 FORMAT(////)
1037 FORMAT(/1H0,*-- INITIAL VALUES --#/(5X,*REY =#,1PE11.3/5X,*NACH =#
1,1PE11.3/5X,*YIN =#,1PE11.3/5X,*YOUT =#,1PE11.3/5X,*RDUCT=#,1PE11
2.3/5X,*PRFSS=#,1PE11.3/5X,*U =#,1PE11.3/5X,*C =#,1PE11.3/5X,
3*T =#,1PE11.3)
1091 FORMAT(4H1XU=,1PE10.3,8H, ISTEP=,I6)
1153 FORMAT(13A6)
1154 FORMAT(6A6)
1155 FORMAT(1X,*RFLOW=#,1PE11.3,1X,*RDUCT=#,1PE11.3,1X,*REXD=#,1PE11.3,
11X,*PRFSS=#,1PE12.4,1X,*DPDX=#,1PE11.3)
C*****
RETURN
END

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COMPILER SPACE


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SUBROUTINE PROFIL (JPROF, TITLE, FIRST, ADD, DIV, FINAL, KPLOT, SYMBOL)
COMMON/GENERAL/ACC, CSALFA, DPDX, DX, ENTH(40), F(10,40), FS(10,40), GAM3,
IGAM1, GAM(40), I, IFIN, INDE(10), INDI(10), ISTEP, IUTRAP, ITEST, KEX, KIN,
2KRAD, N, NEQ, NP1, NM1, OM(40), OMD(40), BOM(40), KAST(10), PEI, PSIE, PSII,
3P(40), R(40), RHO(40), RJE(10), RJI(10), RME, RMI, SD(40), SU(40), WM(10),
4XD, XU, Y(40), YDIF(40), YE, YI, RJTE(10), RJTI(10)
COMMON/CJS/JU, JK, JD, JHS, JA, JG, JTE, JLE, JUV, JB
COMMON/CFS/JH2, JO2, JOH, JH20, JH, JO, JN2
COMMON/TPLOTB/XTAXIS, XTPLT(40), YTAXES(10), YTPLOT(10,40),
1YTMAX(10), YTSYMB(10), OUT(40), IPROF

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C-----
C*****SUBROUTINE TO WRITE PROFILES AND ASSIGN TRANSVERSE PLOT ARRAYS
C-----

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```

      IF(KPLOT) 500,700,700
700  IF(JPROF) 200,200,100

100  DO 101 I=1,NP1
101  OUT(I)=F(JPROF,I)
200  YMAX=1.E-30
      DO 201 I=1,NP1
          YMAX=AMAX1(YMAX,OUT(I))
201  OUT(I)=(OUT(I)+ADD)/DIV
      IF(JPROF.NE.0.AND.IPROF.EQ.1) WRITE(6,900) TITLE,FIRST,(OUT(I),I=2
1,N),FINAL
      IF(JPROF.NE.0.AND.IPROF.EQ.2) WRITE(6,900) TITLE,(F(JPROF,I),I=1,N
1P1)
      IF(KPLOT) 500,600,400
400  DO 401 I=1,NP1
401  YTPLOT(KPLOT,I)=OUT(I)
          YTAXES(KPLOT)=TITLE
          YTSYMB(KPLOT)=SYMBOL
          YTMAX(KPLOT)=YMAX
      RETURN
500  DO 501 I=1,NP1
501  XTPLT(I)=(Y(I)+ADD)/DIV
          XTAXIS=TITLE
          WRITE(6,900) TITLE,FIRST,(XTPLT(I),I=2,N ),FINAL
600  RETURN
900  FORMAT(1H ,A6,1P11E11.3/(7X,1P11E11.3))
      END

```

COMPILER SPACE

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SUBROUTINE PLOTS(X, IDIM, IMAX, XAXIS, Y, YMAX, JDIM, JMAX, YAXES, SYMBOL)
C-----
C SUBROUTINE FOR PLOTTING J CURVES OF Y(J,I) AGAINST X(I)
C-----
C
C X AND Y ARE ASSUMED TO BE IN ANY RANGE EXCEPT THAT NEGATIVE VALUES
C ARE PLOTTED AS ZERO
C X AND Y ARE SCALED TO THE RANGE 0. TO 1. BY DIVISION BY THE MAXIMA
C WHICH ARE ALSO PRINTED
C IDIM IS THE VARIABLE DIMENSION FOR X.
C IMAX IS THE NUMBER OF X VALUES
C XAXIS STORES THE NAME OF THE X-AXIS
C JDIM IS THE VARIABLE DIMENSION FOR Y.
C JMAX IS THE NUMBER OF CURVES TO BE PLOTTED, (UP TO 10).
C THE ARRAY YAXES(J) STORES THE NAME OF THE CURVES.
C THE ARRAY SYMBOL(J) STORES THE SINGLE CHARACTERS USED FOR PLOTTING
C
C*****
      DIMENSION X(IDIM), Y(JDIM, IDIM), YMAX(JDIM), YAXES(JDIM), SYMBOL(JDIM)
      1, A(10))
      DATA DOT, CROSS, BLANK/1H., 1H+, 1H /
C**** 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.
C**** 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=AMAX1(AYMAX, Y(J, I))
      DO 3 I=1, IMAX
3 Y(J, I)=AMAX1((Y(J, I)/AYMAX)*100., 0.)
C**** IDENTIFYING THE VARIOUS CURVES TO BE PLOTTED
      WRITE(6, 103) XAXIS, XMAX
      WRITE(6, 100) (YAXES(I), I=1, JMAX)
      WRITE(6, 106) (SYMBOL(I), I=1, JMAX)
      WRITE(6, 102) (YMAX(I), I=1, JMAX)
      DO 5 I=1, 11
5 A(I)=0.1*FLOAT(I-1)
      WRITE(6, 101) (A(I), I=1, 11)
C**** MAIN LOOP. EACH PASS PRODUCES AN X-CONSTANT LINE
      DO 40 I=1, 51
      IF(I.EQ.1.OR.I.EQ.51) GO TO 32
      GO TO 33
C**** 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
C**** ALLOCATE . OR + MARK ON THE X-AXIS, ALSO THE APPROPRIATE X VALUE
33 A(1)=DOT
      A(10)=DOT
      K=I-1
40 K=K-5
      IF(K) 4R, 47, 46

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47 A(I)=CROSS
   A(101)=CROSS
42 XL=0.02*FLOAT(I-1)
C***** CHECK IF ANY Y( X(I) ) VALUE LIES ON THIS X-CONSTANT LINE
C***** IF YES GO TO 41, OTHERWISE GO TO 42
      DO 43 K=1,IMAX
      IF(IFIX(X(K)+1.5)-I) 43,41,43
C***** LOCATE Y( X(I) )
41 DO 44 J=1,JMAX
   NY=Y(J,K)+1.5
   A(NY)=SYMBOL(J)
42 CONTINUE
   GO TO 42
43 CONTINUE
C***** PRINT X-CONSTANT LINE
42 WRITE(6,105) XL,(A(K),K=1,101),XL
C***** PUTTING BLANKS INTO X-CONSTANT LINE
   DO 49 K=1,101
49 A(K)=BLANK
40 CONTINUE
   DO 50 I=1,11
50 A(I)=.1*FLOAT(I-1)
   WRITE(6,104) (A(J),I=1,11)
   RETURN
100 FORMAT(11H Y-AXES ARE,5X,10(1X,A10))
101 FORMAT(1H0,2X,11F10.1)
102 FORMAT(15H MAXIMUM VALUES,1P10E11.3)
103 FORMAT(11H0X-AXIS IS ,A8.17H ,MAXIMUM VALUE =.1PE10.3)
104 FORMAT(3X,11F10.1/1H1)
105 FORMAT(2H X,F6.2,3X,101A1,F6.2)
106 FORMAT(7H SYMBOL,11X,10(1X,A10))
   END

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SUBROUTINE YINT(FRAC,YFRAC,JJ)
COMMON/GENRAL/ACC,CSALFA,DPDX,DX,ENTH(40),F(10,40),FS(10,40),GAM3,
1GAMN,GAM(40),I,IFIN,INDE(10),INDI(10),ISTEP,IUTRAP,ITEST,KEX,KIN,
2KRAD,N,NE0,NP1,NM1,OM(40),OMD(40),BOM(40),KAST(10),PEI,PSIE,PSII,
3P(40),R(40),RHO(40),RJE(10),RJI(10),RME,RMI,SD(40),SU(40),WM(10),
4XD,XI,Y(40),YDIF(40),YE,YI,RJTE(10),RJTI(10)
COMMON/CJ0/JU,JK,JD,JHS,JA,JG,JTE,JLE,JUV,JB
COMMON/CF0/JH2,J02,JOH,JH20,JH,JO,JN2

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C*****INTERPOLATION SUBROUTINE
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REFDIF=FRAC*ABS(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=,I4,4H XU=,1PE10.3,52H IN SUBROUTINE YINT, REFDIF=
10. 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=,I3,5H NP1=,I4,
1 11H F(JJ,NP1)=,E10.3,9H F(JJ,1)=,E10.3)
RETURN
10 IF(FRAC.GT..5) GO TO 30
DO 20 I=2,N
DIF=ABS(F(JJ,I)-F(JJ,1))
IF(DIF-REFDIF) 20,21,21
21 T=ABS(F(JJ,I)-F(JJ,I-1))
IF(T) 22,23,22
22 T=(DIF-REFDIF)/T
23 YFRAC=Y(I)-T*(Y(I)-Y(I-1))
RETURN
20 CONTINUE
30 DO 40 IDACH=2,N
I=N+2-IDACH
DIF=ABS(F(JJ,I)-F(JJ,1))
IF(DIF-REFDIF) 41,41,40
41 T=ABS(F(JJ,I)-F(JJ,I+1))
IF(T) 42,43,42
42 T=(DIF-REFDIF)/T
43 YFRAC=Y(I)-T*(Y(I+1)-Y(I))
RETURN
40 CONTINUE
RETURN
END

```

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