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PREDICTION OF HYDRODYNAMICS AND CHEMISTRY OF CONFINED TURBULENT METHANE - AIR FLAMES WITH ATTENTION TO FORMATION OF OXIDES OF NITROGEN

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16. Abstract

A formulation of the governing partial differential equations for fluid flow and reacting chemical species in a tubular combustor is presented. A numerical procedure for the solution of the governing differential equations is described and models for chemical-equilibrium and chemical-kinetics calculations are presented. The chemical-equilibrium model is used to characterise the hydrocarbon reactions. The chemical-kinetics model is used to predict the concentrations of the oxides of nitrogen. The combustor considered consists of a cylindrical duct of varying cross-section with concentric streams of gaseous fuel and air entering the duct at one end.

Four sample cases with specified inlet and boundary conditions are considered and the results are discussed.

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1. INTRODUCTION

1.1 Purpose of the Report

The purpose of this report is to present an analysis of the hydrodynamics and the chemical reaction in a duct which is a greatly scaled up and simplified model of a typical flow passage in a porous material surface combustor. The geometry considered is a cylindrical duct of varying cross-section and hence the analysis should be valid for any tubular combustor passage whose radius can be expressed as a parabolic function of axial position.

The analysis involves the mathematical formulation of the flow in terms of partial differential and some auxiliary algebraic equations. Subsequently these equations are cast in their finite-difference form for obtaining numerical solutions. The solution procedure is incorporated in a computer program to produce profiles of velocity, temperature, and species concentrations throughout the combustor.

This report provides details of the formulation and solution procedure as also the results of some sample cases.

1.2 Layout of the Report

The remainder of this report is divided into ten chapters. Chapter 2 is concerned with the mathematical formulation and physical models employed in the solution procedure. Chapter 3 details the numerical solution procedure, and Chapter 4 some further features of the calculation procedure. Thermodynamic and element data are discussed in Chapter 5, and kinetics data in Chapter 6. Results and discussions are provided in Chapter 7 and Chapter 8 provides some concluding remarks. Chapters 9 and 10 include references and nomenclature. Appendices A and B contain the description and the listing of the computer program.

1.3 The Problem Considered

The problem involves the development of a general-purpose computer program for the realistic prediction of the hydrodynamics and chemical reaction in a tubular combustor; special attention being given to pollutant (NO_x) formation and flame stability.

The combustor geometry considered in this study consists of a duct of circular cross-section (Fig. 1), the radius of which varies along the length. Two concentric streams, one of gaseous fuel, and the other of air, enter the duct at one end. On entering the duct, the fuel and air mix together, and the fuel starts burning in the region. Oxides of nitrogen and other combustion products are formed as a result of the chemical reaction.

The flow is two-dimensional, axisymmetric, steady and turbulent, with axial diffusion.

1.4 Connexions with Previous Work

The method of solution employed is based on an already existing computer program, GENMIX (Ref. 1). In the published form of the program, the axial diffusion term is not provided, and only one-dimensional storage of the dependent variables is used, i.e. the problems considered are truly parabolic. In the present work, the GENMIX program has been extended to account for the effects of axial diffusion, and provision is made for repeated marching, since the problem is no longer truly parabolic. The present work has also involved the inclusion of the appropriate chemical-equilibrium and kinetics-calculation schemes.

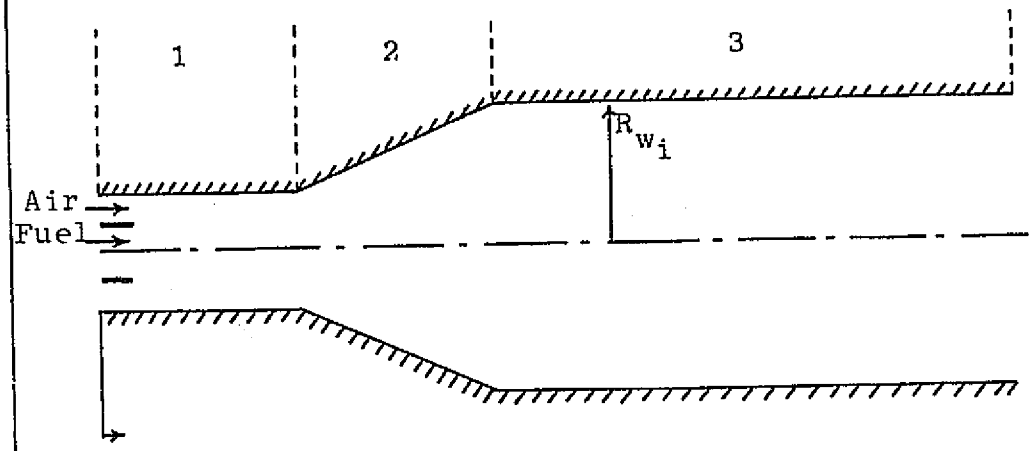

Fig.1. Geometry of the problem (not to scale).

2. PHYSICAL AND MATHEMATICAL ANALYSIS

2.1 Introduction

This Chapter describes the mathematical and physical basis of the problem considered. The physical modelling of properties and processes is discussed in Section 2.2. Section 2.3 outlines the conservation equations for momentum, stagnation enthalpy, and chemical species. Upstream, boundary, and downstream conditions are considered in Sections 2.4, 2.5, and 2.6 respectively. Auxiliary equations for mixture properties and flux calculations are dealt with in Section 2.7. Section 2.8 describes the chemical-equilibrium model, and Section 2.9 the chemical-kinetics model. Finally, the influence of recirculation on the transport properties is discussed in Section 2.10.

2.2 Physical Models

The conservation equations outlined in the next section are based on a physical model which involves certain assumptions regarding properties and processes; these are now described.

2.2.1 Processes

(i) Axial derivatives for conduction, diffusion, and momentum transport are included in the conservation equations.

(ii) The chemistry incorporated into the computer code is as follows:

(1) A single-step reaction for hydrocarbon oxidation according to:

1 kg of fuel + s kg of oxygen → (1 + s)kg products (1)

where s is a fixed stoichiometric ratio, and the rate of the reaction is governed by the Arrhenius relation:

$$\text{Rate} = C_1\ T^{C2} m_{fu}^{C3} m_{ox}^{C4} \exp(-C_5/T)$$

where C_1, C_2,———C_5, are constants, T is the absolute temperature, and m_{fu} and m_{ox} are the concentrations of fuel and oxygen respectively.

(2) The products of the above idealized reaction are assumed to consist of the species: CO, CO_2, H_2O, O, H, H_2, and OH, in such proportions as are appropriate to equilibrium stoichiometric adiabatic combustion at the prevailing pressure and enthalpy. These proportions are represented as algebraic functions of pressure and enthalpy; the constants in these functions being determined from interpolations in equilibrium computations, made external and prior to the main computer code.

(3) Oxides of nitrogen are calculated by reference to the kinetically-controlled reactions involving the species N_2, O_2, O, H, and OH. The scheme consists of nine reactions including the Zeldovich mechanism, as shown in Section 2.9.

2.2.2 Properties

Transport-property assumptions are such as to allow a composite property ξ ($\equiv m_{fu} - m_{ox}/s$) to characterise the composition of the gas-mixture with respect to the products of combustion resulting from the main hydrocarbon oxidation reaction. The quantity ξ obeys a source-free conservation equation, and its transport coefficient is a function of position alone. This means that ξ is influenced by convection and diffusion alone; and underlying its definition is the assumption that the transport properties of oxidant and fuel are everywhere equal.

2.3 Governing Differential Equations

The dependent variables are the u-velocity, mixture fraction f, mass fraction of unburnt fuel m_{fu}, stagnation enthalpy $\tilde{h}$ and the mass fractions of the species involved in the NO_x-reactions (i.e. NO, NO_2, N, and N_2O). As mentioned earlier in Section 2.2.1, the concentrations of the species CO, CO_2, H_2O, O, H, H_2, and OH are determined by a chemical-equilibrium analysis, subsequent to the solution of the governing differential equations for f and m_{fu}.

The differential equations which govern the fluid flow for steady, two-dimensional axisymmetric flow are written* in the x-ψ (Von-Mises) coordinates as:

x-direction momentum equation**:

$$\frac{\partial u}{\partial x} = \frac{\partial}{\partial \psi} (r^2 \rho u \mu \frac{\partial u}{\partial \psi}) + \frac{1}{\rho u} \{- \frac{\partial p}{\partial x} + \frac{\partial}{\partial x} (\mu \frac{\partial u}{\partial x})\} \qquad (3)$$

Conservation equation for species j:

$$\frac{\partial m_j}{\partial x} = \frac{\partial}{\partial \psi} (r^2 \rho u \Gamma_j \frac{\partial m_j}{\partial \psi}) + \frac{1}{\rho u} \{\frac{\partial}{\partial x} (\Gamma_j \frac{\partial m_j}{\partial x}) + S_j\} \qquad (4)$$

where S_j is the mass rate of creation of species j by chemical reaction.

*Symbols are explained in the nomenclature (Chapter 10).

**In the equations presented here and later in the report, μ and Γ are the effective transport coefficients; the subscript 'eff' is however largely omitted for the sake of convenience.

Conservation equation for stagnation enthalpy $\tilde{h}$:

$$\frac{\partial \tilde{h}}{\partial x} = \frac{\partial}{\partial \psi} (r^2 \rho u \Gamma_{\tilde{h}} \frac{\partial \tilde{h}}{\partial \psi}) + \frac{1}{\rho u} \{\frac{\partial}{\partial x} (\Gamma_{\tilde{h}} \frac{\partial \tilde{h}}{\partial x})\}$$

$$+ \frac{\partial}{\partial \psi}\{(\mu - \Gamma_{\tilde{h}})\ r^2\ \rho u \frac{\partial}{\partial \psi} (\frac{u^2}{2})\} + \frac{1}{\rho u} \left[\frac{\partial}{\partial x}\{(\mu - \Gamma_{\tilde{h}}) \frac{\partial}{\partial x}(\frac{u^2}{2})\}\right] \qquad (5)$$

where the last two terms on the right-hand side represent "kinetic heating", i.e. the effect on the enthalpy flux of the viscous stresses.

Conservation equation for mixture fraction f:

$$\frac{\partial f}{\partial x} = \frac{\partial}{\partial \psi} (r^2\ \rho u\ \Gamma_f \frac{\partial f}{\partial \psi}) + \frac{1}{\rho u} \{\frac{\partial}{\partial x} (\Gamma_f \frac{\partial f}{\partial x})\} \qquad (6)$$

where the mixture fraction f is defined as

$$f \equiv (\xi - \xi_{ox}) \ / \ (\xi_{fu} - \xi_{ox}) \qquad (7)^*$$

General form of governing differential equations:

Equations (3 - 6) may be written in a general form as:

$$\frac{\partial \phi}{\partial x} = \frac{\partial}{\partial \psi} (c \frac{\partial \phi}{\partial \psi}) + d + e \qquad (8)$$

*Note: $\xi_{ox} = (-m_{ox})_{inle.}/s$ and $\xi_{fu} = (m_{fu})_{inlet}$, where m_{ox} is the oxygen mass fraction in the incoming oxidant stream and m_{fu} is the fuel mass fraction in the incoming fuel stream.

where

$\phi \equiv$ any one of the dependent variables

and c, d, e are defined as:

$$c \equiv r^2 \rho u \Gamma_\phi \tag{9}$$

$$d \equiv S_\phi / \rho u \tag{10}$$

$$e \equiv \frac{1}{\rho u} \{\frac{\partial}{\partial x} (\Gamma_\phi \frac{\partial \phi}{\partial x})\} \tag{11}$$

Introduction of a non-dimensional stream function $\omega(\equiv\psi/\psi_E)$* as the independent variable gives the general form of the governing equations as:

$$\frac{\partial \phi}{\partial x} = \frac{\partial}{\partial \omega} (c \frac{\partial \phi}{\partial \omega}) + d + e \tag{12}$$

where c is now defined as:

$$c \equiv \frac{\Gamma_\phi}{\psi_E} \tag{13}$$

and the definitions of d and e are as before.

2.4 Upstream Conditions

Integration proceeds from left to right on Fig. 1. The upstream conditions, therefore, are prescribed in the form of values of the dependent variables along the radius at x = 0. The velocities of the incoming air and fuel streams (Fig.1) are uniform and constant, and equal to V_{ao} and V_{fo} respectively. The size of he fuel jet is determined by the overall equivalence ratio ϕ.

*ψ_E refers to the value of the stream function ψ at the duct wall which forms the E (external or outer) boundary of the calculation domain. The value of ψ at the axis of symmetry which forms the I (internal or inner) boundary is set to zero by definition.

2.5 Boundary Conditions

The duct is made of three distinct sections. The radius of the wall at each section is described by an equation of the form:

$$R_{wi} = A_i + B_i (x-x_i) + C_i (x-x_i)^2 \quad (i = 1,2,3) \tag{14}$$

The wall temperatures are prescribed for each section of the duct by an equation of the form:

$$T_{wi} = D_i + E_i (x-x_i) + F_i (x-x_i)^2 \quad (i = 1,2,3) \tag{15}$$

The other boundary is provided by the symmetry axis, through which there is no flux of any quantity at all.

2.6 Downstream Conditions

The downstream condition is assumed to be that of zero gradient at the duct exit for all the dependent variables: i.e.,

$$\frac{\partial \phi}{\partial x} = 0 \text{ at the exit,} \tag{16}$$

where $\phi \equiv$ any dependent variable.

2.7 Auxiliary Relations

In this section some auxiliary relations, and the assumptions associated with their use, are introduced. These relations are used for the calculation of fluxes and certain properties.

2.7.1 Flux laws

Implicit in the differential equations given in Section 2.3 are the flux laws for the transport of momentum, mass and heat. These laws will now be summarised, for laminar and turbulent flows.

(a) Laminar transport properties:

(i) Viscosity: Newton's law of viscosity for momentum transfer, relating the shear stress τ to the local velocity gradient, through the laminar viscosity, μ, can be expressed for simple flows as:

$$\tau = \mu(\partial u/\partial y) \tag{17}$$

The evaluation of laminar viscosity for the present problem is now discussed. In general, the gas mixture at any point is composed of unburnt fuel, oxygen, nitrogen, and combustion products. In the calculation of viscosity, the last two are treated as identical in properties. The proportions of the components are supposed to influence the laminar mixture viscosity in proportion to their mass fractions in the local mixture. The viscosity of each of the components is assumed to increase as the one-half power of the absolute temperature. Thus,

$$\mu_j = \mu_{jo}\, T^{\frac{1}{2}}, \; j = \text{fu, ox, products} \tag{18}$$

and $$\mu_{mixture} = \sum_j m_j\, \mu_j, \; j=\text{fu, ox, products} \tag{19}$$

Any other temperature function can be employed, and also any expression connecting the mixture viscosity to the composition and individual species viscosities.

(ii) Diffusion coefficient: Fick's law of diffusion for mass transfer, relating the diffusion mass flux J_j, to the concentration gradient, through the exchange coefficient, Γ_j, has the form:

$$J_j = -\Gamma_j (\partial m_j/\partial y), \text{ for the species } j \qquad (20)$$

The diffusion coefficient Γ_j is obtained from the definition of Schmidt number. Thus,

$$\Gamma_j = \mu/Sc_j \qquad (21)$$

It has been assumed in the solution procedure that the Schmidt numbers for fuel and oxygen (and all the other species) are equal to each other, and also uniform throughout the flow field.

(iii) Thermal conductivity: Fourier's law of heat conduction, relating the heat flux Q to the temperature gradient, through the exchange coefficient, $\Gamma_{\tilde{h}}$, can be written as:

$$Q = -\Gamma_{\tilde{h}}\, c(\partial T/\partial y) \qquad (22)$$

where c stands for the constant-pressure specific heat of the local gas mixture.

In the present analysis, $\Gamma_{\tilde{h}}$ is obtained from a knowledge of the mixture viscosity μ and the laminar Prandtl number:

$$\Gamma_{\tilde{h}} = \mu/Pr_{\tilde{h}} \qquad (23)$$

In general, the laminar Prandtl number (or the exchange coefficient $\Gamma_{\tilde{h}}$ itself) can, if desired, be specified as any arbitrary function of temperature and composition; this will make $\Gamma_{\tilde{h}}$ depend upon temperature and composition in a way different from μ.

(b) Turbulent transport properties:

For a realistic modelling of the flow, the effect of turbulence has to be included whenever appropriate. The scope of the present contract does not permit the treatment of turbulence by means of a sophisticated model. Instead a simple zero-equation model of turbulence, which gives a realistic distribution of the effective viscosity with radial distance, is employed.

(i) Viscosity: The turbulent shear stresses are linked to the local velocity gradient through a laminar-like stress-strain law:

$$\tau = \mu_{eff} \left| \frac{\partial u}{\partial y} \right| \qquad (24)$$

The turbulent viscosity μ_{eff} is obtained from an empirical distribution of the turbulent shear stress as a function of the radial distance from the wall. The variation of the non-dimensional viscosity $\mu_{eff}/(\bar{\rho}\bar{u}rS^{\frac{1}{2}})$ with distance from the wall is as shown in Fig. 2. It should be noted that $\mu_{eff}/(\bar{\rho}\bar{u}rS^{\frac{1}{2}})$ increases linearly with distance from the duct wall and attains its maximum value at $y/r = 0.15$ whereafter it is assumed to remain constant at this value across the duct.

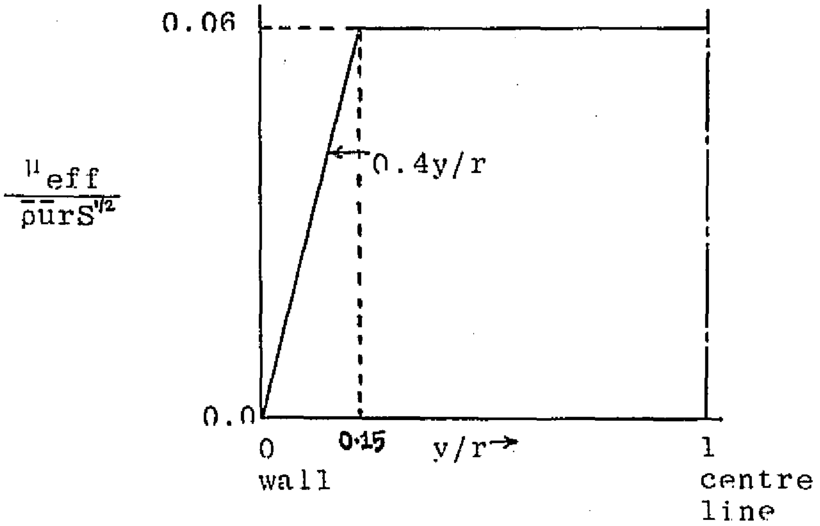

Fig.2. Radial distribution of effective viscosity.

The skin-friction coefficient S is given by:

$$S = 0.0225\ (\bar{\rho}\bar{u}r/\mu_{\ell})^{-\frac{1}{4}} \qquad (25)$$

where μ_{ℓ} is the laminar viscosity.

The flow is approximately one-dimensional except for a small region near the wall extending from $y/r = 0$ to $y/r = 0.15$. This is reflected in Fig. 2 as a constant value of μ_{eff} for the central region of the duct.

(ii) Diffusion coefficient and thermal conductivity:

The effective diffusion coefficients for the transfer of mass and energy are obtained from the definitions of Schmidt and Prandtl numbers respectively.

Thus, for mass transfer, $\Gamma_{eff} = \mu_{eff}/Sc_{eff}$, (26)

and for heat transfer, $\Gamma_{eff} = \mu_{eff}/Pr_{eff}$. (27)

2.7.2 Temperature of the mixture

The temperature of the mixture, T, at a given point in the flow field, is obtained from known local values of the stagnation enthalpy $\tilde{h}$, the velocity u, and the composition of the mixture as follows:

$$\tilde{h} - \tfrac{1}{2}\,u^2 = \sum_{j=1}^{NS} m_j\, h_j \qquad (28)$$

where the species enthalpy h_j is obtained by the method described in Section 5.2 on thermodynamic data.

2.7.3 The ideal-gas equation of state

For a given temperature, the pressure and the density are assumed to be related through the ideal gas-equation

$$p = \frac{\rho RT}{\bar{W}} \tag{29}$$

where $\bar{W}$ the mean molecular weight of the gas mixture is given by

$$\bar{W} = 1/\sum_{j=1}^{NS} (m_j/W_j) \tag{30}$$

2.8 The Chemical-Equilibrium Model

2.8.1 Introduction

The chemistry involved in the hydrocarbon-oxidation process (Sec. 2.2.1) will now be described. The oxidation reaction is assumed to be a single-step one and results in some product species. These species are in chemical equilibrium at the prevailing pressure and enthalpy. Their concentrations are obtained from a model which is based on the minimization of Gibbs free energy. The method has been described by Gordon and McBride (Ref. 2).

2.8.2 Species considered

The equilibrium products of combustion are considered to consist of the following species: CO, CO_2, H_2O, O, OH, H_2, and OH, together with unburnt O_2 and CH_4, and N_2. The last of these is assumed to be inert in the equilibrium reactions*.

*N_2 is of course not inert in the NO_x-formation reactions; but these will be treated separately (Sec.2.9).

2.8.3 Equations of chemical-equilibrium

The chemical-equilibrium equations to obtain the concentrations of the equilibrium-product-species have been discussed in detail in Ref. 2. Here the basis of their derivation will be only briefly described. The condition of chemical equilibrium is the minimization of Gibbs free energy subject to the following constraints: (a) mass balance for the elements present in the system; (b) specified enthalpy; and (c) specified pressure. Since the resulting equations are not all linear, they have to be solved by an iterative procedure. The numerical method of solution of these equations is described in Section 3.5. Here the basic steps for obtaining the chemical-equilibrium composition are considered.

2.8.4 Procedure for obtaining chemical-equilibrium compositions

The basic steps for obtaining the concentrations of the species CO, CO_2, H, H_2, H_2O, O, and OH are:

- The stagnation enthalpy, $\tilde{h}$, the mixture fraction, f, and the mass fraction oi unburnt fuel, m_{fu}, are obtained from the solution of the respective partial differential equations (5, 6, and 4).

- The mass fraction of unburnt oxygen, m_{ox}, is obtained from:

$$m_{ox} = (m_{fu} - \frac{f - f_{st}}{1 - f_{st}})s \qquad (31)$$

  where f_{st} is the stoichiometric value of f. Should the value of m_{ox} be less than zero, during the iterative solution, it is set equal to zero (or a small quantity for programming convenience).

- The mass fraction of the equilibrium-product-species m_{pr}, is given by:

$$m_{pr} = (f - m_{fu})(1 + s) \tag{32}$$

- The mass fraction of nitrogen, m_{N_2}, is given by:

$$m_{N_2} = 1 - m_{fu} - m_{ox} - m_{pr} - \sum_j m_j \tag{33}$$

where the summation is carried out over the species N, NO, NO_2, and N_2O which are determined through rate-controlled reactions.

- The enthalpy of the equilibrium-product-species, h_{pr}, is then:

$$h_{pr} = \{\tilde{h} - \tfrac{1}{2}u^2 - \sum_j h_j m_j\} / m_{pr} \tag{34}$$

where the summation is over all species other than the equilibrium-product-species (CO, CO_2, H, H_2, H_2O, O, and OH).

- For a given value of enthalpy (h_{pr}) and pressure, the equilibrium-product-species concentrations for stoichiometric adiabatic combustion are obtained by means of interpolations using polynomial fits* in accordance with the method described in Section 3.5.4. These concentrations are then multiplied by a factor so that they add to m_{pr}, i.e.

$$m_{CO} + m_{CO_2} + m_H + m_{H_2O} + m_O + m_{OH} = m_{pr} \tag{35}$$

*The determination of the polynomial coefficients is done external and prior to the main computer code.

- At this stage, the mass fractions of all species except the pollutant-species N, NO, NO_2, and N_2O have been determined. Since the latter are present in small amounts, the values of these from the previous iterative sweep are used, and the temperature of the mixture obtained as per Section 3.7.

- The next step is the determination of the mass fractions of the pollutant species N, NO, NO_2, and N_2O. This is considered in the following section.

2.9 Treatment of Chemical-Kinetics

2.9.1 Introduction

Oxides of nitrogen are formed during the course of combustion reactions involving air as oxidant. These species are considered separately from the equilibrium species since their formation is governed by much slower kinetically-controlled reactions. The determination of the concentrations of these pollutant species involves a treatment of chemical-kinetics. This is discussed in the following sub-sections.

2.9.2 Species and reactions

The chemistry involved in the formation of nitrogen oxides will now be described. The model employed incorporates one of the simplest and most widely used mechanisms for calculations involving nitric oxide formation, namely the Zeldovich mechanism:

$$1.\quad N_2 + O \rightleftarrows NO + N \tag{36}$$

$$2.\quad O_2 + N \rightleftarrows NO + O \tag{37}$$

In addition to the above two reactions, the following reactions with the species N_2, O_2, O, H, and OH may be involved in the formation of the oxides of nitrogen, and are considered in the present work:

3. $N + OH \rightleftarrows NO + H$ (38)

4. $H + N_2O \rightleftarrows OH + N_2$ (39)

5. $N_2O + O \rightleftarrows NO + NO$ (40)

6. $N_2O + M \rightleftarrows N_2 + O + M$ (41)

7. $M + N + O \rightleftarrows M + NO$ (42)

8. $NO_2 + O \rightleftarrows NO + O_2$ (43)

9. $NO_2 + M \rightleftarrows O + NO + M$ (44)

The choice of these reactions is based on a study of published literature (e.g. Ref. 5). Although some of these reactions have large rate constants, they usually involve species which are present in very small concentrations; hence their contribution towards the formation of nitric oxide is often small compared to that of reactions (1) and (2). Under fuel-rich conditions, reaction (3) may be significant.

2.9.3 The chemical-kinetics equations

The chemical-kinetics equations have been discussed in detail in Ref. 3. These equations are used to determine the concentrations of the pollutant species. Here the equations will be only briefly described. The conservation equation for species j has been given in Section 2.3 (equation 4). Attention is now centred on the source-term in this equation.

The source S_j of species j is the mass rate of creation of species j by chemical reaction and is given by:

$$S_j = \sum_{j=1}^{M} (\alpha'_{ij} - \alpha''_{ij}) (R_j - R_{-j}) \tag{45}$$ [*]

The forward rate, R_j of reaction j, is given by the Arrhenius expression:

$$R_j = 10^{B_j} \tilde{T}^{N_j} \exp(-T_{actj}/T) (\rho\sigma_m)^{\bar{\alpha}j} \prod_{k=1}^{NS} (\rho\sigma_k)^{(\alpha'_{kj} - \alpha''_{kj})} \tag{46}$$

The backward rate, R_{-j} of reaction j, is given by a similar expression.

In the calculation of rates of production of N, NO, NO_2, and N_2O by means of the above equations, the concentrations of the other species (which have already been determined by a chemical-equilibrium analysis) are assumed to remain unchanged. The justification for this assumption is that these species are mainly produced by reactions which are considerably faster than those involving NO_x production; therefore, the amounts of these species consumed (or produced) by the NO_x - reactions are negligible. The numerical method of solution of the species-conservation equation (4) is presented in Section 3.6.

2.9.4 Procedure for obtaining chemical-kinetics compositions

The steps for obtaining the concentrations of the species N, NO, NO_2, and N_2O, are:

[*] See Nomenclature for explanation of symbols.

- The variables u, $\tilde{h}$, m_{fu}, m_{ox}, and the mass fractions of the chemical-equilibrium products are first obtained (Section 2.8.4).

- The species-conservation equations are solved to obtain the mass fractions of N, NO, NO_2, and N_2O.

- The mass fraction of nitrogen, m_{N_2}, is adjusted so that all the species mass fractions add to unity:

$$m_{N_2} = 1 - \sum_j m_j, \; j = 1,NS \text{ except for } N_2. \qquad (47)$$

2.10 The Influence of Recirculation on Transport Properties

In the diverging section of the duct, there is in reality a zone of recirculation, of extent depending on the angle of divergence. The effect of recirculation is to augment the turbulent transport properties, and to provide additional convective transport. This results in increased heat and mass transfer from the reaction zone to the relatively cold unburnt mixture, thus aiding flame stabilization.

The present solution procedure however, was not designed to handle flow reversals. Therefore the effect of recirculation has to be artificially simulated if the flow is to be correctly modelled. This is done by multiplying the calculated transport coefficient by an arbitrary factor. It is found that a factor of 100 results in the turbulent diffusivities being of the same order of magnitude as in a truly recirculating flow. The resulting flame thickness is also of a magnitude as would be expected under such circumstances (Private communication from A. J. Juhasz, NASA Lewis Research Center, Cleveland, Ohio).

A more satisfactory procedure would be to include a feature permitting the computation of the extent and effects of the recirculation. However, this feature was not called for in the present contract.

3. THE NUMERICAL SOLUTION PROCEDURE

3.1 Introduction

The numerical procedure employed to solve the set of partial differential equations that govern the flow and combustion in the system considered is of the repeated-marching-integration type. If longitudinal diffusion were neglected, downstream effects would not be allowed to propagate upstream, and the solution could be obtained by marching through the integration domain (from the upstream to the downstream end) only once. In this problem, because of the importance of longitudinal diffusion, it is not possible to obtain the solution in one sweep: repeated marching is required, and also two-dimensional storage for the dependent variables $(u, \tilde{h}, m_j)$.

3.2 The Grid and its Numbering

3.2.1 The cross-stream arrangement

The values of the fluid properties are calculated on a grid of which the nodes lie at constant values of the longitudinal distance x and the non-dimensional stream function ω. Fig. 3 shows how the ω coordinate stretches from the value 0 at the I boundary (the symmetry axis) to the value 1 at the E boundary, the wall of the duct. Between ω=0 and ω=1 lie N - 2 "grid points", i.e. arbitrarily chosen locations at which the ϕ values are computed; these are indicated by ●'s along the base of Fig. 3, through which pass vertical full lines. N is the total number of ω nodes, including the boundary values 0 and 1.

Halfway between adjacent pairs of grid points in the range 2 to (N-1) are drawn vertical broken lines, dividing the whole ω range into (N-1) intervals. The value of any dependent variable ϕ is supposed to be uniform within the interval; the fact is illustrated by the step-like

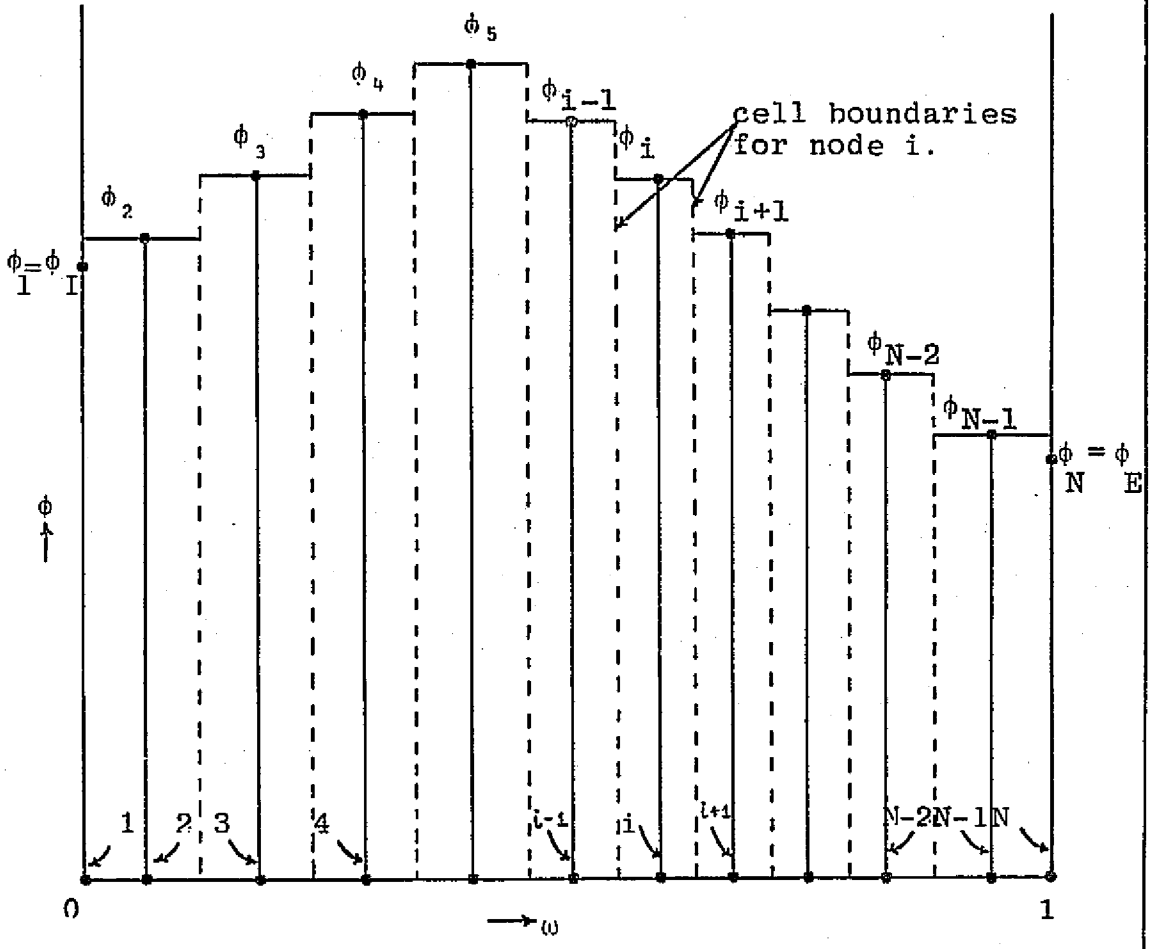

Fig.3. Diagram illustrating, for a fixed x:- the location of grid nodes; the distribution of a variable ϕ; the location of cell boundaries and the numbering system.

ϕ-distribution of Fig. 3; the horizontals stretch from one broken line to the next.

The ϕ's in these intervals are distinguished by subscripts: $\phi_2, \phi_3, \cdot\cdot\phi_{i-1}, \phi_i, \phi_{i+1}\cdot\cdot\cdot\phi_{N-2}, \phi_{N-1}$. The boundary values are ϕ_1 and ϕ_N; and they may also be referred to as ϕ_I and ϕ_E respectively.

3.2.2 The longitudinal dimensions

The grid is a two-dimensional one; thus, corresponding to the ω-array, there is also an x-array. The value of Δx, the increment in x, can be varied at will. As is usual in numerical work, small values of Δx increase accuracy, but also computer time and storage. The right choice always represents a compromise.

3.3 The Finite-Difference Equations

3.3.1 Motive and method

A five-node finite-difference relation will now be derived connecting the value of a dependent variable $\phi_{i,D}$ at a downstream node i, with those of:- (a) its two neighbors at the same x-value, $\phi_{i-1,D}$ and $\phi_{i+1,D}$; (b) its upstream (i.e. previous -x) neighbor $\phi_{i,U}$; and (c) its downstream neighbor $\phi_{i,DD}$. This is to be a linear formula of the form:

$$D_i' \phi_{i,D} = A_i' \phi_{i+1,D} + B_i' \phi_{i-1,D} + E_i' \phi_{i,U} + F_i' \phi_{i,DD} + G_i' \quad (48)$$

where A_i', B_i', etc., will be treated as constants, the expressions for which are derived by integration of the differential equation (12) over a control volume surrounding the node where $\phi_{i,D}$ prevails. There will be an equation like (48) with individual coefficients, for each grid point, other than those on the boundaries, and for each of the dependent variables, u, $\tilde{h}$, m_{fu}, and f.

In equation (48), the ϕ values at the upstream (U) station can be regarded as known. The ϕ values at the DD station are regarded as temporarily known, either from the results of a previous iteration, or from an initial 'guess' or estimate. It is therefore useful to combine the last three terms on the right-hand side into one, thus:

$$C_i' = E_i' \phi_{i,U} + F_i' \phi_{i,DD} + G_i' \tag{49}$$

The result is an equation which focusses all the attention on the unknown ϕ's namely:

$$D_i' \phi_{i,D} = A_i' \phi_{i+1,D} + B_i' \phi_{i-1,D} + C_i' \tag{50}$$

It is now necessary to obtain expressions from which A_i', B_i', C_i' and D_i' can be evaluated, by integrating the differential equation for ϕ over an appropriate control volume.

3.3.2 Integration over a control volume

Now the integration of the differential equation for ϕ, namely equation (12), over a control volume will be considered. Fig. 4 illustrates the control volume and its neighboring one which must be considered. First, some general remarks are made about the locations of the control volume faces. The two control volumes near the boundaries differ from all the others in that, if the lower edge is denoted by $i-\frac{1}{2}$ and the upper by $i+\frac{1}{2}$:

$$\text{for } i = 2 \quad : \quad \omega_{i-\frac{1}{2}} = 0 \tag{51}$$

$$\text{for } i = N-1 \quad : \quad \omega_{i+\frac{1}{2}} = 1 \tag{52}$$

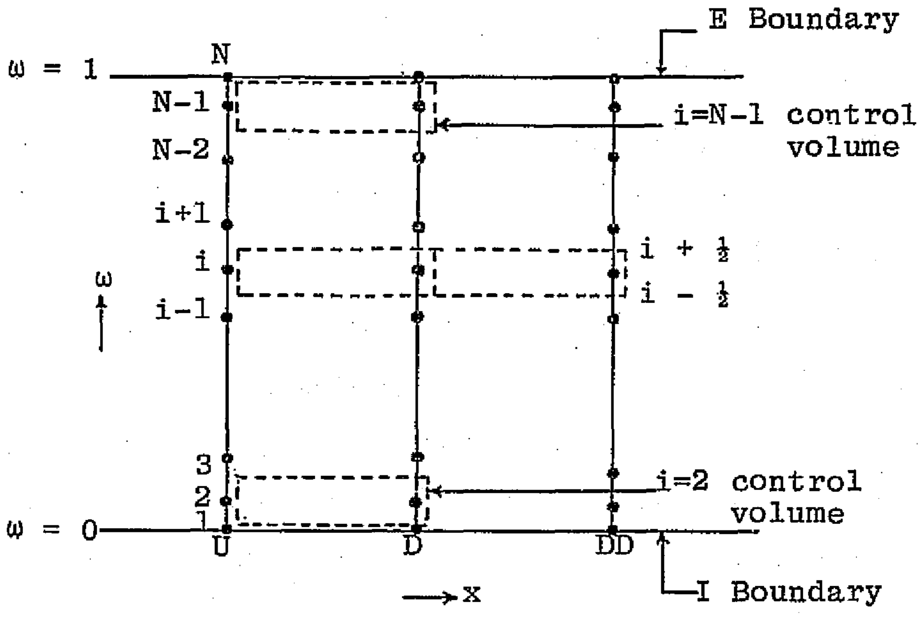

Fig.4. Illustration of a part of the x-ω grid and of control volumes used for the derivations of the finite-difference equations.

whereas for all the other control-volume boundaries the appropriate formulae are:

$$\omega_{i-\frac{1}{2}} = \tfrac{1}{2}\ (\omega_{i-1} + \omega_i) \qquad (53)$$

$$\omega_{i+\frac{1}{2}} = \tfrac{1}{2}\ (\omega_i + \omega_{i+1}) \qquad (54)$$

With these definitions, it follows that the sum of all the control-volume "heights" equals that of the whole grid; thus:

$$\sum_{i=2}^{N-1} (\omega_{i+\frac{1}{2}} - \omega_{i-\frac{1}{2}}) = 1 \qquad (55)$$

Thus, if conservation is satisfied for each of the individual control volumes, it will surely also be satisfied for the flow domain.

For an individual control volume, integration of equation (12) yields, with subscripts U, D and M standing for "upstream", "downstream", and "intermediate":

$$\frac{1}{\delta x} \int_{i-\frac{1}{2}}^{i+\frac{1}{2}} (\phi_D - \phi_U)\ d\omega \qquad \text{Term (i)},$$

$$= \{(c\frac{\partial\phi}{\partial\omega})_{i+\frac{1}{2}} - (c\frac{\partial\phi}{\partial\omega})_{i-\frac{1}{2}}\}_M \qquad \text{Term (ii)},$$

$$+ \{\int_{i-\frac{1}{2}}^{i+\frac{1}{2}} d.d\omega\}_M \qquad \text{Term (iii)},$$

$$+ \{ \int_{i-\frac{1}{2}}^{i+\frac{1}{2}} e.d\omega \}_M \qquad \text{Term (iv).} \qquad (56)$$

It is now necessary to employ the ϕ - profile assumption of Fig. 3 and to introduce further assumptions permitting evaluation of the gradients and other terms in equation (56) so as to arrive at expressions for A', B', C', and D' of equation (50).

(a) The x-direction convection flux, term (i)

Evaluation of term (i) in equation (56) is perfectly straightforward; the profile assumption implies:

$$(i) \quad \equiv \quad \left(\frac{\phi_{i,D} - \phi_{i,U}}{\delta x}\right)(\omega_{i+\frac{1}{2}} - \omega_{i-\frac{1}{2}}) \qquad (57)$$

(b) The ω-direction diffusion flux, term (ii)

The diffusive term (ii) in equation (56) can first be rewritten with the aid of the definition of c, equation (13). There results:

$$\left(c\frac{\partial\phi}{\partial\omega}\right)_{i+\frac{1}{2}} \quad = \quad \frac{1}{\psi_E}\left(r\Gamma_\phi \frac{\partial\phi}{\partial r}\right)_{i+\frac{1}{2},D} \qquad (58)$$

and

$$\left(c\frac{\partial\phi}{\partial\omega}\right)_{i-\frac{1}{2}} \quad = \quad \frac{1}{\psi_E}\left(r\Gamma_\phi \frac{\partial\phi}{\partial r}\right)_{i-\frac{1}{2},D} \qquad (59)$$

where the following relations between ω and r have been used:

$$\delta\omega \;=\; r\rho u\delta r \;/\psi_E \tag{60}$$

and

$$\frac{\partial}{\partial r} \;\equiv\; \frac{r\rho u}{\psi_E}\;\frac{\partial}{\partial\omega} \tag{61}$$

At this point, some simple presumtions are introduced about the values of ϕ, and of the ϕ gradients, at the control volume boundaries. These are:

$$\phi_{i+\frac{1}{2},D} = \tfrac{1}{2}\,(\phi_i + \phi_{i+1})_D \tag{62}$$

$$\left(\frac{\partial\phi}{\partial r}\right)_{i+\frac{1}{2},D} \;=\; \frac{(\phi_{i+1} - \phi_i)_D}{(r_{i+1} - r_i)_U} \tag{63}$$

with similar expressions for the $(i-\frac{1}{2})$ location*.

Then term (ii) becomes:

$$(ii) \;\equiv\; \{T_{i+\frac{1}{2}}\,(\phi_{i+1} - \phi_i)_D - T_{i-\frac{1}{2}}(\phi_i - \phi_{i-1})_D\} \tag{64}$$

Here the definitions have been introduced*:

$$T_{i+\frac{1}{2}} \;\equiv\; (r\Gamma_\phi)_{i+\frac{1}{2}} \;/\; (r_{i+1} - r_i)_U \tag{65}$$

*Modifications will be needed for the cell boundaries at ω=o and at ω=1 (Section 3.3.5).

and

$$T_{i-\frac{1}{2}} \equiv (r\Gamma_{\phi})_{i-\frac{1}{2}} \;/\; (r_i - r_{i-1})_U \qquad (66)$$

(c) The source of ϕ, term (iii)

Term (iii) in equation (56) represents the effect of sources of ϕ within the control volume, per unit increment of x. In conformity with the foregoing preference for downstream values, d_M will be taken as a function of $\phi_{i,D}$; moreover, although sources are non-linear functions of ϕ in general, a linear form will be adopted, by way of the definition:

$$\text{(iii)} \equiv d_{i,D}(\omega_{i+\frac{1}{2}} - \omega_{i-\frac{1}{2}}) = S_i + S_i' \phi_{i,D} \qquad (67)$$

Obviously, S_i and S_i' must be chosen so that as the step shortens and $\phi_{i,D}$ tends to $\phi_{i,U}$ the known upstream source term is recovered;

thus:

$$S_i + S_i' \phi_{i,U} = d_{i,U} (\omega_{i+\frac{1}{2}} - \omega_{i-\frac{1}{2}}) \qquad (68)$$

Otherwise S_i and S_i' are chosen so as to promote physical realism.

(d) The x-direction diffusive flux, term (iv)

The x-direction diffusive term (iv) in equation (56) can be written as:

$$(iv) \equiv \frac{1}{\rho u} \int_{i-\frac{1}{2}}^{i+\frac{1}{2}} \frac{\partial}{\partial x} \left(\Gamma_{\phi} \frac{\partial \phi}{\partial x}\right) d\omega$$

$$= (\omega_{i+\frac{1}{2}} - \omega_{i-\frac{1}{2}}) \left\{\frac{\phi_{i,DD} - \phi_{i,D}}{x_{DD} - x_{D}} \Gamma_{\phi,D}\right.$$

$$\left. - \frac{\phi_{i,D} - \phi_{i,U}}{x_{D} - x_{U}} \Gamma_{\phi,U} \right\} \frac{1}{\rho u \delta x}$$

$$= (\omega_{i+\frac{1}{2}} - \omega_{i-\frac{1}{2}}) \left\{\Gamma_{\phi,D}\left(\frac{\phi_{i,DD}}{x_{DD} - x_{D}}\right) + \Gamma_{\phi,U}\left(\frac{\phi_{i,U}}{x_{D} - x_{U}}\right)\right\} \frac{1}{\rho u \delta x}$$

$$- \phi_{i,D} \left\{(\omega_{i+\frac{1}{2}} - \omega_{i-\frac{1}{2}}) \frac{\Gamma_{\phi,D}}{x_{DD} - x_{D}} + \frac{\Gamma_{\phi,U}}{x_{D} - x_{U}}\right\} \frac{1}{\rho u \delta x} \qquad (69)$$

Thus the axial diffusion term may be written as an appropriately linearised source term $S_i + S_i' \phi_{i,D}$, where:

$$S_i \equiv \frac{(\omega_{i+\frac{1}{2}} - \omega_{i-\frac{1}{2}})}{\rho u \delta x} \left\{\frac{\phi_{i,DD}}{x_{DD} - x_{D}} \Gamma_{\phi,D} + \frac{\phi_{i,U}}{x_{D} - x_{U}} \Gamma_{\phi,U}\right\} \qquad (70)$$

$$S_i' \equiv - \frac{(\omega_{i+\frac{1}{2}} - \omega_{i-\frac{1}{2}})}{\rho u \delta x} \left\{\frac{\Gamma_{\phi,D}}{x_{DD} - x_{D}} + \frac{\Gamma_{\phi,U}}{x_{D} - x_{U}}\right\} \qquad (71)$$

Therefore the linearised parts S_i and S_i' will include the contributions given by equations (70) and (71) respectively, in addition to the usual source term given by equation (68).

3.3.3 The finite-difference equation

It is now possible to derive from the expressions for terms (i) to (iv) a set of definitions of terms A'_i, B'_i, C'_i, and D'_i, of the finite-difference equation (50). They are:

$$A'_i = T_{i+\frac{1}{2}} \tag{72}$$

$$B'_i = T_{i-\frac{1}{2}} \tag{73}$$

$$C'_i = \psi_E(\omega_{i+\frac{1}{2}} - \omega_{i-\frac{1}{2}})\ \phi_{i,U}/\delta x + S_i \tag{74}$$

$$D'_i = A'_i + B'_i + \psi_E(\omega_{i+\frac{1}{2}} - \omega_{i-\frac{1}{2}})/\delta x - S'_i \tag{75}$$

These coefficients can be evaluated from quantities which are known at the upstream station, and from the quantities $\phi_{i,DD}$ which are as yet unknown. For this reason the technique of repeated marching or successive sweeps described in the next section is used.

3.3.4 The technique of repeated marching

The term S_i of equation (74) involves the values of ϕ at a section downstream of the D section, i.e. $\phi_{i,DD}$. For the purpose of solving equation (50) these ϕ values are regarded as temporarily known, either from the results of a previous iteration, or from an initial 'guess'. For this reason, the solution procedure requires several integration sweeps to obtain a converged solution; at each sweep, the values of $\phi_{i,DD}$ from the previous sweep are used. Finally, when the changes in the values of the dependent variables from one sweep to the next one are within a specified tolerance limit, the solution is assumed to have converged.

3.3.5 Special feature relating to transfer across the E and I boundaries

There is a special feature about the diffusive transfer across control-volume sides which lie along the E and I boundaries. (Fig. 4). This is that the terms T_i in equations (72) and (73) must be given a special definition to account for the facts that:

- at the symmetry (I) boundary, the ϕ-gradients are zero;
- at the wall (E) boundary, sharp variations of transport properties may render equations (65) and (66) inaccurate, unless special care is taken to insert an appropriate Γ_ϕ;
- special effects, such as kinetic heating or chemical reaction, sometimes make the diffusive flux proportional not to $\phi_{NM_1} - \phi_N$, but to some other difference.

To account for these, the following definitions are adopted:

$$\text{at } I = NM_1 : T_{i+\frac{1}{2}} \equiv T_E \equiv (rJ_\phi)_E/(\phi_{NM_1} + \delta\phi_E - \phi_N) \qquad (76)$$

where $J_\phi \equiv$ diffusive flux of ϕ.

The T's and $\delta\phi$'s are set equal to zero at the axis of symmetry (I=2).

The expression for T_E has been derived in Ref. 1. (Chapter 6) and is not reproduced here.

3.4 Solution of the Finite-Difference Equations

The equations which have to be solved for the unknown ϕ's (i.e. equation (50)) are of a form which enables the solution to be obtained using the well-known tri-diagonal matrix algorithm (TDMA). Details of this method may be found, for example in Ref. 1.

3.5 Solution of the Chemical-Equilibrium Equations

3.5.1 Solution procedure

The chemical-equilibrium equations were discussed in Section 2.8. They are solved by the procedure given in Ref. 2. The salient features of this technique are described next.

The Newton-Raphson iteration method is used to solve the equilibrium equations. The correction variables are (NLM + 2) in number, where NLM is the number of distinct elements in the system being considered (there are three in the present case, i.e. C, O, and H). The corresponding correction equations are obtained after appropriate linearization as follows.

(a) The correction equations for the conservation of elements are expressed in terms of the non-dimensionalized Lagrange multipliers, π_i as:

$$\sum_{i=1}^{NLM} \left(\sum_{k=1}^{NSE} a^L_{ik}\, a^L_{jk}\sigma_k \right) \pi_i + \left(\sum_{k=1}^{NSE} a^L_{jk}\sigma_k \right) \Delta\log\sigma_m$$

$$+ \left\{ \sum_{k=1}^{NSE} a^L_{jk}\sigma_k \left(\frac{h_k}{RT}\right) \right\} \Delta\log T = \sum_{k=1}^{NSE} a^L_{jk}\sigma_k \left(\frac{g_k}{RT}\right), j=1,NLM \qquad (77)$$

(b) The correction equation for the reciprocal of the mixture molecular weight, σ_m is:

$$\sum_{i=1}^{NLM} \{ \sum_{k=1}^{NSE} a_{ik}^{L} \sigma_k \} \pi_i + \{ \sum_{k=1}^{NSE} \sigma_k - \sigma_m \} \Delta \log \sigma_m$$

$$+ \{ \sum_{k=1}^{NSE} \sigma_k (\frac{h_k}{RT}) \} \Delta \log T = \sigma_m - \sum_{k=1}^{NSE} \sigma_k + \sum_{k=1}^{NSE} \sigma_k (\frac{g_k}{RT}) \qquad (78)$$

(c) The correction equation for temperature is based on an enthalpy balance condition (i.e., enthalpy of the products is specified) and is:

$$\sum_{i=1}^{NLM} \{ \sum_{k=1}^{NSE} a_{ik}^{L} \sigma_k (\frac{h_k}{RT}) \} \pi_i + \{ \sum_{k=1}^{NSE} \sigma_k (\frac{h_k}{RT}) \} \Delta \log \sigma_m$$

$$+ \{ \sum_{k=1}^{NSE} \sigma_k (\frac{C_{pk}}{R}) + \sum_{k=1}^{NSE} \sigma_k (\frac{h_k}{RT})^2 \} \Delta \log T$$

$$= \frac{h_{pr}}{RT} - \sum_{k=1}^{NSE} \sigma_k (\frac{h_k}{RT}) + \sum_{k=1}^{NSE} \sigma_k (\frac{h_k}{RT}) (\frac{g_k}{RT}) \qquad (79)$$

where h_{pr} is the enthalpy (sensible & chemical) of the equilibrium-products and is obtained from equation (34).

The correction equations (77), (78), (79) involve the unknowns π_i (i=1, NLM), $\Delta \log \sigma_m$, and $\Delta \log T$. They are solved by a standard Gaussian elimination procedure. The correction matrix will become singular at the solution point when the coefficient of $\Delta \log \sigma_m$ in equation (78) is identically zero. This potential singularity is avoided by a single interchange between the row involving the zero coefficient of $\Delta \log \sigma_m$ and any other row (in practice, the row with the largest coefficient of $\Delta\log\sigma_m$ is selccted). All other diagonal elements are positive and do not require special treatment.

The new values of the variables are then obtained as:

$$\Delta\log\sigma_k = (\frac{h_k}{RT}) \quad \Delta\log T - (\frac{g_k}{RT}) + \Delta\log\sigma_m + \sum_{i=1}^{NLM} a^L_{ik} \quad \pi_i, k=1,NSE \tag{80}$$

$$\log\sigma_i^{(k+1)} = \log\sigma_i^{(k)} + \eta(\Delta\log\sigma_i)^{(k)}, \ i=1, NSE \tag{81}$$

$$\log\sigma_m^{(k+1)} = \log\sigma_m^{(k)} + \eta(\Delta\log\sigma_m)^{(k)} \tag{82}$$

$$\log T^{(k+1)} = \log T^{(k)} + \eta(\Delta\log T)^{(k)} \tag{83}$$

where the superscripts indicate the iteration number, and η is an under-relaxation parameter ($0<\eta\leqslant1$). The determination of η and the convergence criterion are discussed in Section 3.5.3.

3.5.2 Initial estimate of species mole-numbers and temperature

The initial estimate of the species mole-numbers is based on complete stoichiometric combustion. Thus if x and y are the number of kg-atoms of carbon and hydrogen respectively, per kg of mixture, the initial estimate is given by:

$$\sigma_{CO_2} = x \tag{84}$$

$$\sigma_{H_2O} = y/2 \tag{85}$$

All other mole numbers are set equal to a small number 10^{-6}.

The initial estimate for temperature is obtained from an adiabatic enthalpy balance for the assumed composition and the given mixture enthalpy. The procedure is the same as that described in Section 3.7.

3.5.3 Under-relaxation and convergence criterion

The self-adjusting under-relaxation parameter η similar to that of Ref. 2 is used here. This parameter is determined at each iteration from:

$$\eta = \text{minimum of } (1, \eta_1, \eta_2) \qquad (86)$$

where η_1 and η_2 are quantities which are defined below.

(a) For T, σ_m, and species with $(\sigma_i/\sigma_m) > 10^{-8}$ and $\Delta\log\sigma_i > 0$, η_1 is defined as:

$$\eta_1 \equiv \frac{0.2}{\max\left(|\Delta\log T|, |\Delta\log\sigma_m|, |\Delta\log\sigma_i|\right)} \qquad (87)$$

This causes the correction of the variables T, σ_m, and σ_i to be scaled so that none of the variables is increased by more than a factor of 1.22 (=exp(0.2)) on any one iteration. This is different from the definition of η_1 in Ref 2, which permits maximum increases by a factor of upto 7.39 (=exp(2)) on any one iteration.

(b) For species with $(\sigma_i/\sigma_m) < 10^{-8}$ and $\Delta\log\sigma_i > 0$, η_2 is defined as:

$$\eta_2 \equiv \left| \frac{\log(10^{-4}) - \log(\sigma_i/\sigma_m)}{\Delta\log\sigma_i - \Delta\log\sigma_m} \right| \quad (88)$$

This scales all the corrections so that the species with σ_i initially less than 10^{-8} increase to no more than 10^{-4}.

A convergence criterion similar to that recommended in Ref.2 is used. This is:

$$\left(\frac{\sigma_i}{\sigma_m}\right) \left| \Delta\log\sigma_i \right| \leqslant 1.0\text{x}10^{-10}, \; i=1,\text{NSE} \quad (89)$$

and

$$\left|\Delta\log\sigma_m \right| \leqslant 1.0\text{x}10^{-10} \quad (90)$$

3.5.4 Polynomial fits for equilibrium-product-species concentrations

The equilibrium compositions are represented in terms of polynomials of enthalpy at different pressures. The polynomial coefficients are determined in computations external and prior to the main computer code. The steps for obtaining these polynomials are now described.

The equilibrium compositions are computed by the method of Section 3.5.1 for several values of enthalpy at different pressures. At each pressure, the logarithm of the equilibrium-species mass fraction is represented as a polynomial of enthalpy. There are two distinct polynomials (one over each of two ranges of enthalpy), both of third order, for each of the species and for each pressure considered. The logarithm of the species mass fraction is used since the variation in mass fraction over the enthalpy range is a few orders of magnitude (for species like O, H, OH etc.). In the main code, when the equilibrium composition is required for a particular enthalpy and pressure, the polynomials are used to calculate the species mass fractions at the given enthalpy and two successive pressures P_1 and P_2 adjoining the given pressure P (i.e. $P_1<P<P_2$). The mass fractions at the pressures P_1 and P_2 are then interpolated to give the values at pressure P.

3.6 Solution of the Chemical-Kinetics Equations

3.6.1 Solution procedure

The chemical-kinetics equations were discussed in Section 2.9. They are solved by the procedure described in Ref.3; it will be only briefly described here.

The procedure involves a point-by-point simultaneous solution of all the pollutant concentrations (i.e. N, NO, NO_2, and N_2O). The line-by-line procedure which is used to solve for other dependent variables (u, $\tilde{h}$, f, and m_{fu}) is not suitable for the solution of the chemical-kinetics equations. The reason is that the concentration of any pollutant species at a point depends more strongly on the concentrations of the other pollutant species at the same point rather than its own concentration at neighboring points. The line-by-line procedure would, under such conditions, require an excessively large number of iterations to achieve convergence (e.g. Ref. 4).

The Newton-Raphson method is used to solve the chemical-kinetics equations. The correction equations for the species mole numbers are expressed, after appropriate linearization as:

$$\sum_{k=1}^{NSK} \{A_p \sigma_i \delta_{ik} + \sum_{j=1}^{M} (\alpha'_{ij} - \alpha''_{ij})(R_j \, \alpha'_{kj} - R_{-j} \, \alpha''_{kj}) \, \Delta\log\sigma_k\}$$

$$= A_p(\sigma_i{*}-\sigma_i) - \sum_{j=1}^{M}(\alpha'_{ij}-\alpha''_{ij}) \, (R_j-R_{-j}), \; i=1, \, NSK \qquad (91)$$

Equations (91) involve the unknowns $\Delta\log\sigma_k$ (k=1,NSK). The equations are solved by a standard Gaussian elimination procedure. All the diagonal elements of the correction matrix are positive, so that no matrix conditioning is necessary.

The new values of the variables are then obtained as:

$$\log\sigma_i^{\;(k+1)} = \log\sigma_i^{(k)} + \eta(\Delta\log\sigma_i)^{(k)}, \; i=1,NSK \qquad (92)$$

where the superscripts indicate the iteration number and η is an under-relaxation parameter ($0<\eta\leqslant 1$). The determination of η, and the convergence criterion, are discussed below.

3.6.2 <u>Initial estimate of the mole numbers of pollutant species</u>

The initial estimate is obtained by setting the concentrations of the pollutant species at any grid node equal to those at the corresponding upstream node. For the very first set of cross-stream points, the initial estimates of the concentrations are set to a small number, 10^{-15} to 10^{-20}. This procedure is followed when sweeping through the integration domain for the first time. For subsequent sweeps, the values at the particular grid node from the previous sweep are used as the initial estimates for the solution of the correction equations (91).

3.6.3 Under-relaxation and convergence criterion

The self-adjusting under-relaxation parameter of Ref. 2 is used without modification (see also Section 3.5.3). The solution at any grid node is assumed to have converged when the concentrations of the NO_x-species remain within a certain value from one iteration to the next.

3.7 Solution of the Auxiliary Equations

The auxiliary equations were discussed in Section 2.7. Of these only the equations dealing with the temperature of the mixture require an iterative solution procedure; the other equations involve straightforward algebraic expressions.

The temperature equation (28) is solved by the Newton-Raphson iteration method. The Newton-Raphson correction equation for temperature is:

$$h - \sum_{j=1}^{NS} m_j h_j \; (T_k) = \left(\sum_{j=1}^{NS} C_{pj} \; (T_k) \; m_j \right) \Delta T_k \qquad (93)$$

$$T_{k+1} = T_k + \Delta T_k \qquad (94)$$

where T_k ≡ the temperature at the k^{th} iteration

$h_j(T_k)$ ≡ the enthalpy of species j at temperature T_k

$C_{pj}(T_k)$ ≡ the constant pressure specific heat of species j at temperature T_k (see Section 5.2).

Convergence is monitored by computing $|\Delta T_k/T_{k+1}|$ at each iteration; and, when its value falls below a prespecified limit, the iteration is terminated.

4. FURTHER FEATURES OF THE CALCULATION PROCEDURE

4.1 The Treatment of the Wall Boundary

The treatment of wall boundaries has been discussed in Ref. 1, to which the reader is referred for details. The essential features may be summed up as:

(a) Near the wall, the relation between ρu and ω is not linear as in other regions of the flow field; this is accounted for by modifying the $\rho u \sim \omega$ relation for the near-wall region.

(b) Steep variations in transport properties occur in the near-wall region; this is accounted for by using appropriate values of the Γ_ϕ's in this region.

4.2 The Calculation of Pressure Gradient

4.2.1 The problem

In order to solve the x-direction momentum equation, values must be ascribed to the pressure gradient, dp/dx. The pressure gradient must be such as to make the flow fit the cross-sectional area of the duct at the given downstream section. The procedure involves making an informed guess of the pressure gradient followed by a comparison of the downstream area of the calculated flow with that available in the duct. A correction is then made to the velocity which diminishes the discrepancy of the areas.

4.2.2 The solution adopted

The cross-stream area A_{12}, of the flow bounded by the streamlines ψ_1 and ψ_2, is given by:

$$A_{12} = {}_1\int^2 (\rho u)^{-1} d\psi \qquad (95)$$

Therefore, if the sensitivity of this area to pressure is to be determined, the right-hand side requires to be differentiated with respect to pressure. Thus:

$$\frac{dA_{12}}{dp} = \int_{1}^{2} - (\rho u)^{-2}(\rho\frac{du}{dp} + u\frac{d\rho}{dp}) \quad d\psi \qquad (96)$$

Now the variation of u with p can be estimated by noting that, if the shear stresses are supposed to be uninfluenced by the pressure change, the x-direction momentum equation (3) leads to:

$$\frac{du}{dp} = -\frac{1}{\rho u} \qquad (97)$$

This equation can now be substituted into equation (96), together with introduction of the gas-law relation for isentropic compression:

$$\frac{d\rho}{dp} = \frac{1}{\gamma} \frac{\rho}{p} = \frac{M^2}{u^2} \qquad (98)$$

in which M stands for the Mach number.
The result is:

$$\frac{dA_{12}}{dp} = \int_{1}^{2} \frac{1}{\rho^2 u^3} (1-M^2) \ d\psi \qquad (99)$$

This relation is employed, first to calculate the pressure gradient needed at the beginning of a forward step and second, to provide a pressure adjustment at the end of the step so as to ensure a close fit of the flow area to the actual duct area.

4.2.3 Fine adjustments of the pressure gradient

Fine adjustments of the pressure gradient are required to avoid the calculation of negative velocities when a large adverse pressure gradient is estimated.

This is achieved if the pressure gradient is adjusted to be no greater than $(\alpha\rho u^2_{min})/\Delta x$, where $\alpha \leqslant 0.5$ and u_{min} is the minimum u-velocity at the cross-stream plane upstream of that under consideration.

Similarly, during the adjustment of pressure and velocity to match the flow area with the duct area, the adjustment is made in steps so that at no step is the change in pressure greater than $(\beta\rho u^2_{min})$ where $\beta \leqslant 0.5$.

4.3 The Calculation of Radii

4.3.1 Formula for r

From the definition of ω as:

$$\omega \equiv \psi/\psi_E \tag{100}$$

the following relation is obtained:

$$\omega = \int_o^r r\rho u dr / \int_o^{r_E} r\rho u dr \tag{101}$$

$$\text{and} \quad \int_o^r r dr = \psi_E \int_o^\omega \frac{1}{\rho u} d\omega \tag{102}$$

A quantity I is now defined as:

$$I \equiv \psi_E \int_o^\omega \frac{1}{\rho u} d\omega \tag{103}$$

therefore, $$\frac{r^2}{2} = I \qquad (104)$$

i.e. $$r = (2I)^{\frac{1}{2}} \qquad (105)$$

which gives an expression for the radius. The integral I has to be evaluated in terms of the grid-point values of ρ, u, and ω. This will now be considered for two regions.

4.3.2 Evaluations of I for central regions of the grid

For $2 \leqslant i \leqslant N-2$,

$$\frac{I_{i+1} - I_i}{\psi_E} \equiv \int_{\omega_i}^{\omega_{i+1}} (\rho u)^{-1} d\omega$$

$$= \tfrac{1}{2} \; (\omega_{i+1} - \omega_i) \; \left\{ \frac{1}{(\rho u)_i} + \frac{1}{(\rho u)_{i+1}} \right\} \qquad (106)$$

Equation (106) permits the evaluation of $r_{i+1}-r_i$. Thus the radii may all be calculated once r_2 is known. This will be discussed next, along with the modification necessary in the evaluation of $r_N-r_{NM_1}$.

4.3.3 Distance evaluations for edge regions

r_2 is computed according to the following relation:

$$r_2 = \psi_E \; \omega_2/(\tfrac{1}{2}\{(\rho u)_1 + (\rho u)_2\}) \qquad (107)$$

r_N is obtained from:

$$r_N - r_{NM_1} = \psi_E \; (1-\omega_{NM_1})/(B_{pE}(\rho u)_{NM_1}) \qquad (108)$$

where B_{pE} is evaluated from the stream-function coefficient. For details of the above two equations, the reader is advised to refer to Ref. 1 (Chapter 7).

4.4. The Longitudinal Tri-Diagonal Matrix Algorithm (LTDMA)

4.4.1 Definition and Capability

The LTDMA is an implicit numerical procedure which determines dependent variable values for all nodes at a longitudinal station at a time by solving a set of tri-diagonal equations for each station at each iteration step. The LTDMA overcomes the drawbacks of standard iteration procedures which involve using initial values (or values from the previous iteration) of dependent variables at the transverse section downstream of the section currently being solved for; this restricts the propagation of downstream influences in the upstream direction to only one finite-difference cell for every iterative sweep. Thus with a fine grid it will require a very large number of iterations for downstream effects to propagate upstream and convergence rates will be slow.

4.4.2 Function of the LTDMA

The function of the LTDMA is the adjustment of the average ϕ at each longitudinal (x-) section. This adjustment is done between each forward step, by solution of an equation of the form:

$$d'_j \, \phi'_j = a'_j \, \phi'_{j+1} + b'_j \, \phi'_{j-1} + c'_j \qquad (109)$$

where ϕ'_j is the said adjustment, and j denotes the x-station. The adjustment ϕ'_j is to be added to every ϕ at the x-station.

4.4.3 Derivation of the coefficients a', b', c', and d'

These coefficients are derived in terms of the finite-difference coefficients which are being computed during the course of the normal solution procedure; additional computation is thus minimized.

Let Φ denote the finite-difference solution before application of the LTDMA, and ϕ that after its application. Then,

$$\phi \equiv \Phi + \phi' \qquad (110)$$

The equation satisfied by Φ is of the form:

$$D'_{ij}\,\Phi_{ij} = A'_{ij}\,\Phi_{i+1,j} + B'_{ij}\,\Phi_{i-1,j} + E'_{ij}\,\Phi_{i,j-1}$$

$$+ F'_{ij}\,\Phi^{o}_{i,j+1} + G'_{ij} \qquad (111)^{*}$$

where the subscript i refers to the radial direction and j to the longitudinal direction. There is an equation of the above form for each internal node (i,j).

The coefficient G'_{ij} includes the part of the linearised source term S_i <u>without</u> the axial diffusion contribution. The contribution of the axial diffusion to S'_i is included in D'_{ij} as usual.

Coefficients E'_{ij} and F'_{ij} are given by:

$$E'_{ij} = \frac{\psi_{i+\frac{1}{2}} - \psi_{i-\frac{1}{2}}}{\delta x} + \frac{\psi_{i+\frac{1}{2}} - \psi_{i-\frac{1}{2}}}{\rho u \delta x}\;\frac{\Gamma_{\phi i,j-1}}{x_j - x_{j-1}} \qquad (112)$$

$$F'_{ij} = \frac{\psi_{i+\frac{1}{2}} - \psi_{i-\frac{1}{2}}}{\rho u \delta x}\;\frac{\Gamma_{\phi i,j}}{x_{j+1} - x_j} \qquad (113)$$

*The derivation of the finite-difference coefficients A', B', C', and D', has been discussed in Section 3.3. These coefficients are stored one-dimensionally as A'_i, B'_i, C'_i, and D'_i but are represented by two subscripts here for the sake of clarity.

The solution ϕ after application of the LTDMA satisfies the equation:

$$D'_{ij}\ \phi_{ij} = A'_{ij}\ \phi_{i+1,j} + B'_{ij}\phi_{i-1,j} + E'_{ij}\ \phi_{i,j-1} + F'_{ij}\phi_{i,j+1} + G'_{ij} \tag{114}$$

at each internal node (i,j).

Summation over cross-stream points leads to:

$$\phi'_j \sum_i (D'_{ij} - A'_{ij} - B'_{ij}) = \phi'_{j+1} (\sum_i F'_{ij}) + \phi'_{j-1}(\sum_i E'_{ij})$$

$$+ \sum_i (G'_{ij} + A'_{ij}\ \Phi_{i+1,j} + B'_{ij}\ \Phi_{i-1,j} + E'_{ij}\ \Phi_{i,j-1} + F'_{ij}\ \Phi_{i,j+1}$$

$$- D'_{ij}\ \Phi_{ij}) \tag{115}$$

$$\text{or,}\quad d'_j\phi'_j = a'_j\phi'_{j+1} + b'_j\phi'_{j-1} + c'_j \tag{116}$$

$$\text{where}\quad d'_j \equiv \sum_i(D'_{ij} - A'_{ij} - B'_{ij}) \tag{117}$$

$$a'_j \equiv \sum_i F'_{ij} \tag{118}$$

$$b'_j \equiv \sum_i E'_{ij} \tag{119}$$

$$c'_j \equiv \sum_i (G'_{ij} + A'_{ij}\Phi_{i+1,j} + B'_{ij}\Phi_{i-1,j} + E'_{ij}\ \Phi_{i,j-1}$$

$$+ F'_{ij}\ \Phi^o_{i,j+1} - D'_{ij}\ \Phi_{ij}) \tag{120}$$

The term c_j' is zero for all j except the ones immediately upstream and downstream of the x-station just solved for (by the transverse TDMA of Section 3.4).

Thus $c_j' \;=\; 0$ (121)

except at sections (j-1) and (j+1) where:

$$c_{j-1}' \;=\; \sum_i F_{ij}' \, (\Phi_{ij} - \Phi_{ij}^{o}) \qquad (122)$$

$$c_{j+1}' \;=\; \sum_i E_{ij}' \, (\Phi_{ij} - \Phi_{ij}^{o}) \qquad (123)$$

Equation (116) is solved by the standard TDMA procedure.

4.5 The Iterative Procedure to Determine Fuel Concentration

In the determination of the mass fraction of unburnt fuel, the source of fuel is appropriately linearised; this is done as follows (Ref. 1, Chapter 8).

The source of fuel is given by:

$$S_{fu} \;=\; Pp2 \;\; m_{fu} \, m_{ox} \, \exp\,(-E/RT) \qquad (124)$$

where the term $m_{fu} \, m_{ox}$ is linearised as:

$$m_{fu} \, m_{ox} \;=\; - \frac{m_{fu,U} \, m_{ox}^{*} \, m_{fu,b}}{m_{fu,U} - m_{fu,b}} \;+\; \frac{m_{fu,U} \, m_{ox}^{*}}{m_{fu,U} - m_{fu,b}} m_{fu,D} \qquad (125)$$

Here the following definitions have been used:

U $\equiv$ refers to upstream values (already solved for);

D $\equiv$ refers to downstream values (currently being solved for).

The mass fraction of fuel $m_{fu,b}$ when combustion is complete (i.e. when either all the oxygen or all the fuel has been consumed) is given by:

$$m_{fu,b} \equiv 0 \quad \text{if } \frac{f_D - f_{st}}{1 - f_{st}} \leq 0 \text{ or if } f_D \leq f_{st} \tag{126}$$

$$\equiv \frac{f_D - f_{st}}{1 - f_{st}} \quad \text{if } \frac{f_D - f_{st}}{1 - f_{st}} > 0 \text{ or if } f_D > f_{st} \tag{127}$$

(Note: The mixture fraction f_D at the downstream station D is known at this stage, since the f-equation is solved before the m_{fu}-equation).

f_{st} = Stoichiometric value of the mixture fraction

The mass fraction of oxygen m^*_{ox} used in equation (125) is given by:

$$m^*_{ox} = (m_{fu,U} - \frac{f_D - f_{st}}{1 - f_{st}})s \tag{128}$$

In the solution procedure, the upstream (U) values are used only when sweeping through the integration domain for the first time; on subsequent sweeps, the values from the previous sweep are used instead.

When large forward-step sizes (Δx) are taken, the use of upstream values will result in a loss of accuracy. As a result, an iterative procedure is adopted. When the downstream value is obtained, it is used to re-calculate the source term;

and a new value is thereby obtained. This iteration is carried out until the calculated values do not differ from one iteration to another within a prespecified tolerance limit. The temperature of the gas mixture is also recomputed at each such iteration, as described in Section 3.7.

4.6 The One-Dimensional Calculation Procedure

4.6.1 Purpose of one-dimensional calculations

The purpose of the one-dimensional calculations is to obtain a good initial estimate of the solution before starting the two-dimensional calculations.

4.6.2 Method

The one-dimensional solution is obtained by an iterative procedure involving applications of the TDMA in the longitudinal direction. Once satisfactory convergence is obtained, the solution is inspected; if it is found plausible, the cross-stream (two-dimensional) effects are introduced. The solution procedure thus achieves rapid convergence.

4.6.3 Finite-difference form of the equations solved

Only two dependent variables are solved for: the stagnation enthalpy $\tilde{h}$, and the mass fraction of unburnt fuel, m_{fu}. The mixture fraction f is constant with respect to the longitudinal distance in a one-dimensional situation.

The finite-difference equation to be solved is:

$$d_j\phi_j = a_j\phi_{j+1} + b_j\phi_{j-1} + c_j \tag{129}$$

where $\phi_j \equiv$ value of dependent variable ($\tilde{h}$ or m_{fu}) at section j. (130)

$$a_j \equiv \frac{\Gamma_{\phi,j} A_j}{\delta x \, (x_{j+1} - x_j)} \quad (131)$$

$$b_j \equiv \frac{\Gamma_{\phi,j-1} A_{j-1}}{\delta x \, (x_j - x_{j-1})} \quad (132)$$

$c_j \equiv$ term involving sources and wall fluxes (after linearization) (133)

$$d_j \equiv a_j + b_j - S_i' \quad (134)$$

$A_j \equiv$ duct area at section j (135)

4.6.4 Upstream conditions

Inlet conditions at j=1 are specified as follows. The mass fraction of unburnt fuel is assigned a value corresponding to the specified overall equivalence ratio, ϕ. Thus at j=1,

$$m_{fu} = \frac{1}{1+s/(0.232\phi)} \quad (136)$$

$$m_{ox} = \frac{s}{\phi} m_{fu} \quad (137)$$

$$m_{N_2} = 1 - m_{fu} - m_{ox} \quad (138)$$

The stagnation enthalpy is assigned a value (at j=1) which is the average of the fuel and air enthalpies at inlet weighted by their respective flow rates.

4.6.5 Boundary conditions

There is no flux of fuel at the wall. For the stagnation enthalpy, the diffusive flux $J_{\tilde{h}}$ to the wall is given by an empirical relation of the form:

$$J_{\tilde{h}_j} = 0.0015\ \bar{\rho}\bar{u}r\ (\tilde{h}_j - \tilde{h}_{wall}) \qquad (139)$$

This is incorporated into the finite-difference equation by augmenting the coefficients c_j and d_j:

$$c_j = c_j + 0.0015\ \bar{\rho}\bar{u}r\ \tilde{h}_{wall} \qquad (140)$$

$$d_j = d_j + 0.0015\ \bar{\rho}\bar{u}r \qquad (141)$$

4.6.6 Downstream conditions

A condition of zero gradient (for both $\tilde{h}$ and m_{fu}) at the exit plane is employed.

4.6.7 Transport properties

Transport properties are evaluated as described in Sections 2.7 and 2.10.

4.6.8 Thermodynamic properties

A simplified treatment of the thermodynamic properties is presented for the one-dimensional calculations.

(a) The specific heat at constant pressure $C_{p,j}$ is represented as a linear function of temperature for each species j; and the mixture specific heat $C_{p,mix}$ is obtained by averaging with respect to the mass fractions of the species.

$$C_{p,mix} = A_{mix} + B_{mix}\,T \qquad (142)$$

$$A_{mix} = \sum_j A_j m_j \qquad (143)$$

$$B_{mix} = \sum_j B_j m_j \qquad (144)$$

$$C_{p,j} = A_j + B_j\,T \qquad (145)$$

(b) For given stagnation enthalpy $\tilde{h}$ and composition, the temperature of the mixture is obtained from:

$$h = \tilde{h} - H_{fu}\,m_{fu} = (A_{mix} + B_{mix}\,T)T \qquad (146)$$

4.6.9 Chemistry

The chemistry is represented by a simple chemical reaction:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \qquad (147)$$

The mass fractions of the species are given by:

$$m_{O_2} = \left(m_{fu} - \frac{f - f_{st}}{1 - f_{st}}\right) s, \text{ or zero if this is negative.} \qquad (148)$$

$$m_{CO_2} = \frac{44}{16}\,(f - m_{fu}) \qquad (149)$$

$$m_{H_2O} = \frac{36}{16}\,(f - m_{fu}) \qquad (150)$$

$$m_{N_2} = 1 - m_{fu} - m_{O_2} - m_{CO_2} - m_{H_2O} \qquad (151)$$

4.6.10 Initial guess

For Section 1 of the duct (Fig. 1), the initial guess corresponds to the unburnt conditions; and, for Section 3, the fully-burnt conditions. For Section 2, an exponential variation is employed.

5. THERMODYNAMIC AND ELEMENT DATA

5.1 Element Data

The following information is required to describe the set of elements which make up the chemical species present in the system:

- the element symbol (e.g. C, O, H, and N);
- the corresponding atomic weight.

5.2 Thermodynamic Data

The thermodynamic data for constant pressure specifc heat, enthalpy, and the entropy at one atmosphere for the chemical species are the same as those used in Ref. 2. These properties are expressed as polynomials in temperature:

$$\frac{C_p}{R} = Z_1 + Z_2T + Z_3T^2 + Z_4T^3 + Z_5T^4 \qquad (152)$$

$$\frac{h}{RT} = Z_1 + \frac{Z_2T}{2} + \frac{Z_3T^2}{3} + \frac{Z_4T^3}{4} + \frac{Z_5T^4}{5} + \frac{Z_6}{T} \qquad (153)$$

$$\frac{s^o}{R} = Z_1\log T + Z_2T + \frac{Z_3T^2}{2} + \frac{Z_4T^3}{3} + \frac{Z_5T^4}{4} + Z_7 \qquad (154)$$

There are thus seven coefficients $Z_1 \ldots . Z_7$ for each one of the chemical species for each one of two temperature ranges, 300^oK to 1000^oK, and 1000^oK to 5000^oK.

The enthalpy equation (153) includes both the sensible enthalpy and the standard-state enthalpy of formation. The entropy s^o includes the low-temperature enthalpy of formation as also the chemical and sensible contributions.

The entropy s at any arbitrary pressure is given by:

$$s = s^o - RT\log (p/P_o) \qquad (155)$$

where P_o = standard atmospheric pressure.

6. KINETICS DATA

The following information is required to specify the chemical kinetics of the system considered:

- the set of elementary reactions making up the assumed chemical-kinetic mechanism;
- the Arrhenius constants for each elementary reaction.

In the present study, only reactions of the following types are considered:

$$A + B \rightarrow C + D \quad , \text{MODE=1} \tag{156}$$

$$AB + M \rightarrow A + B + M \quad , \text{MODE=2} \tag{157}$$

$$A + B + M \rightarrow AB + M \quad , \text{MODE=3} \tag{158}$$

The forward reaction rate constant is expressed as:

$$k_{f_j} = A_j \, T^{B_j} \exp\left(-T_{actj}/T\right), \text{ for reaction } j \tag{159}$$

The Arrhenius constants A_j, B_j, and T_{actj} are supplied for each one of the reactions considered.

The reverse reaction rate constant may either be directly specified as above, or it may be calculated from a knowledge of the forward rate constant and the equilibrium constant:

$$k_{bj} = \frac{k_{fj}}{K_{cj}} \tag{160}$$

7. RESULTS AND DISCUSSIONS

7.1 Introduction

In this Chapter, results are presented for:

(i) one-dimensional calculations;
(ii) grid-dependency tests; and,
(iii) four sample cases, specified by NASA Lewis Research Center.

These are now individually discussed below.

7.2 One-Dimensional Calculations

One-dimensional calculations were carried out in accordance with the method described in Section 4.6. These calculations are useful in obtaining preliminary results and for qualitative comparisons; they also involve considerably less computational times than a full two-dimensional calculation.

The problem-specification for the one-dimensional calculations is as for Test Case 1 (Tables 1, 2, 3, and 4 at the end of this Chapter).

7.2.1 The influence of pre-exponential factor on flame position

The pre-exponential factor of the hydrocarbon oxidation reaction (factor C_1 of equation (2)) was varied to test its influence on the position of the flame in the duct. An approximate value of this factor was first obtained from Spalding's centroid rule based on one-dimensional flame theory (Ref. 6), and it was then varied in the neighborhood of this value.

Figure 5 shows the axial temperature distribution for three different values of this factor. Thus a higher value of the pre-exponential factor causes the flame to move

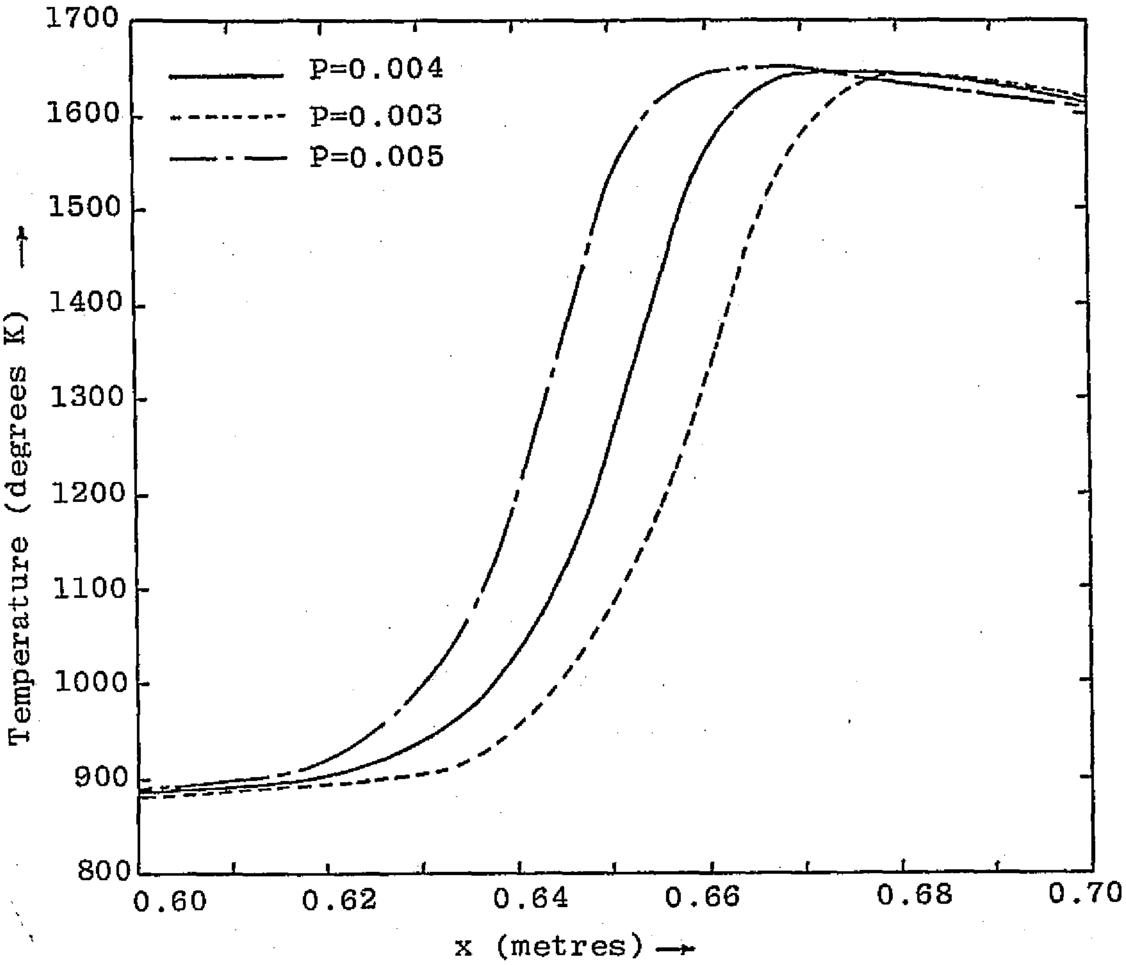

Fig. 5. The dependence of flame position on the preexponential factor P for the hydrocarbon oxidation reaction.

upstream and vice versa. The behaviour is as expected since the onset of chemical reaction is earlier in the duct the higher the value of the pre-exponential factor. A value of 0.003 was chosen for the results described in the following Sections.

7.3 Grid-Dependency Tests

Computations were performed with several different lateral and axial grid distributions to study the grid-dependency of the solution. All these computations were performed for the specifications of Test Case 1 (Tables 1, 2, and 3). Since the main region of interest is the diverging section of the duct wherein the flame exists, the number of longitudinal grid nodes in this section only was varied in these computations. A uniform axial grid distribution in the diverging section was used for all these runs. The lateral grid had five points, non-uniformly distributed.

Figures 6, 7, and 8 show the results of the grid-dependency tests for two-dimensional computations. In Figure 6 are shown the axial temperature distributions along the duct centerline for different numbers of longitudinal grid nodes. Figures 7 and 8 show the influence of changing the number of lateral grid nodes.

The solution is clearly grid-dependent with respect to the axial grid. No general conclusion can be drawn about the influence of the axial grid on the flame position.

The dependence of the solution on the lateral grid is small. This is due to the largely one-dimensional nature of the flow.

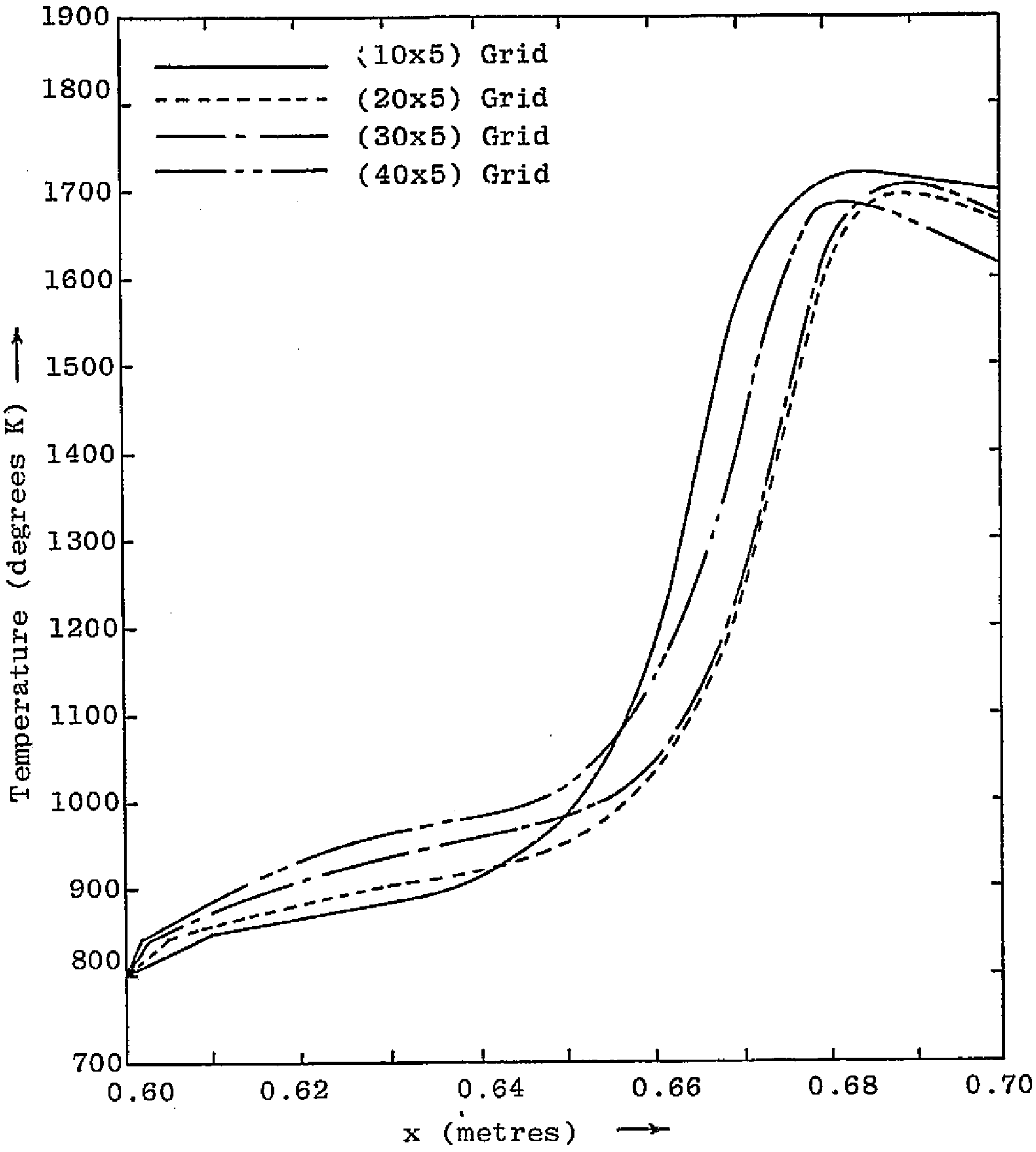

Fig. 6. Grid-dependency tests: effect of longitudinal grid distribution.

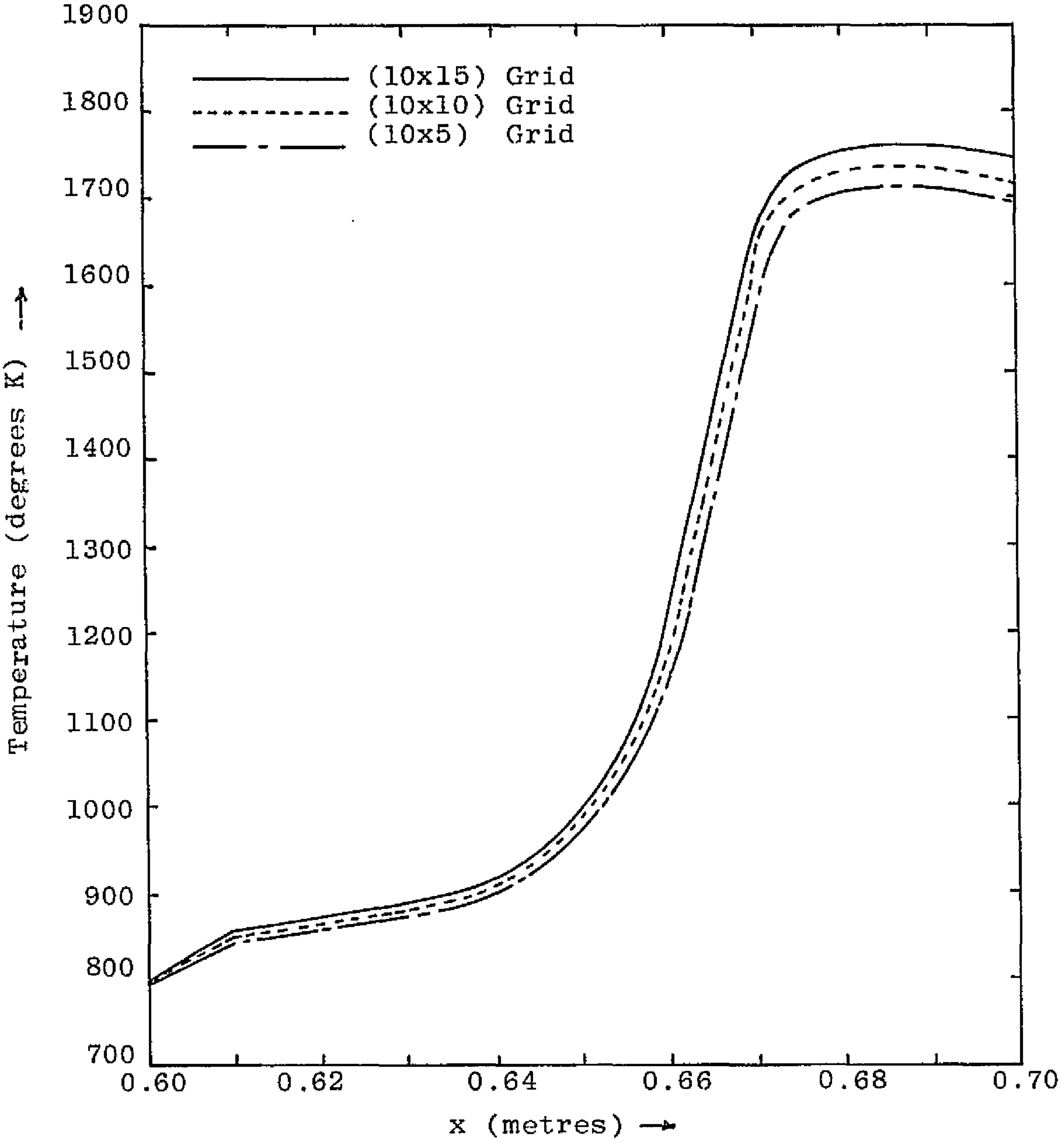

Fig. 7. Grid-dependency tests: effect of transverse grid distribution.

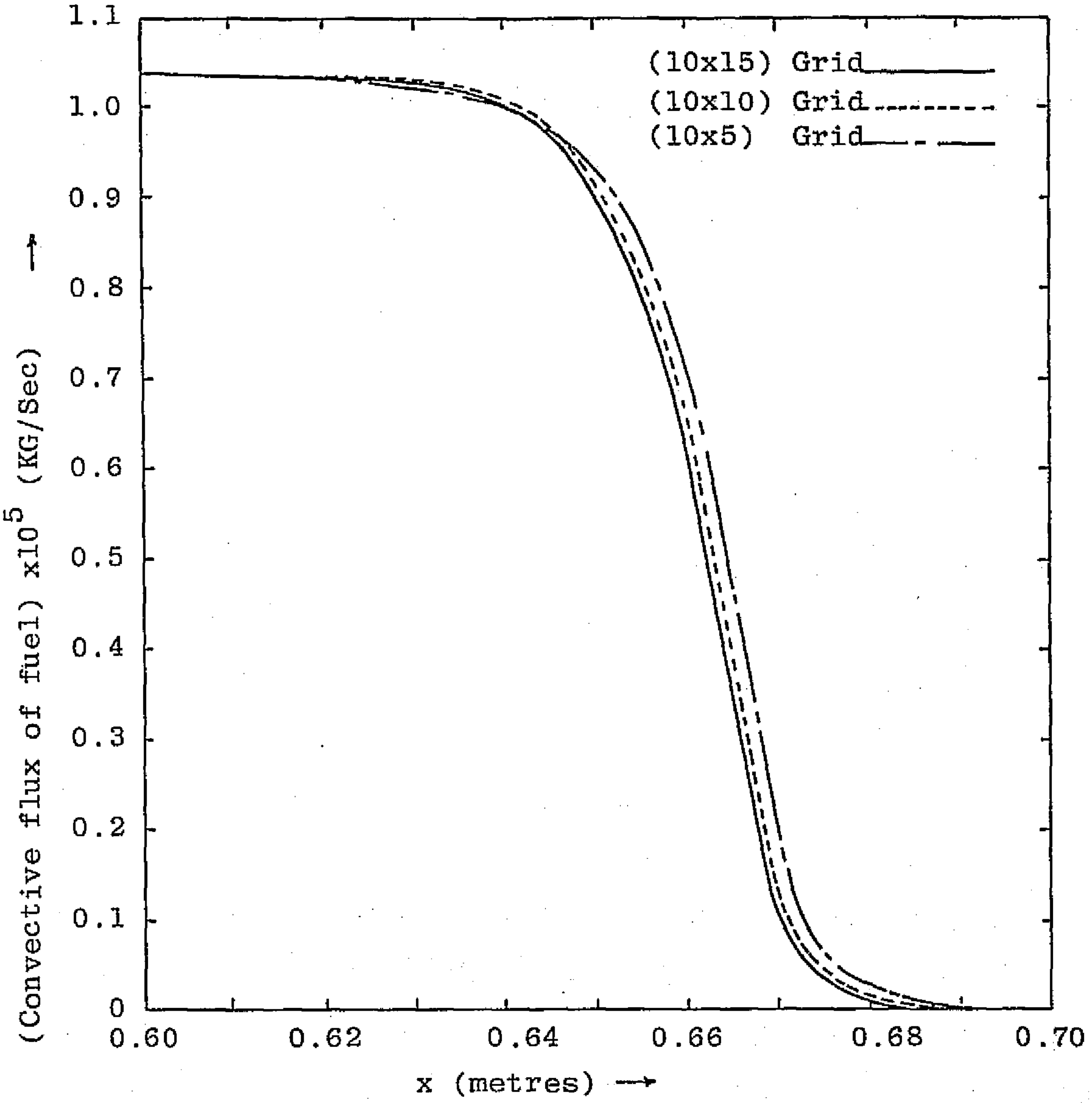

Fig.8. Grid-dependency tests: effect of transverse grid distribution.

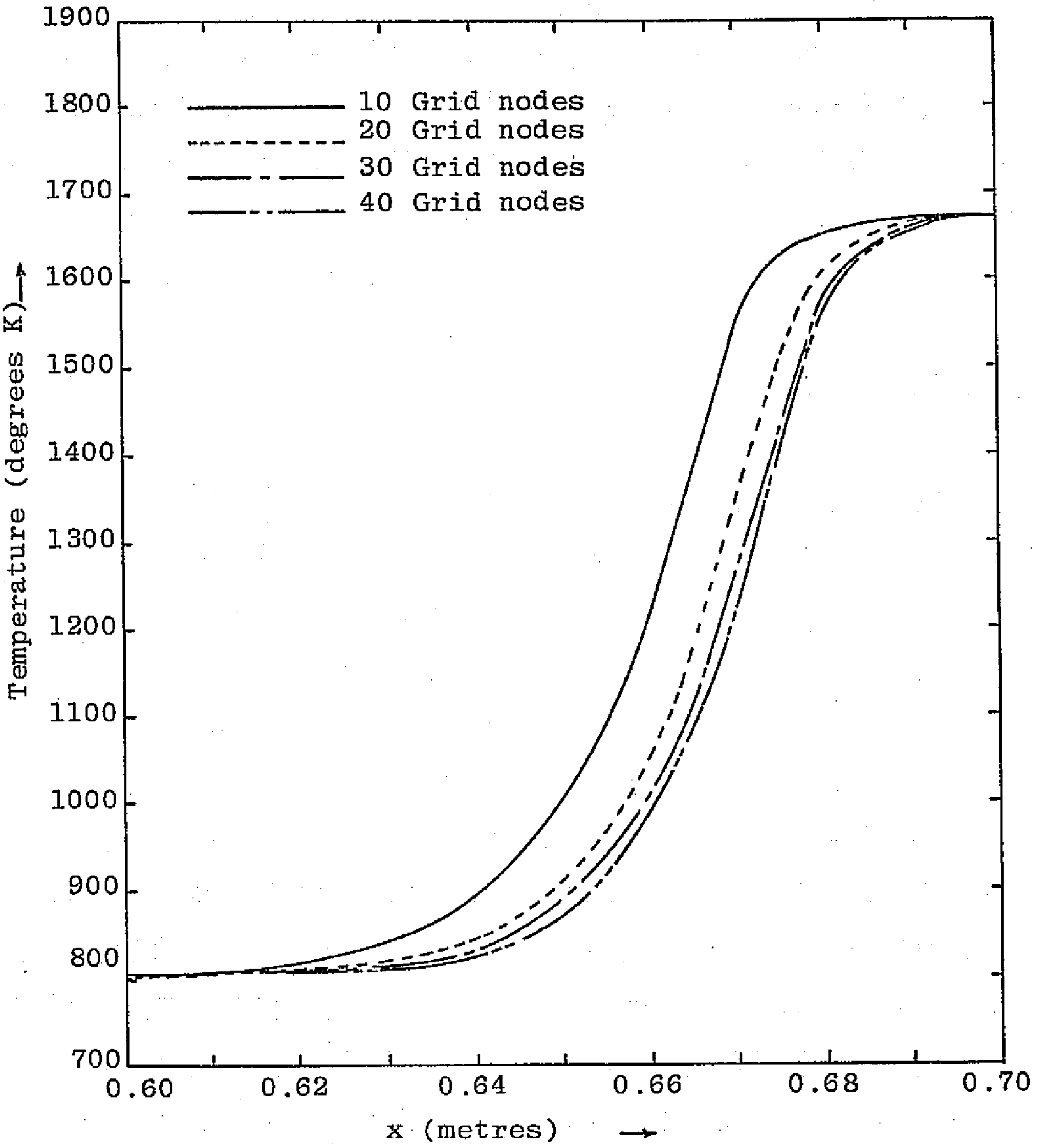

Fig. 9. Grid-dependency tests: one-dimensional calculations.

Figure 9 shows the results of one-dimensional computations for different axial grid distributions. Here again the solution is grid-dependent, though not as strongly as in the corresponding two-dimensional computations. There is not much significant difference in the solutions with 30 and 40 grid nodes; this shows that grid-independency is being approached with increasing number of grid nodes.

7.4 Results and discussions of test cases

In this Section, the results of four test cases are presented. Tables 1, 2, and 3 summarize the geometry, initial conditions, and temperature boundary-conditions for the four cases.

To demonstrate the general capabilities of the solution procedure, the results of the first test case are discussed in detail. The results of the other three cases are discussed in terms of the dependence of temperature and NO-concentration on the overall equivalence ratio which was 0.6, 0.8 and 1.0 for these cases.
First, some computational details which are common to all test cases are described.

7.4.1 Computational details

(i) Variables computed:

At each grid node, 18 variables were computed. The variables obtained from the solution of partial differential equations were: the axial velocity u, the stagnation enthalpy $\tilde{h}$, the mixture fraction f, the mass fraction of unburnt fuel m_{fu}, and the mass fractions of the species N, NO, NO_2 and N_2O. The variables obtained through the use of auxiliary algebraic equations were: the mass fractions of the species CO, CO_2, H, H_2, H_2O, N_2, O, OH, and O_2, and the temperature.

(ii) Grid used:The results of the grid-dependency tests discussed above show that even with fine axial grid distributions (e.g. 40 points in the diverging section of the duct), a grid-independent two-dimensional solution was not obtained. Therefore, to avoid unduly excessive computational times by further axial-grid-refinement, it was not attempted to obtain a grid-independent solution for the test cases. The solution is not strongly dependent on the lateral grid and grid-independency in this direction was achieved easily.

The grid used in all the test cases had 10 nodes in the radial direction and 35 in the axial direction. Twenty nodes were placed in the diverging duct section (Section 2, Fig. 1) and the rest in Sections 1 and 3. The distribution of the nodes was non-uniform in Sections 1 and 3 and uniform in Section 2. The axial distribution of the grid nodes for all the test cases is shown in Table 4. The lateral grid distribution in terms of the non-dimensionalized stream function ω is shown in Table 5. The radial locations of the grid nodes was computed by the program (as in Section 4.3) and varied from one axial location to another.

(iii) Convergence:

The convergence criteria adopted were:

- The variables u, $\tilde{h}$, f, and m_{fu} which were solved by a line-by-line procedure, should remain within 0.5% of their local values from one iteration sweep to the next.

- The mass fractions of N, NO, NO_2, and N_2O which were obtained by a point-by-point solution procedure should remain within 0.1% of their values from one iteration to the next.

(iv) Number of iterations:

Typically, 10 to 20 integration sweeps were necessary to obtain a converged solution for the variables u, $\tilde{h}$, f and m_{fu}. The point-by-point solution for the mass fractions of N, NO, NO_2, and N_2O required approximately 10 iterations at each point.

(v) Computing time:

The computing time for one integration sweep for the grid size employed here was approximately 8.5 seconds on the CDC-6500 computer.

(vi) Program adaptation:

No special program adaptation was necessary for the test cases reported here. The parameters defining the test case were easily incorporated into the program through appropriate Fortran variables.

(vii) Physical and chemical data:

The thermochemical data for all the species were obtained from Ref.2. Reaction rate data are given in Table 6.

7.4.2 Results of Test Case 1

The problem specification for Test Case 1 is given in Tables 1-5. Figures 10-14 show in detail the results of this test case. Since the diverging section of the duct (Section 2, Fig.1) is the region where the phenomena of interest occur, the figures show the details for this section only.

Figure 10 shows the velocity profile at various axial locations in the diverging section of the duct. At any axial location (except the first one),the profile is uniform over a large part of the duct cross-section and decays to zero in a narrow region near the wall. The reason for the uniformity of the velocity profile is the relatively large value of the turbulent viscosity (refer to Section 2.10), which causes rapid mixing of momentum. The predicted velocity profile at entry to this section is as would be expected in a developing turbulent flow.

If recirculation were accounted for, there would be a region of flow reversal near the wall. Consequently the velocities in the central region would be larger in magnitude. The influence of this on flame position is discussed below.

Figure 11 shows the temperature profile at various axial locations. On entry into the diverging section, the cold mixture of fuel and air is heated by conduction from the hot wall. Heat transfer within the fluid is rapid because of the relatively large turbulent diffusivities in this section of the duct. Ignition first occurs in a region close to the duct wall as shown by the temperature profile at x=0.66. Further downstream the profiles are uniform with a small near-wall region wherein a sharp radial gradient of

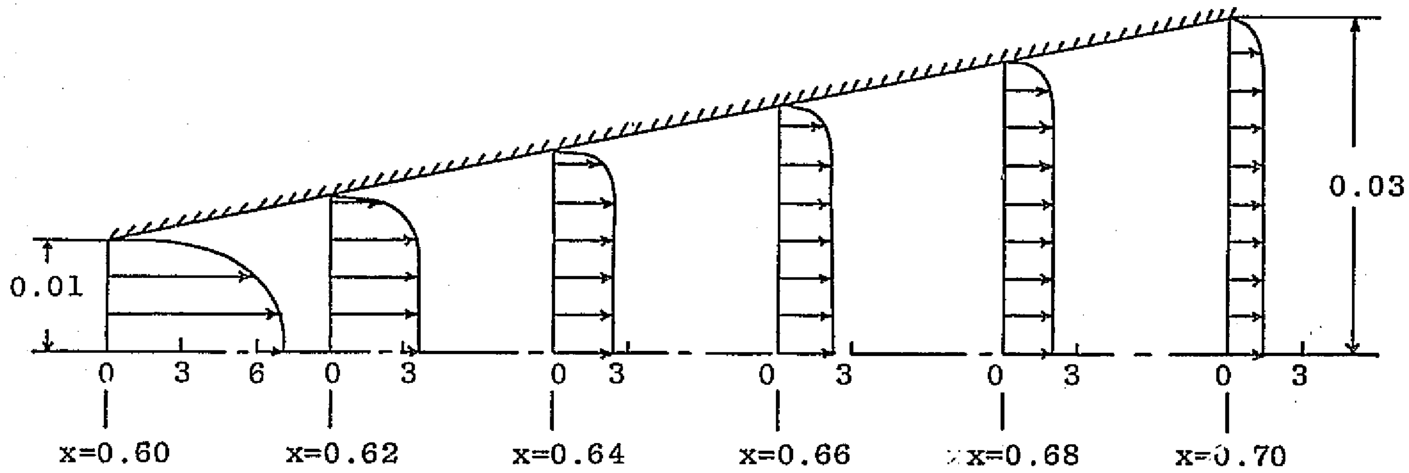

Fig.10. Velocity distribution at various axial locations.

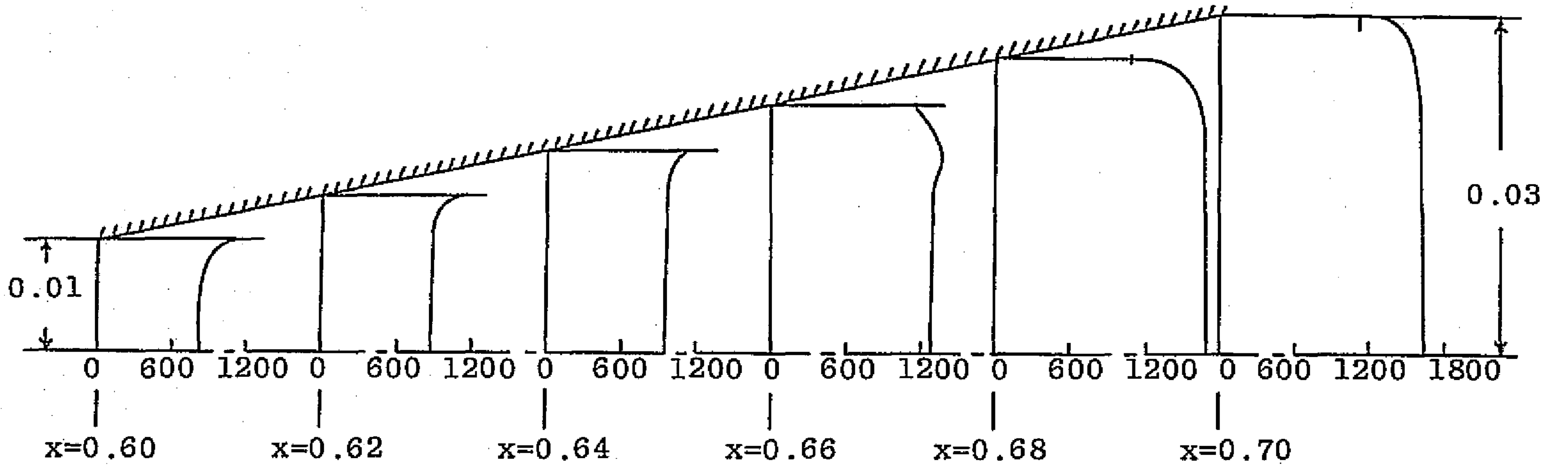

Fig. 11. Temperature distribution at various axial locations.

temperature exists.

Thus both the velocity and temperature profiles of Figures 10 and 11 demonstrate that the solution is essentially one-dimensional over a large region of interest.

Figure 12 shows the longitudinal profiles along the duct centerline of temperature and mass fractions of fuel and oxygen, and the convective fuel flux across cross-stream sections.

There is a sharp rise in temperature immediately after entry into the diverging section of the duct. The reason for this discontinuous behaviour of temperature is the sudden increase in turbulent diffusivity by a factor of 100. The rest of the temperature profile is as expected. There is a gradual rise in temperature in the preheat zone ($x \simeq 0.61-0.66$),and then a rapid rise in the reaction zone ($x \simeq 0.66-0.68$). Towards the end of the diverging section the temperature drops slightly, due to heat loss to the duct wall (temperature $1110^{o}K$).

The flame thus exists at an axial location of approximately x=0.66 to 0.68. The position of the flame is a function of several parameters. With increasing mass flow rates and velocity the flame moves downstream. Thus if recirculation were considered, due to larger velocities in the central region of the duct, the flame would move downstream in this region. However, due to rapid mixing in the near-wall recirculation region, ignition would occur close to the wall and at a point further upstream than would be the case if there were no recirculation. Thus a curved flame would exist in the duct, stretching along the duct wall down to the centerline of the duct.

Like the temperature profile, the fuel profile also exhibits a discontinuity on entry into the diverging section. Due to the sudden large increase in the turbulent diffusivity, there is a rapid mixing in the radial direction, and hence a discontinuity in the axial profile. After this initial mixing, the gases are fairly premixed, and the subsequent decay of fuel concentration with longitudinal distance is similar to the behaviour in a flat premixed flame. The behaviour of fuel concentration is seen to be consistent with the temperature distribution.

The convective flux of fuel, being the integral flow rate of unburnt fuel through a given duct section, does not exhibit any discontinuities. It gradually decays with the passage of the gases through the flame zone, as expected.

The oxygen concentration along the centerline rises initially due to mixing in the radial direction and subsequently decreases as oxygen is consumed due to chemical reaction . Finally it levels off at a value which corresponds to the excess oxygen in the oxidant stream.

Figure 13 shows the longitudinal profiles along the duct axis of the species involved in the NO_x reactions (i.e. N, NO, NO_2, N_2O, O, and OH). The temperature profile is also sketched in for reference

The NO concentration peaks at a point slightly downstream of the main reaction zone (i.e. at x=0.68m). This behaviour is as expected since the formation of NO is governed by kinetically-controlled reactions which are much slower than the hydrocarbon-oxidation reactions which rapidly reach the

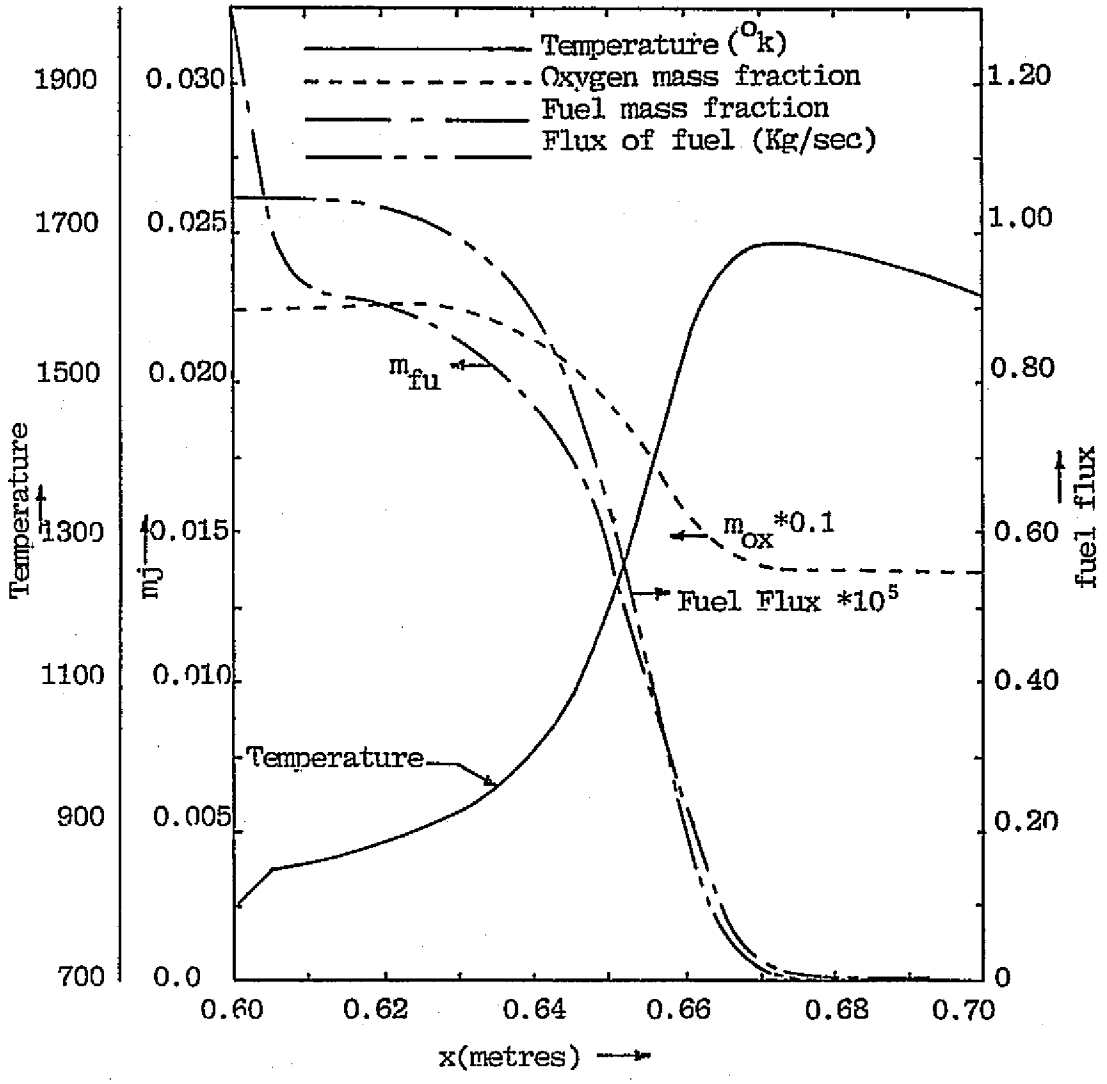

Fig. 12: Longitudinal profiles of temperature, mass fractions of fuel and oxygen along duct axis and of convective flux of fuel(Case 1).

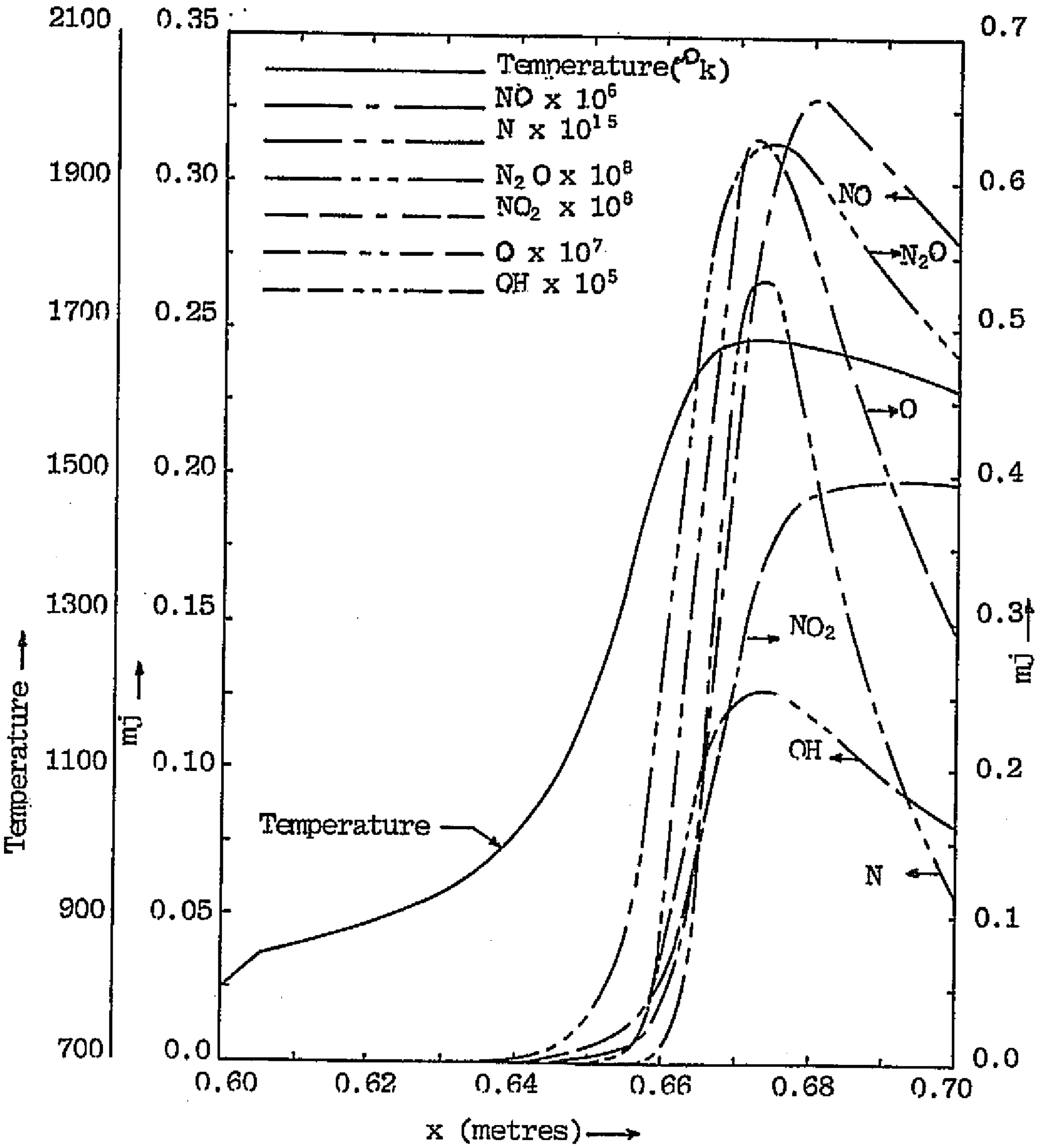

Fig. 13: Logitudinal profiles of temperature and mass fractions of N, NO, NO_2, N_2O, O, and OH along duct axis (Case 1).

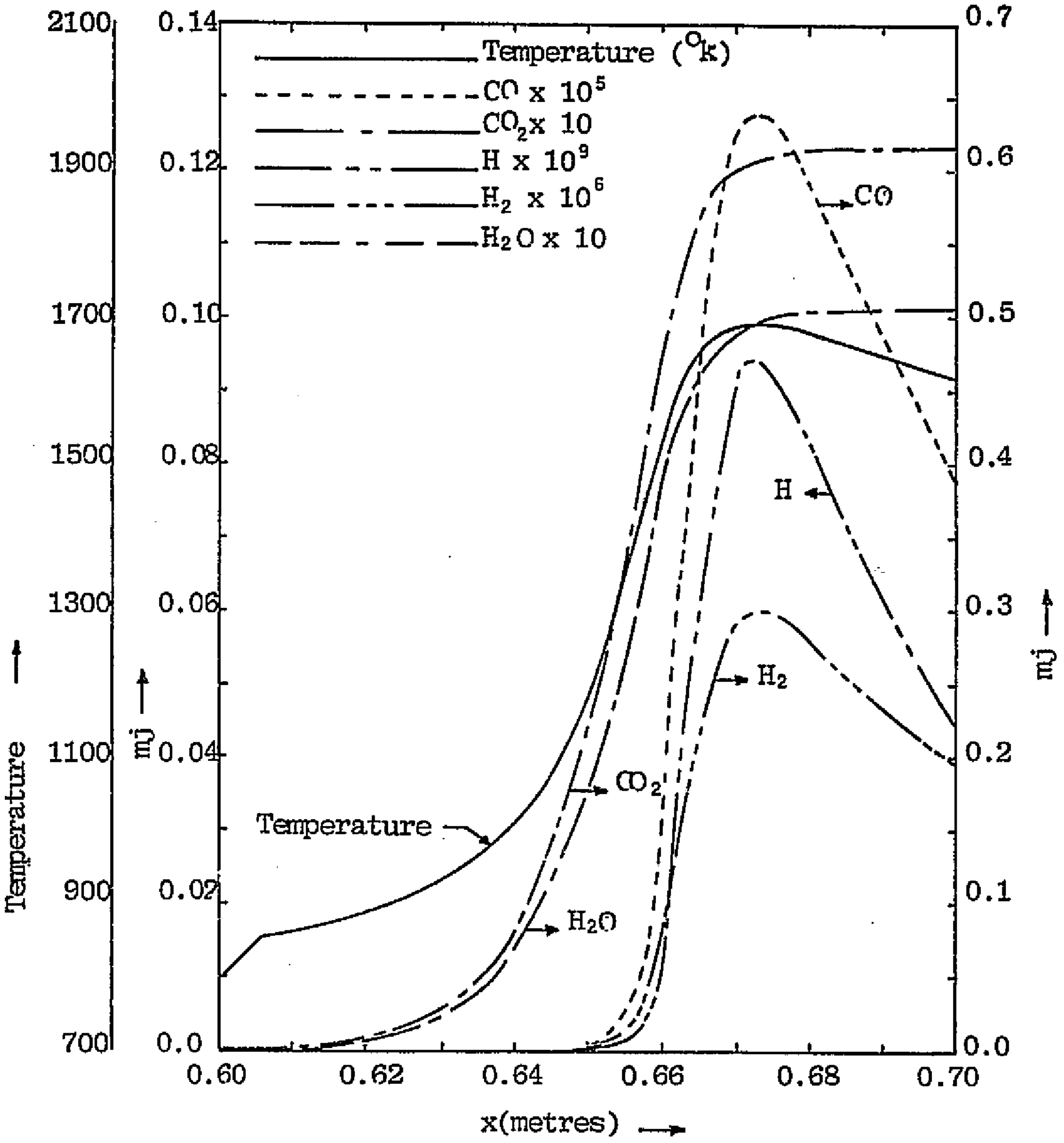

Fig. 14: Longitudinal profiles of temperature and mass fractions of CO, CO_2, H, H_2, and H_2O along duct axis (Case 1).

equilibrium state. After reaching a maximum value of 3.295E-7 at x=0.68m., the NO mass fraction decays slightly towards the end of the diverging section of the duct. This drop is due to the dropping temperature.

Figure 14 shows the longitudinal profiles of some of the equilibrium-product-species. As expected, the concentrations of the intermediate products CO,H, and H_2 (as also O and OH in Figure 13) all have a maximum value within the main reaction zone. The drop in the concentrations of these species from their maximum values as one proceeds further downstream is due to their being converted into the stabler product species CO_2 and H_2O. THe final product-species CO_2 and H_2O show a continuous rise and levelling off in the post-flame region. The formation of these two species is consistent with the temperature rise and fuel consumption through the flame zone.

7.4.3. Comparison of Test Cases 2, 3, and 4

Test Cases 2, 3, and 4 differ from each other in respect of the overall equivalence ratio. This is 0.6, 0.8, 1.0 respectively for the three cases.

Figure 15 shows the longitudinal profiles of temperature and NO mass fraction for the three cases. The behaviour is as expected. The maximum temperature in the flame zone increases as the overall equivalence ratio is increased from 0.6 (fuel-lean) to 1.0 (stoichiometric), and there is an upstream movement of the flame. Thus the onset of chemical reaction occurs earlier in the duct for stoichiometric mixtures than for fuel-lean mixtures, due to the faster reaction rates occuring under stoichiometric conditions.

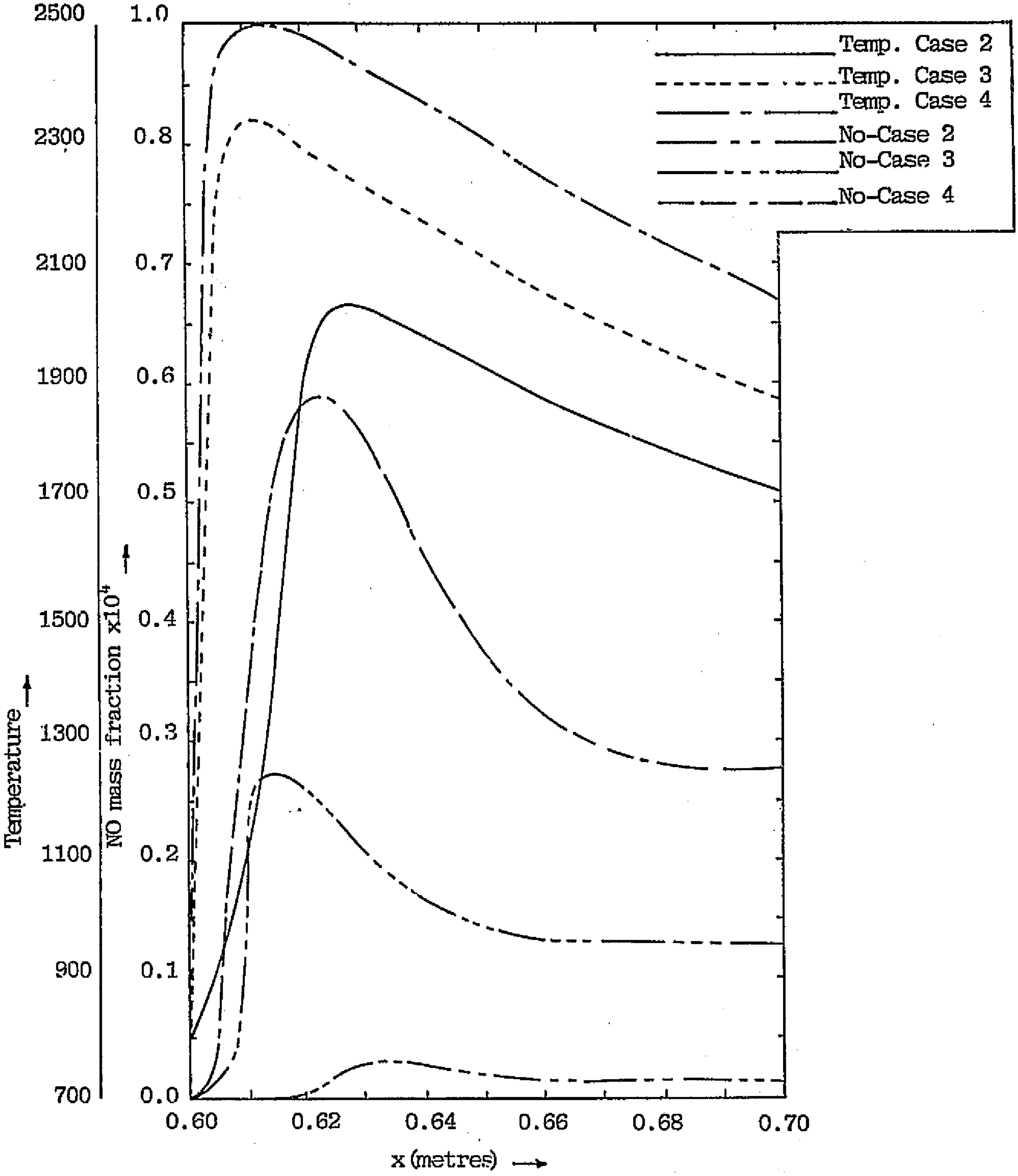

Fig. 15: Longitudinal profiles of temperature and NO mass fraction along duct axis for test cases 2, 3, and 4.

The maximum concentration of nitric oxide increases as the equivalence ratio is increased from 0.6 (fuel-lean) to 1.0 (stoichiometric).

The formation of nitric oxide is influenced by the equivalence ratio through its influence on combustion temperatures and the availability of oxygen, as discussed below:

(a) The combustion temperature: Since nitric oxide is a high-enthalpy species relative to molecular nitrogen and oxygen, its formation is favoured by the existence of high combustion temperatures.

(b) Availability of oxygen: The availability of oxygen is dependent directly on the air-fuel ratio. The formation of nitric oxide is low for low air-fuel ratios and increases to a maximum for mixtures having approximately 10% excess air. as compared to stoichiometric mixtures. This increase is due partly to the increase in the availability of oxygen and partly to increasing combustion temperatures. Further increases in the air-fuel ratio decrease the nitric oxide formation since the lower combustion temperatures offset the increased availability of oxygen.

Figure 16 confirms the above conclusions. The maximum nitric oxide mass fraction increases from $3.05\text{x}10^{-5}$ at $\phi=0.6$ to $5.88\text{x}10^{-4}$ at $\phi=1.0$. In addition it is observed that the formation of NO occurs mostly in the post-flame region in all the cases. This confirms the widely observed behaviour that the formation of NO is kinetically controlled and lags the temperature rise.

Table 1. Geometry specification of Test Cases 1-4

A_1 (m)	A_2 (m)	A_3 (m)	B_2	x_2 (m)	x_3 (m)	x_4 (m)
0.01	0.01	0.03	0.2	0.6	0.7	1.3
$B_1 = B_3 = C_1 = C_2 = C_3 = x_1 = 0$ for all Test Cases.						

(Refer to equation (14) of Section 2.5)

Table 2. Initial conditions of Test Cases

Test	V_{a_o}(m/s)	V_{f_o}(m/s)	T_{a_o}(^oK)	T_{f_o}(^oK)	P_o(atm)	ϕ
1	6	0.6	810	294	4	0.4
2	6	0.6	810	294	4	0.6
3	6	0.6	810	294	4	0.8
4	6	0.6	810	294	4	1.0

Table 3. Temperature boundary-condition of Test Cases 1-4

D_1(^oK)	D_2(^oK)	D_3(^oK)	E_1(^oK/m)	E_2(^oK/m)	E_3(^oK/m)
810	1110	1110	500	0	- 500
$F_1 = F_2 = F_3 = 0$ for all Test Cases.					

(Refer to equation (15) of Section 2.5)

Table 4. Longitudinal grid distribution for Test Cases 1-4.

I	x (m)
1	0.000
2	0.100
3	0.200
4	0.300
5	0.400
6	0.500
7	0.600
8	0.605
9	0.610
10	0.615
11	0.620
12	0.625
13	0.630
14	0.635
15	0.640
16	0.645
17	0.650
18	0.655
19	0.660
20	0.665
21	0.670
22	0.675
23	0.680
24	0.685
25	0.690
26	0.695
27	0.700
28	0.750
29	0.800
30	0.900
31	1.000
32	1.100
33	1.200
34	1.250
35	1.300

Table 5. Transverse grid distribution for Test Cases.

Test Cases	1	2	3	4
I	ω	ω	ω	ω
1	0	0	0	0
2	2.979E-3	4.418E-3	5.826E-3	7.203E-3
3	5.958E-3	8.837E-3	1.165E-2	1.441E-2
4	8.937E-3	1.326E-2	1.748E-2	2.161E-2
5	3.641E-2	5.400E-2	7.121E-2	8.803E-2
6	2.400E-1	2.400E-1	2.400E-1	2.400E-1
7	3.800E-1	3.800E-1	3.800E-1	3.800E-1
8	5.500E-1	5.500E-1	5.500E-1	5.500E-1
9	7.500E-1	7.500E-1	7.500E-1	7.500E-1
10	1.000	1.000	1.000	1.000

Table 6. Reaction rate data (in S.I. Units)

No.	Reaction			A	B	T_{act}	Ref.
1	N+NO	$\rightleftarrows$	N_2+0	1.500E10	0	0	3
2	$N+0_2$	$\rightleftarrows$	NO+0	5.998E6	1.0	3.172E3	3
3	OH+N	$\rightleftarrows$	H+NO	5.998E8	0.5	4.028E3	3
4	$H+N_20$	$\rightleftarrows$	$OH+N_2$	7.998E10	0	7.553E3	3
5	N_20+0	$\rightleftarrows$	NO+NO	1.000E11	0	1.500E4	3
6	N_20+M	$\rightleftarrows$	N_2+0+M	1.000E11	0	2.518E4	3
7	N+0+M	$\rightleftarrows$	NO+M	6.397E10	-0.5	0	5
8	NO_2+0	$\rightleftarrows$	$NO+O_2$	1.000E10	0	3.000E2	5
9	NO_2+M	$\rightleftarrows$	O+NO+M	1.099E13	0	3.300E4	5

Forward rate constant $k_f = AT^B \exp(-T_{act}/T)$
Reverse rate constant obtained from forward rate and equilibrium constants.

Hydrocarbon oxidation reaction rate = $0.003 m_{fu} m_{ox} \exp(-18000/T)$

8. CONCLUDING REMARKS

The present computer program has successfully undergone some tests, e.g., the program has been used to predict the hydrodynamics and chemistry for four cases involving different inlet and boundary conditions. These tests show that the predictions are qualitatively plausible. Detailed experimental data are required to assess quantitatively the validity of the numerical procedure and the physical hypotheses involved.

In concluding this report, some consideration is given to what further developments would be fruitful. The following improvements may be envisaged to make the code approach more towards physical realism.

(a) Turbulence modelling:

The present version of the code incorporates a simple zero-equation model of turbulence. A more sophisticated model would be the two-equation model employing the kinetic energy of turbulence and its dissipation rate, as the dependent variables of differential equations.

(b) Recirculation:

The inclusion of a means of calculating the recirculating flow, if conditions should arise which give rise to it, will be one more step towards physical realism. Techniques to enable the treatment of recirculation with the present stream function coordinate system are under study (Private Communication from D B Spalding of CHAM Ltd., London). Alternatively, recirculation can be treated by a special program accounting for elliptic effects in the recirculation zone. A proper treatment of recirculation will also result in a correct prediction of the transport properties thereby avoiding their augmentation by arbitrary factors as has been done in the present program.

The treatment of recirculating flows using fully elliptic solution procedures is an area where considerable work has already been done at CHAM Ltd. Computer codes (e.g., Ref. 8) based on the SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithm of Patankar and Spalding (Ref. 9) can be easily adapted to handle the present flow situation.

(c) Lateral momentum equation:

In the present solution procedure, pressure has been assumed to be uniform across the duct. The inclusion of the lateral momentum equation allows for the pressure to be non-uniform across the duct. Its chief advantage, in the present context, is that it allows incipient recirculation to be detected.

(d) Wall temperature:

The wall temperature distribution has been specified in the present program. The inclusion of the calculation of wall temperature into the solution procedure represents one step further towards physical realism. The solution method would then involve extending the finite-difference grid into the solid material. When the enthalpy (temperature) equation is being solved, account would be taken of: (i) radial conduction in the solid material; (ii) axial conduction in the solid material; (iii) radiative transfer along the duct; and (iv) heat sources in the solid material.

(e) Hydrocarbon-Air kinetics:

The consideration of detailed hydrocarbon-air kinetics as distinct from a simple Arrhenius expression would shed more light on the processes occuring at a molecular level; the formation of nitric oxide would also be predicted more accurately.

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10. NOMENCLATURE

Symbol	Meaning
a^{L}_{ij}	Number of kg - atoms of element i per kg mole of species j.
a', b', c', d'	LTDMA* coefficients.
A_i, B_i, C_i	Constants in duct wall equation.
$A'_i, B'_i, \ldots G'_i$	Coefficients in the finite-difference equations.
Aj	Duct area at section j.
A_j, A_{-j}	Arrhenius pre-exponential factor.
A_j, B_j	Specific heat coefficients.
AP	$\equiv (A'_i+B'_i+C'_i-S'_i)$
b_j	Number of kg-atoms of element i per kg of mixture.
B_j, B_{-j}	Exponent on temperature in Arrhenius rate expression.
c	Transport-property term in differential equation.
C, C_p	Specific heat at constant pressure of the mixture.

*Longitudinal Tri-Diagonal Matrix Algorithm.

Symbol	Meaning
$C_{p,j}$	Constant-pressure specific heat of chemical species j.
d	Source term in differential equation.
D_i, E_i, F_i	Constants in the duct wall-temperature equation.
e	Axial diffusion term in differential equation.
E	Activation energy.
f	Mixture fraction.
f_{st}	Stoichiometric value of mixture fraction.
g_j	Ideal-gas partial molal specific Gibb's function of species j, per kg-mole.
G	Mass flow rate per unit area.
$\tilde{h}$	Stagnation enthalpy.
H_{fu}	Heat of combustion of fuel.
h_j	Enthalpy of chemical species j.
h_{mix}	Mixture enthalpy (sensible + chemical).
I	Integral appearing in distance calculation.
J_j	Diffusion mass flux.

Symbol	Meaning
k_b	Backward reaction rate constant.
k_f	Forward reaction rate constant.
K_c	Equilibrium constant.
L	Length.
m_{fu}	Mass fraction of unburnt fuel.
m_j	Mass fraction of chemical species j.
m_{ox}, m_{O_2}	Mass fraction of oxygen.
M	Mach number.
M	Number of chemical reactions.
n	Mole number.
n_j'	$\equiv \sum_{i=1}^{NS} \alpha_{ij}'$ = Molecularity of forward reaction j.
n_j''	As n_j', but for backward reaction j.
N	Number of cross-stream grid nodes.
NLM	Number of elements.
NS	Number of chemical species in the system.

Symbol	Meaning
NSE	Number of chemical species whose concentrations are determined by a chemical-equilibrium analysis.
NSK	Number of chemical species whose concentrations are kinetically determined.
p	Pressure.
P	Arrhenius pre-exponential factor.
P_o	Initial pressure.
P_o	Standard atmospheric pressure.
Pr	Laminar Prandtl number.
Pr_{eff}	Effective Prandtl number.
Q	Heat flux.
r	Radius.
R	Universal gas constant.
R_j, R_{-j}	Mass rate of creation of species by forward and reverse reactions j, respectively.
R_{wi}	Radial location of duct wall.
s	Mass of oxygen per unit mass of fuel in stoichiometric combustion.

Symbol	Meaning
s_j	Ideal-gas specific entropy of species j.
s_j^o	One-atmosphere value of s_j.
S	Skin-friction coefficient.
S_c	Schmidt number.
S_i, S_i'	Parts of linearised source term.
S_ϕ	Source term of dependent variable ϕ.
T	Temperature.
T_i	Term representing diffusive effects in finite-difference equations.
$T_{act,j}$	Activation temperature for reaction j, i.e. activation energy divided by the universal gas constant.
T_{ao}	Air temperature at initial axial position.
T_{fo}	Fuel temperature at initial axial position.
u	x-direction velocity.
V_{ao}	Air velocity at initial axial position.
V_{fo}	Fuel velocity at initial axial position.

Symbol	Meaning
$\bar{W}$	Mean molecular weight of gas mixture.
W_j	Molecular weight of chemical species j.
x	Axial distance.
x	Number of kg-atoms of carbon per kg-mole of hydrocarbon fuel.
y	Number of kg-atoms of hydrogen per kg-mole of hydrocarbon fuel.
Z_i (i=1,7)	Coefficients in thermochemical data equations.
Greek Symbols	
$\alpha'_{ij}, \alpha''_{ij}$	Stoichiometric coefficients of species i in chemical reaction j, as a reactant and as a product respectively.
$\bar{\alpha}_j$	Third-body stoichiometric coefficient in reaction j.
γ	Ratio of specific heats (C_p/C_v).
Γ_ϕ	Exchange coefficient for dependent variable ϕ.
δ_{ik}	Kronecker delta function.
δx, δx	Grid distance in x-direction.
$\Delta\psi$	Grid distance in ψ-direction.

Symbol	Meaning
$\Delta\omega$	Grid distance in ω-direction.
η	Under-relaxation parameter.
λ	Thermal conductivity.
μ, μ_{eff}	Effective viscosity.
μ_{ℓ}	Laminar viscosity.
μ_j	Viscosity of chemical species j.
$\mu_{j,o}$	Constant in viscosity law for species j.
ξ	Defined as $(m_{fu} - m_{ox}/s)$.
ξ_{fu}	Defined as $(m_{fu})_{inlet}$.
ξ_{ox}	Defined as $-(m_{ox})_{inlet}/s$.
π_i	Lagrange multipliers in Gibbs function minimisation equation.
ρ	Density.
σ_j	Mole number of species j, kg-moles j/kg mixture.
$\sigma_j{}^*$	Average of σ_j over adjacent nodes, weighted by respective finite-difference coefficient.

Symbol	Meaning
σ_m	Reciprocal of mean molecular weight of gas mixture $\equiv \sum_{i=1}^{NS} \sigma_i$.
ζ	Shear stress.
ϕ	Dependent variable.
ϕ	Equivalence ratio.
ϕ'	LTDMA* correction of dependent variable.
Φ	Solution before application of LTDMA.
ψ	Stream function.
ω	Non-dimensional stream function.

Subscripts

b	Fully burnt.
D	Downstream.
DD	Downstream of D.
E	E (external) boundary of the grid.
$\tilde{h}$	Stagnation enthalpy.
i	i'th location in the grid.

*Longitudinal Tri-Diagonal Matrix Algorithm.

Symbol	Meaning
I	I (internal) boundary of the grid.
j	Chemical species j.
M	Intermediate.
pr	Products.
P	Grid node P.
U	Upstream.
wall	Wall values.
ϕ	Dependent variable ϕ.
o	Previous iteration value.
12	Between streamlines 1 and 2.

APPENDIX A

ORGANISATION OF THE NASCO* COMPUTER PROGRAM

A.1 Introduction

The organisation of the computer program will be looked at in detail in this Appendix. Firstly the structure and the interconnectedness of the different subroutines are described. The subroutines are classified into different categories depending on the function they serve in the program, and then each of the subroutines is described in detail. In the course of this description are mentioned the program changes necessary to solve problems with different initial and boundary conditions, and also incorporation of alternative physical modelling for properties.

The present program has been derived and developed from the GENMIX program of Spalding (Ref. 1). The reader is advised to refer to the description of the GENMIX program for background information.

A.2 Program Structure

A.2.1 Flow diagram

The structure of the computer program can be represented by the flow diagram given on the next page.

There are 13 subroutines: BLOCK DATA, MAIN, OUTPUT, PHYS, WALL, CHEM, SPECE, CALC, CREKO, HCPS, COMP, START and PLOTS. The first three are of major concern to the user and they will require at least minor modifications when a new problem

*NASCO stands for NASA Surface Combustor.

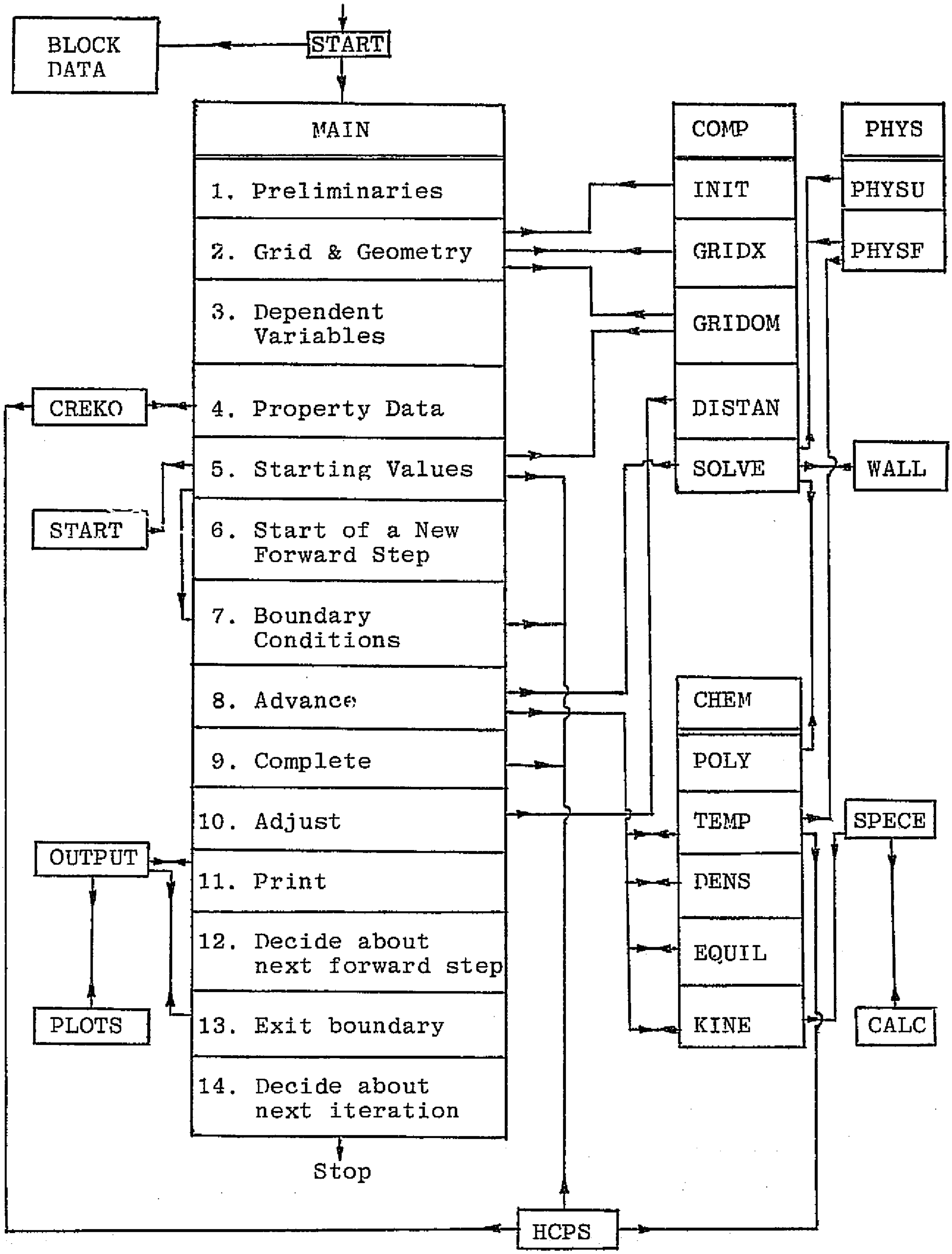

Fig. A.1 Flow diagram of the NASCO computer program

is to be tackled. The other subroutines will in general require no modifications. Subroutines PHYS and WALL embody the physical processes; modifications to these are needed only if alternative physical models are to be considered. Subroutines CHEM, SPECE, and CALC relate to chemical-equilibrium and kinetics calculations; these should not be altered. Subroutine CREKO is for the input of thermochemical and kinetics data and subroutine HCPS for the calculation of certain thermodynamic quantities. Finally subroutines COMP, START and PLOTS, embody the mechanisms for solving the finite-difference equations and plotting the results graphically; these again should not be altered unless major extensions of the program are envisaged.

A.2.2 Flow of control

Inspection of subroutine MAIN in the flow diagram reveals that, apart from calls to subroutines CREKO, START and COMP (ENTRY INIT, GRIDX, and GRIDOM) control proceeds from the start to the end of Chapter 5. Chapter 6 is then skipped. The initial part of Chapter 7 is passed through to specify some boundary-condition information; then Chapter 9 to complete the computation of starting values.

The main computation loop is entered at Chapter 6 after Chapter 12 has been completed. The loop 6-7-8-9-10-11-12-6 is then traversed as many times as there are forward steps. During the course of this traverse, calls are made to subroutines CHEM, COMP, and HCPS. Finally subroutines OUTPUT and PLOTS are called to print and plot the results as indicated in the flow diagram.

The various subroutines will now be described in detail.

A.3 The user-oriented subroutines, BLOCK DATA, MAIN, and OUTPUT

A.3.1 BLOCK DATA

This subroutine is used for the input of some data. It consists of seven chapters, the functions of which are explained by their titles; these will now be briefly described.

Chapter 1. Preliminaries

In this Chapter, identification and control parameters are defined. Examples of these parameters are:- the maximum number of iterations to be performed; whether to obtain diagnostic print out or not; and so on. An inspection of the Glossary of Fortran variables in Appendix C, will reveal the function served by the parameters defined in this Chapter.

Chapter 2. Grid and Geometry

In this Chapter, the user must specify the number of transverse and longitudinal grid points and how they are distributed. Geometrical information relating to the radius of the duct wall is also supplied here.

Chapter 3. Dependent Variables

In this Chapter, the number of dependent variables, NF,is specified. The indices (JH,JP, etc.) defining the location of a variable held in two-dimensional storage in the F-array and the indices (IDN,IDNO, etc.) defining the location of a variable held in one-dimensional storage in the FS-array, are also specified here. It will be cbserved that some of the species concentrations are stored in both the F and FS arrays; this is for programming convenience.

The array ISPEC is also defined here as follows:
ISPEC (I) = J means that the variable which occupies the Ith storage location in the FS-array occupies the Jth location in the F-array. If ISPEC equals zero, the corresponding variable is stored only in the FS-array.

Chapter 4. Property Data

In this Chapter, some of the properties of the fluids are specified. Some control parameters relating to properties and processes are also supplied here. Polynomial coefficients AC, AH, AS, AS1, BS1* are defined in this chapter.

Chapter 5. Starting Values

In this Chapter the velocities, temperatures, fuel and oxygen concentrations of the two incoming streams are specified. The inlet pressure and the overall equivalence ratio are also specified here.

Chapter 6. Boundary Conditions

The parameters which define the temperature of the duct wall are specified here.

Chapter 7. Print

In this Chapter, the parameters controlling the printout and plotting of the various variables are defined. The

*See Appendix C for explanation of Fortran variable names.

reader is again advised to refer to Appendix C for an explanation of the Fortran variable names.

A.3.2 Subroutine MAIN

Subroutine MAIN consists of 14 chapters, the functions of which are explained by their titles, and these will now be briefly described.

Chapter 1. Preliminaries

Here DIMENSION and COMMON statements allocate storage and variable names. Comment cards describing the special features of a particular run are conveniently placed in this Chapter. Arithmetic statement functions for specifying geometrical data (i.e.,radius of duct wall as a function of longitudinal distance) and boundary conditions (i.e., wall temperature as a function of longitudinal distance) are also defined in this Chapter. These functions may be changed readily if different ways of specifiying the geometry and wall temperature are required.

Chapter 2. Grid and Geometry

In this Chapter, the distribution of cross-stream grid points (i.e.,values of OM(I)) are computed using any specified functional relation, e.g., power law, etc.* Calls to subroutine COMP, at ENTRY's INIT, GRIDX, and GRIDOM are made for the initialisation of certain quantities and for the computation of certain grid related quantities.

*In the present listing, the values of OM(I) are specified directly in subroutine BLOCK DATA.

The duct area is computed once for all at various axial locations and stored in the array ADUCT.

Chapter 3. Dependent-variables

In this Chapter comment cards are supplied to state the variables which appear in the differential equations and the auxiliary equations that are to be solved.

Chapter 4. Property Data

In this Chapter the ratio of the specific heats (C_p/C_v), the laminar and the turbulent Prandtl numbers of the various dependent variables, and the stoichiometric mixture fraction are calculated. For simplicity, all the laminar Prandtl numbers are set equal to PRLAM, and all the turbulent Prandtl numbers are set equal to PRTURB. The appropriate place to insert temperature and/or composition dependence is in subroutine PHYS and will be described later.

The array NEWPR(J) is also filled in this Chapter. NEWPR(J) is set to unity if the Prandtl number of a dependent variable denoted by J is equal to that of the variable denoted by (J-1); otherwise NEWPR(J) is set to 2. This is done so as to avoid recomputation of diffusion terms when NEWPR(J) equals unity*.

Chapter 5. Starting Values

The program conducts a marching integration from an upstream

* The variable corresponding to J=0 is the u-velocity.

station to a downstream one until the entire flow field is covered and then the process is repeated. The values of the dependent variables are computed, step-by-step, for all internal nodes of the grid except those lying on the starting line. The latter, which are termed as starting values or initial conditions, must be specified. This is done in Chapter 5.

In this Chapter, firstly the radius of the inner fuel jet (denoted by RDIV) is computed on the basis of the fuel and air velocities and the overall equivalence ratio. Next follows a sequence of statements to set the cell boundary at the radial location RDIV and then a call is made to subroutine COMP at ENTRY'GRIDOM to compute some grid related quantities. Next a call to subroutine OUTPUT at ENTRY OUTP1 results in some initial printout and a call to subroutine START gives the one-dimensional solution.

Finally, at the end of the Chapter is a DO-loop which inserts the appropriate values of the dependent variables at the internal grid nodes. Except for the values specified on the starting line, the values at the other grid nodes, as specified here, are to be regarded as only 'initial guesses' and are over-ridden as integration proceeds. These 'initial guesses' are specified here only for the two cross-stream planes immediately downstream of the inlet plane; thus the DO-loop index JX runs only up to the value 3. The re-specification of the initial guess for JX=3 as also the specification for other internal grid nodes is done in Chapter 6 and is described below.

Chapter 6. Start of a new forward step

This is the first of six chapters in the main integration loop which runs from Chapter 6 through Chapter 12. The magnitude of the forward step DX, and the value of X at the downstream location XD, are set here.

Also done in this Chapter is the updating of 'initial guesses' for the first integration sweep only. The initial guesses for the downstream (D)station (i.e., the station for which solution is about to commence) and the one further downstream (DD) of it are specified as the corresponding upstream (U)station values (i.e., the values which have been just determined). This is done in the DO-602 loop. Only the D- and the DD- station values are the as yet undetermined ones which will be required when solving at the D-station. This updating of the initial guesses to obtain faster convergence, is done for all variables except mass fraction of unburnt fuel (J=JF) and temperature (J=JTE) which are obtained from a preliminary one-dimensional analysis (subroutine START).

Chapter 7. Boundary Conditions

The boundary conditions at the walls of the duct are specified in this Chapter. The boundary values of some of the dependent variables are specified by inserting the appropriate values at the boundary grid nodes in the various arrays.

Chapter 8. Advance

In this Chapter the pressure gradient is at first computed. This is an estimated value based on the rate of area increase of the duct. The effect of the wall shear on the pressure is next considered. The detailed steps in the computation of the pressure gradient are;

- The downstream duct area ADUCTD is obtained by reference to the duct geometry. (Note: The duct areas at the different longitudinal grid locations are calculated only once in Chapter 2 and stored in the array ADUCT.)

- The downstream duct area is compared with the upstream flow area (AFLOWU), which is equal to the downstream flow area appropriate to the previous step.

- The pressure gradient DPDX is then computed as equal to the difference in areas (ADUCT-AFLOWU) divided by the step size DX and by DADP (which itself is computed in Chapter 10 at the downstream location of the previous step). This pressure gradient is that which should produce the correct area change, provided the neglect of shear stresses at the wall is justified.

- The shear stresses at the duct wall are then accounted for partly, by the addition to the computed DPDX of terms involving TAUE; for the pressure gradient must also balance the forces on the walls.

- Finally the pressure gradient is restricted to be no greater than $\alpha\rho u^2_{min}/\Delta x$ (where α = a factor which may be varied at will by the user and is denoted by the Fortran symbol BFRAC; BFRAC is assigned a value in BLOCK DATA). This restriction is imposed to avoid the occurrence of negative velocities and is done as per the discussion presented in Section 4.2.3. (Note: BFRAC $\leqslant$ 0.5)

- This pressure gradient is used in subroutine PHYS (ENTRY PHYSU) for the calculation of momentum sources.

This completes the computation of the pressure gradient. Next a call to subroutine COMP at ENTRY SOLVE is involved. This results in the execution of a forward step and the computed values of the dependent variables: u-velocity, enthalpy, mass fraction of unburnt fuel, and mixture fraction are stored at the appropriate location in the respective arrays. Some other variables such as temperature, mass fraction of oxygen, etc. are also computed in the process; details will be described when the appropriate subroutine is being discussed.

Chapter 8 is completed by calls to subroutine CHEM (only for INERT=2, reacting flows):

(a) at ENTRY TEMP to compute the temperature;

(b) at ENTRY DENS to compute the density ;

(c) at ENTRY EQUIL for chemical-equilibrium computations (only for IEQUIL=1) ;

(d) at ENTRY KINE for chemical-kinetics computations (only for KNTCS=1, and NITER $\geqslant$ NITERK).

The variables IX, IXX, XU, ISTEP and AREAU are then updated to represent the new step values.

Chapter 9. Complete

In this Chapter, variables which are not obtained directly from the differential equations are computed. Thus the computation of temperature, density, and mass fraction of oxygen is performed here for INERT=1 (i.e., non-reacting flows). For INERT=2 (reacting flows), subroutine CHEM (ENTRY's TEMP and DENS)is called in Chapter 8 and these operations are performed in this subroutine itself.

Firstly, the radial locations of the grid nodes are computed by a call to subroutine COMP at ENTRY DISTAN. The solution obtained is now 'improved' by adjusting the pressure and the corresponding velocity and density distributions. Since the pressure gradient is guessed at the beginning of a forward step, this adjustment is necessary at the end of the step so as to ensure a close fit of the downstream area (AFLOWD) of the calculated flow with that available in the duct (ADUCTD). This is achieved in the following steps:

- A quantity DA1, which is a dimensionless measure of the extent by which the flow area (AFLOWD) differs from the duct area (ADUCTD), is first calculated.

- The dependence of area on pressure as expressed by the Fortran variable DADP is now calculated in the DO-loop ending at statement number 1025; this amounts to performing the integration indicated in equation (96) of Section 4.2.2.

- If ABS(DA1) is greater than DAMIN, the value of pressure is adjusted accordingly. (DAMIN is assigned a value in BLOCK DATA). The consequent increments to velocity and density are then calculated and applied in the DO-1027 loop. This is done in accordance with equations (97) and (98) of Section 4.2.2.

- The increment of pressure is restricted to be no greater than $\beta\rho u_{min}^2$ (where β = a factor which may be varied at will by the user and is denoted by the Fortran symbol PFRAC: PFRAC is assigned a value in BLOCK DATA, and PFRAC ≤ 0.5). This restriction is imposed to avoid the occurrence of negative velocities due to over-correction and is done as per the discussion presented in Section 4.2.3. The increments to velocity and density are also scaled down correspondingly.

- The result of the preceding operations is a new flow area AFLOWD, and a new measure of the area discrepancy, DA2. The latter should be nearer to zero than DA1,

- If ABS(DA2) is larger than DAMIN, the previous steps are repeated, but in no case more than NDAMAX times. (NDAMAX is assigned a value in BLOCK DATA.) When repeating the above steps, the increment of pressure is taken to be half of that given by $\beta\rho u^2_{min}$, if DA2 has a sign different from that of DA1. The reason for doing so is that a change of sign from DA1 to DA2 implies an over-correction, and hence the necessity to scale down the subsequent corrections.

Chapter 11. Print

The function of this Chapter is calling subroutine OUTPUT (ENTRY OUTP2).

Chapter 12. Decide about next forward step

The function of this Chapter is to decide whether to terminate the integration or continue it. Firstly, a check is made to see if the final x-station in the flow field has been reached. If not control is returned to statement 600 at the start of Chapter 6 and then another forward step is taken; otherwise control proceeds to Chapter 13.

Chapter 13. Exit Boundary

This Chapter is entered if the entire flow field has been covered. The boundary condition of zero gradient at the exit as represented by equation (16) of Section 2.6 is applied in the DO-1206 loop. A call to subroutine OUTPUT (ENTRY OUTP2) is made to obtain complete printout of the dependent variables at the exit plane.

Chapter 14. Decide about next iteration

In this Chapter a check is made to see if the number of sweeps or iterations, NITER, exceeds the specified maximum value of NITMAX. If yes, then the iteration is terminated. Otherwise, a call to subroutine COMP at ENTRY INIT is made to reinitialize certain variables, and another sweep of the flow field started by transferring control to statement 700. If the next iterative sweep is to be started at an intermediate x-station IX=ISTRT, the reinitialization is done by transferring control to statement number 1210.

A.3.3. Subroutine OUTPUT

Subroutine OUTPUT is divided into six chapters which are now briefly described. It has two entry points, ENTRY OUTP1 in Chapter A, and ENTRY OUTP2 in Chapter B.

Chapter A. Initial printout

This Chapter provides, by way of DATA statements, titles for the dependent variables the cross-stream distributions of which are to be printed out in Chapter E below. Information required by subroutine PLOTS for the line-printer display of profiles is also provided in this Chapter by way of DATA statements. This is divided into two categories: transverse (cross-stream) plot data and longitudinal (down-stream) plot data. Finally some initial printout describing the problem is obtained. This subprogram is called from Chapter 5 of subroutine MAIN.

Chapter B. Headings

This Chapter is used for the printout of the iteration number at the beginning of each marching sweep.

Chapter C. Tests for printout

In this Chapter the index IPRINT, which decides what printout is obtained, is set a value depending on the values of ISTEP, NSTAT, NPROF,...etc. Thus for IPRINT=0 there is no printout; if it equals 1, "station" variables are printed; if it equals 2, "profile" variables are printed; and for IPRINT=3, the variations of the "profile" variables in the cross-stream direction are plotted by the line-printer. These different kinds of printout are discussed below.

Chapter C is also used to insert into the appropriate arrays (XLPLOT, YLPLOT) the variables which are to be employed in the "longitudinal plot"; and for the computation of the convective fluxes of the dependent variables.

If IPRINT equals zero, control returns to the calling program without any further printout.

Chapter D. Station Variables

This Chapter is entered when IPRINT is greater than zero, i.e. whenever ISTEP is a multiple of either NSTAT, NPROF, or NPLOTC.

Variables having a single value for the x-station under consideration are termed as "station variables". These include the longitudinal distance, x, the index IX specifying the location of a grid node in the x-direction, the forward step size DX, the pressure PRESSD (non-dimensionalized as p/p_{inlet} -1), the convective fluxes UFLUX and FLUX(J), and the non-dimensional area errors, DA1 and DA2. All these quantities are printed in this Chapter.

Chapter E. Cross-stream profiles

This Chapter is entered when IPRINT is greater than 1, i.e., whenever ISTEP is a multiple of either NPROF or NPLOTC.

"Profile variables" are those which may be represented as distributions with respect to the cross-stream distance r, and are printed as a consequence of the operations in this Chapter. Thus the u-velocity, temperature, fuel and oxygen concentrations, and the mixture fraction are printed in the DO-1091 loop. The DO-1207 loop results in the printout of the nitrogen concentration, density, viscosity, and enthalpy. Just before this loop, the centerline viscosity is set equal to that at the neighboring radial node; this is for printout purposes only and does not affect the computations. This completes the printout of profile variables for chemically inert flows (INERT=1). For reacting flows the chemical-equilibrium concentrations are printed in the DO-1202 and DO-1203 loops (for IEQUIL=1) and finally for KNTCS=1 the chemical-kinetics concentrations are printed in the DO-1302 loop.

The next section is entered only on the last iteration when IPRINT=3, i.e., when ISTEP is a multiple of NPLOTC. This section provides cross-stream plots of various dependent variables; the programming sequence is easy to interpret.

Chapter F. Longitudinal plots and return

This Chapter is entered when IFIN=2 (i.e., the entire flow field has been covered at a given iteration) and when NITER is a multiple of NPLOTL. Longitudinal plots of the various dependent variables are obtained as a result of the operations in this Chapter.

Finally the maximum changes in the dependent variables from one iteration to the next one are printed out in this Chapter.

A.4 The physical-model subroutines, PHYS and WALL

These two subroutines incorporate the physical models describing the flow situation.

A.4.1 Subroutine PHYS

This subroutine is divided into two chapters, each having its own ENTRY and RETURN statements.

Chapter A. ENTRY PHYSU

The function of this subprogram is to compute the viscosity and the source terms of the u-momentum equation.

Two sections are provided for the computation of viscosity, one for laminar flows and the other for turbulent. After entry into this Chapter, control is transferred to the appropriate section depending on the value of the variable MODEL.

(a) Laminar viscosity:

The laminar viscosity is computed according to the square-root formula and weighted with the mass fractions of the species as discussed in Section 2.7.1. This computation is carried out in the DO-110 loop for all cross-stream points at two planes: the one under consideration (EMUD) and the one upstream of it (EMUU).

(b) Turbulent viscosity:

The turbulent viscosity is computed according to the formulae discussed in Section 2.7.1. Here again as for the laminar case, the EMUD and EMUU arrays are filled with the appropriate viscosity values. In addition, the laminar viscosity at the wall temperature is computed for use in subroutine WALL. For points lying in Sections 2 and 3 of the duct (Fig. 1)the viscosities are multiplied by a factor of 100; this is done as per the discussion of Section 2.10.

In the calculation of turbulent viscosities, the upstream values (EMUU) for the current x-location are set equal to the downstream values (EMUD) of the previous x-location. This avoids recalculation of the same quantitiy.*

* In the computation of laminar viscosities, EMUU is based on the current iteration values of the mixture composition and temperature, and EMUD on the previous iteration values. Therefore EMUU of the current x-location is not set equal to EMUD of the previous x-location; the two will however be equal in the converged state.

Finally in the DO-203 loop the viscosities for the cell boundaries in the ω-direction are obtained by an averaging process; this computation is common to both laminar and turbulent viscosities.

Next the momentum sources are computed. These comprise of the pressure gradient and the axial diffusion term. The contributions to the parts S_i and S_i' of the linearised source term are computed in the DO-210 loop and stored in the arrays SI and SIP respectively.

The DO-210 loop incorporates certain other operations. The diffusion coefficient occurs with the variables AREA, XDIF, and DX for all the dependent variables. Therefore to avoid recomputation, this group of variables is computed only once here and the result stored in the EMUU and EMUD arrays for the upstream and downstream locations respectively. SUMA and SUMB, denoting the summation of EMUD and EMUU respectively over the cross-stream points, are also computed here; these will be required for the longitudinal TDMA for some of the dependent variables.

Subprogram PHYSU is called from subroutine COMP (ENTRY SOLVE, u-velocity section).

Chapter B. ENTRY PHYSF

The function of this subprogram is to compute the transport properties and source terms for the dependent variables stored in the F-array (i.e., stagnation enthalpy, mass fraction of unburnt fuel, and mixture fraction). The three dependent variables are considered individually below.

Firstly after entry into Chapter B, the transport properties are computed in the DO-313 loop. This computation is by-passed when NEWPR for the corresponding dependent variable equals unity (see also Chapter 4 of subroutine MAIN). The computation of diffusion coefficients is straightforward: the diffusion coefficient for a variable J equals that for variable (J-1) multiplied by the ratio of the Prandtl numbers for variables (J-1) and J. When J equals unity, the variable (J-1) is the velocity for which the Prandtl number is treated as being equal to unity. Now the source-term computations are described.

(a) <u>The source of stagnation enthalpy (J=JH)</u>

The programming sequence for computing the source term of the stagnation enthalpy equation begins at statement number 314. The source term is composed of two parts: the kinetic heating term and the axial diffusion term.

First the kinetic heating term corresponding to $\frac{\partial}{\partial\omega}\{(\mu-\Gamma_{\tilde{h}})\frac{\partial}{\partial\omega}(\frac{u^2}{2})\}$ is computed in the DO-322 loop and stored in the SI array. Next the other part of the kinetic heating term corresponding to $\frac{\partial}{\partial x}\{(\mu-\Gamma_{\tilde{h}})\frac{\partial}{\partial x}(\frac{u^2}{2})\}$ is computed in the DO-323 loop and added on to the SI array. Finally the contributions of the axial diffusion term to the two parts S_i and S_i' of the linearised source term are computed. Control is then transferred to statement number 5000 where the LTDMA coefficients ALF and BLF (corresponding to a' and b' of Section 4.4)are obtained.

When $\mu=\Gamma_{\tilde{h}}$, the kinetic heating term vanishes. The source term then consists of only the axial diffusion term. The corresponding programming sequence is contained in the DO-324 loop which is accessed when NEWPR (JH) equals unity, i.e. when $\mu = \tilde{\Gamma}_h$.

(b) The source of fuel (J=JF)

The computation of the source term of the fuel equation begins at statement number 3000. The computation is done according to the linearised source-term expressions described in Section 4.5. The programming sequence is contained in the DO-344 loop and is easy to interpret. The computation of the axial diffusion contribution is also performed here.

It will be noted that an additional entry point, ENTRY SORFU is provided here. This entry point is used during the iterative procedure to determine the fuel concentration for all iterations except the first. A call to subroutine CHEM (ENTRY TEMP) is made at each such iteration to obtained the latest values of the temperature.

Finally control is transferred to statement number 5000 to obtain the LTDMA coefficients ALF and BLF (a' and b' of Section 4.4).

(c) The source of mixture fraction (J=JP)

The source term for this variable consists of only the axial diffusion term. This is computed in the DO-360 loop; the computation is similar to that for the variables discussed above.

Subprogram PHYSF is calle: from subroutine COMP (ENTRY SOLVE, F-Section) once for each of the three variables: $\hat{h}$, f, and m_{fu}.

A.4.2 Subroutine WALL

The function of this subroutine is the calculation of the quantities required for the modification of the finite-difference coefficients for the nodes adjacent to the duct wall. Subroutine WALL has two arguments (OUT1, OUT2), both of which are output quantities from it. OUT1 and OUT2 stand for ϕ and T_E (of equation (76)) respectively when velocity is in question (J=0), they stand for $\delta\phi_E$ and T_E (of the same equation) respectively when enthalpy is the variable in question (J>0).

There are three chapters in this subroutine. Chapter A involves some preliminaries where certain quantities are given values through data statements. A decision is then made depending on the value of J whether to enter Chapter B (J=0) or Chapter C (J>0).

Chapter B is entered for J=0 when velocity is the variable in question. Here some 'reference' values are chosen for density, viscosity, velocity and radius. These are chosen rather arbitrarily. Then if laminar flow is indicated either by MODEL being equal to 1 or the Reynolds number (based on the 'reference' values) being less than 132.25($\equiv 11.5^2$) control is transferred to statement number 110. Here quantities related to laminar flow are computed. Otherwise the turbulent flow section is accessed. The programming sequence for the calculation of OUT1 and OUT2 is easy to interpret and is the Fortran equivalent of the formulae derived in Ref.1 (Chapter 6).

Chapter C is entered for J >0, when enthalpy is the variable in question. Here again there are separate sections for laminar and turbulent flows. The programming sequence follows closely the formulae derived in Ref.1 (Chapter 6).

Subroutine WALL is called from subroutine COMP (ENTRY SOLVE) once for u-velocity and once for enthalpy.

A.5 The chemical-model subroutines, CHEM, SPECE, and CALC

These subroutines incorporate the computations involved with the chemistry of the flow. The chemical-kinetics computations are mainly incorporated in subroutines SPECE and CALC which are simplified versions of those given in Ref.3. These subroutines have been simplified from their original general version to make them more particular to the problem considered here.

A.5.1 Subroutine CHEM

This subroutine is divided into five chapters, each having its own ENTRY and RETURN statements.

Chapter A. ENTRY POLY

The function of this subprogram is to compute the polynomial coefficients at the prevailing pressure by linear interpolation between two neighboring pressure values. Polynomıal coefficients for enthalpy, specific heat, and reciprocal mean molecular weight of the equilibrium-product-species, as functions of temperature are thus obtained.

This subprogram is called from subroutine COMP (ENTRY SOLVE, F-section) when INERT equals 2 (i.e. reacting flows).

Chapter B. ENTRY TEMP

The function of this subprogram is to compute the temperature of the gas mixture for specified stagnation enthalpy, velocity, and composition. The method described in Section 3.7 is followed. On entry into this subprogram indices NS1 and NS2 are set appropriate values depending on whether the chemical-kinetics solution is required (KNTCS=1) or not required (KNTCS=0). In the former case the concentrations of the NO_x-species (which are kinetically determined) at the cross-stream plane under consideration are stored in the FS-array. This is done in the DO-103 loop. These concentrations are those obtained from the previous iteration, since they have not yet been determined at the current iteration. However, since the NO_x-species are present in relatively small amounts, not much error is introduced.

The DO-100 loop spans all the internal cross-stream points. Firstly the mass fraction of unburnt fuel is restricted to be no greater than the mixture fraction. Next the concentrations of oxygen and products (considered as one species) are obtained, the concentration of nitrogen is obtained by a process of subtraction in the DO-102 loop. Finally, the DO-110 loop incorporates the Newton-Raphson iteration scheme for temperature. At each iteration the enthalpy (HPR) and the specific heat (CPR) of the equilibrium-product-species are obtained using polynomial fits; thus the computation of each individual species-concentration is avoided. The number of iterations is restricted to NTMAX or less if the normalised change in temperature from one iteration to the next is less than EPST. Both NTMAX and EPST are defined in Chapter 4 of BLOCK DATA.

Subprogram TEMP is called from subroutine MAIN (Chapter 8) and from subroutine PHYS (the m_{fu} section in ENTRY PHYSF) during the iterative procedure to determine the fuel concentration (Section 4.5) .

Chapter C. ENTRY DENS

The function of this subprogram is to determine the density of the gas mixture. The updating of certain values is also performed here. The density is computed in the DO-200 loop which spans all internal cross-stream points. In obtaining the mean molecular weight of the gas mixture, the contribution of the equilibrium-product-species is obtained by means of a polynomial involving temperature.

The density values at the cross-stream plane corresponding to (ISTRT-1) are stored in the array RHO2; these values will be required if the next iterative sweep is started at an intermediate section IX=ISTRT.

Next the centerline values of the concentrations of oxygen, fuel and nitrogen, and temperature are updated, as also their wall values (except temperature). The updating is done by setting the boundary value equal to that at the neighboring internal node. Finally the wall enthalpy is computed to fit the composition. Subprogram DENS is called from subroutine MAIN (Chapter 8), when INERT equals 2 (reacting flows).

Chapter D. ENTRY EQUIL

The function of this subprogram is to obtain the concentrations of the equilibrium-product-species. This is done by using polynomial expressions described in Section 3.5.4.

The programming sequence is easy to interpret and involves (a) the determination of the polynomial coefficients at the prevailing pressure by linear interpolation between two neighboring pressure values; (b) the selection of the coefficients for the appropriate enthalpy-range; (c) determination of the equilibrium concentrations; and (d) the updating of the boundary values of these concentrations by setting them equal to the values at the neighboring internal node.

This subprogram is called from subroutine MAIN (Chapter 8), when INERT equals 2 (reacting flows), and IEQUIL equals unity.

Chapter E. ENTRY KINE

This subprogram is used to obtain the concentrations of the NO_x-species by reference to kinetically-controlled reactions.

Firstly inital estimates for the concentrations of the NO_x-species are specified at the cross-stream plane being solved for and the one downstream of it. This is done by simply setting these values equal to those at the corresponding upstream grid node. This is done in the DO-482 loop which is accessed only during the first iterative sweep for the solution of the NO_x-species (i.e. NITER= NITERK); the chemical-kinetics solution is started after other variables have undergone NITERK number of iterative sweeps and have stabilized to a certain extent.

Next the finite-difference coefficients A and B expressing the links to the neighboring cross-stream points are computed. This is done in the DO-470 loop which is accessed only when the variable NEWPR is not equal to unity (see also Subroutine MAIN, Chapter 4).

The DO-487 loop spans all the internal cross-stream points. In this loop the following operations are performed at each grid node :

- computation of finite-difference coefficients C and D which express the links with the neighboring upstream and downstream grid nodes respectively;

- computation of the mole numbers of all the species and storing them in the S2-array (DO-486 loop) ;

- computation of the weighted averages of the mole numbers of the NO_x- species at the four neighboring nodes and storing them in the S1-array (DO-488 loop) (this corresponds to σ_i^* of equation (91), Section 3.6.1);

- a call to subroutine SPECE to obtain the chemical-kinetics solution (i.e.mole numbers of the NO_x-species) for temperatures greater than 550°K;

- conversion of the mole numbers to mass fractions (DO-489 and DO-490 loops);

- adjusting the mass fraction of nitrogen to ensure that all mass fractions add to unity (DO-493 loop).

It will also be noted that should a converged solution be not obtained from subroutine SPECE (as indicated by CONVG= .FALSE.) a warning message is printed out and the NO_x-species-concentrations set equal to the weighted averages of their concentrations at the four neighboring nodes (DO-502 loop). This is also done for temperatures not greater than 550°K.

Finally the values of the NO_x-species-concentrations at the boundary nodes are updated by setting them equal to the values at the corresponding neighhboring internal node.

Subprogram KINE is called subroutine MAIN (Chapter 8) when NITER ≥ NITERK and KNTCS=1.

A.5.2 Subroutine SPECE

The function of this subroutine is to control the Newton-Raphson iteration procedure for the solution of the chemical-kinetics equations as described in Section 3.6. This subroutine consists of five chapters.

In Chapter 1 the logarithms of the species mole-numbers are computed in the DO-10 loop. The sum of the species mole-numbers and its logarithm are also computed here. The size of the correction matrix, IMAT, is then specified.

In Chapter 2 the main iteration loop (DO-170) is started. The elements of the Newton-Raphson correction matrix are set up by a call to subroutine CALC. Subsequent statements in Chapter 2 involve the standard Gaussial pivotal elimination solution procedure for the correction matrix.

In Chapter 3 the under-relaxation parameter ETA is computed as described in Ref.2.

In Chapter 4 the species mole numbers are corrected, the corrections being scaled by the factor ETA.

In Chapter 5 the convergence criterion is applied (Section 3.6. 3). If all the species mole numbers have converged to within a user-specified tolerance limit EPSS, the variable CONVG is set equal to .TRUE., and iteration is stopped. Otherwise the same set of operations is repeated until convergence is achieved; the maximum number of iterations being restricted to ITMAX. Values of both ITMAX and EPSS are set in BLOCK DATA (Chapter 4).

Provision is made for printout of several quantities for diagnostic purposes at various stages of this subroutine. This printout is triggered by setting IDEBUG equal to two in Chapter 4 of BLOCK DATA.

Subroutine SPECE is called from subroutine CHEM (ENTRY KINE).

A.5.3 Subroutine CALC

The function of this subroutine is to construct the Newton-Raphson correction matrix for the solution of the chemical-kinetics equations as described in Section 3.6. This subroutine consists of three chapters.

In Chapter 1 all the elements of the correction matrix are initialised to zero. The mixture density is also computed.

In Chapter 2 the forward and reverse rates for each reaction are computed in the DO-100 loop. Only three different types of reactions have been considered:

MODE = 1 : $A + B \rightarrow C + D$
MODE = 2 : $AB + M \rightarrow A + B + M$
MODE = 3 : $A + B + M \rightarrow AB + M$

Relevant Fortran statements are provided to determine the reaction type and for MODES 2 and 3, control is transferred to statements 20 and 30 respectively. Subsequent statements compute the correction matrix elements as per the equations given in Section 3.6. All these operations are performed for each reaction in the DO-100 loop.

Chapter 3 completes the calculation of the matrix elements; the term $A_p\sigma_i$ of equation (91) is added to the diagonal elements and the term A_p $(\sigma_i - \sigma_i*)$ of equation (91) is added to the last column of the correction matrix.

Subroutine CALC is called from Chapter 2 of subroutine SPECE.

A.6 The computational subroutines, COMP, START, and PLOTS

A.6.1. Subroutine COMP

This subroutine is divided into five chapters, each having its own ENTRY and RETURN statements.

Chapter A. ENTRY INIT

The function of this subprogram is to perform some initializing operations at the beginning of an integration sweep. Default values are also set in this Chapter.

This subprogram is called from Chapter 2 of subroutine MAIN at the beginning of the computations, and then again from Chapter 14, just before the start of the next integration sweep.

Chapter B. ENTRY GRIDX

The function of this subprgram is to compute quantites associated with the x-(or longitudinal) grid.
These quantities are:

- XS(J), the width of a finite-difference cell at grid node J, in terms of x-distance;

- XDIF(J), the difference in the values of x at grid nodes J and J+1.

It will be noted that appropriate modifications are made for the finite-difference cells located at the boundaries of the flow domain. (J=2, J=LM1). This subprogram is called from Chapter 2 of subroutine MAIN.

Chapter C. ENTRY GRIDOM

The function of this subprogram is to compute quantities associated with the ω-grid. These quantities are:

- OMINT(I), the value of ω for a finite-difference cell interface between grid nodes I and I+1;

- BOM(I), the width of a finite-difference cell in terms of ω;

- OMDIF(I), the difference in the values of ω at grid nodes I and I-1.

It will be noted that appropriate modifications are made to these quantities for the cells located at the boundaries of the calculation domain (i.e., I=2 and N-1).

This subprogram is called from Chapter 2 of subroutine MAIN. It is called again from Chapter 5 of subroutine MAIN in case the ω -grid has been redistributed so as to locate a cell boundary at the interface between the streams of fuel and air entering the duct.

Chapter D. ENTRY DISTAN

The function of this subprogram is the computation of the product (ρu) and the radius r for each grid node, and the cell areas. The computation is incorporated in the DO-231 loop. The computation of (ρu)'s and cell areas is straightforward. These are stored in the arrays RU and AREA respectively. The computation of the radii is done according to the equations given in Section 4.3.

The quantity B_{pE} of equation (108) required during these computations is available from an earlier visit to subroutine WALL. The variable B_{pE} is assigned a value of unity in Chapter A of subroutine COMP; this is the value used when DISTAN is called for the very first time. When a intergration sweep is started at an intermediate x-station (IX=ISTRT), the value of B_{pE} appropriate to this x-station is obtained from BPSAVE (which was stored during the previous integration sweep; see statement towards end of u-velocity section, Chapter E, subroutine COMP)

Subprogram DISTAN is called from Chapter 10 of subroutine MAIN at two different stages. The first call is to obtain the (ρu) values which are used subsequently to compute DADP, the dependence of area on pressure. The second call is made during the course of adjustment of the calculated flow area to match the duct area.

Chapter E. ENTRY SOLVE

The function of this subprogram is to compute the finite-difference coefficients and solve the resulting finite-difference equations. Because the u-velocity is treated differently from the other dependent variables, there are two sections in this subprogram: one solves for the u-velocity, the other solves for the other dependent variables (stored in the F-array). These two sections are now discussed separately.

(a) The u-velocity section:

After entrv into this Section, the variable RSUMAX which denotes the maximum normalised change in u-velocity from one iteration to the next, is initialised to zero. This initialisation is done only at the start of the integration sweep which may be either at the start of the flow domain or at an intermediate x-station (IX=ISTRT).

Next a call to subroutine PHYS at ENTRY PHYSU is made to compute the viscosities and the source terms. The subsequent computation of the finite-difference coefficients A,B in the DO-413 loop, and C,D in the DO-418 loop is straightforward. The programming sequence is the Fortran equivalent of equations (72)-(75) of Section 3.3.3. During the course of these computations a call to subroutine WALL is made and the coefficient A at the wall boundary is correspondingly modified (See Chapter 4 of Ref.1).

A provision is made for the printout of the coefficients A,B,C,D, SI and SIP for diagnostic purpose, this print-out is triggered by setting a value of 2 for the index ITEST in BLOCK DATA.

The next step is the solution of the finite-difference equations. This involves a standard application of the TDMA; the programming is contained in the DO-421 and DO-420 loops. The computation of the velocities for the downstream points is performed in the DO-420 loop.

The shear stress at the wall is then computed. The u-velocity at the centerline is updated on the basis of the zero-gradient condition at the symmetry axis. This is done by simply setting the centerline value equal to that at the neighboring radial grid node. It should be mentioned that the computation of symmetry axis values is a purely 'decorative' exercise and does not influence any further computations. Alternative practices of determining the centerline values (e.g. by extrapolation) may be introduced by the user if so desired.

(b) The F-Section:

The structure of this section is similar to that already described for the u-velocity. This section is embedded in the DO-480 loop, which causes the index J to run from 1 to NF. The index J denotes the particular dependent variable in question (i.e., 1 for stagnation enthalpy, 2 for mixture fraction, etc.) and NF stands for the number of dependent variables (excluding u-velocity and the species concentrations determined by kinetically-controlled reactions) for which a differential equation is solved.

The computation of the finite-difference coefficients (DO-484 and DO-485 loops), the modifications of the coefficients at the wall, the TDMA solution (DO-465 and DO-466 loops), the updating of F-values at the boundaries, are all similar to the operations performed for u-velocity. The corresponding programming sequence is easy to interpret. Provision for diagnostic printout is made here also.

There are four additional features in the F-section which will now be described.

(i) The computation of the coefficients A and B in the DO-484 loop is skipped if NEWPR(J) (defined in Chapter 4 of subroutine MAIN) equals unity.

(ii) The iterative procedure to determine the fuel concentration is contained in this section. This involves performing the operations described above several times, subject to a maximum number NFUMAX, or less if the normalised change in the fuel concentration from one iteration to the next is less than FUTEST (FUTEST and NFUMAX are specified in BLOCK DATA).

(iii) The longitudinal TDMA: The programming sequence incorporating the LTDMA commences at statement number 4314. The LTDMA operations are not performed when solving for the mixture fraction (J=JP) since this would not significantly enhance convergence rates. The LTDMA coefficients CLF and DLF (corresponding to c' and d' of Section 4.4) are computed in the DO-492 loop; coefficients ALF and BLF (corresponding to a' and b') are computed earlier in subroutine PHYS. The TDMA solution and the incrementing of the dependent variables by the LTDMA corrections are incorporated in the DO-4310 and DO-4320 loops.

(iv) For non-reacting flows (INERT=1), control is transferred from the early part of the F-section to statement number 4410 towards the end of this section, when the fuel concentration is the variable in question (J=JF). Here the fuel concentration is simply set equal to the mixture fraction in the DO-4411 loop and the solution sequence for the fuel concentration is skipped. It will also be noted that the call to subroutine CHEM at ENTRY POLY (before commencement of the DO-480 loop) to set up polynomial coefficients relating to equilibrium-product-species is skipped if INERT equals 1.

Subprogram SOLVE is called from Chapter 8 of subroutine MAIN.

A.6.2 Subroutine START

The function of this subroutine is to obtain a one-dimensional solution which will be used as the initial guess for the two-dimensional solution. There are seven chapters in this subroutine. The coding follows the discussion of Section 4.6.

Chapter 1. Preliminaries

Preliminary operations are performed in this Chapter. Some thermodynamic-property-data required for the one-dimensional computations are supplied through DATA statements. Properties at the inlet plane are computed as an average of those of the entering fuel and air streams (weighted by the respective mass flow rates). The temperature and composition of fully-burnt gas are also computed.

Chapter 2. Initial guess

In this Chapter the initial guess for the one-dimensional solution is specified. In section 1 (Fig.1) of the duct this corresponds to the unburnt condition; in Section 3 to the fully-burnt condition. In section 2 an exponential variation of the fuel mass fraction and temperature between the unburnt and the fully-burnt values is employed.

Chapter 3. Transport Properties

In this Chapter the laminar or turbulent viscosities are computed depending on the type of flow. The sequence of Fortran statements is similar to that described in Subroutine PHYS (ENTRY PHYSU).

Chapter 4. Main Solution Loop

This Chapter incorporates the main solution procedure in the DO-335 loop. The solution sequence is entirely skipped when the mixture fraction (J=JP) is the variable in question since the one-dimensional solution for it is a uniform value throughout the flow field.

Firstly the finite-difference coefficients ALF and BLF, expressing the links to the downstream and upstream neighboring points are computed. Next the source terms are computed and control is transferred to the appropriate section depending upon the variable being solved for. For the stagnation enthalpy (J=JH) equation, the effect of heat transfer to the duct wall is included. The source terms for the fuel equation (J=JF) are computed as already described in subroutine PHYS (ENTRY PHYSF).

The solution of the finite-difference equations commences at statement number 331. This involves a standard application of the TDMA and is carried out in the DO-332 and DO-333 loops. The maximum normalised changes of the variables from the previous iteration are also computed in the DO-333 loop.

Chapter 5. Completion of an iteration

In this Chapter an iteration is completed after the computation of some auxiliary quantities. These are: the mass fractions of oxygen and the product species and the temperature. This is done in DO-440 loop. Next the exit boundary condition of zero gradient is applied.

Chapter 6. Print

In this Chapter the solution is printed out as decided by the value of N1DPR (assigned in BLOCK DATA). The printout occurs at the first and last iterations and every N1DPR intermediate iterations. If the maximum changes in the dependent variables are less than a user-specified convergence criterion EPS1D, the value of N1DMAX (denoting maximum number of one-dimensional iterations) is set equal to the current number of iterations NIT. This causes the solution to be terminated in Chapter 7.

Chapter 7. Complete

In this chapter the one-dimensional solution is stored at all cross-stream grid nodes (for given axial distance). This will now form the starting point for the two-dimensional solution.

Subroutine START is called from Chapter 5 of subroutine MAIN.

A.6.3 Subroutine PLOTS

The function of this subroutine is to generate an on-line plot of a dependent variable Y as a function of radius r (cross-tream plots) or axial distance x (longitudinal plots). Both the abscissa and the ordinate are normalised in this subroutine before plotting, so as to fall within the range 0 to 1.

Information is conveyed to the subroutine by way of its 8 arguments. The subroutine itself requires no alteration by the user, except to change the horizontal and the vertical dimensions of the plots. This is done by specifying appropriate values for the variables XSIZE and YSIZE. On each plot the following information is provided: the location of the plot, the maximum and minimum values of the abscissa and all the ordinates. For further details, the reader is asked to refer to the comment cards in the listing of the subroutine (Appendix B).

A.7 The thermochemical property subroutines, CREKO and HCPS

These subroutines are concerned with the input and calculation of certain thermodynamic quantities. They have been adapted from Ref.3 with some changes.

A.7.1. Subroutine CREKO

The function of this subroutine is to read, store and process thermochemical data. This subroutine is divided into 4 chapters.

In Chapter 1 certain quantities are defined through data statements. Then follow statements which cause control to be transferred to the appropriate chapter. This depends on which of the words ELEMENTS, THERMO, MECHANISM, or a blank card is encountered in the data deck. Data cards must be in this order, since element data is needed to process thermodynamic data, and thermodynamic data for kinetic-mechanism data. If the chemical-kinetics solution is not required (i.e,KNTCS=0), the kinetic-mechanism data is not read.

Chapter 2 deals with element data. Here one data card is read for each element considered. The contents and format of each data card are given in Table A.1. The total number of elements is designated by NLM.

Chapter 3 deals with thermochemical data. Entry into Chapter 3 occurs after completion of Chapter 2 and via statement number 5. Four data cards are read for each chemical species considered. The contents and format of each data card are given in Table A.2 . After the data cards for each species are read, its molecular weight is computed in the DO-24 loop. The total number of species is designated by NS.

The polynomial coefficients Z(I,J,K) for the thermodynamic properties are divided by the respective molecular weights in the DO-27 loop. Since the present program performs computations with species mass fractions rather than mole numbers, the coefficients will be required in this modified form.

Chapter 4 deals with kinetic-mechanism data. Entry into Chapter 4 occurs after completion of Chapter 3 and via statement number 5. One data card is read for each reaction considered. The contents and format of each data card are given in Table A.3 . In statements 33 to 38, the numbers to be stored in the ID (N,J) array are calculated. ID (N,J) is equal to the species index number I (I=1,NS) of the Nth (N=1,4) species which appears in the Jth (J=1,JJ) reaction.

TABLE A.1

ELEMENT DATA CARDS

Order of data cards	Contents	Format	Card Columns
First	ELEMENTS	3A4	1 to 8
Any order	One card for each element present in the system. Each card contains:		
	(i) Atomic symbol of element.	A2	1 to 2
	(ii) Atomic weight of element.	F10.6	8 to 17
	(iii) Valence or oxidation state of the element (positive, negative. or zero).	F10.6	18 to 27
Last	Blank card.	-	-

TABLE A.2

THERMOCHEMICAL DATA CARDS

Order of data cards	Contents	Format	Card Columns
First	THERMO	3A4	1 to 6
Any order	A set of four data cards for each species considered. The cards in sequence and contain:		
	(1)(a) Molecular symbol or name of species.	3A4	1 to 12
	(b) Date.	2A3	19 to 24
	(c) Atomic symbols & formula	4(A2,F3.0)	25 to 44
	(d) Phase (gas only, letter G).	A1	45
	(e) Temperature range, degrees K.	2F10.3	46 to 65
	(f) Card number.	I15	80
	(2)(a) Coefficients $Z_i (i=1,5)$ for upper temperature range.	5E15.8	1 to 75
	(b) Card number.	I5	80
	(3)(a) Coefficients Z_6 and Z_7 for upper temperature range, and Z_1, Z_2, and Z_3 for the lower range.	5E15.8	1 to 75
	(b) Card number.	I5	80
	(4)(a) Coefficients $Z_i (i=4,7)$ for the lower temperature range.	4E15.8	1 to 60
	(b) Card number	I20	80
Last	Blank Card.	-	-

TABLE A.3

REACTION MECHANISM DATA CARDS

Order of data card	Contents	Format	Card Columns
First	MECHANISM	3A4	1 to 9
Any order	One data card for each forward (or optionally, reverse) reaction considered. Each card contains:		
	(i) Molecular symbols of upto three reactant species*.	3(2A4)	1 to 24
	(ii) Molecular symbols of upto three product species*.	3(2A4)	25 to 48
	(iii) Exponent B_j**.	F8.3	49 to 56
	(iv) Exponent N_j**.	F8.3	57 to 64
	(v) Activation temperature T_{actj}**.	F8.3	65 to 72
	(vi)(a) For forward reactions, date or comments.	2A4	73 to 80
	(b) For reverse reactions, REVERSE+.	2A4	73 to 79
Last	Blank card.	-	-

*Molecular symbols must be identical to those used in thermochemical data cards.

**Quantities as defined in:

$k_{fj} = 10^{B_j} T^{N_j} \exp(-T_{actj}/T)$ with units

$m^3/$ (kg-mole-sec) for bimolecular reactions,

and $m^6/$ (kg-mole)^{2}sec for termolecular reactions.

+When REVERSE is specified, Columns 1 to 48 are ignored. The data card with reverse rate data must follow immediately the card with the corresponding forward rate data.

Thus for the reaction

$N + NO = N_2 + O$ (Jth reaction),

ID (1,J)=IDN, ID(2,J)=IDNO, ID(3,J)=IDN2, ID(4,J)=IDO. IDN, IDNO, etc., which identify the different species are defined in Chapter 3 of subroutine BLOCK DATA.

The rest of Chapter 4 is devoted to the computation of the reverse reaction rates, for each forward reaction rate just read in. The reverse reaction rate constant is obtained from the ratio of the forward reaction rate constant and the equilibrium constant. This is done for fifteen temperatures between $1000^{O}K$ and $3000^{O}K$ and the reverse rate parameters are obtained by a least-square linear regression analysis. Details of this computational procedure are given in Ref.3.

If however, the reverse rate data is also supplied on a data card which is subsequently read, the calculated reverse rate parameters are overwritten. This is indicated by the statements just preceding statement number 32.

Subroutine CREKO is called from Chapter 4 of subroutine MAIN.

A.7.2 Subroutine HCPS

The function of this subroutine is to compute certain thermodynamic quantities (See Section 5.2).

On entry into this subroutine a check is made to see if the temperature is less than $1000^{O}K$; this is to decide whether to use the coefficients for the lower (temperature $< 1000^{O}K$) or the higher (temperature $\geq 1000^{O}K$) temperature range. Depending on the value assigned to the variable IHCPS, the following properties are computed:

(i)   IHCPS = 1: The non-dimensional species enthalpy HO(I) and the non-dimensional mixture enthalpy

HSUM are computed in the DO-5 loop.

(ii) IHCPS = 2: The non-dimensional species enthalpy HO(I), the non-dimensional mixture enthalpy HSUM and the non-dimensional mixture specific heat CPSUM are computed in the DO-10 loop.

(iii)IHCPS = 3: The non-dimensional species enthalpy HO(I), and the non-dimensional species entropy SO(I) at one-atmosphere are computed in the DO-20 loop.

Subroutine HCPS is called from:

(a) Subroutine CREKO, Chapter 4, during the computation of reverse reaction rate parameters, with IHCPS=3;

(b) Subroutine MAIN:

- Chapter 5, to obtain inlet enthalpies of the fuel and air streams, with IHCPS=1;
- Chapter 7, to obtain the wall enthalpy, with IHCPS=1;
- Chapter 9, to obtain the mixture enthalpy and specific heat, with IHCPS=2;

(c) Subroutine CHEM;

- Chapter B (ENTRY TEMP), to obtain the mixture enthalpy and specific heat, with IHCPS=2;
- Chapter C (ENTRY DENS), to obtain the wall enthalpy with IHCPS=1.

APPENDIX B

LISTING OF THE NASCO COMPUTER PROGRAM

```
      COMA     PROC
              COMMON
             1 ADUCT(35),ALF(35,3),BLF(35,3),CLF(35),DLF(35,3),
             2 ELF(35),F(350,9),U(350),XDIF(35),XS(35),
             3 ARFA(10),ARFAU(10),BOM(10),DIF(10),DIFU(10),EMU(10),EMUD(10),
             4 EMUU(10),FS(10,15),OMINT(10),R(10),RESIDU(10),RESU(10),RHO(10),
             5 RHO1(10),RHO2(10),RU(10),SI(10),SIP(10)
              COMMON /COMA/ OM(10),X(35),
             6 AK,BFRAC,BIG,DAMIN,DPDX,DX,EPSF,EPST,EPS1D,
             7 EWAL,FMIN,FSTOIC,FSTOIM,FUTEST,H,IPEX(3),IDEBUG,IEND,IFIN,IGN,
             8 IMAX,IPLOT(30),IPLOTL,IPLOTM,ISPEC(14),IRMFX(3),IRMFY(3),IRHUX,
             9 IRMUY,ISTEP,ISTRT,ISWP,ITEST,IX,IXY,IY,J,JF,JH,JMAX,JN,JNO,JNO2,
             1 JN2O,JOX,JP,JTE,L,LM1,LM2,MODEL,N,NDAMAX,NEWPR(7),NF,NFUMAX,
             2 NITER,NITERK,NITMAX,NM1,NM2,NM3,NPRINT,NTMAX,N1DMAX,N1DPR,PFRAC,
             3 PRLT(7,2),PSIE,RE,RI,RSFMAX(3),RSUMAX,TAUE,TMAX,THIN,XD,XU
              DIMENSION AMUD(35),AMUU(35),PR(35),PRL(7),PRT(7)
              EQUIVALENCE (PRLT(1),PRL(1)),(PRLT(8),PRT(1))
              EQUIVALENCE (ALF(1,2),AMUD(1)),(BLF(1,2),AMUU(1)),(DLF(1,2),PR(1))
        END

      COMB     PROC
              COMMON/COMB/
             1 ARRCON,DA1,DA2,EQRAT,INERT,PREEXP,PRESS,STOICH,UBAR,
             2 VISFU,VISMIX,VISOX,VISPR
        END

      COMC     PROC
              COMMON/COMC/
             1 AREX(3),BREX(3),CREX(3),DWALL(3),EWALL(3),FWALL(3),XD(3),
             2 CMIX,ENTHB,ENTHC,FLOB,FLOC,FUB,FUC,GAMMA,IPRINT,KASE,NSTAT,
             3 NPROF,NPLOTC,NPLOTL,OXB,OXC,PRLAM,PRTURB,RDIV,REXD,REY,TB,TC,UB,
             4 UC,UFLUX,WMIX
        END

      COMD     PROC
              LOGICAL CONVG,DEBUG
              COMMON /INDEX/ IDCO,IDCO2,IDF,IDH,IDH2,IDH2O,IDO,IDOH,IDO2,IDN,
             1 IDNO,IDNO2,IDN2,IDN2O,IEQUIL,IHCPS,IMAT,IPP,ITER,JJ,KNTCS,NA,NLM,
             2 NS,NSE1,NSE2,NSK,NSM,NS1,NS2,ID(4,15)
             3/PARAMS/ CONVG,DEBUG,FMV,EPSS,GASCON,ITMAX,PA,SH,TINY,TINYK,TK,
             4 TLN,TNY
             5/SPECES/ASUB(20,3),CPSUM,HSUM,HO(14),SMW(14),SO(14),S1(14),
             6 S2(14),Z(2,7,14)
             7 /CEQUIL/AC(4,5),AFS(4,7,2),AH(4,5),AS(4,5),AS1(4,7,5),BS1(4,7,5),
             8 HDIV,HMAX,HMIN,PMAX,PMIN
             9/REACTS/BX(15),BX2(15),TACT(15),TACT2(15),TEN(15),TEN2(15)
        END
```

```
C
C-----------------------------------------------------------------------
CHAPTER 1  1  1  1  1  1  1  1  PRELIMINARIES  1  1  1  1  1  1  1  1
C-----------------------------------------------------------------------
C
C ---------- DIMENSIONS AND COMMON BLOCKS.
      INCLUDE COMA,LIST
      INCLUDE COMB,LIST
      INCLUDE COMC,LIST
      INCLUDE COMD,LIST
C
C     ------------------------------------------------------------------
C ---------- ARITHMETIC STATMENT FUNCTIONS.
      REX(X,I)=AREX(I)+(BREX(I)+CREX(I)*(X-XD(I)))*(X-XD(I))
      TWALL(X,I)=DWALL(I)+(EWALL(I)+FWALL(I)*(X-XD(I)))*(X-XD(I))
C-----------------------------------------------------------------------
CHAPTER 2  2  2  2  2  2  2  GRID AND GEOMETRY  2  2  2  2  2  2  2  2
C-----------------------------------------------------------------------
C
C ----------SEE BLOCK DATA FOR THE SPECIFICATION OF GRID AND GEOMETRY.
      CALL INIT
      CALL GRIDX
      CALL GRIDDM
      DO 225 JX=1,L
      XJX=X(JX)
      DO 215 I=1,3
      IF (XJX.LT.XD(I)) GO TO 220
  215 CONTINUE
      I=4
  220 ISEC=I-1
      REXD=REX(XJX,ISEC)
  225 ADUCT(JX)=0.5*REXD**2
C
C-----------------------------------------------------------------------
CHAPTER 3  3  3  3  3  3  3  DEPENDENT VARIABLES  3  3  3  3  3  3  3
C-----------------------------------------------------------------------
C
C ---------- SEE BLOCK DATA FOR DEPENDENT VARIABLE SPECIFICATION.
C           U(I)       = VELOCITY.
C           F(I,JH)    = STAGNATION ENTHALPY.
C           F(I,JP)    = MIXTURE FRACTION.
C           F(I,JF)    = MASS FRACTION OF UNBURNT FUEL.
C           F(I,JOX)   = MASS FRACTION OF OXYGEN.
C           F(I,JTE)   = ABSOLUTE TEMPERATURE.
C           F(I,JN)    = MASS FRACTION OF SPECIES N.
C           F(I,JNO)   = MASS FRACTION OF SPECIES NO.
C           F(I,JNO2)  = MASS FRACTION OF SPECIES NO2.
C           F(I,JN2O)  = MASS FRACTION OF SPECIES N2O.
C
C-----------------------------------------------------------------------
CHAPTER 4  4  4  4  4  4  4  4  PROPERTY DATA  4  4  4  4  4  4  4  4
C-----------------------------------------------------------------------
C
C ---------- SEE BLOCK DATA FOR SPECIFICATION OF PROPERTIES.
      CALL CREKO
      GAMMA=CMIX/(CMIX-GASCON/WMIX)
      DO 40 J=1,JN20
      PRL(J)=PRLAM
   40 PRT(J)=PRTURB
      NEWPR(1)=2
      IF (ABS(PRLT(1,MODEL)-1.0).LT.TINY) NEWPR(1)=1
      DO 41 J=2,JN20
      NEWPR(J)=2
      IF (ABS(PRLT(J,MODEL)-PRLT(J-1,MODEL)).LT.TINY) NEWPR(J)=1
   41 CONTINUE
      FSTOIC=OXC/(OXC+STOICH)
      FSTOIM=1.0-FSTOIC
C
C-----------------------------------------------------------------------
CHAPTER 5  5  5  5  5  5  5  STARTING VALUES  5  5  5  5  5  5  5  5
C-----------------------------------------------------------------------
C
C ---------- SEE BLOCK DATA FOR SPECIFICATION OF STARTING VALUES.
      INSAVE=INERT
      ADUCTD=ADUCT(1)
      PRESS1=PRESS
      PR(1)=PRESS
      PDGSCN=PRESS/GASCON
      PRB=1.0-OXB-FUB
      PRC=1.0-OXC-FUC
      WB=OXB/SMW(IDO2)+FUB/SMW(IDF)+PRB/SMW(IDN2)
      WC=OXC/SMW(IDO2)+FUC/SMW(IDF)+PRC/SMW(IDN2)
      RHOB=PDGSCN/(WB*TB)
      RHOC=PDGSCN/(WC*TC)
      REXD=REX(0.0,1)
      REXDSQ=REXD**2
      FLOB=RHOB*UB*0.5
      FLOC=RHOC*UC*0.5
      RDIVSQ=REXDSQ/(1.0+FLOB*STOICH/((FLOC+TINY)*EQRAT*OXC))
      RDIV=SQRT(RDIVSQ)
      FLOB=FLOB*RDIVSQ
      FLOC=FLOC*(REXDSQ-RDIVSQ)
      OMDIV=FLOB/(FLOB+FLOC)
      PSIE=FLOB+FLOC
C ---------- SEQUENCE TO PUT CELL BOUNDARY AT OMDIV.
      IF(OMDIV.LE.1.E-10.OR.OMDIV.GE.(1.-1.E-10)) GO TO 53
      DO 52 I=2,NM1
      IF(OMINT(I)-OMDIV) 52,53,57
   57 IDIV=I+1
      GO TO 58
   52 CONTINUE
   58 FAC=OMDIV/OMINT(IDIV-1)
      DO 59 I=2,IDIV
   59 OM(I)=OM(I)*FAC
      CALL GRIDOM
      CALL OUTP1
C ---------- ONE-DIMENSIONAL SOLUTION OBTAINED FROM SUBROUTINE START.
   53 IF(NF.NE.0) CALL START
      TK=TB
      IHCPS=1
      NS1=IDN2
      NS2=IDO2
      S2(IDN2)=PRB
      S2(IDF)=FUB
      S2(IDO2)=OXB
      CALL HCPS
      ENTHB=(HO(IDO2)*OXB+HO(IDF)*FUB+HO(IDN2)*PRB)*GASCON*TB
      TK=TC
      CALL HCPS
      ENTHC=(HO(IDO2)*OXC+HO(IDF)*FUC+HO(IDN2)*PRC)*GASCON*TC
C ---------- INSERTION INTO ARRAYS.
      DO 501 IY=1,N
      DO 506 JX=2,3
      IXY=IY+(JX-1)*N
      F(IXY,JN)=1.0E-20
      F(IXY,JNO)=1.0E-15
      F(IXY,JNO2)=1.0E-20
  506 F(IXY,JN2O)=1.0E-20
      IF (OM(IY).GT.OMDIV) GO TO 503
      DO 504 JX=1,3
      IXY=IY+(JX-1)*N
      U(IXY)=UB
      F(IXY,JH)=ENTHB
      F(IXY,JOX)=OXB
  504 F(IXY,JP)=FUB
      F(IY,JF)=FUB
      F(IY,JTE)=TB
      FS(IY,IDN2)=PRB
      FS(IY,IDO2)=OXB
      FS(IY,IDF)=FUB
      RHO(IY)=RHOB
      RHO1(IY)=RHOB
      RHO2(IY)=RHOB
      GO TO 501
  503 CONTINUE
      DO 505 JX=1,3
      IXY=IY+(JX-1)*N
      U(IXY)=UC
      F(IXY,JH)=ENTHC
      F(IXY,JOX)=OXC
  505 F(IXY,JP)=FUC
      F(IY,JF)=FUC
      F(IY,JTE)=TC
      FS(IY,IDN2)=PRC
      FS(IY,IDO2)=OXC
      FS(IY,IDF)=FUC
      RHO(IY)=RHOC
      RHO1(IY)=RHOC
      RHO2(IY)=RHOC
  501 CONTINUE
      IF(NF.GT.0) GO TO 700
      JXX=0
      DO 510 JX=2,L
      JXX=JXX+N
      DO 510 IY=1,N
      IXY=IY+JXX
      F(IXY,JF)=F(IY,JF)
      F(IXY,JOX)=F(IY,JOX)
  510 F(IXY,JTE)=F(IY,JTE)
C
```

```
C ---------- ENTER MAIN LOOP AT CHAPTER 7.
      GO TO 700
C----------------------------------------------------------------------
CHAPTER 6  6  6  6  6  6 START OF A NEW FORWARD STEP 6  6  6  6  6  6  6
C----------------------------------------------------------------------
C
  600 DX=XS(IX+1)
      XD=XU+DX
      IF (NITER.GT.0) GO TO 70
      INERT=1
      IF(Y(IX+1).GT.XD(2)) INERT=INSAVE
      IF (IX.EQ.1) GO TO 70
      IXN=IX*N
      IXNU=IXN-N
      IXND=IXN+N
      DO 602 IY=1,N
      UU=U(IY+IXNU)
      U(IY+IXN)=UU
      U(IY+IXND)=UU
      DO 602 J=1,JMAX
      IF (J.EQ.JF.OR.J.EQ.JTE) GO TO 602
      FU=F(IY+IXNU,J)
      F(IY+IXN,J)=FU
      F(IY+IXND,J)=FU
  602 CONTINUE
      GO TO 70
C
C----------------------------------------------------------------------
CHAPTER 7  7  7  7  7  7  7 BOUNDARY CONDITIONS 7  7  7  7  7  7  7  7
C----------------------------------------------------------------------
C
C ---------- BOUNDARY CONDITIONS AT E BOUNDARY(DUCT WALL).
  700 TAUE=0.0
      IF (MOD(NITER,ISWP).NE.0.AND.ISTRT.NE.1) TAUE=TAUSAV
      IF (NITER.GT.0) GO TO 900
      IBEX(JH)=1
      DO 7413 J=2,NF
 7413 IBEX(J)=2
      IHCPS=1
      NS1=IDN2
      NS2=IDO2
      DO 7414 JX=1,L
      DO 705 I=1,3
      IF (X(JX).LT.XD(I)) GO TO 710
  705 CONTINUE
      I=4
  710 ISEC=I-1
      IXY=JX*N
      U(IXY)=0.0
      TK=TWALL(X(JX),ISEC)
      F(IXY,JTE)=TK
      IF(JX.GT.2) GO TO 7414
      CALL HCPS
      F(IXY,JH)=(HO(IDO2)*OXC+HO(IDF)*FUC+HO(IDN2)*PRC)*GASCON*TK
 7414 CONTINUE
      GO TO 900
C----------------------------------------------------------------------
```

```
CHAPTER 8  8  8  8  8  8  8  8  ADVANCE  8  8  8  8  8  8  8  8  8  8
C-----------------------------------------------------------------------
C
C ---------- ESTIMATED PRESSURE GRADIENT.
C           PRESSURE GRADIENT DUE TO AREA CHANGE.
   70 AFLOWU=AFLOWD
      ADUCTD=ADUCT(IX+1)
      DA=ADUCTD-AFLOWU
      DPDX=DA/(DADP*DX)
C ---------- PRESSURE GRADIENT DUE TO WALL SHEAR.
      DPDX=DPDX-TAUE*R(N)/ADUCTD
      DPDXM=ABS(DPDX)*DX
      DO 823 IY=2,NM1
      IXY=IY+IXX
      RESU(IY)=U(IXY+N)
      RU2=BFRAC*RHO(IY)*U(IXY)**2
  823 DPDXM=AMIN1(DPDXM,RU2)
      DPDX=DPDXM*ABS(DPDX)/(DX*(DPDX+TINY))
C ---------------------- CALL SUBROUTINE SOLVE ----------------------
      CALL SOLVE
      IF (INERT.EQ.1) GO TO 825
      CALL TEMP
      CALL DENS
      IF (IEQUIL.EQ.1) CALL EQUIL
      IF (KNTCS.EQ.1.AND.NITER.GE.NITERK) CALL KINE
  825 XU=XD
      ISTEP=ISTEP+1
      IXX=IXX+N
      IX=IX+1
      DO 824 IY=2,NM1
  824 AREAU(IY)=AREA(IY)
      IF (IX.EQ.ISTRT) TAUSAV=TAUE
C
C-----------------------------------------------------------------------
CHAPTER 9  9  9  9  9  9  9  9  COMPLETE  9  9  9  9  9  9  9  9  9  9
C-----------------------------------------------------------------------
C
  900 PRESS=PRESS+DPDX*DX
      IF (NF.EQ.0) GO TO 9410
      IF (INERT.EQ.2) GO TO 9410
      IF (IX.EQ.1) GO TO 9410
      IF (MOD(NITER,ISWP).NE.0.AND.ISTRT.NE.1.AND.IX.EQ.ISTRT)
     1.GO TO 9410
      PDGSCN=PRESS/GASCON
      IHCPS=2
      NS1=IDN2
      NS2=ID02
      DO 907 IY=1,N
      IXY=IY+IXX
      FFU=F(IXY,JF)
      FOX=OXC*(1.0-FFU)
      F(IXY,JOX)=FOX
      FPR=1.0-FFU-FOX
      FS(IY,IDN2)=FPR
      FS(IY,IDF)=FFU
      FS(IY,ID02)=FOX
      TK=F(IXY,JTE)
      IF(IY.EQ.N) GO TO 9412
      ENTH=(F(IXY,JH)-0.5*U(IXY)**2)/GASCON
      DO 9417 I=NS1,NS2
 9417 S2(I)=FS(IY,I)
      DO 9414 IT=1,NTMAX
      CALL HCPS
      FACTOR=1.0+(ENTH/TK-HSUM)/CPSUM
      TK=TK*FACTOR
      TK=AMIN1(TMAX,TK)
      TK=AMAX1(TMIN,TK)
      DTEMP=(FACTOR-1.0)/FACTOR
      IF (ABS(DTEMP).LE.EPST) GO TO 9413
 9414 CONTINUE
      IT=IT-1
      WRITE (6,9415) IX,IY,IT,TK,DTEMP
 9415 FORMAT (1H0,10(1H-),2X,31HPOOR CONVERGENCE OF TEMPERATURE/13X,
     1 7HAT IX =,I3,10H, AND IY =,I3/13X,22HNUMBER OF ITERATIONS =,I3/
     2 13X,13HTEMPERATURE =,1PE15.6/13X,7HDTEMP =,1PE15.6/13X,
     3 18H***MAIN PROGRAM***/)
      GO TO 9413
 9412 IHCPS=1
      CALL HCPS
      F(IXY,JH)=HSUM*GASCON*TK
 9413 F(IXY,JTE)=TK
      VMIY=FFU/SMW(IDF)+FOX/SMW(IDO2)+FPR/SMW(IDN2)
      RHO(IY)=PDGSCN/(TK*VMIX)
      IF (IX.EQ.ISTRT) RHO2(IY)=RHO(IY)
  907 CONTINUE
C
C-----------------------------------------------------------------------
CHAPTER 10  10  10  10  10  10  10  ADJUST  10  10  10  10  10  10  10
C-----------------------------------------------------------------------
C
 9410 CALL DISTAN
      AFLOWD=0.5*R(N)**2
      DA1=ADUCTD/AFLOWD-1.
      ALPHA=1.0
C ---------- DEPENDENCE OF AREA ON PRESSURE.
      NIT=0
 1024 NIT=NIT+1
      GAMPRS=1.0/(GAMMA*PRESS)
      SUM=0.0
      DO 1025 IY=2,NM1
      IXY=IY+IXX
      RU2=PU(IY)*U(IXY)
      FACTOR=1.0-PU2*GAMPRS
 1025 SUM=SUM+BCM(IY)*FACTOR/(RU2*RU(IY))
      DADP=PSIE*SUM
      IF(MOD(NITER,ISWP).NE.0.AND.ISTRT.NE.1.AND.IX.EQ.ISTRT) GO TO 1022
      IF (ABS(DA1).LT.DAMIN) GO TO 1022
C ---------- ADJUSTMENT OF PRESSURE,VELOCITIES,AND DENSITIES.
      DP=DA1*AFLOWD/DADP
      DPMIN=ABS(DP)
      DO 1021 IY=2,NM1
      RU2=PFRAC*RHO(IY)*U(IY+IXX)**2
 1021 DPMIN=AMIN1(RU2,DPMIN)
      DP=DPMIN*ABS(DP)/DP
      DP=DP*ALPHA
      PRESS=PRESS+DP
      RHOFAC=1.D+DP*GAMPRS
      DO 1027 IY=2,NM1
      IXY=IY+IXX
      U(IXY)=U(IXY)-DP/RU(IY)
 1027 RHO(IY)=RHO(IY)*RHOFAC
      RHO(1)=RHO(2)
      RHO(N)=RHO(NM1)
      U(1+IXX)=U(2+IXX)
      CALL DISTAN
      AFLOWD=0.5*R(N)**2
      DA2=ADUCTD/AFLOWD-1.
      ALPHA=1.D
      IF (DA2*DA1.LE.0.D) ALPHA=0.5
      IF (ABS(DA2).LT.DAMIN) GO TO 1022
      IF (NIT.GE.NDAMAX) GO TO 1022
      DA1=DA2
      GO TO 1024
 1022 PR(IX)=PRESS
      IF (IX.EQ.1) GO TO 1030
      DO 1029 IY=2,NM1
      IXY=IY+IXX
      RESU(IY)=U(IXY)-RESU(IY)
      STORE=ABS(RESU(IY))/U(IXY)
      IF (STORE.LE.RSUMAX) GO TO 1029
      RSUMAX=STORE
      IRMUX=IX
      IRMUY=IY
 1029 CONTINUE
 1030 CONTINUE
C-----------------------------------------------------------------------
CHAPTER 11 11 11 11 11 11 11 11 11 11  PRINT  11  11  11  11  11  11
C-----------------------------------------------------------------------
C
C ---------- SEE BLOCK DATA FOR SPECIFICATION OF PARAMETERS FOR CONTROL
C            OF PRINTOUT.
      CALL OUTP2
C
C-----------------------------------------------------------------------
CHAPTFR 12  12  12  12 DECIDE ABOUT NEXT FORWARD STEP 12  12  12  12  12
C-----------------------------------------------------------------------
C
      IF(IX.EQ.IEND.AND.MOD(NITER,ISWP).NE.0) GO TO 1211
      IF (IX.NE.LM1) GO TO 600
      IFIN=2
C     -----------------------------------------------------------------
CHAPTER 13  13  13  13  13  13 EXIT BOUNDARY 13  13  13  13  13  13  13
C-----------------------------------------------------------------------
C
      LN=LM1*N
      DO 1207 IY=1,N
      IXY=IY+LN
      U(IXY)=U(IXY-N)
      DO 1207 J=1,JMAX
      F(IXY,J)=F(IXY-N,J)
 1207 CONTINUE
```

```
      PR(L)=PR(L-1)
      IX=L
      IXX=LN
      CALL OUTP2
C
C-----------------------------------------------------------------------
CHAPTER 14  14  14  14  14 DECIDE ABOUT NEXT ITERATION 14  14  14  14
C-----------------------------------------------------------------------
C
 1211 NITER=NITER+1
      IF (NITER.GT.NITMAX) GO TO 1205
      IF (RSUMAX.GT.EPSF) GO TO 1208
      IF (NF.EQ.0) GO TO 1202
      DO 1209 J=1,NF
      IF (RSFMAX(J).GT.EPSF) GO TO 1208
 1209 CONTINUE
 1202 NITMAX=NITER
 1208 IF (NITER.NE.NITMAX) GO TO 1212
      NPROF=1
      ISTRT=1
      IEND=L
 1212 IF (MOD(NITER,ISWP).NE.0.AND.ISTRT.NE.1) GO TO 1210
      CALL INIT
      PRESS=PRESS1
      ADUCTD=ADUCT(1)
      DO 1220 IY=1,N
      RHO(IY)=RHO1(IY)
      FS(IY,IDF)=F(IY,JF)
      FS(IY,IDO2)=F(IY,JOX)
 1220 FS(IY,IDN2)=1.0-FS(IY,IDF)-FS(IY,IDO2)
      GO TO 700
 1210 IX=ISTRT
      ISTEP=IX-1
      IXX=ISTEP*N
      IFIN=1
      PRESS=PR(ISTRT)
      ADUCTD=ADUCT(ISTRT)
      DO 1221 IY=1,N
 1221 RHO(IY)=RHO2(IY)
      DPDX=0.0
      XU=0.5*(X(ISTRT)+X(ISTRT+1))
      GO TO 700
 1205 CONTINUE
      STOP
      END
      BLOCK DATA
      INCLUDE COMA,LIST
      INCLUDE COMB,LIST
      INCLUDE COMC,LIST
      INCLUDE COMD,LIST
C
C-----------------------------------------------------------------------
CHAPTER 1  1  1  1  1  1  1  1  PRELIMINARIES  1  1  1  1  1  1  1  1
C-----------------------------------------------------------------------
C
      DATA KASE/1/
      DATA ITEST/1/
      DATA NITER/0/
      DATA NITMAX/19/
      DATA EPS1D/0.01/,N1DMAX/25/
      DATA EPSF/0.005/,FMIN/1.0E-4/
      DATA ISTRT,IEND,ISWP/20,86,1/
      DATA BFRAC,PFRAC/0.1,0.2/,NDAMAX/15/,DAMIN/1.0E-3/
      DATA BIG,TINY,TINYK,TNY/1.0E20,1.0E-10,1.0E-30,-69.0776/
C
C-----------------------------------------------------------------------
CHAPTER 2  2  2  2  2  2  2  GRID AND GEOMETRY  2  2  2  2  2  2  2  2
C-----------------------------------------------------------------------
C
C ---------- GRID
      DATA L/35/
      DATA N/10/
      DATA X/0.0,0.1,0.2,0.3,0.4,0.5,0.6,0.605,0.61,.615,.62,0.625,0.63,
     1 0.635,0.64,0.645,0.65,0.655,0.66,0.665,0.67,0.675,0.68,0.685,
     2 0.69,0.695,0.7,0.75,0.8,0.9,1.0,1.1,1.2,1.25,1.3/
      DATA OM/0.0,0.009,0.018,0.027,0.11,0.24,0.38,0.55,0.75,1.0/
C ---------- GEOMETRY
      DATA AREX/0.01,0.01,0.03/,BREX/0.0,0.2,0.0/,CREX/3*0.0/,
     1 XD/0.0,0.6,0.7/
C
C-----------------------------------------------------------------------
CHAPTER 3  3  3  3  3  3  3  DEPENDENT VARIABLES  3  3  3  3  3  3  3
C-----------------------------------------------------------------------
C
      DATA NF/3/
      DATA IMAX,IPR,JMAX/15,15,9/
      DATA JH,JP,JF,JN,JNO,JNO2,JN2O,JOX,JTE/1,2,3,4,5,6,7,8,9/
      DATA IDN,IDNO,IDNO2,IDN2O,IDN2,IDF,IDO2,IDCO,IDCO2,IDH,IDH2,IDH2O,
     1      IDO,IDOH/1,2,3,4,5,6,7,8,9,10,11,12,13,14/
      DATA ISPEC/4,5,6,7,0,3,8,7*0/
      DATA NSK/4/,NSE1/8/,NSE2/14/
C
C-----------------------------------------------------------------------
CHAPTER 4  4  4  4  4  4  4  4  PROPERTY DATA  4  4  4  4  4  4  4  4
C-----------------------------------------------------------------------
C
C ---------- S. I. UNITS
C ---------- THERMODYNAMIC PROPERTIES.
      DATA GASCON/8314.4/
      DATA NTMAX/10/,EPST/0.001/
      DATA CMIX/1100.0/
      DATA WMIX/29.0/
C ---------- CHEMICAL PROPERTIES.
      DATA STOICH,ARRCON,PREEXP/4.0,18000.0,0.003/
      DATA TMAX,TMIN/4000.0,273.0/
      DATA NFUMAX/10/,FUTEST/0.01/
      DATA EPSS/0.001/,ITMAX/50/
      DATA NITERK/1/
      DATA IDEBUG/1/
      DATA IEQUIL/1/
      DATA KNTCS/1/
      DATA INERT/2/
      DATA HDIV,HMAX,HMIN,PMAX,PMIN/-8.24F6,-2.16E6,-1.0E7,5.0E5,1.0E5/
C ---------- POLYNOMIAL COEFFICIENTS FOR SPECIFIC HEAT OF EQUILIBRIUM-
C                PRODUCT-SPECIES - CUBIC FUNCTIONS OF TEMPERATURE.
      DATA AC/
     1 1.294E-01, 9.890E-05,-2.498E-08, 2.126E-12, 1.294E-01, 9.895E-05,
     2-2.507E-08, 2.163E-12, 1.294E-01, 9.898E-05,-2.512E-06, 2.183E-12,
     3 1.294E-01, 9.899E-05,-2.516E-08, 2.196E-12, 1.294E-01, 9.900E-05,
     4-2.518E-08, 2.207E-12/
C ---------- POLYNOMIAL COEFFICIENTS FOR ENTHALPY.
      DATA AH/
     1-1.608E+03, 8.313E-01,-5.153E-04, 1.281E-07,-1.579E+03, 7.412E-01,
     2-4.360E-04, 1.075E-07,-1.563E+03, 6.928E-01,-3.940E-04, 9.669E-08,
     3-1.5[illegible]2E+03, 6.6[illegible]4E-01,-3.661E-04, 8.960E-08,-1.544E+03, 6.362E-01,
     4-3.4[illegible]E-04, 8.441E-08/
C ---------- POLYNOMIAL COEFFICIENTS FOR RECIPROCAL OF MEAN MOLECULAR
C                WEIGHT.
      DATA AS/
     1 3.368E-02, 1.075E-05,-8.588E-09, 2.042E-12, 3.415E-02, 9.316E-06,
     2-7.330E-09, 1.716E-12, 3.440E-02, 8.544E-06,-6.665E-09, 1.547E-12,
     3 3.457E-02, 8.027E-06,-6.224E-09, 1.435E-12, 3.470E-02, 7.643E-06,
     4-5.898E-09, 1.354E-12/
C ---------- POLYNOMIAL COEFFICIENTS FOR CONCENTRATIONS OF EQUILIBRIUM-
C                PRODUCT-SPECIES  -  LOG(CONCENTRATION) AS A CUBIC FUNCTION
C                OF ENTHALPY.
C                COEFFICIFNTS AS1 FOR ENTHALPY .GE. HMIN, AND .LE. HDIV.,
C                COEFFICIENTS BS1 FOR ENTHALPY .GT. HDIV, AND .LE. HMAX.
      DATA (((AS1(I,J,K),I=1,4),J=1,7),K=1,3)/
     1-2.103E+01, 1.293E+02,-4.792E+02, 7.870E+02,-5.981E-01,-6.903E-03,
     2 1.258E-01,-5.925E-01,-3.480E+01, 1.849E+02,-6.624E+02, 1.067E+03,
     3-2.233E+01, 1.088E+02,-3.985E+02, 6.526E+02,-7.981E-01,-5.743E-03,
     4 1.074E-01,-5.285E-01,-3.085E+01, 1.853E+02,-6.477E+02, 1.021E+03,
     5-1.927E+01, 1.140E+02,-4.006E+02, 6.337E+02,-2.126E+01, 1.293E+02,
     6-4.798E+02, 7.899E+02,-5.981E-01,-5.580E-03, 1.015E-01,-4.767E-01,
     7-3.526E+01, 1.850E+02,-6.634E+02, 1.072E+03,-2.256E+01, 1.089E+02,
     8-3.990E+02, 6.552E+02,-7.981E-01,-4.693E-03, 8.745E-02,-4.284E-01,
     9-3.131E+01, 1.853E+02,-6.487E+02, 1.026E+03,-1.950E+01, 1.140E+02,
     X-4.013E+02, 6.375E+02,-2.140E+01, 1.294E+02,-4.803E+02, 7.918E+02,
     A-5.981E-01,-4.918E-03, 8.938E-02,-4.192E-01,-3.553E+01, 1.850E+02,
     B-6.640E+02, 1.075E+03,-2.270E+01, 1.089E+02,-3.995E+02, 6.570E+02,
     C-7.981E-01,-4.159E-03, 7.736E-02,-3.781E-01,-3.158E+01, 1.853E+02,
     D-6.491E+02, 1.030E+03,-1.964E+01, 1.140E+02,-4.015E+02, 6.391E+02/
      DATA (((AS1(I,J,K),I=1,4),J=1,7),K=4,5)/
     1-2.150E+01, 1.294E+02,-4.806E+02, 7.930E+02,-5.981E-01,-4.494E-03,
     2 8.161E-02,-3.825E-01,-3.573E+01, 1.850E+02,-6.643E+02, 1.077E+03,
     3-2.279E+01, 1.089E+02,-3.997E+02, 6.580E+02,-7.981E-01,-3.813E-03,
     4 7.085E-02,-3.459E-01,-3.178E+01, 1.853E+02,-6.493E+02, 1.032E+03,
     5-1.973E+01, 1.140E+02,-4.017E+02, 6.402E+02,-2.157E+01, 1.295E+02,
     6-4.811E+02, 7.944E+02,-5.981E-01,-4.188E-03, 7.603E-02,-3.561E-01,
     7-3.588E+01, 1.851E+02,-6.647E+02, 1.079E+03,-2.287E+01, 1.090E+02,
     8-4.002E+02, 6.593E+02,-7.981E-01,-3.563E-03, 6.615E-02,-3.225E-01,
     9-3.192E+01, 1.853E+02,-6.492E+02, 1.033E+03,-1.981E+01, 1.140E+02,
     X-4.016E+02, 6.407E+02/
C
      DATA (((BS1(I,J,K),I=1,4),J=1,7),K=1,3)/
     1-1.356E+01, 3.797E+01,-4.566E+01, 1.922E+01,-6.409E-01, 4.487E-01,
     2-1.269E+00, 4.565E-01,-2.402E+01, 5.678E+01,-6.813E+01, 2.885E+01,
     3-1.611E+01, 3.302E+01,-3.918E+01, 1.649E+01,-8.034E-01, 1.444E-01,
     4-5.913E-01, 2.307E-01,-1.975E+01, 5.715E+01,-7.005E+01, 2.987E+01,
     5-1.245E+01, 3.493E+01,-4.297E+01, 1.831E+01,-1.396E+01, 3.888E+01,
     6-4.642E+01, 1.943E+01,-6.482E-01, 4.791E-01,-1.261E+00, 4.391E-01,
     7-2.478E+01, 5.841E+01,-6.959E+01, 2.931E+01,-1.648E+01, 3.380E+01,
     8-3.982E+01, 1.668E+01,-8.100E-01, 1.802E-01,-6.237E-01, 2.417E-01,
     9-2.056E+01, 5.916E+01,-7.200E+01, 3.053E+01,-1.289E+01, 3.615E+01,
     X-4.415E+01, 1.871E+01,-1.418E+01, 3.934E+01,-4.674E+01, 1.949E+01,
     A-6.517E-01, 4.909E-01,-1.245E+00, 4.241E-01,-2.520E+01, 5.924E+01,
     B-7.025E+01, 2.948E+01,-1.670E+01, 3.419E+01,-4.009E+01, 1.673E+01,
     C-8.135E-01, 1.989E-01,-6.380E-01, 2.457E-01,-2.102E+01, 6.020E+01,
     D-7.291E+01, 3.080E+01,-1.314E+01, 3.678E+01,-4.470E+01, 1.887E+01/
      DATA (((BS1(I,J,K),I=1,4),J=1,7),K=4,5)/
     1-1.434E+01, 3.963E+01,-4.690E+01, 1.951E+01,-6.538E-01, 4.965E-01,
     2-1.229E+00, 4.114E-01,-2.549E+01, 5.976E+01,-7.062E+01, 2.956E+01,
     3-1.684E+01, 3.443E+01,-4.023E+01, 1.674E+01,-8.159E-01, 2.110E-01,
     4-6.456E-01, 2.473E-01,-2.133E+01, 6.088E+01,-7.346E+01, 3.095E+01,
     5-1.331E+01, 3.719E+01,-4.503E+01, 1.895E+01,-1.445E+01, 3.983E+01,
     6-4.700E+01, 1.951E+01,-6.552E-01, 4.992E-01,-1.214E+00, 4.003E-01,
     7-2.572E+01, 6.014E+01,-7.086E+01, 2.959E+01,-1.695E+01, 3.460E+01,
     8-4.032E+01, 1.674E+01,-8.177E-01, 2.196E-01,-6.501E-01, 2.478E-01,
     9-2.157E+01, 6.136E+01,-7.382E+01, 3.103E+01,-1.344E+01, 3.748E+01,
     X-4.524E+01, 1.900E+01/
C ---------- TRANSPORT PROPERTIES.
      DATA VISFU,VISOX,VISPP,VISMIX/4*1.E-6/
      DATA PRLAM,PRTURB/0.70,0.86/
      DATA AK,EWAL/0.435,9.0/
      DATA MODEL/2/
      DATA H/0.9/
C
C-----------------------------------------------------------------------
CHAPTER 5  5  5  5  5  5  5  STARTING VALUES  5  5  5  5  5  5  5  5
C-----------------------------------------------------------------------
C
C ---------- TWO STREAMS ENTERING - STREAM B IS PURE FUEL, AND STREAM
C                C IS AIR.
      DATA UB,UC/ .6, 6.0/,TB,TC/294.0,810.0/
      DATA FUB,FUC/1.,0./, OXB,OXC/0.,.232/
      DATA PRESS/4.053E5/
      DATA EQRAT/0.4/
C
C-----------------------------------------------------------------------
CHAPTER 6  6  6  6  6  6  6 BOUNDARY CONDITIONS 6  6  6  6  6  6  6  6
C-----------------------------------------------------------------------
C
C ---------- PARAMETERS DEFINING DUCT WALL TEMPERATURE.
      DATA DWALL/810.0,1110.0,1110.0/,EWALL/500.0,0.0,-500.0/,
     1 FWALL/3*0.0/
C
C-----------------------------------------------------------------------
CHAPTER 7  7  7  7  7  7  7  7  7 PRINT 7  7  7  7  7  7  7  7  7  7  7
C-----------------------------------------------------------------------
C
      DATA NSTAT,NPROF,NPLOTC,NPLOTL/3*10000,1/
      DATA NPRINT/20/
      DATA N1DPR/25/
      DATA IPLOT/     30*35/,IPLOTH/0/
      DATA IPLOTL/1/
C
      END
      SUBROUTINE START
      INCLUDE COMA,LIST
      INCLUDE COMB,LIST
      INCLUDE COMC,LIST
      DIMENSION ISOLVE(3),FDUM1(100),FDUM2(100),FDUM3(100)
      TWALL(X,I)=DWALL(I)+(FWALL(I)+FWALL(I)*(X-XD(I)))*(X-XD(I))
C
C-----------------------------------------------------------------------
CHAPTER 1  1  1  1  1  1  1  1 PRELIMINARIES 1  1  1  1  1  1  1  1  1
C-----------------------------------------------------------------------
C
      DATA AFU,AOX,AH20,AC02,AN2/2113.9,976.9,2088.2,988.6,1102.5/
      DATA BFU,BOX,BH20,BC02,BN2/1.9996,0.10755,0.36872,0.238,0.09525/
      DATA HFU,C02H20/5.50E7,1.2222222/
      DATA ISOLVE/5,10000,1/
      DATA TINY/1.0E-10/
      DATA NIT/0/
      CFH20=(1.0+STOICH)/(1.0+C02H20)
      STORE=STOICH/(EORAT*OXC)
      FUUNB=1.0/(1.0+STORE)
      FOXUNB=OXC*STORE*FUUNB
      FPRUNE=1.0-FUUNB-FOXUNB
      PRB=1.0-FUB-OXB
      PRC=1.0-OXC-FUC
      AMIX=AFU*FUP+AOX*OXB+AN2*PRB
      BMIX=BFU*FUR+BOX*OXB+BN2*PRB
      CMIXB=AMIX+BMIX*TB
      AMIX=AFU*FUC+AOX*OXC+AN2*PRC
      BMIX=AFU*FUC+BOX*OXC+BN2*PRC
      CMIXC=AMIX+BMIX*TC
      ENTHB=CMIXB*TB+HFU*FUB
      ENTHC=CMIXC*TC+HFU*FUC
      ENTH=(FLOB*ENTHP+FLOC*ENTHC)/PSIE
      AMIX=AFU*FUUNB+AOX*FOXUNB+AN2*FPRUNB
      BMIX=BFU*FUUNP+POX*FOXUNB+BN2*FPRUNB
      TUNP=(-AMIX+SQRT(AMIX**2-4.0*BMIX*(HFU*FUUNB-ENTH)))/(2.0*BMIX)
      T1=PREEXP*PRESS**2
      FJP=FUUNB
      PHI=(FJP-FSTOIC)/FSTOIH
      FUBRN=AMAX1(0.0 PHI)
      NN=NF
      IF (INERT.EQ.2) GO TO 101
      NN=JH
      FUBRN=FUUNB
      NIDMAX=1
  101 FOXBRN=AMAX1(TINY,(FUBRN-PHI)*STOICH)
      FH20=CFH20*(FJP-FUBRN)
      FC02=C02H20*FH20
      FN2=1.0-FUBRN-FOXBRN-FH20-FC02
      AMIX=AFU*FUBRN+AOX*FOXBRN+AH20*FH20+AC02*FC02+AN2*FN2
      BMIX=BFU*FUBRN+BOX*FOXBRN+BH20*FH20+BC02*FC02+BN2*FN2
      TBRN=(-AMIX+SQRT(AMIX**2-4.0*BMIX*(HFU*FUBRN-ENTH)))/(2.0*BMIX)
C
C-----------------------------------------------------------------------
CHAPTER 2  2  2  2  2  2  2  2 INITIAL GUESS 2  2  2  2  2  2  2  2  2
C-----------------------------------------------------------------------
```

```
C
      XDIFF=XD(3)-XD(2)
      TDIFF=TBRN-TUNB
      FDIFF=FUBRN-FUUNB
      DENOM=1.0/(EXP(XDIFF)-1.0)
      XDIFF=1.0/XDIFF
      F(1,JOX)=FOXUNB
      IXX=-N
      DO 125 JX=1,L
      IXX=IXX+N
      IXY=IXX+1
      F(IXY,JH)=ENTH
      DO 100 I=1,3
      IF (X(JX).LT.XD(I)) GO TO 102
  100 CONTINUE
  102 ISEC=I-1
      F(IXX+N,JTE)=TWALL(X(JX),ISEC)
      IF (ISEC-2) 103,104,105
C ---------- SECTION 1 - UNBURNT CONDITIONS.
  103 F(IXY,JF)=FUUNB
      F(IXY,JTE)=TUNB
      F(IXY,JOX)=FOXUNB
      GO TO 125
C ---------- SECTION 2 - EXPONENTIAL VARIATION OF TEMPERATURE AND FUEL
C                        CONCENTRATION.
  104 ZETA=X(JX)-XD(2)
      RATIO=(EXP(ZETA)-1.0)*DENOM
      F(IXY,JTE)=TDIFF*RATIO+TUNB
      F(IXY,JF)=FDIFF*RATIO+FUUNB
      F(IXY,JOX)=AMAX1((F(IXY,JF)-PHI)*STOICH,TINY)
      GO TO 125
C ---------- SECTION 3 - ALL-BURNT CONDITIONS.
  105 F(IXY,JF)=FUBRN
      F(IXY,JTE)=TBRN
      F(IXY,JOX)=FOXBRN
  125 CONTINUE
      IF (ITEST.EQ.1) GO TO 130
      DO 126 JX = 1,L
      JDUM = (JX-1) * N + 1
      FDUM1(JX) = F(JDUM,JH)
      FDUM2(JX) = F(JDUM,JF)
      FDUM3(JX) = F(JDUM,JTE)
  126 CONTINUE
      WRITE(6,127) JH,(FDUM1(JX), JX=1,L)
      WRITE(6,127) JF,(FDUM2(JX), JX=1,L)
      WRITE(6,127)JTE,(FDUM3(JX), JX=1,L)
  127 FORMAT (1H0,20HINITIAL GUESS, F(IX,,I2,1H)/(3X,1P6E11.3))
C
C-----------------------------------------------------------------------
CHAPTER 3   3   3   3   3   3 TRANSPORT PROPERTIES 3   3   3   3   3   3   3   3   3
C-----------------------------------------------------------------------
C
  130 IF (MODEL.EQ.1) GO TO 215
C ---------- MODEL=2, TURBULENT FLOW.
      PSIE12=0.12*PSIE
      AMUL=VISMIX*SQRT(F(N,JTE))
      SQAPEA=SQRT(0.5*ADUCT(1))
      SHALF=0.15*(PSIF/(AMUL*SQAREA))**(-0.125)
      AMUTP=PSIE12*SHALF*ADUCT(1)/(2.0*SQAREA*XDIF(1))
      IXX=0
      DO 210 JX=2,LM1
      IXX=IXX+N
      AMUT=AMUTP
      AMUL=VISMIX*SQRT(F(IXX+N,JTE))
      SQAREA=SQRT(0.5*ADUCT(JX))
      SHALF=0.15*(PSIE/(AMUL*SQAREA))**(-0.125)
      AMUTP=PSIE12*SHALF*ADUCT(JX)/(2.0*SQAREA*XDIF(JX))
      IF (X(JX).GT.XD(2).AND.X(JX).LE.XD(3)) AMUTP=100.0*AMUTP
      AMUU(JX)=AMUT/XS(JX)
  210 AMUD(JX)=AMUTP/XS(JX)
      GO TO 220
  215 AMUL1=(FUUNB*VISFU+FOXUNB*VISOX+FPRUNB*VISPR)*SQRT(TUNB)*ADUCT(1)
     1 /XDIF(1)
  220 NIT=NIT+1
      IF (MODEL.EQ.2) GO TO 235
C ---------- MODEL=1, LAMINAR FLOW.
      AMULP=AMUL1
      IXX=0
      DO 230 JX=2,LM1
      IXX=IXX+N
      IXY=IXX+1
      AMUL=AMULP
      AMULP=(VISFU*F(IXY,JF)+VISOX*F(IXY,JOX)+VISPR*(1.0-F(IXY,JF)
     1 -F(IXY,JOX)))*SQRT(F(IXY,JTE))*ADUCT(JX)/XDIF(JX)
      AMUD(JX)=AMULP/XS(JX)
  230 AMUU(JX)=AMUL/XS(JX)
C
C-----------------------------------------------------------------------
CHAPTER 4  4  4  4  4  4  4  4 MAIN SOLUTION LOOP 4  4  4  4  4  4  4  4
C-----------------------------------------------------------------------
C
  235 DO 335 J=1,NN
      RSFMAX(J)=0.0
      IRMFX(J)=0
      IF (MOD(NIT-1,ISOLVE(J)).NE.0) GO TO 335
      IF (J.EQ.JP) GO TO 335
      IXX=0
      PRCON=1.0/PRLT(J,MODEL)
      DO 330 JX=2,LM1
      IXX=IXX+N
      IXYD=IXX+1
      P=PSIE/XS(JX)
      FFU=F(IXYD,JF)
      FOX=AMAX1((FFU-PHI)*STOICH,TINY)
      ALF(JX,J)=AMUD(JX)*PRCON
      BLF(JX,J)=AMUU(JX)*PRCON+P
C ---------- STAGNATION ENTHALPY EQUATION(J=JH).
      IF (J.NE.JH) GO TO 305
      TW=F(IXX+N,JTE)
      TEF=0.0015*PSIE*SQRT(2.0/ADUCT(JX))
      FH2O=CFH2O*(FJP-FFU)
      FCO2=CO2H2O*FH2O
      FN2=1.0-FFU-FOX-FH2O-FCO2
      AMIX=AFU*FFU+AOX*FOX+AH2O*FH2O+ACO2*FCO2+AN2*FN2
```

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      BMIX=BFU*FFU+BOX*FOX+BH2O*FH2O+BCO2*FCO2+BN2*FN2
      HWALL=(AMIX+BMIX*TW)*TW+HFU*FFU
      DLF(JX,J)=ALF(JX,J)+BLF(JX,J)+TEF
      CLF(JX)=TEF*HWALL
      GO TO 330
C ---------- FUEL EQUATION (J=JF).
  305 IF (J.NE.JF) GO TO 330
      FUEX=FFU-FUBRN
      IF (FUEX.GT.0.0) GO TO 346
      DLF(JX,J)=BIG
      GO TO 344
  346 TERM=T1*EXP(-ARPCON/F(IXYD,JTE))*ADUCT(JX)*FOX
      DLF(JX,J)=TERM*FFU/FUEX
  344 CLF(JX)=DLF(JX,J)*FUBRN
      DLF(JX,J)=DLF(JX,J)+ALF(JX,J)+BLF(JX,J)
  330 CONTINUE
      IF (ITEST.EQ.1) GO TO 331
      WRITE (6,3100) J,(ALF(JX,J),JX=2,LM1)
      WRITE (6,3101) (BLF(JX,J),JX=2,LM1)
      WRITE (6,3102) (CLF(JX),JX=2,LM1)
      WRITE (6,3103) (DLF(JX,J),JX=2,LM1)
 3100 FORMAT (20H SUBROUTINE START,F(,I2,1H)/8H ALF(IX)/(3X,1P6E11.3))
 3101 FORMAT (8H BLF(IX)/(3X,1P6E11.3))
 3102 FORMAT (8H CLF(IX)/(3X,1P6E11.3))
 3103 FORMAT (8H DLF(IX)/(3X,1P6E11.3))
C ---------- TDMA SOLUTION.
  331 CLF(2)=(BLF(2,J)*F(1,J)+CLF(2))/DLF(2,J)
      ELF(2)=ALF(2,J)/DLF(2,J)
      DO 332 JX=3,LM1
      T=DLF(JX,J)-BLF(JX,J)*ELF(JX-1)
      ELF(JX)=ALF(JX,J)/T
  332 CLF(JX)=(BLF(JX,J)*CLF(JX-1)+CLF(JX))/T
      DO 333 JXJ=1,LM2
      JX=L-JXJ
      IXY=(JX-1)*N+1
      FOLD=F(IXY,J)
      F(IXY,J)=ELF(JX)*F(IXY+N,J)+CLF(JX)
      ABSF=ABS(F(IXY,J))
C ---------- MAXIMUM NORMALISED CHANGES FROM PREVIOUS ITERATION.
      IF (ABSF.LE.FMIN) GO TO 333
      STORE2=ABS(F(IXY,J)-FOLD)/ABSF
      IF (STORE2.LE.RSFMAX(J)) GO TO 333
      RSFMAX(J)=STORE2
      IRMFX(J)=JX
  333 CONTINUE
  335 CONTINUE
C
C-----------------------------------------------------------------------
CHAPTER 5  5  5  5  5  5  5 COMPLETION OF AN ITERATION 5  5  5  5  5  5
C-----------------------------------------------------------------------
C
      IXX=0
      DO 440 JX=2,LM1
      IXX=IXX+N
      IXY=IXX+1
      FFU=F(IXY,JF)
      FOX=AMAX1((FFU-PHI)*STOICH,TINY)
      FH2O=CFH2O*(FJP-FFU)
      FCO2=CO2H2O*FH2O
      F(IXY,JOX)=FOX
      FN2=1.0-FFU-FOX-FH2O-FCO2
      AMIX=AFU*FFU+AOX*FOX+AH2O*FH2O+ACO2*FCO2+AN2*FN2
      BMIX=BFU*FFU+BOX*FOX+BH2O*FH2O+BCO2*FCO2+BN2*FN2
  440 F(IXY,JTE)=(-AMIX+SQRT(ABS(AMIX**2-4.0*BMIX*(HFU*FFU-F(IXY,JH)))))
     1 /(2.0*BMIX)
C ---------- EXIT BOUNDARY, ZERO GRADIENT CONDITION.
      IXY=(L-1)*N+1
      IXYU=IXY-N
      F(IXY,JH)=F(IXYU,JH)
      F(IXY,JF)=F(IXYU,JF)
      F(IXY,JOX)=F(IXYU,JOX)
      F(IXY,JTE)=F(IXYU,JTE)
C
C-----------------------------------------------------------------------
CHAPTER 6  6  6  6  6  6  6  6  6 PRINT 6  6  6  6  6  6  6  6  6  6  6
C-----------------------------------------------------------------------
C
C ---------- CHECK IF MAXIMUM CHANGES IN DEPENDENT VARIABLES .LE.
C            SPECIFIED CONVERGENCE LIMIT, EPS1D.
      DO 516 J=1,NF
      IF (RSFMAX(J).GT.EPS1D) GO TO 517
  516 CONTINUE
      N1DMAX=NIT
      GO TO 519
  517 IF(NIT.EQ.1) GO TO 519
      IF(MOD(NIT,N1DPR).NE.0.AND.NIT.NE.N1DMAX) GO TO 514
  519 WRITE (6,520) NIT
  520 FORMAT (1H1,20(1H*),6X,17HITERATION NUMBER ,I3,6X,20(1H*)/1H0,
     1 9(2H-+),6X,24HONE-DIMENSIONAL SOLUTION,6X,9(2H+-)//8X,3H IX,5X,
     2 1HX,7X,8HENTHALPY,5X,4HFUEL,6X,6HOXYGEN,6X,4HTEMP/)
      IXX=-N
      DO 500 JX=1,L
      IXX=IXX+N
      IXY=IXX+1
  500 WRITE (6,510) JX,X(JX),F(IXY,JH),F(IXY,JF),F(IXY,JOX),F(IXY,JTE)
  510 FORMAT (8X,I3,1P5E11.3)
      WRITE(6,511)
  511 FORMAT(1H0,24(3H-+-))
  514 WRITE (6,515) NIT,(J,RSFMAX(J),IRMFX(J),J=1,NF)
  515 FORMAT(1H0,3X,4HNIT=,I3/(12X,7HRSFMAX(,I2,3H) =,1PE10.3,
     1 18H AT GRID NODE IX =,I3))
      IF (NIT.LT.N1DMAX) GO TO 220
C
C-----------------------------------------------------------------------
CHAPTER 7  7  7  7  7  7  7  7  7 COMPLETE 7  7  7  7  7  7  7  7  7  7
C-----------------------------------------------------------------------
C
C ---------- ONE-DIMENSIONAL SOLUTION STORED AT ALL CROSS-STREAM GRID
C            NODES - STARTING VALUES FOR THE 2-D SOLUTION.
      IXX=0
      DO 605 JX=2,L
      IXX=IXX+N
      CLF(JX)=0.0
      IXY1=IXX+1
      FTE=F(IXY1,JTE)
      FFU=F(IXY1,JF)
      FJH=F(IXY1,JH)
      DO 605 IY=2,N
      IXY=IY+IXX
      F(IXY,JTE)=FTE
      F(IXY,JH)=FJH
      F(IXY,JP)=FJP
  605 F(IXY,JF)=FFU
      IXX=0
      RETURN
      END
      SUBROUTINE OUTPUT
      INCLUDE COMA,LIST
      INCLUDE COMB,LIST
      INCLUDE COMC,LIST
      INCLUDE COMD,LIST
C
      DIMENSION DATA(6),FLUX(3),LAB(6),LABK(14),XLPLOT(26),
     1 XTPLOT(15),YLAXIS(18),YLPLOT(26,18),YTPLOT(15,7),YAXIS1(7),
     2 YAXIS2(7),YAXIS3(7),YAXISL(18)
      ENTRY OUTP1
C
C-----------------------------------------------------------------------
CHAPTER A ---------------- INITIAL PRINTOUT ----------------------------
C-----------------------------------------------------------------------
C
C ---------- CROSS-STREAM OUTPUT (PROFILE) DATA.
      DATA (LAB(K),K=1,6)/'P','U VEL','TEMP','FUEL','OXYG',' F    '/
      DATA KOUT/6/
      DATA LABK1/'R'/
      DATA(LABK(K),K=1,4)/' N    ',' NO  ',' NO2 ',  ' N2O '/
      DATA (LABK(K),K=8,14)      /' CO    ',  ' CO2 ','  H  ',' H2    ',
     1                           ' H2O ','  O  ',' OH    '/
      DATA (LABK(K),K=5,7)       /'  N2  ','  FUEL','     O2'/
      DATA LABKR/ ' RHO   '/,LABKH/'ENTLPY'  /,LABKV/     'VISC'/
C
C ---------- TRANSVERSE (CROSS-STREAM) PLOT DATA.
      DATA ITDIM,JTDIM/15,7/
C ---------- ASSIGN LABELS FOR PLOT AXES.
      DATA XTAXIS/'R(I)'/
      DATA (YAXIS1(K),K=1,7)/'U VEL','TEMP','FUEL','OXYG',3*0.0/
      DATA (YAXIS2(K),K=1,7)/'8,O','9,OH','0,N2','N    ','*,NO','1,NO2',
     1 '2,N2O'/
      DATA (YAXIS3(K),K=1,7)/'3,CO','4,CO2','5,H','6,H2','7,H2O',2*0.0/
C
C ---------- LONGITUDINAL (DOWN-STREAM) PLOT DATA.
      DATA ILDIM,JLDIM/26,18/
C ---------- ASSIGN LABELS FOR PLOT AXES.
      DATA XLAXIS/'X   '/
      DATA (YLAXIS(K),K=1,18)/'U(1)','T','DPDX','GF(JF)',
     1 'FUEL','OXYG','3,CO','4,CO2','5,H','6,H2','7,H2O','8,O','9,OH',
     2 '0,N2','N    ','*,NO','1,NO2','2,N2O'/
      DATA BLANK/4H    /,THIRD/4HM   /
      NSE3=NSE1+4
      NSE4=NSE3+1
C
      PRESS1=PRESS
      EMU1 = (VISFU*FUB+VISOX*OXB+VISPR*(1.0-FUB-OXB))*SQRT(TB)
      REY=PSIE/(EMU1*0.5*REXO)
C
      WRITE (6,1087)
 1087 FORMAT (1H1)
      WRITE (6,1013)
 1013 FORMAT (11X,51(1H*)/11X,1H*,49X,1H*/11X,1H*,49X,1H*/11X,1H*,49X,
     1 1H*/11X,  51H*          PREDICTION OF HYDRODYNAMICS AND            */
     262H            *          
     362H            *         CHEMISTRY OF CONFINED METHANE-AIR          */
     462H             *                                                 */
     562H             *          FLAMES WITH ATTENTION TO FORMATION     */
     662H             *                                                 */
     762H             *                  OF NITROGEN OXIDES             */
     8 11X,1H*,49X,1H*/11X,1H*,49X,1H*/11X,1H*,49X,1H*/11X,1H*,49X,1H*/
     9 11X,1H*,49X,1H*/11X,1H*,49X,1H*)
      WRITE (6,1015)
 1015 FORMAT(11X,1H*,11X,    39HTHE NASCO COMPUTER PROGRAM              */
     162H             *                                                 */
     242H             *                        PREPARED BY,19X,1H*/11X,1H*,49X,
     3 1H*/11X,1H*, 5X,45H  CONCENTRATION HEAT AND MOMENTUM LTD.        */
     4 11X,1H*,49Y,1H*/11X,1H*,23X,3HFOR,23X,1H*/11X,1H*,49X,1H*/
     562H             *  NATIONAL AERONAUTICS AND SPACE ADMINISTRATION  */
     662H             *                                                 */
     762H             *               NASA LEWIS RESEARCH CENTER        */
     8 11X,1H*,49X,1H*/11X,1H*,49X,1H*/11X,1H*,49X,1H*/11X,1H*,49X,1H*/
     9 11X,1H*,15X,19HCONTRACT NAS3-18940,15X,1H*/11X,1H*,49X,1H*)
      WRITE (6,1016) KASE
 1016 FORMAT(11X,1H*,19X,10HAPRIL 1977,20X,1H*/
     1 11X,1H*,49X,1H*/11X,1H*,49X,1H*/11X,1H*,49X,1H*/11X,1H*,49X,1H*/
     2 11X,1H*,49X,1H*/11X,1H*,49X,1H*/11X,1H*,49(1H-),1H*/
     3 11X,1H*,49X,1H*/11X,1H*,49X,1H*/11Y,1H*,49Y,1H*/11X,1H*,49X,1H*/
     445H             *                RESULTS FOR TEST CASE,I5,11X,1H*/11X,
     5 1H*,49X,1H*/11X,1H*,10X,30HS.I. UNTITS ARE USED THROUGHOUT,9X,1H*/
     6 11X,1H*,49X,1H*/11X,1H*,49X,1H*/11X,1H*,49X,1H*/11X,1H*,49X,1H*/
     7 11X,51(1H*))
      WRITE (6,1020)
 1020 FORMAT (1H1,15HFLOW CONDITIONS/1X,15(1H=))
      IF (MODEL.EQ.1) WRITE (6,1021)
 1021 FORMAT (1H0,4X,16HLAMINAR, MODEL=1)
      IF (MODEL.EQ.2) WRITE (6,1022)
 1022 FORMAT (1H0,4X,18HTURBULENT, MODEL=2)
      IF (INERT.EQ.1) WRITE (6,1023)
 1023 FORMAT (1H0,4X,21HNON-REACTING, INERT=1//)
      IF (INERT.EQ.2) WRITE (6,1024)
 1024 FORMAT (1H0,4X,28HCHEMICALLY REACTING, INERT=2//)
      WRITE (6,1019)
 1019 FORMAT (1H0,8HGEOMETRY/1X,8(1H=))
      WRITE (6,1025) RDIV,REXO,X(L)
 1025 FORMAT (1H0,4X,29HRADIUS OF FUEL JET AT INLET  ,1PE10.3//5X,
     1 29HRADIUS OF DUCT AT INLET      ,1PE10.3//5X,  20HTOTAL LENGTH OF
     2 DUCT,9X,1PE10.3//)
      WRITE (6,1026) (I,XO(I),AREX(I),BREX(I),CREX(I),I=1,3)
 1026 FORMAT(1H0,4X,21HDUCT WALL CONSTANTS -//11X,1HI,8X,2HXO,9X,4HAREX,
     1 8X,4HBREX,9X,4HCREX//(10X,I2,2X,1P4E12.3))
      WRITE (6,1027) UB,UC,TB,TC,PRESS,REY,EQRAT,PSIE
 1027 FORMAT (//1H0,16HINLET CONDITIONS/1X,16(1H=)//5X,   27HVELOCITY OF
     1 FUEL STREAM, UB,7X,1PE10.3//5X,26HVELOCITY OF AIR STREAM, UC,8X,
     2 1PE10.3//5X,30HTEMPERATURE OF FUEL STREAM, TB,4X,1PE10.3//5X,
     3 29HTEMPERATURE OF AIR STREAM, TC,5X,1PE10.3//5X,21HINLET PRESSURE
     4, PRESS,13X,1PE10.3//5X,15HREYNOLDS NUMBER,19X,1PE10.3//5X,
     5 34HOVERALL EQUIVALENCE RATIO, EQRAT  ,1PE10.3//5X,  26HTOTAL MASS
     6 FLOW RATE, PSIE,8X,1PE10.3//)
      WRITE (6,1028) (I,DWALL(I),EWALL(I),FWALL(I),I=1,3)
 1028 FORMAT(1H0,19HBOUNDARY CONDITIONS/1X,19(1H=)//5X,28HWALL TEMPERATU
     1RE CONSTANTS -//11X,1HI,6X,5HDWALL,7X,5HEWALL,7X,5HFWALL//(10X,I2,
     2 2X,1P3E12.3))
```

```
      WRITE (6,1029) (OM(I),I=1,N)
 1029 FORMAT (//1H0,4HGRID/1X,4(1H=)//13H OMEGA GRID -/(3X,1P6E11.3))
      WRITE (6,1080) (X(I),I=1,L)
 1080 FORMAT(//9H X GRID -/(3X,1P6E11.3))
      WRITE (6,1081)
 1081 FORMAT(1H1,53HPOLYNOMIAL COEFFICIENTS FOR THERMODYNAMIC PROPERTIES
     1./61H 14 COEFFICIENTS ((Z(K,J,I),J=1,7),K=1,2) FOR EACH SPECIES I.
     2//)
      DO 1088 I=1,NSE2
 1088 WRITE (6,1082) ASUB(I,1),((Z(K,J,I),J=1,7),K=1,2)
 1082 FORMAT (1H0,A4/(3X,1P6E11.3))
      IF (KNTCS.EQ.0) GO TO 1085
      WRITE (6,1083)
 1083 FORMAT (1H1,18HREACTION MECHANISM/1X,18(1H=))
      DO 1061 J=1,JJ
      DO 1060 KK=1,6
      LL=KK
      IF (KK.GT.3) LL=KK-1
      DATA (KK)=BLANK
      IF (KK.EQ.3) GO TO 1060
      IF (KK.EQ.6) GO TO 1060
      IDLLJ=ID(LL,J)
      IF (IDLLJ.EQ.0) GO TO 1060
      DATA (KK)=ASUB(IDLLJ,1)
 1060 CONTINUE
      IF (ID(2,J).EQ.0) GO TO 1062
      IF (ID(4,J).EQ.0) GO TO 1062
      GO TO 1063
 1062 DATA(3)=THIRD
      DATA(6)=THIRD
      WRITE (6,1064) J,(DATA(K),K=1,6)
 1064 FORMAT (I3,2H. ,A4,2H+ ,A4,2H+ ,A4,2H= ,A4,2H+ ,A4,2H+ ,A4,
     1 1P3E11.3)
      GO TO 1061
 1063 WRITE (6,1065) J,(DATA(K),K=1,6)
 1065 FORMAT (I3,2H. ,A4,2H+ ,A4,2X,A4,2H= ,A4,2H+ ,A4,2X,A4,1P3E11.3)
 1061 CONTINUE
      WRITE (6,1084) (J,BX(J),TEN(J),TACT(J),BX2(J),TEN2(J),TACT2(J),
     1                                                            J=1,JJ)
 1084 FORMAT (1H0,2X,24HRATE CONSTANT PARAMETERS/5X,37HRATE CONSTANT =
     1 A*T**B*EXP(-TACT/T),10X,15H(T=TEMPERATURE)///17X,12HFOPWARD RATE,
     2 21X,13HBACKWARD RATE//9X,1HA,10X,1HB,8X,4HTACT,9X,1HA,10X,1HB,8X,
     3 4HTACT/(I3,1H.,1P6E11.3))
 1085 WRITE (6,1086) FMIN
 1086 FORMAT (1H0,7(10H   ****   )/
     162H ***** NOTE - THE MAXIMUM CHANGES IN THE FIELD VALUES OF      /
     262H U-VELOCITY, STAGNATION ENTHALPY, MIXTURE FRACTION, AND MASS  /
     362H FRACTION OF UNBURNT FUEL BETWEEN SUCCESSIVE ITERATIONS ARE   /
     462H PRINTED AT EACH ITEPATION.  THESE VALUES ARE COMPUTED AS THE /
     562H MAXIMUM OF ABS(CUPRENT VALUE - PREVIOUS VALUE)/CURRENT VALUE./
     650H THIS IS DONE IF THE CURRENT VALUE IS GREATER THAN,1PE8.1,1H./
     762H THE FOLLOWING SYMBOLS DENOTE THE MAXIMUM CHANGES -            /
     862H         RSUMAX FOR U-VELOCITY,                                /
     962H         RSFMAX(J) FOR VARIABLE J,                             /
     *62H             J=1 FOR STAGNATION ENTHALPY,                      /
     162H             J=2 FOR MIXTURE FRACTION, F,                      /
     262H             J=3 FOR MASS FRACTION OF UNBURNT FUEL.            /
     3 7(10H   ****   )/7(10H   ****   )/1H1)
      RETURN
C
C-----------------------------------------------------------------------
CHAPTER B------------------------- HEADINGS -------------------------
C-----------------------------------------------------------------------
C
      ENTRY OUTP2
      IF (MOD(NITFR,ISWP).NE.0.AND.ISTRT.NE.1.AND.IX.EQ.ISTRT)RETURN
      IF (MOD(NITER,NPRINT).EQ.0) GO TO 1000
      IF (NITER.EQ.NITMAX) GO TO 1000
      GO TO 1052
 1000 IF (IX.EQ.1) GO TO 1109
      IF (MOD(NITER,ISWP).NE.0.AND.IX.EQ.(ISTRT+1).AND.ISTRT.NE.1)
     1 GO TO 1109
      GO TO 1110
 1109 NITER1=NITER+1
      DO 1089 IY=1,N
 1089 EMU(IY)=EMU1
      JXPLOT=0
      WRITE (6,1106) NITER1
 1106 FORMAT(1H1,20(1H*),6X,17HITERATION NUMBER ,I3,6X,20(1H*)/
     1         1H0,9(2H-+),6X,24HTWO-DIMENSIONAL SOLUTION,6X,9(2H-+)//)
C
C-----------------------------------------------------------------------
CHAPTER C------------------- TESTS FOR PRINTOUT ---------------------
C-----------------------------------------------------------------------
C
 1110 UBAR=0.0
      DO 110 IY=2,NM1
      IXY=IY+IXX
  110 UBAR=UBAR+BOM(IY)*U(IXY)
      UFLUX=PSIE*UBAR
C
      DO 115 J=1,NF
      FLUX(J)=0.
      DO 116 IY=2,NM1
  116 FLUX(J)=FLUX(J)+BOM(IY)*F(IY+IXX,J)
  115 FLUX(J)=PSIF*FLUX(J)
C
      PRESSD=PR(IX)/PRESSI-1.0
C
      IF (MOD(NITER,NPLOTL).NE.0) GO TO 1105
C ---------- ASSIGN VALUES FOR DOWNSTREAM PLOT.
      IF(X(IX).GT.XD(3).OR.X(IX).LT.XD(2)) GO TO 1105
      JXPLOT=JXPLOT+1
      IF(JXPLOT.EQ.1) ISLP=IX-1
      IF(MOD(JXPLOT,IPLOTL).NE.0.AND.JXPLOT.NE.1) GO TO 1105
      IL=JXPLOT/IPLOTL+1
      IF (IPLOTL.EQ.1) IL=IL-1
      XLPLOT(IL)=X(IX)
      IXY=1+IXX
      YLPLOT(IL,1)=U(IXY)
      YLPLOT(IL,2)=0.0
      DO 1104 IY=2,NM1
 1104 YLPLOT(IL,2)=AMAX1(YLPLOT(IL,2),F(IY+IXX,JTE))
      YLPLOT(IL,3)=DPDX
      NYL=3
      IF (INERT.EQ.1) GO TO 1105
      NYL=6
      YLPLOT(IL,4)=FLUX(JF)
      YLPLOT(IL,5)=0.0
      YLPLOT(IL,6)=0.0
      DO 1103 IY=2,NH1
      IXY=IY+IXX
      YLPLOT(IL,5)=AMAX1(YLPLOT(IL,5),F(IXY,JF))
 1103 YLPLOT(IL,6)=AMAX1(YLPLOT(IL,6),F(IXY,JOX))
      IF (IEQUIL.EQ.0) GO TO 1105
      DO 1102 I=7,18
 1102 YLPLOT(IL,I)=0.0
      DO 1107 IY=2,NH1
      YLPLOT(IL,7)=AMAX1(YLPLOT(IL,7),FS(IY,IDCO))
      YLPLOT(IL,8)=AMAX1(YLPLOT(IL,8),FS(IY,IDCO2))
      YLPLOT(IL,9)=AMAX1(YLPLOT(IL,9),FS(IY,IDH))
      YLPLOT(IL,10)=AMAX1(YLPLOT(IL,10),FS(IY,IDH2))
      YLPLOT(IL,11)=AMAX1(YLPLOT(IL,11),FS(IY,IDH2O))
      YLPLOT(IL,12)=AMAX1(YLPLOT(IL,12),FS(IY,IDO))
      YLPLOT(IL,13)=AMAX1(YLPLOT(IL,13),FS(IY,IDOH))
 1107 YLPLOT(IL,14)=AMAX1(YLPLOT(IL,14),FS(IY,IDN2))
      IF (KNTCS.EQ.0) GO TO 1105
      DO 1119 IY=2,NH1
      IXY=IY+IXX
      YLPLOT(IL,15)=AMAX1(YLPLOT(IL,15),F(IXY,JN))
      YLPLOT(IL,16)=AMAX1(YLPLOT(IL,16),F(IXY,JNO))
      YLPLOT(IL,17)=AMAX1(YLPLOT(IL,17),F(IXY,JNO2))
 1119 YLPLOT(IL,18)=AMAX1(YLPLOT(IL,18),F(IXY,JN2O))
C
C     ----- TESTS FOR PRINTOUT
C     ----- IPRINT=1 GIVES SINGLE (STATION) VARIABLES,
C           IPRINT=2 ADDS THE ARRAY (PROFILE) VARIABLES,
C           IPRINT=3 ADDS THE CROSS-STREAM PLOTS.
C
 1105 IPRINT=0
      IF(MOD(ISTEP,NSTAT).EQ.0) IPRINT=1
      IF (MOD(ISTEP,NPROF).EQ.0.OR.ITEST.NE.1) IPRINT=2
      IF ((MOD(ISTEP,NPLOTC).EQ.0.AND.ISTEP.NE.0).OR.IFIN.NE.1) IPRINT=3
C
      DO 1108 I=1,IPLOTM
      IF (IX.EQ.IPLOT(I)) IPRINT=3
 1108 CONTINUE
      IF (IPRINT.EQ.0) GO TO 1052
C
C-----------------------------------------------------------------------
CHAPTER D ------------------ STATION VARIABLES ------------------------
C-----------------------------------------------------------------------
C
      WRITE (6,1032)
 1032 FORMAT (1H0,72(1H-))
      WRITE (6,1030) X(IX),IX,DX,PRESSD,(J,J=1,3),UFLUX,(FLUX(J),J=1,NF)
 1030 FORMAT (1H0,5H***  ,2HX=,1PE10.3,2X,3HIX=,I5,5X,3HDX=,1PE10.3/6X,
     1 7HPRESSD=,1PE10.3/25X,3HJ =,3(I6,5X)/7H UFLUX=,E10.3,9H FLUX(J)=,
     2 (3E11.3))
C
      WRITE (6,1047) DA1,DA2
 1047 FORMAT (5H DA1=,1PE10.3,5H DA2=,E10.3)
C
C----------------------------------------------------------------------
CHAPTER E ---------------- CROSS-STPEAM PROFILES ----------------------
C----------------------------------------------------------------------
C
      IF (IPRINT.EQ.1) GO TO 1050
C
      WRITE (6,1099) (LAB(K),K=1,KOUT)
      DO 1091 IY=1,N
      IXY=IY+IXX
 1091 WRITE (6,1098) IY,R(IY),U(IXY),F(IXY,JTE),F(IXY,JF),F(IXY,JOX),
     1 F(IXY,JP)
      WRITE (6,1099)LABK1,LABK(IDN2),LABKR,LABKV,LABKH
      EMU(1)=EMU(2)
      DO 1207 IY=1,N
 1207 WRITE(6,1098)IY,R(IY),FS(IY,IDN2),RHO(IY),EMU(IY),F(IY+IXX,JH)
      IF (INERT.EQ.1) GO TO 1092
      IF (IEQUIL.EQ.0) GO TO 1092
      WRITE (6,1201)
 1201 FORMAT (1H0,5(2H-+),10X,29HCHEMICAL-EQUILIBRIUM SOLUTION,10X,
     1 5(2H+-))
      WRITE (6,1099) LABK1,(LABK(K),K=NSE1,NSE3)
      DO 1202 IY=1,N
 1202 WRITE (6,1098) IY,R(IY),(FS(IY,K),K=NSE1,NSE3)
      WRITE (6,1099) LABK1,(LABK(K),K=NSE4,NSE2)
      DO 1203 IY=1,N
 1203 WRITE (6,1098) IY,R(IY),(FS(IY,K),K=NSE4,NSE2)
      IF (KNTCS.EQ.0) GO TO 1092
      IF (NITER.LT.NITERK) GO TO 1092
      WRITE (6,1301)
 1301 FORMAT (1H0,5(2H-+),11X,26HCHEMICAL-KINETICS SOLUTION,11X,5(2H+-))
      WRITE (6,1099) LABK1,(LABK(K),K=1,NSK)
      DO 1302 IY=1,N
 1302 WRITE (6,1098) IY,R(IY),(FS(IY,K),K=1,NSK)
 1092 WRITE (6,1032)
C
      IF (IPRINT.EQ.2) GO TO 1052
C ---------- ASSIGN CPOSS-STREAM PLOTS.
      IF (NITER.NE.NITMAX) GO TO 1050
      DO 1073 IY=1,N
      IXY=IY+IXX
      XTPLOT(IY)=R(IY)
      YTPLOT(IY,1)=U(IXY)
 1073 YTPLOT(IY,2)=F(IXY,JTE)
      NYT=2
      IF (INERT.EQ.1) GO TO 1074
      NYT=4
      DO 1075 IY=1,N
      IXY=IY+IXX
      YTPLOT(IY,3)=F(IXY,JF)
 1075 YTPLOT(IY,4)=F(IXY,JOX)
      WRITE (6,1096) Y(IX),IX
      CALL PLOTS (XTPLOT,ITDIM,N,XTAXIS,YTPLOT,JTDIM,NYT,YAXIS1)
      IF (IEQUIL.EQ.0) GO TO 1050
      NYT=5
      DO 1077 IY=1,N
      XTPLOT(IY)=R(IY)
      YTPLOT(IY,1)=FS(IY,IDCO)
      YTPLOT(IY,2)=FS(IY,IDCO2)
      YTPLOT(IY,3)=FS(IY,IDH)
      YTPLOT(IY,4)=FS(IY,IDH2)
 1077 YTPLOT(IY,5)=FS(IY,IDH2O)
      WRITE (6,1096) X(IX),IX
      CALL PLOTS (XTPLOT,ITDIM,N,XTAXIS,YTPLOT,JTDIM,NYT,YAXIS3)
      NYT=3
      DO 1076 IY=1,N
      XTPLOT(IY)=R(IY)
      YTPLOT(IY,1)=FS(IY,IDO)
      YTPLOT(IY,2)=FS(IY,IDOH)
 1076 YTPLOT(IY,3)=FS(IY,IDN2)
      IF (KNTCS.EQ.0) GO TO 1078
      NYT=7
      DO 1079 IY=1,N
      IXY=IY+IXX
      YTPLOT(IY,4)=F(IXY,JN)
      YTPLOT(IY,5)=F(IXY,JNO)
      YTPLOT(IY,6)=F(IXY,JNO2)
 1079 YTPLOT(IY,7)=F(IXY,JN2O)
 1078 WRITE (6,1096) X(IX),IX
      CALL PLOTS (XTPLOT,ITDIM,N,XTAXIS,YTPLOT,JTDIM,NYT,YAXIS2)
      GO TO 1050
C ---------- CROSS-STREAM PLOT OUTPUT.
 1074 WRITE (6,1096) X(IX),IX
 1096 FORMAT (19H1CROSS-STREAM PLOT,,4H XU=,1PE10.3,4H IX=,I4)
      CALL PLOTS (XTPLOT,ITDIM,N,XTAXIS,YTPLOT,JTDIM,NYT,YAXIS1)
C
C-----------------------------------------------------------------------
CHAPTER F ---------  LONGITUDINAL PLOTS AND RETURN  -------------------
C-----------------------------------------------------------------------
C
 1050 IF (IFIN.EQ.1) GO TO 1052
      IF (JXPLOT.EQ.0) GO TO 1052
      IF (NITER.EQ.NITMAX) GO TO 1053
C
C ---------- LONGITUDINAL PLOT OUTPUT.
      IF (NITER.EQ.0) GO TO 1052
      IF (MOD(NITER,NPLOTL).NE.0) GO TO 1052
 1053 WRITE (6,1054) X(L),L
 1054 FORMAT (19H1LONGITUDINAL PLOT,,4H XU=,1PE10.3,4H IX=,I4)
      CALL PLOTS(XLPLOT,ILDIM,IL,XLAXIS,YLPLOT,JLDIM,NYL,YLAXIS)
      IF (INERT.EQ.1) GO TO 1052
      IF (IEQUIL.EQ.0) GO TO 1052
      NYL=5
      DO 1055 KX=1,JXPLOT
      IF (MOD(KX,IPLOTL).NE.0.AND.KX.NE.1) GO TO 1055
      JX=KX/IPLOTL+1
      IF (IPLOTL.EQ.1) JX=JX-1
      XLPLOT(JX)=X(KX+ISLP)
      DO 1056 I=1,NYL
      YAXISL(I)=YLAXIS(I+6)
 1056 YLPLOT(JX,I)=YLPLOT(JX,I+6)
 1055 CONTINUE
      WRITE (6,1054) X(L),L
      CALL PLOTS(XLPLOT,ILDIM,IL,XLAXIS,YLPLOT,JLDIM,NYL,YAXISL)
      NYL=7
      IF (KNTCS.EQ.0) NYL=3
      DO 1057 KX=1,JXPLOT
      IF (MOD(KX,IPLOTL).NE.0.AND.KX.NE.1) GO TO 1057
      JX=KX/IPLOTL+1
      IF (IPLOTL.EQ.1) JX=JX-1
      XLPLOT(JX)=X(KX+ISLP)
      DO 1058 I=1,NYL
      YAXISL(I)=YLAXIS(I+11)
 1058 YLPLOT(JX,I)=YLPLOT(JX,I+11)
 1057 CONTINUE
      WRITE (6,1054) X(L),L
      CALL PLOTS(XLPLOT,ILDIM,IL,XLAXIS,YLPLOT,JLDIM,NYL,YAXISL)
 1052 IF (IX.NE.L) RETURN
      WRITE (6,1032)
      WRITE (6,1205) NITER,RSUMAX,(RSFMAX(J),J=1,NF)
      WRITE (6,1206) IRMUX,IRMUY,(IRMFX(J),IRMFY(J),J=1,NF)
 1205 FORMAT (1H0,6HNITER=,I2,1X,23HRSUMAX,RSFMAX(J),J=1,3,,1P4E10.3)
 1206 FORMAT (10X,23HAT GRID NODES, IX, IY =,8I5)
      RETURN
C     ----------------------------------------
 1098 FORMAT(1X,I3,1P7E11.3)
 1099 FORMAT(1H0,2X,1HI ,7A11)
      END
      SUBROUTINE PHYS
      INCLUDE COMA,LIST
      INCLUDE COMB,LIST
      INCLUDE COMC,LIST
      INCLUDE COMD,LIST
C
C------------------------------------------------------------------------
CHAPTER A ---------- PHYSU ---------- PHYSU ---------- PHYSU -----------
C------------------------------------------------------------------------
      ENTRY PHYSU
C     ---------------------------------------- LAMINAR VISCOSTTY
C     SQUARE-ROOT FORMULA, WITH WEIGHTING ACCORDING TO MASS FRACTION
      IXD=IX+1
      IF (MODEL.EQ.2) GO TO 200
      DO 110 IY=1,N
      IXY=IY+IXX
      IXYD=IXY+N
      FOX=F(IXY,JOX)
      FJF=F(IXY,JF)
      FPR=1.0-FJF-FOX
      EMUU(IY)=(VISFU*FJF+VISOX*FOX+VISPR*FPR)*SQRT(F(IXY,JTE))
      FOX=F(IXYD,JOX)
      FJF=F(IXYD,JF)
      FPR=1.0-FJF-FOX
      EMUD(IY)=(VISFU*FJF+VISOX*FOX+VISPR*FPR)*SQRT(F(IXYD,JTE))
  110 EMU(IY)=EMUD(IY)
      GO TO 201
C
C ---------- TURBULENT VISCOSITY.
  200 IXY=IXX+N
      IXYD=IXY+N
      ALPHA=1.0
      IF (X(IXD).GT.XD(2)) ALPHA = 100.
      IF (IX.EQ.1) GO TO 107
      IF (MOD(NITER,ISWP).NE.0.AND.ISTRT.NE.1.AND.IX.EQ.ISTRT) GO TO 107
      GO TO 109
  107 PSIE12=0.12*PSIE
      EMUNU=(VISFU*F(IXY,JF)+VISOX*F(IXY,JOX)+VISPR*(1.0-F(IXY,JF)
     1 -F(IXY,JOX)))*SQRT(F(IXY,JTE))
      SQIX=SQRT(0.5*ADUCT(IX))
      SHALFU=0.15*(PSIE/(EMUNU*SQIX))**(-0.125)
      AMUTU=ALPHA*PSIE12*SHALFU/(2.0*SQIX)
      AMUTU1=6.6666667*AMUTU
      GO TO 108
  109 AMUTU=AMUTD
      AMUTU1=AMUTD1
  108 EMU(N)=(VISFU*F(IXYD,JF)+VISOX*F(IXYD,JOX)+VISPR*(1.0-F(IXYD,JF)
     1 -F(IXYD,JOX)))*SQRT(F(IXYD,JTE))
      SQIXD=SQRT(0.5*ADUCT(IXD))
      SHALFD=0.15*(PSIE/(EMU(N *SQIXD))**(-0.125)
      AMUTD=ALPHA*PSIE12*SHALFD/(2.0*SQIXD)
      AMUTD1=6.6666667*AMUTD
      DO 104 IY=2,NM1
      YDR=1.0-R(IY)/R(N)
      IF (YDR.LT.0.15) GO TO 106
      EMUU(IY)=AMUTU
      EMUD(IY)=AMUTD
      GO TO 104
  106 EMUU(IY)=AMUTU1*YDR
      EMUD(IY)=AMUTD1*YDR
  104 EMU(IY)=EMUD(IY)
  201 DO 203 IY=2,NM2
  203 EMU(IY)=0.5*(EMU(IY)+EMU(IY+1))
C
C     ---------------------------------------------- MOMENTUM SOURCE
      STOPE=1.0/(XDIF(IXD)*DX)
      STOPE1=1.0/(XDIF(IX)*DX)
      SUMA=0.0
      SUMP=0.0
      DO 210 IY=2,NM1
      IXY=IY+IXX
      IXYDD=IXY+N+N
      EMUD(IY)=EMUD(IY)*AREA(IY)*STORE
      EMUU(IY)=EMUU(IY)*AREAU(IY)*STORE1
      SUMA=SUMA+EMUD(IY)
      SUMB=SUMB+EMUU(IY)
      SI(IY)=-DPDX*AREA(IY)+EMUD(IY)*U(IXYDD)+EMUU(IY)*U(IXY)
  210 SIP(IY)=-(EMUD(IY)+EMUU(IY))
      RETURN
C
C----------------------------------------------------------------------
CHAPTER 6 ---------- PHYSF ---------- PHYSF ---------- PHYSF ----------
C----------------------------------------------------------------------
      ENTRY PHYSF
      IF (NEWPR(J).EQ.1) GO TO 314
      PRCON=1.0/PPLT(J,MODEL)
      PRRAT=PRCON
      IF (J.NE.1) PRRAT=PRLT(J-1,MODEL)*PRCON
      DO 313 IY=2,NM2
      EMUU(IY)=EMUU(IY)*PRRAT
      EMUD(IY)=EMUD(IY)*PRRAT
  313 DIF(IY)=DIFU(IY)*PRCON
      EMUU(NM1)=EMUU(NM1)*PRRAT
      EMUD(NM1)=EMUD(NM1)*PPRAT
      SUMA=SUMA*PRRAT
      SUMB=SUMB*PRRAT
C     ----------------------------------------- KINETIC HEATING SOURCE
  314 IF (J.NE.JH) GO TO 3000
      IF (NEWPR(J).EQ.1) GO TO 303
      PPCON1=0.5*(PRLT(J,MODEL)-1.0)
      IXXD=IXX+N
      DUSQP=0.0
      USQP=U(2+IXXD)**2
      DO 322 IY=2,NM2
      USQ=U(IXXD+IY+1)**2
      DUSQ=(DIFU(IY)-DIF(IY))*(USQ-USQP)
      SI(IY)=0.5*(DUSQ-DUSQP)
      DUSQP=DUSQ
  322 USQP=USQ
      SI(NM1)=-DUSQ
      DO 323 IY=2,NM1
      IXY=IY+IXX
      IXYD=IXY+N
      IXYDD=IXYD+N
      USQ=U(IXY)**2
      UDSQ=U(IXYD)**2
      UDDSQ=U(IXYDD)**2
      SI(IY)=SI(IY)+PPCON1*(EMUD(IY)*(UDDSQ-UDSQ)-EMUU(IY)*(UDSQ-USQ))
     1        +EMUD(IY)*F(IXYDD,J)+EMUU(IY)*F(IXY,J)
  323 SIP(IY)=-EMUD(IY)-EMUU(IY)
      GO TO 5000
  303 DO 324 IY=2,NM1
      IXY=IY+IXX
      SI(IY)=EMUD(IY)*F(IXY+N+N,J)+EMUU(IY)*F(IXY,J)
  324 SIP(IY)=-EMUD(IY)-EMUU(IY)
      GO TO 5000
C
C     ------------------------------------------------ FUEL SOURCE
 3000 IF (J.NE.JF) GO TO 4000
      T1=PREEXP*PRESS*PRESS
      GO TO 342
      ENTRY SORFU
      CALL TEMP
  342 DO 344 IY=2,NM1
      IXY=IXX+IY
      IXYD=IXY+N
      FJF=F(IXYD,JF)
      PHI=(F(IXYD,JP)-FSTOIC)/FSTOIM
      FUBRNT=AMAX1(0.0,PHI)
      FUEX=FJF-FUBRNT
      IF (FUEX.GT.0.0) GO TO 346
      SIP(IY)=-BIG
      GO TO 345
  346 FOX=AMAX1((FJF-PHI)*STOICH,TINY)
      SIP(IY)=-T1*EXP(-ARRCON/F(IXYD,JTE))*AREA(IY)*FOX*FJF/FUEX
  345 SI(IY)=-SIP(IY)*FUBRNT
      SI(IY)=SI(IY)+EMUD(IY)*F(IXYD+N,JF)+EMUU(IY)*F(IXY,JF)
  344 SIP(IY)=SIP(IY)-(EMUU(IY)+EMUD(IY))
      GO TO 5000
C
C     ---------------------------------------------------  JP (F)
 4000 IF (J.NE.JP) GO TO 6000
      DO 360 IY=2,NM1
      IXY=IY+IXX
      SI(IY)=EMUD(IY)*F(IXY+N+N,J)+EMUU(IY)*F(IXY,J)
  360 SIP(IY)=-(EMUD(IY)+EMUU(IY))
      GO TO 6000
 5000 ALF(IXD,J)=SUMA
      BLF(IXD,J)=SUMB
 6000 RETURN
      END
      SUBROUTINE CHEM
      COMMON /COEFF/ A(10),B(10),C(10),D(10),POM(10),OMDIF(10)
      INCLUDE COMA,LIST
      INCLUDE COMB,LIST
      INCLUDE COMC,LIST
      INCLUDE COMD,LIST
C
C-----------------------------------------------------------------------
CHAPTER  A  - + - + - + - + - + - +   POLY  + - + - + - + - + - + - + -
C-----------------------------------------------------------------------
C
      ENTRY POLY
      PP=AMAX1(PRESS,PMIN)
      PP=AMIN1(PP,PMAX)
      PP=PP*1.0E-05
      IP=PP
      IP1=IP+1
      FACTR2 =PP-IP
      FACTR1 =1.0-FACTR2
      AH1=AH(1,IP)*FACTR1 +AH(1,IP1)*FACTR2
      AH2=AH(2,IP)*FACTR1 +AH(2,IP1)*FACTR2
      AH3=AH(3,IP)*FACTR1 +AH(3,IP1)*FACTR2
      AH4=AH(4,IP)*FACTR1 +AH(4,IP1)*FACTR2
      AC1=AC(1,IP)*FACTR1 +AC(1,IP1)*FACTR2
      AC2=AC(2,IP)*FACTR1 +AC(2,IP1)*FACTR2
      AC3=AC(3,IP)*FACTR1 +AC(3,IP1)*FACTR2
      AC4=AC(4,IP)*FACTR1 +AC(4,IP1)*FACTR2
      ASM1=AS(1,IP)*FACTR1 +AS(1,IP1)*FACTR2
      ASM2=AS(2,IP)*FACTR1 +AS(2,IP1)*FACTR2
      ASM3=AS(3,IP)*FACTR1 +AS(3,IP1)*FACTR2
      ASM4=AS(4,IP)*FACTR1 +AS(4,IP1)*FACTR2
      RETURN
C
C-----------------------------------------------------------------------
CHAPTER  B  - + - + - + - + - + - +   TEMP  + - + - + - + - + - + - + -
C-----------------------------------------------------------------------
C
      ENTRY TEMP
      SP1=1.0+STOICH
      IHCPS=2
      NS2=IDO2
      NS1=IDN2
      IF(KNTCS.EQ.0) GO TO 101
      NS1=1
      DO 103 IY=2,NM1
      IXYD=IXX+N+IY
      DO 103 I=1,NSK
      KK=ISPEC(I)
  103 FS(IY,I)=F(IXYD,KK)
  101 DO 100 IY=2,NM1
      IXYD=IXX+N+IY
      FFU=F(IXYD,JF)
      FJP=F(IXYD,JP)
      FFU=AMIN1(FFU,FJP)
      F(IXYD,JF)=FFU
      PHI=(FJP-FSTOIC)/FSTOIM
      FO2=AMAX1((FFU-PHI)*STOICH,TINY)
      FPR=AMAX1((FJP-FFU)*SP1,TINY)
      FS(IY,IPR)=FPR
      F(IXYD,JOX)=FO2
      FS(IY,IDO2)=FO2
      FS(IY,IDF)=FFU
      FS(IY,IDN2)=FPR
      FN2=1.0
      DO 102 I=NS1,NS2
      S2(I)=FS(IY,I)
  102 FN2=FN2-S2(I)
      FS(IY,IDN2)=FN2
      S2(IDN2)=FN2
      TK=F(IXYD,JTE)
      ENTH=(F(IXYD,JH)-0.5*U(IXYD)**2)/GASCON
      DO 110 IT=1,NTMAX
      HPR=(AH1+(AH2+(AH3+AH4*TK)*TK)*TK)*FPR
      CPR=(AC1+(AC2+(AC3+AC4*TK)*TK)*TK)*FPR
      CALL HCPS
      CPMIX=CPSUM+CPR
      HMIX=HSUM*TK+HPR
      FACTOR=1.0+(ENTH-HMIX)/(TK*CPMIX)
      TK=TK*FACTOR
      TK=AMIN1(TK,TMAX)
      TK=AMAX1(TK,TMIN)
      DTEMP=(FACTOR-1.0)/FACTOR
      IF (ABS(DTEMP).LE.EPST) GO TO 100
  110 CONTINUE
      IT=IT-1
      WRITE(6,9415) IX,IY,IT,TK,DTEMP
 9415 FORMAT (1H0,10(1H-),2X,31HPOOR CONVFRGENCE OF TEMPERATURE/13X,
     1 7HAT IX =,I3,10H, AND IY =,I3/13X,22HNUMBEP OF ITERATIONS =,I3/
     2 13X,13HTEMPERATURE =,1PE15.6/13X,7HDTEMP =,1PE15.6/13X,
     3 25H**** SUBROUTINE TEMP ****)
  100 F(IXYD,JTE)=TK
      RETURN
C
C------------------------------------------------------------------------
CHAPTER  C  - + - + - + - + - + - +   DENS  + - + - + - + - + - + - + -
C------------------------------------------------------------------------
C
      ENTRY DENS
      PDGSCN=PRESS/GASCON
      DO 200 IY=2,NM1
      TK=F(IXX+IY+N,JTE)
      SM=(ASM1+(ASM2+(ASM3+ASM4*TK)*TK)*TK)*FS(IY,IPR)
      DO 217 I=NS1,NS2
  217 SM=SM+FS(IY,I)/SMW(I)
  200 RHO(IY)=PDGSCN/(TK*SM)
      RHO(1)=RHO(2)
      RHO(N)=RHO(NM1)
      IF (IX.NE.(ISTRT-1)) GO TO 218
      DO 219 IY=1,N
  219 RHO2(IY)=RHO(IY)
  218 IXY=IXX+N+1
      IXY1=IXY+1
      F(IXY,JF)=F(IXY1,JF)
      F(IXY,JOX)=F(IXY1,JOX)
      F(IXY,JTE)=F(IXY1,JTE)
      IXY=IXX+N+N
      IXY1=IXY-1
      F(IXY,JF)=F(IXY1,JF)
      F(IXY,JOX)=F(IXY1,JOX)
      DO 227 I=IDN2,IDO2
      FS(1,I)=FS(2,I)
  227 FS(N,I)=FS(NM1,I)
      TK=F(IXY,JTE)
      HPR=(AH1+(AH2+(AH3+AH4*TK)*TK)*TK)*FS(NM1,IPR)
      IHCPS=1
      DO 220 I=NS1,NS2
  220 S2(I)=FS(NM1,I)
      CALL HCPS
      F(IXY,JH)=(HSUM*TK+HPR)*GASCON
      RETURN
C
C-----------------------------------------------------------------
CHAPTER  D  - + - + - + - + - + - +   EQUTL  + - + - + - + - + - + - + -
C-----------------------------------------------------------------
C
      ENTRY EQUIL
      HDIFF=1.0/(HMAX-HMIN)
      DO 30 II=NSE1,NSE2
      LL=II-NSE1+1
      DO 30 KK=1,4
      AFS(KK,LL,1)=AS1(KK,LL,IP)*FACTR1 +AS1(KK,LL,IP1)*FACTR2
   30 AFS(KK,LL,2)=BS1(KK,LL,IP)*FACTR1 +BS1(KK,LL,IP1)*FACTR2
      DO 300 IY=2,NM1
      SUM=0.0
      FPR=FS(IY,IPR)
      TK=F(IXX+N+IY,JTE)
      HPR=(AH1+(AH2+(AH3+AH4*TK)*TK)*TK)*GASCON
C-----OBTAIN EQUILIBRIUM COMPOSITIONS FROM POLYNOMIAL FITS.
C
      HPR=AMAX1(HPR,HMIN)
      HPR=AMIN1(HPR,HMAX)
      MM=1
      IF (HPR.GT.HDIV) MM=2
      HPR=(HPR-HMIN)*HDIFF
      DO 30002 II=NSE1,NSE2
      LL=II-NSE1+1
      FSII=AFS(1,LL,MM)+(AFS(2,LL,MM)+(AFS(3,LL,MM)+AFS(4,LL,MM)*HPR)
     1 *HPR)*HPR
      FS(IY,II)=FPR*EXP(FSII)
30002 SUM=SUM+FS(IY,II)
      SUM=SUM+FS(IY,IDF)+FS(IY,IDO2)
      IF (KNTCS.EQ.0) FS(IY,IDN2)=AMIN1(1.0-SUM,1.0-OXC)
  300 CONTINUE
      DO 397 I=IDN2,NSE2
      FS(1,I)=FS(2,I)
  397 FS(N,I)=FS(NM1,I)
      RETURN
C
C-----------------------------------------------------------------
CHAPTER  E  - + - + - + - + - + - +   KINE  + - + - + - +   + - + - + -
```

```
C-----------------------------------------------------------------------
C
      ENTRY KINE
      IXD=IX+1
      PA=PRESS
      IF (NITER.NE.NITERK.OR.IX.EQ.1) GO TO 483
      IXN=IX*N
      IXNU=IXN-N
      IXND=IXN+N
      DO 482 I=1,NSK
      KK=ISPEC(I)
      DO 482 IY=1,N
      FU=F(IY+IXNU,KK)
      F(IY+IXN,KK)=FU
  482 F(IY+IXND,KK)=FU
  483 DEBUG=.FALSE.
      IF (IDEBUG.EQ.2) DERUG=.TRUE.
      IF (NEWPR(JN).EQ.1) GO TO 471
      PRCON=1.0/PRLT(JN,MODEL)
      PRRAT=PRLT(JN-1,MODEL)*PRCON
      DO 470 IY=2,NM2
      EMUU(IY)=EMUU(IY)*PRRAT
      EMUD(IY)=EMUD(IY)*PRRAT
      A(IY)=DIFU(IY)*PRCON
  470 B(IY+1)=A(IY)
      EMUU(NM1)=EMUU(NM1)*PRRAT
      EMUD(NM1)=EMUD(NM1)*PRRAT
  471 DO 487 IY=2,NM1
C
C
      C(IY) = POM(IY) + EMUU(IY)
      D(IY) = EMUD(IY)
C
C
      EMV=A(IY)+B(IY)+C(IY)+D(IY)
      DO 486 I=ION2,NSE2
  486 S2(I)=FS(IY,I)/SMW(I)
      IXYD=IXX+N+IY
      TK=F(IXYD,JTE)
      DO 488 I=1,NSK
      KK=ISPEC(I)
      S1(I)=(A(IY)*F(IXYD+1,KK)+B(IY)*F(IXYD-1,KK)+C(IY)*F(IXYD-N,KK)
     1 +D(IY)*F(IXYD+N,KK))/(EMV*SMW(I))
  488 S2(I)=F(IXYD,KK)/SMW(I)
      PWR=EQRAT-0.10
      EMV=EMV/(AREA(IY))**PWR
      IF (TK.LE.550.0) GO TO 500
      CALL SPECE
      IF (CONVG) GO TO 510
      IX1=IX+1
      WRITE (6,981) IX1,IY
  981 FORMAT (10X,68HCHEMICAL KINETICS SOLUTION FAILED...AVG INLET PROPE
     1RTIES RETURNED    /10X,6HAT IX=,I3,9H,AND, IY=,I3/)
  500 DO 502 I=1,NSK
  502 S2(I)=S1(I)
  510 SUM=0.0
      DO 489 I=1,NSE2
  489 SUM=SUM+S2(I)*SMW(I)
      DO 490 I=1,NSK
      KK=ISPEC(I)
      FS(IY,I)=S2(I)*SMW(I)/SUM
  490 F(IXYD,KK)=FS(IY,I)
C----- LUMP ALL ERRORS INTO N2-MASS FRACTION
      SUM=0.D
      DO 493 I=1,NSE2
  493 SUM=SUM+FS(IY,I)
      FS(IY,IDN2)=AMIN1(1.0+FS(IY,IDN2)-SUM,1.D-0XC)
  487 CONTINUE
      IXYN=IXX+N+N
      IXYN1=IXYN-1
      IXY1=IXX+N+1
      IXY2=IXY1+1
      DO 494 I=1,NSK
      FS(1,I)=FS(2,I)
      FS(N,I)=FS(NM1,I)
      KK=ISPEC(I)
      F(IXYN,KK)=F(IXYN1,KK)
  494 F(IXY1,KK)=F(IXY2,KK)
      FS(N,IDN2)=FS(NM1,IDN2)
      FS(1,IDN2)=FS(2,IDN2)
      RETURN
      END
      SUBROUTINE COMP
      COMMON /COEFF/ A(10),B(10),C(10),D(10),POM(10),OMDIF(10)
      INCLUDE COMA,LIST
      INCLUDE COMB,LIST
      INCLUDE COMD,LIST
C
CHAPTER A - + - + - + - + - + - + - INIT - + - + - + - + - + - + - + - + - +
C
      DIMENSION FOUM(100)
      ENTRY INIT
C     ------------------------ INITIAL VALUES AND DEFAULT VALUES
      NM1=N-1
      NM2=N-2
      NM3=N-3
      LM1=L-1
      LM2=L-2
      IX=1
      IXX=0
      ISTEP=0
      IFIN=1
      DX=TINY
      R(I)=0.0
      BPE=1.
      DPDX=0.
      XD=0.0
      XU=0.0
      DA2=0.0
      DO 12 IY=1,N
      DO 11 I=1,NSK
      KK=ISPEC(I)
      F(IY,KK)=0.0
   11 FS(IY,I)=0.0
      DO 14 I=NSE1,NSE2
   14 FS(IY,I)=0.0
   12 CONTINUE
      RETURN
CHAPTER B - + - + - + - + - + - + - GRIDX - + - + - + - + - + - + - + - + -
C
      ENTPY GRIDX
      XS(2)=0.5*(X(3)+X(2))
      XS(LM1)=X(L)-0.5*(X(LM1)+X(LM2))
      XDIF(1)=X(2)-X(1)
      XDIF(2)=X(3)-X(2)
      XDIF(LM1)=X(L)-X(LM1)
      DO 201 JX=3,LM2
      XS(JX)=0.5*(X(JX+1)-X(JX-1))
  201 XDIF(JX)=X(JX+1)-X(JX)
      XS(1)=XS(2)
      XS(L)=XS(LM1)
      RETURN
C
CHAPTER  C  - + - + - + - + - + - +  GRIDOM  + - + - + - + - + - + - + -
C
      ENTRY GRIDOM
      OMI=OM(2)
      OME=1.-OM(NM1)
      BOM(2)=.5*(OM(2)+OM(3))
      OMINT(1)=0.
      OMINT(2)=BOM(2)
      DO 202 I=3,NM2
      OMINT(I)=.5*(OM(I)+OM(I+1))
      BOM(I)=OMINT(I)-OMINT(I-1)
  202 OMDIF(I)=OM(I)-OM(I-1)
      BOM(NM1)=1.-OMINT(NM2)
      OMINT(NM1)=1.
      OMDIF(NM1)=OM(NM1)-OM(NM2)
      RETURN
C
CHAPTER  D  - + - + - + - + - + - +  DISTAN  + - + - + - + - + - + - + -
C
      ENTRY DISTAN
      IF (MOD(NITER,ISWP).NE.0.AND.ISTRT.NE.1.AND.IX.EQ.ISTRT)BPE=BPSAVE
      RU(2)=RHO(2)*U(2+IXX)
      RU(1)=RU(2)
      RU(N)=0.0
      RECI=1.0/RU(2)
      RI=PSIE*RECI
      AREA(2)=(BOM(2)*0.5+OMI)*RI
      RI=RI*OMI
      R(2)=SQRT(2.0*RI)
      RIPP=RI
      HPEI=0.5*PSIE
      DO 231 IY=3,NM1
      RU(IY)=RHO(IY)*U(IY+IXX)
      RECIM1=RECI
      RECI=1.0/RU(IY)
      AREA(IY)=PSIE*BOM(IY)*RECI
      RIP=RIPP+HPEI*OMDIF(IY)*(RECIM1+RECI)
      R(IY)=SQRT(RIP*2.0)
  231 RIPP=RIP
      RE=PSIE*OME/(BPE*RU(NM1))
      R(N)=SQRT((RIP+RE)*2.0)
      AREA(NM1)=0.5*AREA(NM1)+RE
      RI=SQRT(RI*2.0)
      RE=R(N)-R(NM1)
      IF(NITER.NE.0) GO TO 232
      DO 233 IY=2,NM1
  233 AREAU(IY)=AREA(IY)
  232 IF(ITEST.EQ.1) RETURN
      WRITE(6,225) (RU(IY),IY=1,N)
  226 FORMAT(19H COMP DISTAN TESTS,,8H RU(IY)=/(3X,1P5E11.3))
      WRITE(6,236) (R(IY),IY=1,N)
  236 FORMAT(8H  R(IY)=/(3X,1P5E11.3))
      WRITE(6,242) (AREA(IY),IY=2,NM1)
  242 FORMAT(11H  AREA(IY)=/(3X,1P5E11.3))
      RETURN
C
CHAPTER  E  - + - + - + - + - + - +  SOLVE   + - + - + - + - + - + - + -
C
      ENTRY SOLVE
C     ------------------------------------------ PRELIMINARIES
      IXD=IX+1
      IXDD=IX+2
      IF (IX.EQ.1) RSUMAX=0.0
      IF (MOD(NITER,ISWP).NE.0.AND.ISTRT.NE.1.AND.IX.EQ.ISTRT)
     1 RSUMAX=0.0
      CALL PHYSU
      P=PSIE/DX
      DO 411 I=2,NM1
  411 POM(I)=P*BOM(I)
C     ----------------------------------------- COEFFICIENTS FOR U
      DO 413 I=2,NM2
      DIFU(I)=EMU(I)*0.5*(R(I+1)+R(I))/(R(I+1)-R(I))
      A(I)=DIFU(I)
  413 B(I+1)=A(I)
      J=0
      CALL WALL (BPE,TE)
      B(2)=0.0
      A(NM1)=TE
C     ------------------------------------------- C'S AND D'S
      DO 418 IY=2,NM1
      C(IY)=U(IY+IXX)*POM(IY)+SI(IY)
  418 D(IY)=A(IY)+B(IY)+POM(IY)-SIP(IY)
      IF (ITEST.EQ.1) GO TO 404
      WRITE (6,405) (A(I),I=2,NM1)
      WRITE(6,406) (B(I),I=2,NM1)
      WRITE(6,407) (C(I),I=2,NM1)
      WRITE(6,408) (D(I),I=2,NM1)
  405 FORMAT(17H COMP SOLVE TESTS/6H  A(I)/(3X,1P6E11.3))
  406 FORMAT(6H  B(I)/(3X,1P6E11.3))
  407 FORMAT(6H  C(I)/(3X,1P6E11.3))
  408 FORMAT(6H  D(I)/(3X,1P6E11.3))
C----------------------------   SOLVE FOR DOWNSTREAM U 'S  -------------
  404 C(2)=C(2)/D(2)
      D(2)=A(2)/D(2)
      DO 421 I=3,NM1
      T=D(I)-B(I)*D(I-1)
      D(I)=A(I)/T
  421 C(I)=(B(I)*C(I-1)+C(I))/T
      IXXP1=IXX+N
      DO 420 IDASH=1,NM2
      I=N-IDASH
      IXY=I+IXXP1
  420 U(IXY)=D(I)*U(IXY+1)+C(I)
  415 FORMAT (7H BL(IX)/(3X,1P6E11.3))
  416 FORMAT (7H CL(IX)/(3X,1P6E11.3))
  417 FORMAT (7H DL(IX)/(3X,1P6E11.3))
C     ------------------------------------------------
      U(1+IXXP1)=U(2+IXXP1)
      TAUE=TE*U(NM1+IXXP1)/R(N)
      IF (ITEST.EQ.1) GO TO 442
      WRITE (6,443) (U(IY+IXXP1),IY=1,N)
  443 FORMAT(17H COMP SOLVE TESTS/6H  U(I)/(3X,1P6E11.3))
C     -------------------------------------------
  442 IF (IX.EQ.(ISTRT-1)) BPSAVE=BPE
C----------------------------------------------------------  F SECTION
      IF (NF.EQ.0) RETURN
      IF (INERT.EQ.2) CALL POLY
      DO 480 J=1,NF
      IF (IX.EQ.1) RSFMAX(J)=0.0
      IF (MOD(NITER,ISWP).NE.0.AND.ISTRT.NE.1.AND.IX.EQ.ISTRT)
     1 RSFMAX(J)=0.0
      IF(INERT.EQ.1.AND.J.EQ.JF) GO TO 4410
C     ------------------------------- SUBROUTINE PHYS ICS
      CALL PHYSF
C     ---------------------------------------------- A'S AND B'S
      IF (NEWPR(J).EQ.1) GO TO 479
      DO 484 IY=2,NM2
      A(IY)=DIF(IY)
  484 B(IY+1)=A(IY)
      B(2)=0.0
  479 TEF=0.0
      FDIFE=0.0
      IF(J.EQ.JH)CALL WALL(FDIFE,TEF)
      A(NM1)=TEF
      DO 477 IY=2,NM1
  477 RESIDU(IY)=F(IXX+IY+N,J)
C     ---------------------------------------------- C'S AND D'S
      NIT=0
  483 NIT=NIT+1
      IF(NIT.GT.1) CALL SORFU
      DO 485 IY=2,NM1
      D(IY)=A(IY)+B(IY)+POM(IY)-SIP(IY)
  485 C(IY)=F(IY+IXX,J)*POM(IY)+SI(IY)
      C(NM1)=C(NM1)-TEF*FDIFE
      IF(ITEST.EQ.1) GO TO 464
      WRITE (6,409) (SI(I),I=2,NM1)
      WRITE(6,410) (SIP(I),I=2,NM1)
  409 FORMAT(17H COMP SOLVE TESTS/6H SI(I)/(3X,1P6E11.3))
  410 FORMAT(7H SIP(I)/(3X,1P6E11.3))
      WRITE(6,405) (A(I),I=2,NM1)
      WRITE(6,406) (B(I),I=2,NM1)
      WRITE(6,407) (C(I),I=2,NM1)
      WRITE(6,408) (D(I),I=2,NM1)
C     ------------------------------ SOLVE FOR DOWNSTREAM F 'S
  464 C(2)=C(2)/D(2)
      D(2)=A(2)/D(2)
      DO 465 I=3,NM1
      T=D(I)-B(I)*D(I-1)
      D(I)=A(I)/T
  465 C(I)=(B(I)*C(I-1)+C(I))/T
      DO 466 IDASH=1,NM2
      I=N-IDASH
      IXY=I+IXXP1
      SI(I)=F(IXY,J)
  466 F(IXY,J)=D(I)*F(IXY+1,J)+C(I)
      IF (J.NE.JF) GO TO 489
      FMAX=0.0
      DO 462 IY=2,NM1
      IXY=IY+IXXP1
      IF (F(IXY,J).LE.FMIN) GO TO 462
      FMAX=AMAX1(ABS(SI(IY)-F(IXY,J))/(F(IXY,J)+TINY),FMAX)
  462 CONTINUE
      IF (FMAX.LT.FUTEST) GO TO 489
      IF (NIT.LE.NFUMAX) GO TO 483
  489 DO 461 I=2,NM1
      IXY=I+IXXP1
      ABSF=ABS(F(IXY,J))
      RESIDU(I)=F(IXY,J)-RESIDU(I)
      IF(ABSF.LE.FMIN) GO TO 461
      STOPE2=ABS(RESIDU(I))/ABSF
      IF (STORE2.LE.RSFMAX(J)) GO TO 461
      RSFMAX(J)=STORE2
      IRMFX(J)=IX+1
      IRMFY(J)=I
  461 CONTINUE
      IF(ITEST.EQ.1) GO TO 4314
      WRITE(6,476) J,(F(IY+IXXP1,J),IY=1,N)
  476 FORMAT(8H  F(IXY,,I2,1H)/(3X,1P6E11.3))
 4314 IF(J.EQ.JP) GO TO 4317
C ---------- LONGITUDINAL TDMA.
      BLF(IXD,J)=BLF(IXD,J)+P
      CLF(IX)=0.0
      CLF(IXDD)=0.0
      DLF(IXD,J)=0.0
      DO 492 IY=2,NM1
      DLF(IXD,J)=DLF(IXD,J)+POM(IY)-SIP(IY)
      CLF(IX)=CLF(IX)+EMUU(IY)*RESIDU(IY)
  492 CLF(IXDD)=CLF(IXDD)+(EMUD(IY)+POM(IY))*RESIDU(IY)
      CLF(Ix)=CLF(IX)*DX/XS(IX)
      CLF(IXDD)=CLF(IXDD)*DX/XS(IXDD)
      IF (ITEST.EQ.1) GO TO 4720
      WRITF (6,4140) J,(ALF(JX,J),JX=2,LM1)
      WRITE (6,415) (BLF(JX,J),JX=2,LM1)
      WRITE (6,416) (CLF(JX),JX=2,LM1)
      WRITE (6,417) (DLF(JX,J),JX=2,LM1)
 4140 FORMAT (16H LTDMA TESTS, F(,I2,1H)/7H AL(IX)/(3X,1P6E11.3))
      WRITE'6,4323)
 4323 FORMAT(1H0,21HSOLUTION BEFORE LTDMA/)
      DO 4780 IY=2,NM1
      DO 999 JX = 1,L
      IDUM = IY + (JX-1) * N
  999 FDUM(JX) = F(IDUM,J)
 478C WRITF (6,476) J, (FDUM(JX),JX = 1,L)
 4720 CLF(2)=CLF(2)/DLF(2,J)
      ELF'2)=ALF(2,J)/DLF(2,J)
      DO 4310 JX=3,LM1
      T=DLF(JX,J)-BLF(JX,J)*ELF(JX-1)
      ELF(JX)=ALF(JX,J)/T
 4310 CLF(JX)=(BLF(JX,J)*CLF(JX-1)+CLF(JX))/T
      CORR=0.0
      DO 4320 JXJ=1,LM2
      JX=L-JXJ
      JXN=(JX-1)*N
      CORR=ELF(JX)*CORR+CLF(JX)
      DO 4325 IY=2,NM1
      IXY=IY+JXN
      F(IXY,J)=F(IXY,J)+CORP
      IF (J.NE.JF) GO TO 4325
      F(IXY,J)=AMAX1(TINY,F(IXY,J))
      F(IXY,J)=AMIN1(F(IXY,JP),F(IXY,J))
 4325 CONTINUE
 4320 CLF(JX)=0.0
      IF (ITEST.EO.1) GO TO 4317
      WRITE (6,4322)
 4322 FORMAT (1H0,20HSOLUTION AFTER LTDMA/)
      DO 4770 IY=2,NM1
      DO 998 JX = 1,L
      IDUM = IY + (JX-1) * N
  998 FDUM(JX) = F(IDUM,J)
 4770 WRITE (6,476) J, (FDUM(JX),JX = 1,L)
 4317 F(1+IXXP1,J)=F(2+IXXP1,J)
      IF (IBEX(J).EQ.1) GO TO 480
      F(N+IXXP1,J)=F(NM1+IXXP1,J)
      GO TO 480
 4410 DO 4411 IY=1,N
      IXY=IY+IXXP1
 4411 F(IXY,JF)=F(IXY,JP)
  480 CONTINUE
C     ------------------------------------------
      RETURN
      END
      SUBROUTINE CREKD
      INCLUDE COMD,LIST
      INCLUDE COME,LIST
      DIMENSION DATA(12),AT(4),B(4)
C
CHAPTER  1    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1
C
      DATA GAZ/1HG/
      DATA ELEM/4HELEM/
      DATA RVRS/4HREVE/,THIRD/4HH   /
      DATA THRM/4HTHER/,AMCH/4HMECH/,BLANK/4H    /
      DATA TENLN/2.302585/,XMAX/0.001/,XMIN/0.000333333/
    5 READ (5,901) (DATA(I),I=1,12)
  901 FORMAT (12A4)
      IF (DATA(1).EQ.BLANK) GO TO 5
      IF (DATA(1).EQ.ELEM) GO TO 10
      IF (DATA(1).EQ.THRM) GO TO 20
      IF (KNTCS.EQ.0) RETURN
      IF (DATA(1).EQ.AMCH) GO TO 30
C
CHAPTER  2    2    2    2    2    2    2    2    2    2    2    2    2    2    2    2
C
   10 NLM=1
   11 READ (5,950) (ATOM(K,NLM),K=1,3)
  950 FORMAT (A2,7X,2F10.6)
      IF (ATOM(1,NLM).EQ.BLANK) GO TO 12
      NLM=NLM+1
      GO TO 11
   12 NLM=NLM-1
      GO TO 5
C
CHAPTER  3    3    3    3    3    3    3    3    3    3    3    3    3    3    3    3
C
   20 NS=1
   21 READ (5,920) (DATA(I),I=1,3),DT1,DT2,(AT(J),B(J),J=1,4),PHAZ,
     1T1,T2,NCD
  920 FORMAT (3A4,6X,2A3,4(A2,F3.0),A1,2F10.3,I15)
      IF (DATA(1).EQ.BLANK) GO TO 26
      IF (PHAZ.NE.GAZ) WRITE(6,919) (DATA(I),I=1,3),PHAZ
  919 FORMAT (1H0,10X,29H WARNING...DATA FOR SPECIES   ,3A4,19H   NOT GA
     1S, BUT     ,A1 //)
      READ(5,922) (Z(1,J,NS),J=1,5),NCD
  922 FORMAT(5E15.8,I5)
      READ(5,922) (Z(1,J,NS),J=6,7),(Z(2,K,NS),K=1,3),NCD
      READ(5,923) (Z(2,J,NS),J=4,7),NCD
  923 FORMAT(4E15.8,I20)
      DO 22 L=1,NLM
   22 AL(L,NS)=0.0
      SUM=0.0
      DO 24 K=1,4
      IF (B(K).EQ.0.) GO TO 24
      DO 23 L=1,NLM
      IF (ATOM(1,L).NE.AT(K)) GO TO 23
      AL(L,NS)=AL(L,NS)+B(K)
      SUM=SUM+ATOM(2,L)*B(K)
   23 CONTINUE
   24 CONTINUE
      SMW(NS)=SUM
      DO 25 I=1,3
   25 ASUB(NS,I)=DATA(I)
      NS=NS+1                                                           CRK00141
      GO TO 21                                                          CRK00142
   26 NS=NS-1
      NSM=NS+1                                                          CRK00146
      NA=NS+1
      DO 27 I=1,NS
      RSMW=1.0/SMW(I)
      DO 27 J=1,7
      DO 27 K=1,2
   27 Z(K,J,I)=Z(K,J,I)*RSMW
      GO TO 5                                                           CRK00149
C
CHAPTER  4   4   4   4   4   4   4   4   4   4   4   4   4   4   4   4
C
   30 JJ=1
   31 READ (5,930) (DATA(I),I=1,12),BX(JJ),TEN(JJ),TACT(JJ),DT1,DT2
  930 FORMAT (12A4,3F8.3,2A4)                                           CRK00164
      IF (DATA(1).EQ.BLANK) GO TO 39                                    CRK00165
      IF(DT1.NE.RVRS) GO TO 32                                          CRK00167
      J=JJ-1                                                            CRK00168
      BX2(J)=BX(JJ)                                                     CRK00169
      TEN2(J)=TEN(JJ)                                                   CRK00170
      TACT2(J)=TACT(JJ)                                                 CRK00171
      BX2(J)=10.**BX2(J)                                                CRK00175
      GO TO 31                                                          CRK00176
   32 BX(JJ)=10.0**BX(JJ)
      DO 33 I=1,4                                                       CRK00188
   33 ID(I,JJ)=0
      ND=1                                                              CRK00192
      DO 38 N=1,6                                                       CRK00193
      K=N*2-1                                                           CRK00194
      IF (DATA(K).EQ.BLANK) GO TO 38                                    CRK00195
      IF (DATA(K).NE.THIRD) GO TO 34                                    CRK00196
      DATA(K)=BLANK                                                     CRK00197
      GO TO 38                                                          CRK00198
   34 DO 35 I=1,NS
      IF (DATA(K).NE.ASUB(I,1)) GO TO 35                                CRK00201
      IF (DATA(K+1).NE.ASUB(I,2)) GO TO 35                              CRK00202
      II=I                                                              CRK00203
      GO TO 36                                                          CRK00204
   35 CONTINUE                                                          CRK00205
   36 IF (K.GT.3) GO TO 37
      ID(ND,JJ)=II                                                      CRK00208
      ND=ND+1                                                           CRK00209
      GO TO 38                                                          CRK00210
   37 IF (ND.EQ.2) ND=3
      ID(ND,JJ)=II                                                      CRK00213
      ND=ND+1                                                           CRK00214
   38 DX=(XMAX-XMIN)*7.142857E-2
      SUMX=0.0                                                          CRK00227
      SUMY=0.0                                                          CRK00228
      IHCPS=3
      NS1=1
      NS2=NS
      DO 381 N=1,15                                                     CRK00230
      X(N)=XMIN+DX*FLOAT(N-1)                                           CRK00231
      SUMX=SUMX+X(N)                                                    CRK00232
      TK=1./X(N)                                                        CRK00233
      TLN=ALOG(TK)                                                      CRK00234
      CALL HCPS                                                         CRK00235
      SUM1=0.0                                                          CRK00236
      DO 382 ND=1,4                                                     CRK00237
      K=ID(ND,JJ)                                                       CRK00238
      IF (K.EQ.0) GO TO 382                                             CRK00239
      GF=(HO(K)-SO(K))*SMW(K)
      IF (ND.LT.3) SUM1=SUM1+GF                                         CRK00241
      IF (ND.GE.3) SUM1=SUM1-GF                                         CRK00242
  382 CONTINUE                                                          CRK00243
      SUM1=EXP(SUM1)                                                    CRK00244
      TM1=1.0                                                           CRK00245
      IF (ID(2,JJ).EQ.0) TM1=0.082057*TK                                CRK00246
      IF (ID(4,JJ).EQ.0) TM1=1.0/(0.082057*TK)                          CRK00247
      AK=BX(JJ)                                                         CRK00248
      IF (TEN(JJ).NE.0.0) AK=AK*TK**TEN(JJ)                             CRK00249
      IF (TACT(JJ).NE.0.0) AK=AK*EXP(-TACT(JJ)/TK)                      CRK00250
      AK=AK*TM1/SUM1                                                    CRK00251
      Y(N)=ALOG(AK)                                                     CRK00252
      SUMY=SUMY+Y(N)                                                    CRK00253
  381 CONTINUE                                                          CRK00254
      XBAR=SUMX*6.6666667E-2
      YBAR=SUMY*6.6666667E-2
      SUMX=0.0                                                          CRK00257
      SUM1=0.0                                                          CRK00258
      SUMY=0.0                                                          CRK00259
      DO 383 N=1,15                                                     CRK00260
      SUMX=SUMX+Y(N)*(X(N)-XBAR)                                        CRK00261
      SUM1=SUM1+(X(N)-XBAR)**2                                          CRK00262
  383 SUMY=SUMY+(Y(N)-YBAR)**2
      TEN2(JJ)=0.0                                                      CRK00265
      TACT2(JJ)=-SUMX/SUM1                                              CRK00266
      BX2(JJ)=(YBAR+TACT2(JJ)*XBAR)/TENLN                               CRK00267
      SUMX=0.0                                                          CRK00268
      DO 384 N=1,15                                                     CRK00269
  384 SUMX=SUMX+(Y(N)+TACT2(JJ)*X(N)-TENLN*BX2(JJ))**2
      SUMY=SQRT(1.-SUMX/SUMY)                                           CRK00272
      SUMX=SQRT(SUMX*7.142857E-2)
      BX2(JJ)=10.**BX2(JJ)                                              CRK00278
      JJ=JJ+1                                                           CRK00281
      GO TO 31                                                          CRK00282
   39 JJ=JJ-1
      RETURN                                                            CRK00309
      END                                                               CRK00398
      SUBROUTINE SPECE                                                  SPEC0001
      INCLUDE COMD,LIST
      INCLUDE COME,LIST
C
CHAPTER  1    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1
C
      CONVG=.FALSE.                                                     SPEC0021
      SM=0.0                                                            SPEC0022
      DO 10 I=1,NS
      S2(I)=AMAX1(S2(I),TINYK)
      Y(I)=ALOG(S2(I))                                                  SPEC0026
      SM=SM+S2(I)
   10 X(I)=0.0
      X(NSM)=0.0
      Y(NSM)=ALOG(SM)                                                   SPEC0028
      IMAT=NSK
      KMAT=IMAT+1
C
CHAPTER  2    2    2    2    2    2    2    2    2    2    2    2    2    2    2    2
C
      DO 170 ITER=1,ITMAX                                               SPEC0037
      CALL CALC                                                         SPEC0040
      IF (.NOT.DEBUG) GO TO 12                                          SPEC0045
      WRITE (6,911)                                                     SPEC0046
  911 FORMAT (1H0,10X,38H ELEMENTS A(I,K) OF CORRECTION MATRIX  /)      SPEC0047
      DO 11 K=1,IMAT                                                    SPEC0048
   11 WRITE (6,912) (A(K,I),I=1,KMAT)
  912 FORMAT (1H ,1P16E8.0)                                             SPEC0050
   12 DO 50 NN=1,IMAT
      K=NN+1                                                            SPEC0056
      DO 20 J=K,KMAT                                                    SPEC0057
   20 A(NN,J)=A(NN,J)/A(NN,NN)
      IF (K.EQ.KMAT) GO TO 50                                           SPEC0061
      DO 40 I=K,IMAT                                                    SPEC0062
      DO 40 J=K,KMAT
   40 A(I,J)=A(I,J)-A(I,NN)*A(NN,J)
   50 CONTINUE                                                          SPEC0069
      K=IMAT                                                            SPEC0072
   60 J=K+1
      SUM=0.0                                                           SPEC0075
      X(K)=0.0                                                          SPEC0076
      IF (IMAT .LT.J) GO TO 80                                          SPEC0077
      DO 70 I=J,IMAT                                                    SPEC0078
   70 SUM=SUM+A(K,I)*X(I)
   80 X(K)=A(K,KMAT)-SUM
      K=K-1                                                             SPEC0084
      IF (K.NE.0) GO TO 60                                              SPEC0085
C
CHAPTER  3    3    3    3    3    3    3    3    3    3    3    3    3    3    3    3
C
      ETA=1.0                                                           SPEC0109
      ETA1=1.                                                           SPEC0110
      SUM=TINYK
      DO 130 I=1,NSK
      IF (X(I).LE.0.0) GO TO 130
      SUM=AMAX1(X(I),SUM)
      IF (S2(I)/SM.GT.1.0E-8) GO TO 130
      TST1=ABS((Y(NSM)-Y(I)-9.212)/X(I))
      ETA1=AMIN1(TST1,ETA1)
  130 CONTINUE                                                        SPEC0124
      ETA=AMIN1(1.0,2.0/SUM)
      ETA=AMIN1(ETA,ETA1)
C
CHAPTER  4   4   4   4   4   4   4   4   4   4   4   4   4   4   4   4
C
      DO 150 I=1,NSK
      Y(I)=Y(I)+ETA*X(I)                                              SPEC0149
      Y(I)=AMAX1(Y(I),TNY)
      S2(I)=EXP(Y(I))                                                 SPEC0151
  150 CONTINUE                                                        SPEC0157
      IF (DEBUG) WRITE(6,998) ITER,ETA,(ASUB(K,1),S2(K),Y(K),X(K),
     1 K=1,NSK)
C
CHAPTER  5   5   5   5   5   5   5   5   5   5   5   5   5   5   5   5
C
      IF (ETA.LT.1.) GO TO 170                                        SPEC0169
      DO 160 I=1,NSK
      IF (S2(I).LE.TINYK*1.001) GO TO 160
      IF (ABS(X(I)).GT.EPSS) GO TO 170
  160 CONTINUE                                                        SPEC0182
      CONVG=.TRUE.                                                    SPEC0183
  998 FORMAT(1H0,6HITER =,I3,5X,5HETA =,1PE10.3//17X,2HS2,12X,5HLOGS2,
     1 8X,8HD(LOGS2)//(5X,A4,1P3E15.6))
      RETURN                                                          SPEC0189
  170 CONTINUE                                                        SPEC0191
      RETURN                                                          SPEC0193
      END                                                             SPEC022P
      SUBROUTINE CALC                                                   CALC0001
      INCLUDE COMD,LIST
      INCLUDE COME,LIST
C
CHAPTER  1    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1
C
      NSK1=NSK+1
      DO 5 I=1,NS
      DO 5 K=1,NA                                                       CALC0024
    5 A(I,K)=0.0
      RHSM=PA/(GASCON*TK)
      RECTK=1.0/TK
      RHOP=RHSM/SM                                                      CALC0045
      RHSQ=RHOP*RHOP                                                    CALC0046
      RHSMP=RHSM*RHOP
      RHSMSQ=RHSM*RHSQ
C
CHAPTER  2    2    2    2    2    2    2    2    2    2    2    2    2    2    2    2
C
      DO 100 J=1,JJ                                                     CALC0048
      R1=DX(J)*EXP(-TACT(J)*RECTK)
      R2=DX2(J)*EXP(-TACT2(J)*RECTK)
      IF (TEN(J).NE.0.) R1=R1*TK**TEN(J)                               CALC0059
      IF (TEN2(J).NE.0.) R2=R2*TK**TEN2(J)                             CALC0060
      I=ID(1,J)                                                         CALC0062
      K=ID(2,J)                                                         CALC0063
      M=ID(3,J)                                                         CALC0064
      N=ID(4,J)                                                         CALC0065
      IF (K.EQ.0) GO TO 20                                              CALC0067
      IF (N.EQ.0) GO TO 30                                              CALC0068
      MODE=1                                                            CALC0072
      R1=(RHSQ*S2(I))*(R1*S2(K))                                        CALC0073
      R2=(RHSQ*S2(M))*(R2*S2(N))                                        CALC0074
      GO TO 40                                                          CALC0079
   20 MODE=2
      R1=RHSMP*R1*S2(I)
      R2=RHSMSQ*S2(M)*R2*S2(N)
      GO TO 40                                                          CALC0092
   30 MODE=3
      R1=RHSMSQ*S2(I)*R1*S2(K)
      R2=RHSMP*R2*S2(M)
   40 TM1=R1-R2
      A(I,I)=A(I,I)+R1                                                  CALC0114
      A(M,I)=A(M,I)-R1                                                  CALC0115
      A(I,M)=A(I,M)-R2                                                  CALC0116
      A(M,M)=A(M,M)+R2                                                  CALC0117
      A(I,NA)=A(I,NA)-TM1                                               CALC0122
      A(M,NA)=A(M,NA)+TM1                                               CALC0123
      IF (MODE.EQ.3) GO TO 50                                           CALC0124
      A(N,I)=A(N,I)-R1                                                  CALC0126
      A(N,M)=A(N,M)+R2                                                  CALC0127
      A(I,N)=A(I,N)-R2                                                  CALC0128
      A(M,N)=A(M,N)+R2                                                  CALC0129
      A(N,N)=A(N,N)+R2                                                  CALC0130
      A(N,NA)=A(N,NA)+TM1                                               CALC0133
      IF (MODE.EQ.2) GO TO 100                                          CALC0134
   50 A(K,I)=A(K,I)+R1
      A(I,K)=A(I,K)+R1                                                  CALC0138
      A(K,K)=A(K,K)+R1                                                  CALC0139
      A(M,K)=A(M,K)-R1                                                  CALC0140
      A(K,M)=A(K,M)-R2                                                  CALC0141
      A(K,NA)=A(K,NA)-TM1                                               CALC0144
      IF (MODE.EQ.3) GO TO 100                                          CALC0145
      A(N,K)=A(N,K)-R1                                                  CALC0146
      A(K,N)=A(K,N)-R2                                                  CALC0147
  100 CONTINUE
C
CHAPTER   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3
C
      DO 110 I=1,NSK
      A(I,I)=A(I,I)+EMV*S2(I)                                           CALC0197
  110 A(I,NSK1)=A(I,NA)+EMV*(S1(I)-S2(I))
      RETURN                                                            CALC0212
      END                                                               CALC0287
```

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```
      SUBROUTINE HCPS                                                   HCPS0001
      INCLUDE COMD,LIST
      K=1                                                               HCPS0013
      IF (TK.LT.1000.) K=2                                              HCPS0014
      TK1=1.0/TK
      TK3=TK*TK                                                         HCPS0016
      TK4=TK3*TK                                                        HCPS0017
      TK5=TK4*TK                                                        HCPS0018
      TM2=TK*.5                                                         HCPS0019
      TM3=TK3*.333333333                                                HCPS0020
      TM4=TK4*.25                                                       HCPS0021
      TM5=TK5*.2                                                        HCPS0022
      IF (IHCPS-2) 100,200,300
  100 HSUM=0.0
      DO 5 I=NS1,NS2
      HO(I)=TM5*Z(K,5,I)+TM4*Z(K,4,I)+TM3*Z(K,3,I)+TM2*Z(K,2,I)+
     1 Z(K,1,I)+Z(K,6,I)*TK1
    5 HSUM=HSUM+HO(I)*S2(I)
      RETURN
  200 HSUM=0.0
      CPSUM=0.0                                                         HCPS0023
      DO 10 I=NS1,NS2
      ZK5I=Z(K,5,I)
      ZK4I=Z(K,4,I)
      ZK3I=Z(K,3,I)
      ZK2I=Z(K,2,I)
      ZK1I=Z(K,1,I)
      HO(I)=TM5*ZK5I+TM4*ZK4I+TM3*ZK3I+TM2*ZK2I+ZK1I+Z(K,6,I)*TK1
      CPSUM=(TK5*ZK5I+TK4*ZK4I+TK3*ZK3I+TK*ZK2I+ZK1I)*S2(I)+CPSUM
   10 HSUM=HSUM+HO(I)*S2(I)
      RETURN
  300 TK3=TK3*0.5
      TK4=TK4*0.3333333
      TK5=TK5*0.25
      DO 20 I=NS1,NS2
      ZK5I=Z(K,5,I)
      ZK4I=Z(K,4,I)
      ZK3I=Z(K,3,I)
      ZK2I=Z(K,2,I)
      ZK1I=Z(K,1,I)
      SO(I)=TK5*ZK5I+TK4*ZK4I+TK3*ZK3I+TK*ZK2I+TLN*ZK1I+Z(K,7,I)
   20 HO(I)=TM5*ZK5I+TM4*ZK4I+TM3*ZK3I+TM2*ZK2I+ZK1I+Z(K,6,I)*TK1
      RETURN                                                            HCPS0040
      END                                                               HCPS0041
      SUBROUTINE WALL (OUT1,OUT2)
      INCLUDE COMA,LIST
      INCLUDE COMB,LIST
C                                                                       WALL   7
C     FOR VELOCITY,  OUT1=BP,     OUT2=T                                WALL  10
C     FOR F 'S,      OUT1=FIDIF,  OUT2=T                                WALL  11
C                                                                       WALL  12
CHAPTER A ------------------------------ PRELIMINARIES ----------------WALL  13
      DATA BPLAST,SHALF/1.0,0.04/
      DATA TINY/1.0E-20/
      IF (J.GT.0) GO TO 200
CHAPTER B -------------------------------- VELOCITY ------------------WALL  19
      IXY=NM1+IXX
      UREF=U(IXY)
      RHOREF=RHO(NM1)
      RUREF=RHOREF*UREF                                                 WALL  22
      RREF=R(NM1)
      VREF=EMU(N)
      YREF=RE
      REY=RUREF*YREF/VREF
      RRUREF=RREF*RUREF                                                 WALL  27
      EF=YREF*DPDX/(RUREF*UREF)                                         WALL  29
      IF (MODEL.EQ.1) GO TO 110
      IF (REY.LT.132.25) GO TO 110
      ER=REY*EWAL
      ARGMIN=11.5*EWAL
      NIT=0
  101 SHALF1=SHALF
      S=SHALF**2
      SLOC=S+EF
      IF (SLOC.GT.0.0) GO TO 104
      SLOC=TINY
      SHALF=SQRT(ABS(EF))
  104 BEE=SQRT(SLOC)/AK
      ARG=ER*(SHALF+0.5*EF/SHALF)
      IF (ARG.LT.ARGMIN) GO TO 110
      SHALF=AK/ALOG(ARG)
      IF (ABS(SHALF-SHALF1).LT.0.0001) GO TO 102
      NIT=NIT+1
      IF (NIT.LT.11) GO TO 101
  102 S=SHALF**2
      SAV=0.5*(S+SLOC)
      BP=1.0/(1.0+BEE)
      GO TO 103
  110 CONTINUE
      FRE=EF*REY
      SRE=0.5*(2.0-FRE)
      BP=SRE*0.5+FRE*0.1666667
      IF (SRE.GT.TINY) GO TO 113
      SRE=TINY                                                          WALL  69
      BP=0.3333333
  113 S=SRE/REY
      SAV=S                                                             WALL  72
  103 T=S*RRUREF
C     ---------- UNDER-RELAX BP.
      BP=0.5*(BP+BPLAST)
      BPLAST=BP
      OUT1=BP
      OUT2=T
      S11=SAV
      S22=RRUREF
      S3=UREF
      S4=REY
      GO TO 900
C-----------------------------------------------------------------------
CHAPTER C -------------------- ENTHALPY ------------------------------
  200 SAV=S11
      RRUREF=S22
      UREF=S3
      REY=S4
      IF (MODEL.EQ.1) GO TO 210
      PRRAT=PRL(J)/PRT(J)
      PJAY=9.0*(PRRAT-1.0)/PRRAT**0.25
      S=SAV/(PRT(J)*(1.0+AMAX1(-0.99999,PJAY*SQRT(ABS(SAV)))))
      OUT2=S*RRUREF
      OUT1=(H-1.0)*0.5*UREF**2
      GO TO 900
  210 S=1.0/(PRL(J)*REY)
      OUT2=S*RRUREF
      OUT1=(PRL(JH)-1.0)*0.5*UREF**2
C-----------------------------------------------------------------------
  900 IF (ITEST.EQ.1) RETURN
      WRITE (6,9000) J,OUT1,OUT2
 9000 FORMAT (12H WALL TESTS,,3H J=,I3,6H OUT1=,1PE10.3,6H OUT2=,1PE10.3
     1 )
      RETURN
      END
      SUBROUTINE PLOTS(X,IDIME,IMAX,XAXIS,Y,JDIME,JMAX,YAXIS)           PLOT   2
C/OCT.1975/GENMIX/---------------- D.B.SPALCING, IMPERIAL COLLEGE -----*PLOT   3
C                                                                      *PLOT   4
C  SUBROUTINE FOR PLOTTING J CURVES OF Y(I,J) AGAINST X(I).            *PLOT   5
C                                                                      *PLOT   6
C  X AND Y ARE SCALED TO THF RANGE 0. TO 1., FOR PLOTTING AS           *PLOT   7
C    (Y-YMIN)/(YMAX-YMIN), THE MAXIMUM AND MINIMUM VALUES ARE PRINTED  *PLOT   8
C    N.B. THE X AND Y ARRAYS MUST BE REDEFINED BEFORE EACH CALL PLOTS. *PLOT   9
C  IDIME IS THE VARIABLE DIPENSION FOR X.                              *PLOT  10
C  IMAX IS THE NUMBER OF X VALUES.                                     *PLOT  11
C  XAXIS STORES THE NAME OF THE X-AXIS.                                *PLOT  12
C  JDIME IS THE VARIAPLE DIMENSION FOR Y.                              *PLOT  13
C  JMAX IS THE NUMBER OF CURVES TO BE PLOTTED, (UP TO 30).             *PLOT  14
C  THF ARRAY YAXIS(J) STORES THE NAMES OF THE CURVES,                  *PLOT  15
C    THE FIRST CHARACTER OF EACH CURVE-NAME IS USED FOR PLOTTING.      *PLOT  16
C  XSIZE ALTERS THE X-PLOT SIZE BY A FACTOR OF .2 TO 1., IN STEPS OF .1*PLOT  17
C  YSIZE IS THE Y-PLOT SIZE FACTOR OF .2 UPWARDS IN STEPS OF .2        *PLOT  18
C    XSIZE=1., YSIZE=1. GIVES NORMAL SIZE PLOT.                        *PLOT  19
C                                                                      *PLOT  20
C**********************************************************************PLOT  21
      DIMENSION X(IDIME),Y(IDIME,JDIME),YAXIS(JDIME),                   PLOT  22
     1 A(101),YMAX(30),YMIN(30),DIGIT(11)                               PLOT  23
      EQUIVALENCE (YMAX(1),A(1)),(YMIN(1),A(31))                        PLOT  24
      DATA  DOT,CROSS,BLANK/1H.,1H+,1H /                                PLOT  25
     1,DIGIT/1H0,1H1,1H2,1H3,1H4,1H5,1H6,1H7,1H8,1H9,1H1/               PLOT  26
C***** SET PLOT SIZE FACTORS                                            PLOT  27
      XSIZE=0.5
      YSIZE=0.8
C***** SCALING X-ARRAY TO RANGE 0 TO 100*XSIZE                          PLOT  30
      XR=100.*XSIZE                                                     PLOT  31
      XMAX=-1.E30                                                       PLOT  32
      XMIN=+1.E30                                                       PLOT  33
      IM=IMAX                                                           PLOT  34
      DO 1 I=1,IM                                                       PLOT  35
      XMAX=AMAX1(XMAX,X(I))                                             PLOT  36
    1 XMIN=AMIN1(XMIN,X(I))                                             PLOT  37
      S=XR/(XMAX-XMIN+1.E-30)                                           PLOT  38
      DO 2 I=1,IM                                                       PLOT  39
    2 X(I)=(X(I)-XMIN)*S                                                PLOT  40
C***** SCALING Y-ARRAY TO RANGE 0 TO 50*YSIZE                           PLOT  41
      YR=50.*YSIZE                                                      PLOT  42
      JM=JMAX                                                           PLOT  43
      DO 4 J=1,JM                                                       PLOT  44
      YMAX(J)=-1.E30                                                    PLOT  45
      YMIN(J)=+1.E30                                                    PLOT  46
      DO 4 I=1,IM                                                       PLOT  47
      YMIN(J)=AMIN1(YMIN(J),Y(I,J))                                     PLOT  48
    4 YMAX(J)=AMAX1(YMAX(J),Y(I,J))                                     PLOT  49
      DO 3 J=1,JM                                                       PLOT  50
      S=YR/(YMAX(J)-YMIN(J)+1.E-30)                                     PLOT  51
      DO 3 I=1,IM                                                       PLOT  52
    3 Y(I,J)=(Y(I,J)-YMIN(J))*S                                         PLOT  53
C***** WRITE CURVE NAMES, WITH ACTUAL MIN AND MAX VALUES                PLOT  54
      J=1                                                               PLOT  55
      L=IFIX(XR/10.)                                                    PLOT  56
      K=L                                                               PLOT  57
      GO TO 6                                                           PLOT  58
    5 J=J+L                                                             PLOT  59
      K=K+L                                                             PLOT  60
    6 K=MIN0(JM,K)                                                      PLOT  61
      WRITE(6,101) (YAXIS(I),I=J,K)                                     PLOT  62
      WRITE(6,103) (YMIN(I),I=J,K)                                      PLOT  63
      WRITE(6,104) (YMAX(I),I=J,K)                                      PLOT  64
      IF(K-JM) 5,7,7                                                    PLOT  65
    7 WRITE(5,106)                                                      PLOT  66
C***** MAIN LOOP - EACH PASS PRODUCES A Y-CONSTANT LINE                  PLOT  67
      IX=IFIX(XSIZE*10.)                                                PLOT  68
      KX=IFIX(XR)+1                                                     PLOT  69
      IY=IFIX(YR*.1)                                                    PLOT  70
      KY=IFIX(YR)+1                                                     PLOT  71
      N=KY+1                                                            PLOT  72
      DO 40 M=1,KY                                                      PLOT  73
      L=N-M                                                             PLOT  74
      IF(L.EQ.1.OR.L.EQ.KY) GO TO 32                                    PLOT  75
      GO TO 33                                                          PLOT  76
C***** PUT . OR + ALONG THE X-AXIS                                       PLOT  77
   32 DO 30 K=1,KX                                                      PLOT  78
   30 A(K)=DOT                                                          PLOT  79
      DO 31 K=1,KX,IX                                                   PLOT  80
   31 A(K)=CROSS                                                        PLOT  81
      GO TO 45                                                          PLOT  82
C***** PUT . OR + AND Y-VALUES ALONG Y-AXIS                              PLOT  83
   33 A(1)=DOT                                                          PLOT  84
      A(KX)=DOT                                                         PLOT  85
      K=L-1                                                             PLOT  86
   46 K=K-IY                                                            PLOT  87
      IF(K) 48,47,46                                                    PLOT  88
   47 A(1)=CROSS                                                        PLOT  89
      A(KX)=CROSS                                                       PLOT  90
   45 YL=FLOAT(L-1)/YR                                                  PLOT  91
      GO TO 35                                                          PLOT  92
   48 YL=-1.                                                            PLOT  93
C***** SEARCH FOR POINTS ALONG Y-CONSTANT LINE                           PLOT  94
   35 DO 42 J=1,JM                                                      PLOT  95
      DO 42 I=1,IM                                                      PLOT  96
      IF(IFIX(Y(I,J)+1.5)-L) 42,41,42                                   PLOT  97
C***** POINT FOUND- ASSIGN SYMBOL- SEARCH FOR MORE                       PLOT  98
   41 NX=X(I)+1.5                                                       PLOT  99
      A(NX)=YAXIS(J)                                                    PLOT 100
   42 CONTINUE                                                          PLOT 101
C***** PRINT Y-CONSTANT LINE                                             PLOT 102
      IF(YL) 36,37,37                                                   PLOT 103
   36 WRITE(5,106) (A(K),K=1,KX)                                        PLOT 104
      GO TO 38                                                          PLOT 105
   37 WRITE(5,107) YL,(A(K),K=1,KX)                                     PLOT 106
C***** FILL ARRAY A WITH BLANKS                                          PLOT 107
   38 DO 49 K=1,KX                                                      PLOT 108
   49 A(K)=BLANK                                                        PLOT 109
   40 CONTINUE                                                          PLOT 110
C***** PRINT BLANK OR X-VALUE FOR X-AXIS                                 PLOT 111
      L=1                                                               PLOT 112
      K=KX-1                                                            PLOT 113
      A(1)=DIGIT(1)                                                     PLOT 114
    DO 51 I=IX,K,IX                                                     PLOT 115
    L=L+1                                                               PLOT 116
    A(I)=DOT                                                            PLOT 117
 51 A(I+1)=DIGIT(L)                                                     PLOT 118
    A(K)=BLANK                                                          PLOT 119
    WRITE(6,106) (A(K),K=1,KX)                                          PLOT 120
    WRITE(6,100) XAXIS,XMIN,XMAX                                        PLOT 121
    RETURN                                                              PLOT 122
100 FORMAT (1H0,12HABSCISSA IS ,A8,5H MIN=,1PE9.2,5H MAX=,E9.2/)
101 FORMAT(1H0,9HORDINATE ,12(A8,2X))                                   PLOT 124
103 FORMAT(1H ,7H    MIN ,1P11E10.2)                                    PLOT 125
104 FORMAT(1H ,7H    MAX ,1P11E10.2)                                    PLOT 126
106 FORMAT(6X,101A1)                                                    PLOT 127
107 FORMAT(2H  ,F3.1,1X,101A1)                                          PLOT 128
    END                                                                 PLOT 129
```

LISTING OF DATA CARDS FOR THE NASCO PROGRAM

```
ELEMENTS                                                                    0001
C          12.01115  4.0                                                    0002
H           1.00797  1.0                                                    0003
O          15.9994  -2.0                                                    0004
N          14.0067   0.0                                                    0005
                                                                            0006
THERMO  FOR CH4/AIR COMBUSTION WITH NOX                                     0007
N                    J 3/61N  1.00 0.00 0.00 0.G   300.000  5000.000        0008
 0.24502678E 01 0.10661458E-03-0.74653315E-07 0.18796520E-10-0.10259837E-14 0009
 0.56116035E 05 0.44487572E 01 0.25030699E 01-0.21800181E-04 0.54205284E-07 0010
-0.56475602E-10 0.20999038E-13 0.56098898E 05 0.41675749E 01                0011
NO                   J 6/63N  1.0  1.00 0.00 0.G   300.000  5000.000        0012
 0.31889992E 01 0.13382279E-02-0.52899316E-06 0.95919314E-10-0.64847928E-14 0013
 0.98[illegible]3242E 04 0.67458115E 01 0.40459509E 01-0.34181783E-02 0.79819174E-05 0014
-0.61139254E-08 0.15919072E-11 0.97453867E 04 0.29974976E 01                0015
NO2                  J 9/64N  1.0  2.00 0.00 0.G   300.000  5000.000        0016
 0.46240759E 01 0.25260330E-02-0.10609483E-05 0.19879239E-09-0.13799380E-13 0017
 0.22899900E 04 0.13324137E 01 0.34589224E 01 0.20647063E-02 0.66966060E-05 0018
-0.95556665E-08 0.36195873E-11 0.28152261E 04 0.83116980E 01                0019
N2O                  J12/64N  2.0  1.00 0.00 0.G   300.000  5000.000        0020
 0.47306662E 01 0.28258264E-02-0.11558104E-05 0.21263681E-09-0.14564081E-13 0021
 0.81617617E 04-0.17151070E 01 0.26189194E 01 0.86439550E-02-0.68110612E-05 0022
 0.22275877E-08-0.80650276E-13 0.87590078E 04 0.92266951E 01                0023
N2                   J 9/65N  2.0  0.0  0.0  0.G   300.000  5000.000        0024
 0.28963194E 01 0.15154863E-02-0.57235275E-06 0.99807385E-10-0.65223536E-14 0025
-0.90586182E 03 0.61615143E 01 0.36748257E 01-0.12081496E-02 0.23240100E-05 0026
-0.63217520E-09-0.22577253E-12-0.10611587E 04 0.23580418E 01                0027
CH4                  J 3/61C   1H   400  000  0G   300.000  5000.000       10028
 0.15027072E 01 0.10416790E-01-0.39181522E-05 0.67777899E-09-0.44283706E-13 20029
-0.99787078E 04 0.10707143E 02 0.38261932E 01-0.39794581E-02 0.24558340E-04 30030
-0.22732926E-07 0.69626957E-11-0.10144950E 05 0.86690073E 00               40031
O2                   J 9/65O  2.0  0.0  0.0  0.G   300.000  5000.000        0032
 0.36219521E 01 0.73618256E-03-0.19652219E-06 0.36201556E-10-0.28945623E-14 0033
-0.12019822E 04 0.36150942E 01 0.36255907E 01-0.18782183E-02 0.70554543E-05 0034
-0.67635071E-08 0.21555977E-11-0.1047522[illegible]E 04 0.43052769E 01                0035
CO                   J 9/65C  1.0  1.00 0.00 0.G   300.000  5000.000        0036
```

```
 0.29840689E 01 0.14891387E-02-0.57899678E-06 0.10364376E-09-0.69353499E-14       _0037
-0.14245227E 05 0.63479147E 01 0.37100916E 01-0.16190964E-02 0.36923584E-05       _0038
-0.20319673E-08 0.23953344E-12-0.14356309E 05 0.29555340E 01                      _0039
CO2                 J 9/65C  1.0  2.00 0.00 0.G   300.000  5000.000               _0040
 0.44608040E 01 0.30981717E-02-0.12392566E-05 0.22741323E-09-0.15525948E-13       _0041
-0.48961438E 05-0.98635978E 00 0.24007788E 01 0.87350905E-02-0.66070861E-05       _0042
 0.20021860E-08 0.63274039E-15-0.48377520E 05 0.96951447E 01                      _0043
H                   J 9/65H  1.00 0.00 0.00 0.G   300.000  5000.000               _0044
 0.25000000E 01 0.0            0.0            0.0            0.0                  _0045
 0.25471625E 05-0.46011758E 00 0.25000000E 01 0.0            0.0                  _0046
 0.0            0.0            0.25471625E 05-0.46011758E 00                      _0047
H2                  J 3/61H  2.0  0.0  0.0  0.G   300.000  5000.000               _0048
 0.31001883E 01 0.51119458E-03 0.52644204E-07-0.34909964E-10 0.36945341E-14       _0049
-0.87738013E 03-0.19629412E 01 0.30574446E 01 0.26765198E-02-0.58099149E-05       _0050
 0.55210343E-08-0.18122726E-11-0.98890430E 03-0.22997046E 01                      _0051
H2O                 J 3/61H  2.0  1.00 0.00 0.G   300.000  5000.000               _0052
 0.27167616E 01 0.29451370E-02-0.80224368E-06 0.10226681E-09-0.48472104E-14       _0053
-0.29905820E 05 0.66305666E 01 0.40701275E 01-0.11084499E-02 0.41521180E-05       _0054
-0.29637404E-08 0.80702101E-12-0.30279719E 05-0.32270038E 00                      _0055
O                   J 6/62O  1.00 0.00 0.00 0.G   300.000  5000.000               _0056
 0.25420580E 01-0.27550603E-04-0.31028029E-08 0.45510670E-11-0.43680494E-15       _0057
 0.29230801E 05 0.49203072E 01 0.29464283E 01-0.16381664E-02 0.24210303E-05       _0058
-0.16028432E-08 0.38906964E-12 0.29147641E 05 0.29639931E 01                      _0059
OH                  J 3/66O  1.0  1.00 0.00 0.G   300.000  5000.000               _0060
 0.29106417E 01 0.95931627E-03-0.19441700E-06 0.13756646E-10 0.14224542E-15       _0061
 0.39353811E 04 0.54423428E 01 0.38375931E 01-0.10778855E-02 0.96830354E-06       _0062
 0.18713971E-09-0.22571089E-12 0.36412820E 04 0.49370009E 00                      _0063
                                                                                  _0064
MECHANISM                                                                         _0065
N         NO                  N2      O              10.1760  0.0     0.0     WALD7/74_0066
N         O2                  NO      O              6.778   1.0     3172.   WALD7/74_0067
OH        N                   H       NO             8.778   0.5     4028.   WALD7/74_0068
H         N2O                 OH      N2             10.903   0.0    7553.   WALD7/74_0069
N2O       O                   NO      NO             11.000   0.0    15000.  WALD7/74_0070
N2O                 M         N2      O       M      11.000  0.0     25176.  WALD7/74_0071
N         O         M         NO      M              10.806  -0.5                 _0072
NO2       O                   NO      O2             10.000   0.0     300.        _0073
NO2       M                   O       NO      M      13.041   0.0    33000.       _0074
                                                                                  _0075
```

APPENDIX C - GLOSSARY OF FORTRAN VARIABLES

NAME	LOCATION	TYPE	MEANING
A	COMP	Array	Finite-difference coefficient.
A	PLOTS	Array	One line of printed characters.
A	CALC	Array	Elements of the correction matrix.
ABSF	COMP, START		Absolute value of F.
AC	BLOCK DATA	Array	Polynomial coefficients for specific heat of equilibrium-product-species. Specific heat at pressure IP*1.0E5 is given by AC(1,IP)+AC(2,IP)*T +AC(3,IP)*T*T+AC(4,IP)*T**3 (T = temperature).
ACO2	START		Specific heat coefficient for CO_2.
AC1-AC4	CHEM		Temporary storage for coefficients AC.
ADUCT	MAIN	Array	Area of the duct.
ADUCTD	MAIN		Downstream duct area.
AFLOWD	MAIN		Downstream flow area.
AFLOWU	MAIN		Upstream flow area.

NAME	LOCATION	TYPE	MEANING
AFS	CHEM	Array	Temporary storage for polynomial coefficients for concentrations of equilibrium-product-species (see CHEM, ENTRY EQUIL).
AFU	START		Specific heat coefficient for fuel.
AH	BLOCK DATA	Array	Polynomial coefficients for enthalpy of equilibrium-product-species (definition as for AC).
AH1-AH4	CHEM		Temporary storage for coefficients AH.
AH2O	START		Specific heat coefficient for H2O.
AK	BLOCK DATA		Von Karman constant.
AK	CREKO		Temporarily stored quantity.
AL	CREKO	Array	Atomic stoichiometric coefficients; AL (I,J) is the kg-atoms of element I per kg-mole of species J.
ALF	COMP	Array	LTDMA Coefficient.
ALPHA	MAIN, PHYS		Temporarily stored quantity.
AMCH	CREKO		Alphanumeric storage for 'MECH'.
AMIX	START		Specific heat coefficient for gas mixture.

NAME	LOCATION	TYPE	MEANING
AMUD	START	Array	Downstream viscosity *AREA/(Δx)**2 .
AMUL	START		Laminar viscosity *AREA/Δx.
AMULP	START		Temporary storage for AMUL.
AMUL1	START		AMUL at inlet plane.
AMUT	START		Turbulent viscosity *AREA/Δx.
AMUTP	START		Temporary storage for AMUT.
AMUTD	PHYS		Downstream turbulent viscosity.
AMUTD1	PHYS		AMUTD/0.15 .
AMUTU	PHYS		Upstream turbulent viscosity.
AMUTU1	PHYS		AMUTU/0.15.
AMUU	START	Array	Upstream viscosity *AREA/(Δx)**2.
AN2	START		Specific heat coefficient for N2.
AOX	START		Specific heat coefficient for oxygen.
AREA	COMP	Array	Downstream cell area in the transverse direction.

NAME	LOCATION	TYPE	MEANING
AREAU	COMP	Array	Upstream cell area in the transverse direction.
AREX	BLOCK DATA	Array	Duct wall coefficient.
ARG	WALL		Logarithm of argument.
ARGMIN	WALL		Smallest value of ARG.
ARRCON	BLOCK DATA		Arrhenius constant, E/R.
AS	BLOCK DATA	Array	Polynomial coefficients for reciprocal mean molecular weight of equilibrium-product - species(definition as for AC).
ASM1.. ASM4	CHEM		Temporary storage for coefficients AS.
ASUB	CREKO	Array	Molecular symbol for species.
AS1	BLOCK DATA	Array	Polynomial coefficients for concentration of equilibrium-product-species over enthalpy range HMIN $\leqslant$ H$\leqslant$ HDIV. For species J, at pressure IP*1.0E5, $\ell n\ (m_j) = \sum_{I=1}^{4}$ AS1(I,J,IP)*H**(I-1).
AT	CREKO	Array	Atomic symbol for species.

ATOM	CREKO	Array	For element K,
			ATOM (1,K) = Atomic symbol;
			ATOM (2,K) = Atomic weight;
			ATOM (3,K) = Valence or oxidation state.

NAME	LOCATION	TYPE	MEANING
B	COMP	Array	Finite-difference coefficient.
BCO2	START		Specific heat coefficient for CO2 .
BEE	WALL		Exponent.
BFRAC	MAIN		Estimated pressure gradient limited to BFRAC $(\frac{1}{2}\rho u^2)/\Delta x$; BFRAC ≤ 0.5 .
BFU	START		Specific heat coefficient for H20 .
BIG	BLOCK DATA		A large number.
BH20	START		Specific heat coefficient for H20 .
BLANK	OUTPUT, CREKO		Alphanumeric storage for 4 blank spaces.
BLANK	PLOTS		A printer space.
BLF	COMP		LTDMA coefficient.
BMIX	START		Specific heat coefficientfor gas mixture.
BN2	START		Specific heat coefficient for N2 .
BOM	COMP	Array	Omega-width of a cell.
BOX	START		Specific heat coefficient for oxygen.

NAME	LOCATION	TYPE	MEANING
BP	WALL		Big psi, stream function coefficient.
BPE	COMP		Big psi at E boundary.
BPLAST	WALL		Last value of BP.
BPSAVE	COMP		Value of BP saved at IX=ISTRT.
BREX	BLOCK DATA	Array	Duct wall constant.
BS1	BLOCK DATA	Array	As AS1, but over enthalpy range HDIV < H ≤HMAX.
BX	CREKO	Array	Arrhenius pre-exponential factor for forward reaction.
BX2	CREKO	Array	Arrhenius pre-exponential factor for backward reaction.
C	COMP	Array	Finite-difference coefficient.
CFH20	START		Mass of H20 produced per unit mass of fuel burnt.
CLF	COMP	Array	LTDMA Coefficient.
CMIX	START		Specific heat of mixture.
CMIXB	START		Specific heat of B stream.

NAME	LOCATION	TYPE	MEANING
CMIXC	START		Specific heat of C stream.
CONVG	SPECE		Parameter to indicate convergence of chemical-kinetics solution.
CO2H20	START		Mass ratio of CO2 to H20 produced by complete oxidation of fuel.
CORR	COMP		LTDMA corrections.
CPMIX	CHEM		Specific heat of mixture.
CPR	CHEM		Specific heat of equilibrium-product-species.
CPSUM	HCPS		Specific heat of mixture.
CREX	BLOCK DATA	Array	Duct wall constant.
CROSS	PLOTS		A printer symbol.
D	COMP	Array	Finite-difference coefficient.
DA	MAIN		Area increment.
DADP	MAIN		Rate of change of area with pressure.
DAMIN	BLOCK DATA		Maximum permissible non-dimensional area error.

NAME	LOCATION	TYPE	MEANING
DATA	OUTPUT	Array	Temporary storage before printout.
DATA	CREKO	Array	Temporary storage for reading in data.
DA1	MAIN		Non-dimensional area error before correction.
DA2	MAIN		Non-dimensional area error after correction.
DEBUG	CHEM		Trigger for diagnostic output of chemical-kinetics calculations.
DENOM	START		Temporarily stored value.
DIF	PHYS	Array	Diffusion quantity.
DIFU	PHYS	Array	Diffusion quantity related to velocity.
DIGIT	PLOTS		Number printed beside x-axis.
DLF	COMP	Array	LTDMA coefficient.
DOT	PLOTS		A printer symbol.
DP	MAIN		Pressure increment.
DPDX	MAIN		Pressure gradient.

NAME	LOCATION	TYPE	MEANING
DPDXM	MAIN		Temporarily stored value.
DPMIN	MAIN		Temporarily stored value.
DTEMP	MAIN, CHEM		Fractional temperature increment.
DT1	CREKO		Quantities used during input of thermochemcial data.
DT2	CREKO		
DUSQ	PHYS		Diffusion quantity times the square of velocity.
DUSQP	PHYS		Temporary storage for DUSQ.
DWALL	BLOCK DATA	Array	Duct-wall-temperature constant.
DX	MAIN		Increment in x.
EF	WALL		Non-dimensional pressure gradient.
ELEM	CREKO		Alphanumeric storage for 'ELEM'.
ELF	COMP	Array	Array for back-substition of LTDMA.
EMU	PHYS	Array	Effective viscosity.

NAME	LOCATION	TYPE	MEANING
EMUD	PHYS	Array	Effective downstream viscosity.
EMUNU	PHYS		Laminar viscosity at upstream wall temperature.
EMUU	PHYS	Array	Effective upstream viscosity.
EMU1	OUTPUT		Laminar viscosity at inlet.
EMV	CHEM		Total convective and diffusive mass inflow to a cell.
ENTH	MAIN, CHEM, START		Enthalpy.
ENTHB	MAIN		Enthalpy of B-stream.
ENTHC	MAIN		Enthalpy of C-stream.
EPSF	BLOCK DATA		Convergence criterion for dependent variables u, $\tilde{h}$, f, and $\dot{m}_{fu}$.
EPSS	BLOCK DATA		Convergence criterion for species concentrations.
EPST	BLOCK DATA		Convergence criterion for temperature.
EPS1D	BLOCK DATA		Convergence criterion for one-dimensional solution.

NAME	LOCATION	TYPE	MEANING
EQRAT	BLOCK DATA		Equivalence ratio .
ER	WALL		EWAL * Reynolds number.
ETA	SPECE		Under-relaxation parameter.
ETA1	SPECE		Under-relaxation parameter.
EWAL	BLOCK DATA		Constant in wall function.
EWALL	BLOCK DATA	Array	Duct-wall-temperature constant.
F	MAIN	Array	General variable, ϕ.
FAC	MAIN		Factor.
FACTOR	MAIN, CHEM		Temporarily stored quantity.
FACTR1	CHEM		Temporarily stored quantities.
FACTR2	CHEM		
FCO2	START		Mass fraction of CO2.
FDIFE	COMP		F-increment at E Boundary.
FDIFF	START		Temporarily stored quantity.
FFU	MAIN, CHEM		Mass fraction of fuel.

NAME	LOCATION	TYPE	MEANING
FH20	START		Mass fraction of H20.
FJF	PHYS		Mass fraction of fuel.
FJP	CHEM, START		Mixture fraction.
FLOB	MAIN		Flow rate in B-stream.
FLOC	MAIN		Flow rate in C-stream.
FLUX	OUTPUT	Array	Convective flux of general variable ϕ.
FMAX	COMP		Temporarily stored quantity.
FMIN	BLOCK DATA		Smallest value of F for which the convergence criterion is applied.
FN2	START, CHEM		Mass fraction of N2.
FOLD	START		Previous iteration value of F.
FOX	START, MAIN		Mass fraction of oxygen.
FOXBRN	START		Mass fraction of oxygen in fully-burnt gas.
FOXUNB	START		Mass fraction of oxygen in unburnt gas.
FO2	CHEM		Mass fraction of oxygen.

NAME	LOCATION	TYPE	MEANING
FPR	CHEM, PHYS, START		Mass fraction of equilibrium-product-species.
FPRUNB	START		Mass fraction of products in unburnt gas
FRE	WALL		EF * Reynolds number ·
FS	MAIN	Array	Mass fractions of species.
FSII	CHEM		Temporary storage for FS.
FSTOIC	MAIN		Stoichiometric mixture fraction.
FSTOIM	MAIN		1.0 - FSTOIC·
FTE	START		Temperature.
FU	CHEM , MAIN		Upstream value of F.
FUB	BLOCK DATA		Fuel mass-fraction in B-stream.
FUBRN	START		Fuel mass-fraction in fully-burnt gas.
FUBRNT	PHYS		Fuel mass-fraction in fully-burnt gas ·
FUC	BLOCK DATA		Fuel mass-fraction in C-stream .
FUEX	PHYS, START		Excess fuel.

NAME	LOCATION	TYPE	MEANING
FUTEST	BLOCK DATA		Convergence criterion for fuel mass-fraction.
FUUNB	START		Fuel mass-fraction in unburnt gas.
FWALL	BLOCK DATA	Array	Duct-wall-temperature constant.
GAMMA	MAIN		Specific heat ratio.
GAMPRS	MAIN		Reciprocal of GAMMA times pressure.
GASCON	BLOCK DATA		Universal gas constant.
GAZ	CREKO		Alphanumeric storage for 'G'(for gas).
GF	CREKO		Temporarily stored quantity.
H	BLOCK DATA		Recovery factor.
HDIFF	CHEM		Reciprocal of (HMAX-HMIN).
HDIV	BLOCK DATA		Intermediate enthalpy value for the coefficients AS1 and BS1.
HFU	START		Heat of combustion of fuel.
HMAX	BLOCK DATA		Maximum enthalpy value for the coefficients AS1 and BS1 .
HMIN	BLOCK DATA		Minimum enthalpy value for the coefficients AS1 and BS1 .

NAME	LOCATION	TYPE	MEANING
HMIX	CHEM		Mixture enthalpy.
HPEI	COMP		0.5 * PSIE .
HPR	CHEM		Enthalpy of eouilibrium-product-species.
HSUM	MAIN		Enthalpy of mixture.
HWALL	START		Wall enthalpy.
HO	MAIN	Array	Enthalpy of species.
I			Index.

IBEX	MAIN	Array	Index for E boundary condition;
			= 1, boundary value specified;
			= 2, boundary flux specified.

ID	CREKO		ID (K,J) is the species index number of species K in reaction J.
IDASH	COMP		Index in back-substitution for TDMA.
IDCO	BLOCK DATA		Index for CO.
IDCO2	BLOCK DATA		Index for CO2.

IDEBUG	BLOCK DATA		Index for chemical-kinetics diagnostic output;
			=1, no output;
			=2, output obtained.

NAME	LOCATION	TYPE	MEANING
IDF	BLOCK DATA		Index for fuel.
IDH	BLOCK DATA		Index for H.
IDH2	BLOCK DATA		Index for H2.
IDH20	BLOCK DATA		Index for H20.
IDIME	PLOTS		Dimension for arrays.
IDIV	MAIN		I of division between B and C streams.
IDN	BLOCK DATA		Index for N.
IDNO	BLOCK DATA		Index for NO.
IDNO2	BLOCK DATA		Index for NO2.
IDN2	BLOCK DATA		Index for N2.
IDN20	BLOCK DATA		Index for N20.
IDO	BLOCK DATA		Index for 0.
IDOH	BLOCK DATA		Index for 0H.
IDO2	BLOCK DATA		Index for 02.

NAME	LOCATION	TYPE	MEANING
IEND	BLOCK DATA		Index for last x-station in iterative sweep.
IEQUIL	BLOCK DATA		=0, equilibrium concentrations not obtained. =1, equilibrium concentrations obtained.
IFIN	COMP		Index triggering finish of integration.
IHCPS	MAIN		Index to control calculation of thermodynamic properties.
IL	OUTPUT		Number of x-stations in longitudinal plot.
ILDIM	OUTPUT		Variable dimension for longitudinal plot.
IMAT	SPECE		Number of rows in Newton-Raphson correction matrix.
IM	PLOTS		Index in PLOT.
IMAX	BLOCK DATA		Maximum index number for species concentrations.
IMAX	PLOTS		Number of values to be plotted.
INERT	BLOCK DATA		Indicator of chemically-inert/reacting flow: = 1, Chemically inert; = 2, Chemically reacting.
INSAVE	MAIN		Temporarily stored value of INERT.

NAME	LOCATION	TYPE	MEANING
IP	CHEM		Integer value of PP.
IPLOT	BLOCK DATA	Array	x-locations where cross-stream plot is required.
IPLOTL	BLOCK DATA		Number of intervals between x-station values used for longitudinal plot.
IPLOTM	BLOCK DATA		Maximum number of cross-stream plots.
IPR	BLOCK DATA		Index number for products.
IPRINT	BLOCK DATA		Index to control type of printout required.
IP1	CHEM		IP + 1.
IRMFX		Array	x-location of RSFMAX .
IRMFY	COMP	Array	y-location of RSFMAX .
IRMUX	MAIN		x-loaction of RSUMAX .
IRMUY	MAIN		y-location of RSUMAX .
ISEC	MAIN, START		Index to denote section of duct.
ISLP	OUTPUT		Temporarily stored quantity for longitudinal plot.

NAME	LOCATION	TYPE	MEANING
ISOLVE	START	Array	Number of iterations after which the particular variable is to be solved.
ISPEC	BLOCK DATA	Array	Index to establish correpsondence between concentrations stored in F and FS arrays.
ISTEP	COMP		Counter of forward steps.
ISTRT	BLOCK DATA		Index for first x-station for iterative sweep.
ISWP	BLOCK DATA		Number of iterations after which a complete sweep of the flow domain is made.
IT	MAIN, CHEM		Number of iterations on temperature.
ITDIM	OUTPUT		Variable dimension for cross-stream plot.
ITER	SPECE		Number of iterations during chemical-kinetics computations.
ITEST	BLOCK DATA		Trigger for diagnostic output; =1, no output, =2, output obtained.
ITMAX	BLOCK DATA		Maximum number of iterations of chemical-kinetics computations.
IX	COMP		Index for x grid location.

NAME	LOCATION	TYPE	MEANING
IXD			IX + 1.
IXN IXND IXNU			Quantities used for temporary storage.
IXX			(IX-1)*N.
IXXD IXXP1			Used for temporary storage of (IXX+N)·
IXY			IY + IXX.
IXYD			IXY + N.
IXYDD			IXYD + N.
IXYU			IXY - N.
IXYU IXY1			Temporarily stored quantities.
IY			Index for ω-grid location.
J			Index, usually associated with dependent variable.
JDIME	PLOT		Dimension for arrays.
JF	BLOCK DATA		Index for fuel.

NAME	LOCATION	TYPE	MEANING
JH	BLOCK DATA		Index for stagnation enthalpy.
JJ	CREKO		Number of chemical reactions.
JLDIM	OUTPUT		Variable dimension for longitudinal plot.
JMAX	BLOCK DATA		Maximum index number for variables stored in F-array.
JMAX	PLOT		Number of curves to be plotted.
JN	BLOCK DATA		Index for N.
JNO	BLOCK DATA		Index for NO.
JNO2	BLOCK DATA		Index for NO2.
JN2O	BLOCK DATA		Index for N2O.
JOX	BLOCK DATA		Index for oxygen.
JP	BLOCK DATA		Index for mixture fraction.
JTDIM	OUTPUT		Variable dimension for transverse plot.
JTE	BLOCK DATA		Index for temperature.
JX			Index for x-grid location.
JXJ			Temporarily stored quantity.

NAME	LOCATION	TYPE	MEANING
JXPLOT	OUTPUT		Number of x-stations in longitudinal plot.
JXX			Temporarily stored quantity.
K	OUTPUT		Index.
KASE			Index denoting problem .
KK	CHEM		Index.
KMAT	SPECE		IMAT + 1 .
KNTCS	BLOCK DATA		=0, chemical-kinetics computations supressed; =1, chemical-kinetics computations performed.
KOUT	OUTPUT		Index during printing of profiles.
KX	OUTPUT		Index during longitudinal plot.
L	BLOCK DATA		Number of x grid points.
LAB	OUTPUT	Array	Labels for cross-stream profiles .
LABK	OUTPUT	Array	Labels for cross-stream profiles.
LABKH	OUTPUT		Label for enthalpy.

NAME	LOCATION	TYPE	MEANING
LABKR	OUTPUT		Label for density.
LABKV	OUTPUT		Label for viscosity.
LABK1	OUTPUT		Label for radius.
LL	OUTPUT CHEM		Index.
LM1	COMP		L-1.
LM2	COMP		L-2.
LN	MAIN		L*N.
MM	CHEM		Index.
MODE	CALC		Type of reaction.
MODEL	BLOCK DATA		Indicator of transport-process type: =1, laminar; =2, turbulent.
N	BLOCK DATA		Number of transverse grid points.
NA	SPECE		NS + 1
NCD	CREKO		Index used during input of thermochemical data.

NAME	LOCATION	TYPE	MEANING
ND	CREKO		Index during computation of ID.
NDAMAX	BLOCK DATA		Maximum number of iterations to match flow area with duct area.
NEWPR	MAIN	Array	=1, Prandtl number equals that at previous J; =2, Prandtl numbers are unequal.
NF	BLOCK DATA		Number of dependent variables excluding u-velocity and pollutant species.
NFUMAX	BLOCK DATA		Maximum number of iterations for fuel concentration.
NIT	START, COMP, WALL		Number of iterations.
NITER	BLOCK DATA		Number of iterations.
NITERK	BLOCK DATA		Number of iterations after which chemical-kinetics computations are started.
NITER1	OUTPUT		NITER + 1.
NITMAX	BLOCK DATA		Maximum number of iterations.
NLM	CREKO		Number of elements.
NM1	COMP		N - 1.

NAME	LOCATION	TYPE	MEANING
NM2	COMP		N - 2.
NM3	COMP		N - 3.
NN	START, SPECE		Index.
NPLOTC	BLOCK DATA		Number of steps after which cross-stream plots are to be printed.
NPLOTL	BLOCK DATA		Number of iterations after which longitudinal plots are to be printed.
NPRINT	BLOCK DATA		Number of iterations after which printout is obtained, regardless of convergence.
NPROF	BLOCK DATA		Number of steps after which profiles are printed .
NS	BLOCK DATA		Number of chemical species.
NSE1	BLOCK DATA		Index for first equilibrium-product-species.
NSE2	BLOCK DATA		Index for the last equilibrium-product-species.
NSE3	OUTPUT		NSE1 + 4.
NSE4	OUTPUT		NSE3 + 1.

NAME	LOCATION	TYPE	MEANING
NSK	BLOCK DATA		Number of species whose concentrations are kinetically determined.
NSK1	CALC		NSK + 1
NSM	CREKO		NS + 1
NSTAT	BLOCK DATA		Number of stations after which profiles are to be printed.
NS1	MAIN		First and last species numbers for computation of thermodynamic properties.
NS2	MAIN		
NTMAX	BLOCK DATA		Maximum number of iterations on temperature.
NYL	OUTPUT		Number of variables for longitudinal plot.
NYT	OUTPUT		Number of variables for transverse plot.
N1DMAX	BLOCK DATA		Maximum number of iterations in 1-D computations.
N1DPR	BLOCK DATA		Number of iterations after which printout of 1-D solution is obtained.
OM	BLOCK DATA	Array	ω.
OMDIF	COMP	Array	ω - difference.

NAME	LOCATION	TYPE	MEANING
OMDIV	MAIN		ω for division between streams.
OME	COMP		ω difference in the E boundary.
OMI	COMP		ω difference in the I boundary.
OMINT	COMP	Array	ω for cell interfaces.
OXB	BLOCK DATA		Oxygen mass-fraction in B-stream.
OXC	BLOCK DATA		Oxygen mass-fraction in C-stream.
P	COMP		PSIE/DX.
PA	CHEM		Pressure.
PDGSCN	MAIN, CHEM		Pressure ÷ Gas constant.
PFRAC	BLOCK DATA		Pressure corrections during matching of flow and duct areas limited to PFRAC * ($\frac{1}{2}$ ρu^2); PFRAC $\leqslant 0.5$.
PHAZ	CREKO		Phase of species for which thermochemical data is read.
PHI	CHEM		Temporary storage for $(f-f_{st})/(1-f_{st})$.
PJAY	WALL		Jayatillaka's P function (Ref.10).

NAME	LOCATION	TYPE	MEANING
PMAX	BLOCK DATA		Maximum pressure for which polynomial coefficients AC, AH, AS, AS1, BS1 are defined.
PMIN	BLOCK DATA		Minimum pressure for which polynomial coefficients AC, AH, AS, AS1, BS1 are defined.
POM	COMP	Array	P* BOM.
PP	CHEM		Pressure * 1.0E-5.
PR	MAIN	Array	Pressure.
PRB	MAIN, START		Mass fractions of (products +N2) in B-stream.
PRC	MAIN, START		Mass fractions of (products +N2) in C-stream.
PRCON	PHYS, CHEM		Temporary storage for reciprocal Prandtl number.
PRCON1	PHYS		Temporarily stored quantity.
PREEXP	BLOCK DATA		Arrhenius pre-exponential factor.
PRESS	BLOCK DATA		Pressure.
PRESSD	OUTPUT		Downstream pressure, expressed as $(p/p_{inlet}{}^{-1})$.
PRESS1	MAIN, OUTPUT		Inlet pressure.

NAME	LOCATION	TYPE	MEANING
PRL	MAIN	Array	Laminar Prandtl number.
PRLAM	BLOCK DATA		Laminar Prandtl number.
PRLT	MAIN	Array	Array to store laminar and turbulent Prandtl numbers.
PRRAT	WALL, PHYS, CHEM	Array	Prandtl number ratio.
PRTURB	BLOCK DATA		Turbulent Prandtl number.
PSIE	MAIN		ψ_E.
PSIEI2	START, PHYS		0.12 * PSIE.
R	COMP	Array	Radius.
RATIO	START		Temporarily stored quantity..
RDIV	MAIN		R of division between B and C streams.
RDIVSQ	MAIN		RDIV**2.
RE	COMP		Width of half interval close to E boundary.
RECI	COMP		Reciprocal of density-velocity product.

NAME	LOCATION	TYPE	MEANING
RECIMI	COMP		Temporary storage for RECI.
RECTK	CALC		Reciprocal of TK.
RESIDU	COMP	Array	Change in general variable ϕ from one iteration to next.
RESU	MAIN	Array	Change in u-velocity from one iteration to next.
REXD	MAIN		Duct Radius.
REXO	MAIN		Duct radius at inlet.
REXOSQ	MAIN		REXO**2.
REY	WALL		Reynolds number.
RHO	MAIN	Array	Density.
RHOB	MAIN		Density of B-stream.
RHOC	MAIN		Density of C-stream.
RHOFAC	MAIN		Density factor.
RHOP	CALC		Density.

NAME	LOCATION	TYPE	MEANING
RHOREF	WALL		Reference density .
RHO1	MAIN	Array	Density at inlet plane .
RHO2	MAIN	Array	Density at plane IX=ISTRT .
RHSM	CALC		Density ÷ Molecular weight .
RHSMP	CALC		RHSM* Density
RHSMSQ	CALC		RHSM* square of density .
RHSQ	CALC		Square of density .
RI	COMP		Distance of half-internal near I boundary.
RIP	COMP		Integral distance evaluations.
RIPP	COMP		Integral in distance evaluations.
RREF	WALL		Reference radius .
RRUREF	WALL		Reference value of radius * density -velocity product.
RSFMAX	COMP	Array	Maximum normalised change of general variable ϕ from one iteration to next
RSMW	CREKO		Reciprocal of SMW .

NAME	LOCATION	TYPE	MEANING
RSUMAX	MAIN		Maximum normalised change of u-velocity from one iteration to next.
RU	COMP	Array	Density-velocity product.
RUREF	WALL		Reference value of RU.
RU2	MAIN		ρu^2.
RVRS	CREKO		Alphanumeric storage for 'REVE'.
R1	CALC		Forward reaction rate.
R2	CALC		Backward reaction rate .
S	WALL		Friction-factor of Prandtl number.
SAV	WALL		Average value of S.
SHALF	WALL		Square root of S.
SHALF	START		Square root of S.
SHALFD	PHYS		Downstream value of SHALF.
SHALFU	PHYS		Upstream value of SHALF.
SHALF1	WALL		Square root of S.

NAME	LOCATION	TYPE	MEANING
SI	PHYS	Array	Source term.
SIP	PHYS	Array	Second component of source term.
SLOC	WALL		Local value of S .
SM	CREKO		Reciprocal of mean molecular weight of mixture.
SMW	CREKO	Array	Molecular weight of species.
SP1	CHEM		STOICH + 1.0 .
SQAREA	START		Square root of half the duct area (=radius).
SQIX	PHYS		SQAREA at upstream station.
SQIXD	PHYS		SQAREA at downstream station.
SRE	WALL		S* Reynolds number.
STOICH	BLOCK DATA		Stoichiometric ratio.
STORE STORE1 STORE2			Used for temporarily stored quantities.
SUMA	PHYS		Summation (over cross-stream points) of downstream diffusion coefficients.

NAME	LOCATION	TYPE	MEANING
SUMB	PHYS		SUMA for upstream station.
SUMX	CREKO		Sum of x's* .
SUMY	CREKO		Sum of y's* .
SUM1	CREKO		Temporarily stored quantity.
SO	HCPS	Array	One-atmosphere, ideal gas entropy of species.
S1	CHEM	Array	Species mole-numbers averaged over four neighboring nodes.
S11	WALL		Stored value of SAV .
S2	CHEM	Array	Species mole-number.
S22	WALL		Stored value of RRUREF.
S3	WALL		Stored value of UREF .
S4	WALL		Stored value of REY .
T	WALL		Temporarily stored value.
T	START, COMP		Temporarily stored value .

* x and y are used for temporary storage of some quantities in subroutine CREKO .

NAME	LOCATION	TYPE	MEANING
TACT	CREKO	Array	Activation temperature (E/R) for forward reaction.
TACT2	CREKO	Array	Activation temperature (E/R) for backward reaction.
TAUE	MAIN		Shear stress at E boundary.
TAUSAV	MAIN		Saved value at TAUE at IX=ISTRT:
TB	BLOCK DATA		Temperature of B-stream.
TBRN	START		Temperature of fully burnt gas.
TC	BLOCK DATA		Temperature of C-stream.
TDIFF	START		Temporarily stored quantity.
TE	COMP		Transport coefficient at E boundary (u-velocity).
TEF	COMP		Transport coefficient at E boundary (general variable ϕ).
TEN	CREKO	Array	Exponent on temperature in forward reaction rate expression.
TENLN	CREKO		ℓn (10).
TEN2	CREKO	Array	Exponent on temperature in backward reaction rate expression.

NAME	LOCATION	TYPE	MEANING
TERM	START		Temporarily stored quantity.
THIRD	CREKO, OUTPUT		Alphanumeric storage for 'M' (third body in chemical reaction).
THRM	CREKO		Alphanumeric storage for 'THER'.
TINY	BLOCK DATA		A small number.
TINYK	BLOCK DATA		A small number for chemical-kinetics calculations.
TK	CHEM		Temperature.
TK1.. TK5	HCPS		Temporarily stored quantities.
TLN	CREKO		ℓn (temperature) .
TMAX	BLOCK DATA		Maximum temperature in the calculations.
TMIN	BLOCK DATA		Minimum temperature in the calculations.
TM1	CREKO		Temporarily stored quantity.
TM1	CALC		R1 - R2.
TM2.. TM5	HCPS		Temporarily stored quantities.
TNY	BLOCK DATA		ℓn (TINYK).

NAME	LOCATION	TYPE	MEANING
TST1	SPECE		Temporarily stored quantity.
TUNB	START		Unburnt gas temperature.
TW	START		Wall temperature.
T1	START, PHYS		Temporarily stored quantity (= PREEXP*PRESS**2).
T1	CREKO		Quantities used during input of thermochemical data.
T2	CREKO		
U	MAIN	Array	Longitudinal velocity.
UB	BLOCK DATA		Velocity of B-stream.
UBAR	OUTPUT		Average velocity.
UC	BLOCK DATA		Velocity of C-stream.
UDDSQ	PHYS		Square of UDD (= velocity downstream of D location).
UDSQ	PHYS		Square of UD (=velocity at downstream, D, location).
UFLUX	OUTPUT		Convective flux of momentum.
UREF	WALL		Reference velocity.

NAME	LOCATION	TYPE	MEANING
USQ	PHYS		Square of U.
USQP	PHYS		Temporarily stored value of USQ.
UU	MAIN		Upstream value of U.
VISFU	BLOCK DATA		Viscosity constant of fuel.
VISMIX	BLOCK DATA		Viscosity constant of mixture.
VISOX	BLOCK DATA		Viscosity constant of oxygen.
VISPR	BLOCK DATA		Viscosity constant of product.
VMIX	MAIN		Specific volume of mixture.
VREF	WALL		Reference viscosity.
WB	MAIN		Reciprocal molecular weight of B-stream.
WC	MAIN		Reciprocal molecular weight of C-stream.
WMIX	MAIN		Molecular weight of mixture.
X	COMA	Array	Longitudinal distance x.
X	PLOTS	Array	Abscissa x in PLOT.
X	CALC	Array	Corrections in chemical-kinetics calculations.

NAME	LOCATION	TYPE	MEANING
XBAR	CREKO		Average value of X .
XD	MAIN		Downstream distance.
XDIF	COMP	Array	x-difference .
XJX	MAIN		Temporary storage for X(JX).
XLAXIS	OUTPUT		Label for abscissa in longitudinal plot.
XLPLOT	OUTPUT		Downstream distance array for longitudinal plot.
XMAX	CREKO		Maximum x-value .
XMAX	PLOTS		Maximum x in PLOT
XMIN	CREKO		Minimum x value .
XMIN	PLOTS		Minimum x in PLOT .
XS	COMP	Array	Width of cell in x direction .
XTAXIS	OUTPUT		Label for abscissa in cross-stream PLOT .
XTPLOT	OUTPUT	Array	Cross-stream distance array for transverse PLOT.

NAME	LOCATION	TYPE	MEANING
XU	COMP		Upstream distance.
XO	BLOCK DATA	Array	x-location of start of a duct-section.
Y	SPECE	Array	Logarithms of species mole-numbers.
Y	PLOTS	Array	Plotted ordinate values.
YAXISL	OUTPUT	Array	Labels for plotted values.
YAXIS1	OUTPUT	Array	Labels for plotted values (PLOT 1).
YAXIS2	OUTPUT	Array	Labels for plotted values (PLOT 2).
YAXIS3	OUTPUT	Array	Labels for plotted values (PLOT 3).
YBAR	CREKO		Average value of Y.
YDR	PHYS		y divided by R(N).
YLAXIS	OUTPUT	Array	Labels for ordinate of longitudinal plot.
YLPLOT	OUTPUT	Array	Values to be plotted (longitudinal plot)
YREF	WALL		Reference distance.
YTPLOT	OUTPUT	Array	Values to be plotted (cross-stream plot).

NAME	LOCATION	TYPE	MEANING
Z	CREKO	Array	Coefficients for calculation of thermochemical data.
ZETA	START		Temporarily stored quantity.
ZK1I... ZK5I	HCPS		Temporarily stored quantities.

APPENDIX D

A PARTIAL LISTING OF THE OUTPUT FROM THE NASCO PROGRAM

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*                                                *
*         PREDICTION OF HYDRODYNAMICS AND        *
*                                                *
*        CHEMISTRY OF CONFINED METHANE-AIR       *
*                                                *
*        FLAMES WITH ATTENTION TO FORMATION      *
*                                                *
*               OF NITROGEN OXIDES               *
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*                                                *
*          THE NASCO COMPUTER PROGRAM            *
*                                                *
*                 PREPARED BY                    *
*                                                *
*      CONCENTRATION HEAT AND MOMENTUM LTD.      *
*                                                *
*                     FOR                        *
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* NATIONAL AERONAUTICS AND SPACE ADMINISTRATION  *
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*          NASA LEWIS RESEARCH CENTER            *
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*                                                *
*           RESULTS FOR TEST CASE    1           *
*                                                *
*         S.I. UNITS ARE USED THROUGHOUT         *
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```

```
FLOW CONDITIONS
===============

     TURBULENT, MODEL=2

     CHEMICALLY REACTING, INERT=2


GEOMETRY
========

     RADIUS OF FUEL JET AT INLET     3.626-03

     RADIUS OF DUCT AT INLET         1.000-02

     TOTAL LENGTH OF DUCT            1.300+00


     DUCT WALL CONSTANTS -

          I       XO          AREX        BREX        CREX

          1    0.000       1.000-02    0.000       0.000
          2    6.000-01    1.000-02    2.000-01    0.000
          3    7.000-01    3.000-02    0.000       0.000


INLET CONDITIONS
================

     VELOCITY OF FUEL STREAM, UB            6.000-01

     VELOCITY OF AIR STREAM, UC             6.000+00

     TEMPERATURE OF FUEL STREAM, TB         2.940+02

     TEMPERATURE OF AIR STREAM, TC          8.100+02

     INLET PRESSURE, PRESS                  4.053+05

     REYNOLDS NUMBER                        5.398+03

     OVERALL EQUIVALENCE RATIO, EQRAT       4.000-01

     TOTAL MASS FLOW RATE, PSIE             4.628-04


BOUNDARY CONDITIONS
===================

     WALL TEMPERATURE CONSTANTS -

          I       DWALL       EWALL       FWALL
```

```
                1      8.100+02    5.000+07     0.000
                2      1.110+03    0.000        0.000
                3      1.110+03   -5.000+02     0.000


    GRID
    ====

    OMEGA GRID -
         0.000       2.979-03    5.958-03    8.937-03    3.641-02    2.400-01
         3.800-01    5.500-01    7.500-01    1.000+00

    X GRID -
         0.000       1.000-01    2.000-01    3.000-01    4.000-01    5.000-01
         6.000-01    6.050-01    6.100-01    6.150-01    6.200-01    6.250-01
         6.300-01    6.350-01    6.400-01    6.450-01    6.500-01    6.550-01
         6.600-01    6.650-01    6.700-01    6.750-01    6.800-01    6.850-01
         6.900-01    6.950-01    7.000-01    7.500-01    8.000-01    9.000-01
         1.000+00    1.100+00    1.200+00    1.250+00    1.300+00
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POLYNOMIAL COEFFICIENTS FOR THERMODYNAMIC PROPERTIES.
14 COEFFICIENTS ((Z(K,J,I),J=1,7),K=1,2) FOR EACH SPECIES I.

N
         1.749-01   7.612-06   -5.330-09   1.342-12   -7.325-17    4.006+03
         3.176-01   1.787-01   -1.556-06   3.870-09   -4.032-12    1.499-15
         4.005+03   2.975-01

NO
         1.063-01   4.460-05   -1.763-08   3.197-12   -2.161-16    3.275+02
         2.248-01   1.348-01   -1.139-04   2.660-07   -2.038-10    5.305-14
         3.248+02   9.990-02

NO2
         1.005-01   5.491-05   -2.306-08   4.321-12   -3.000-16    4.978+01
         2.896-02   7.518-02    4.488-05   1.453-07   -2.077-10    7.868-14
         6.119+01   1.807-01

N2O
         1.075-01   6.420-05   -2.626-08   4.831-12   -3.309-16    1.854+02
        -3.897-02   5.950-02    1.964-04  -1.548-07    5.061-11   -1.832-15
         1.990+02   2.096-01

N2
         1.034-01   5.410-05   -2.043-08   3.563-12   -2.328-16   -3.234+01
         2.199-01   1.312-01   -4.313-05   8.296-08   -2.257-11   -8.059-15
        -3.788+01   8.418-02

CH4
         9.367-02   6.493-04   -2.442-07   4.725-11   -2.760-15   -6.220+02
         6.674-01   2.385-01   -2.480-04   1.531-06   -1.417-09    4.340-13
        -6.324+02   5.404-02

O2
         1.132-01   2.301-05   -6.142-09   1.131-12   -9.046-17   -3.756+01
         1.130-01   1.133-01   -5.870-05   2.205-07   -2.114-10    6.736-14
        -3.274+01   1.345-01

CO
         1.065-01   5.316-05   -2.067-08   3.700-12   -2.476-16   -5.086+02
         2.266-01   1.325-01   -5.780-05   1.318-07   -7.254-11    8.552-15
        -5.125+02   1.055-01

CO2
         1.014-01   7.040-05   -2.816-08   5.167-12   -3.528-16   -1.113+03
        -2.241-02   5.455-02    1.985-04  -1.501-07    4.549-11    1.438-17
        -1.099+03   2.203-01

H
         2.480+00   0.000       0.000      0.000       0.000        2.527+04
        -4.565-01   2.480+00    0.000      0.000       0.000        0.000
         2.527+04  -4.565-01

H2
         1.538+00   2.536-04    2.611-08  -1.732-11    1.833-15   -4.352+02
        -9.737-01    1.517+00    1.328-03   -2.882-06    2.739-09   -8.990-13
        -4.905+02   -1.141+00

    820
         1.508-01    1.635-04   -4.453-08    5.677-12   -2.691-16   -1.660+03
         3.681-01    2.259-01   -6.153-05    2.305-07   -1.645-10    4.480-14
        -1.681+03   -1.791-02

    0
         1.589-01   -1.722-06   -1.939-10    2.845-13   -2.730-17    1.827+03
         3.075-01    1.842-01   -1.024-04    1.513-07   -1.002-10    2.432-14
         1.822+03    1.853-01

    OH
         1.711-01    5.641-05   -1.143-08    8.089-13    8.364-18    2.314+02
         3.200-01    2.256-01   -6.338-05    5.693-08    1.100-11   -1.327-14
         2.141+02    2.903-02
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ORIGINAL PAGE IS
OF POOR QUALITY

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REACTION MECHANISM
==================
 1. N    + NO           = N2  + O
 2. N    + O2           = NO  + O
 3. OH   + N            = H   + NO
 4. H    + N2O          = OH  + N2
 5. N2O  + O            = NO  + NO
 6. N2O  +        + M   = N2  + O     + M
 7. N    + O      + M   = NO  +       + M
 8. NO2  + O            = NO  + O2
 9. NO2  +        + M   = O   + NO    + M

  RATE CONSTANT PARAMETERS
    RATE CONSTANT =   A*T**B*EXP(-TACT/T)           (T=TEMPERATURE)

                    FORWARD RATE                          BACKWARD RATE

            A          B           TACT         A           B          TACT
   1.   1.500+10   0.000       0.000       6.753+10    0.000       3.786+04
   2.   5.998+06   1.000+00    3.172+03    5.856+09    0.000       2.087+04
   3.   5.998+08   5.000-01    4.328+03    1.102+11    0.000       2.898+04
   4.   7.998+10   0.000       7.553+03    3.842+09    0.000       4.047+04
   5.   1.000+11   0.000       1.500+04    2.805+09    0.000       3.422+04
   6.   1.000+11   0.000       2.518+04    2.678+06    0.000       6.573+03
   7.   6.397+10  -5.000-01    0.000       4.598+12    0.000       7.488+04
   8.   1.000+10   0.000       3.300+02    3.187+09    0.000       2.393+04
   9.   1.099+13   0.000       3.300+04    1.533+08    0.000      -2.950+03

     ****      ****      ****      ****      ****      ****      ****
  ***** NOTE - THE MAXIMUM CHANGES IN THE FIELD VALUES OF
  U-VELOCITY, STAGNATION ENTHALPY, MIXTURE FRACTION, AND MASS
  FRACTION OF UNBURNT FUEL BETWEEN SUCCESSIVE ITERATIONS ARE
  PRINTED AT EACH ITERATION.  THESE VALUES ARE COMPUTED AS THE
  MAXIMUM OF ABS(CURRENT VALUE - PREVIOUS VALUE)/CURRENT VALUE.
  THIS IS DONE IF THE CURRENT VALUE IS GREATER THAN  1.0-04.
  THE FOLLOWING SYMBOLS DENOTE THE MAXIMUM CHANGES -
       RSUMAX FOR U-VELOCITY,
       RSFMAX(J) FOR VARIABLE J,
          J=1 FOR STAGNATION ENTHALPY,
          J=2 FOR MIXTURE FRACTION, F,
          J=3 FOR MASS FRACTION OF UNBURNT FUEL.
    ****      ****      ****      ****      ****      ****      ****
    ****      ****      ****      ****      ****      ****      ****
    ****************         ITERATION NUMBER  20        *******************

    -+-+-+-+-+-+-+-+-+      TWO-DIMENSIONAL SOLUTION      -+-+-+-+-+-+-+-+-+

    ----------------------------------------------------------------------------

    ***  X=  0.000      IX=      1      DX=  1.000-10
         PRESSD=  0.000
                                 J =      1          2          3
    UFLUX=  2.720-03 FLUX(J)=   1.944+02   1.049-05   1.049-05
    DAI=  4.470-08 DA2=  0.000

       I      R           U VEL       TEMP        FUEL        OXYG        F
       1   0.000        6.000-01    2.940+02    1.000+00    0.000       1.000+00
       2   1.314-03     6.000-01    2.940+02    1.000+00    0.000       1.000+00
       3   1.859-03     6.000-01    2.940+02    1.000+00    0.000       1.000+00
       4   2.277-03     6.000-01    2.940+02    1.000+00    0.000       1.000+00
       5   3.791-03     6.000+00    8.100+02    0.000       2.320-01    0.000
       6   5.698-03     6.000+00    8.100+02    0.000       2.320-01    0.000
       7   6.701-03     6.000+00    8.100+02    0.000       2.320-01    0.000
       8   7.747-03     6.000+00    8.100+02    0.000       2.320-01    0.000
       9   8.820-03     6.000+00    8.100+02    0.000       2.320-01    0.000
      10   1.000-02     0.000       8.100+02    0.000       2.320-01    0.000

       I      R           N2          RHO         VISC        ENTLPY
       1   0.000        0.000       2.660+00    1.715-05   -4.676+06
       2   1.314-03     0.000       2.660+00    1.715-05   -4.676+06
       3   1.859-03     0.000       2.660+00    1.715-05   -4.676+06
       4   2.277-03     0.000       2.660+00    1.715-05   -4.676+06
       5   3.791-03     7.680-01    1.736+00    1.715-05    5.383+05
       6   5.698-03     7.680-01    1.736+00    1.715-05    5.383+05
       7   6.701-03     7.680-01    1.736+00    1.715-05    5.383+05
       8   7.747-03     7.680-01    1.736+00    1.715-05    5.383+05
       9   8.820-03     7.680-01    1.736+00    1.715-05    5.383+05
      10   1.000-02     7.680-01    1.736+00    1.715-05    5.383+05

    -+-+-+-+-+         CHEMICAL-EQUILIBRIUM SOLUTION          +-+-+-+-+-+-

       I      R           CO          CO2         H           H2          H2O
       1   0.000        0.000       0.000       0.000       0.000       0.000
       2   1.314-03     0.000       0.000       0.000       0.000       0.000
       3   1.859-03     0.000       0.000       0.000       0.000       0.000
       4   2.277-03     0.000       0.000       0.000       0.000       0.000
       5   3.791-03     0.000       0.000       0.000       0.000       0.000
       6   5.698-03     0.000       0.000       0.000       0.000       0.000
       7   6.701-03     0.000       0.000       0.000       0.000       0.000
       8   7.747-03     0.000       0.000       0.000       0.000       0.000
       9   8.820-03     0.000       0.000       0.000       0.000       0.000
      10   1.000-02     0.000       0.000       0.000       0.000       0.000

       I      R           O           OH
       1   0.000        0.000       0.000
       2   1.314-03     0.000       0.000
       3   1.859-03     0.000       0.000
       4   2.277-03     0.000       0.000
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     5   3.791-03   0.000       0.000
     6   5.698-03   0.000       0.000
     7   6.701-03   0.000       0.000
     8   7.747-03   0.000       0.000
     9   8.820-03   0.000       0.000
    10   1.000-02   0.000       0.000

 -+-+-+-+-+             CHEMICAL-KINETICS SOLUTION              +-+-+-+-+-

     I    R           N           NO          NO2         N2O
     1   0.000       0.000       0.000       0.000       0.000
     2   1.314-03    0.000       0.000       0.000       0.000
     3   1.859-03    0.000       0.000       0.000       0.000
     4   2.277-03    0.000       0.000       0.000       0.000
     5   3.791-03    0.000       0.000       0.000       0.000
     6   5.698-03    0.000       0.000       0.000       0.000
     7   6.701-03    0.000       0.000       0.000       0.000
     8   7.747-03    0.000       0.000       0.000       0.000
     9   8.820-03    0.000       0.000       0.000       0.000
    10   1.000-02    0.000       0.000       0.000       0.000

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 ***  X=  1.000-01  IX=     2      DX=  1.500-01
      PRESSD= -1.112-05
                             J =      1           2           3
 UFLUX=  2.587-03 FLUX(J)=   1.998+02    1.049-05    1.049-05
 DA1= -3.998-03 DA2=  2.074-04

     I    R           U VEL       TEMP        FUEL        OXYG        F
     1   0.000       5.240+00    6.343+02    1.720-01    1.921-01    1.720-01
     2   5.196-04    5.240+00    6.343+02    1.720-01    1.921-01    1.720-01
     3   7.343-04    5.301+00    6.430+02    1.609-01    1.947-01    1.609-01
     4   8.983-04    5.361+00    6.519+02    1.500-01    1.972-01    1.500-01
     5   1.798-03    5.831+00    7.310+02    6.639-02    2.166-01    6.640-02
     6   4.590-03    5.936+00    7.802+02    2.607-02    2.259-01    2.607-02
     7   5.797-03    5.840+00    7.951+02    1.617-02    2.282-01    1.617-02
     8   7.029-03    5.623+00    8.061+02    1.049-02    2.296-01    1.049-02
     9   8.327-03    5.195+00    8.164+02    7.263-03    2.303-01    7.266-03
    10   9.999-03    0.000       8.600+02    7.263-03    2.303-01    7.266-03

     I    R           N2          RHO         VISC        ENTLPY
     1   0.000       6.359-01    1.949+00    3.043-04   -3.552+05
     2   5.196-04    6.359-01    1.949+00    3.043-04   -3.552+05
     3   7.343-04    6.444-01    1.938+00    3.043-04   -2.972+05
     4   8.983-04    6.528-01    1.926+00    3.043-04   -2.400+05
     5   1.798-03    7.170-01    1.827+00    3.043-04    1.962+05
     6   4.590-03    7.480-01    1.766+00    3.043-04    4.084+05
     7   5.797-03    7.556-01    1.746+00    3.043-04    4.623+05
     8   7.029-03    7.599-01    1.730+00    2.719-04    4.956+05
     9   8.327-03    7.624-01    1.713+00    2.395-04    5.190+05
    10   9.999-03    7.624-01    1.713+00    2.933-05    5.685+05

 -+-+-+-+-+             CHEMICAL-EQUILIBRIUM SOLUTION           +-+-+-+-+-
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  I      R            CO          CO2           H           H2          H2O
  1   0.000       6.341-15    7.610-06    4.172-21    1.745-15    6.230-06
  2   5.196-04    6.341-15    7.610-06    4.172-21    1.745-15    6.230-06
  3   7.343-04    6.405-15    7.687-06    4.214-21    1.762-15    6.293-06
  4   8.983-04    6.469-15    7.763-06    4.256-21    1.780-15    6.356-06
  5   1.798-03    6.843-15    8.211-06    4.502-21    1.883-15    6.723-06
  6   4.590-03    8.005-15    9.606-06    5.266-21    2.202-15    7.865-06
  7   5.797-03    8.200-15    9.841-06    5.395-21    2.256-15    8.057-06
  8   7.029-03    8.253-15    9.904-06    5.430-21    2.271-15    8.109-06
  9   8.327-03    8.406-15    1.009-05    5.530-21    2.313-15    8.258-06
 10   9.999-03    8.406-15    1.009-05    5.530-21    2.313-15    8.258-06

  I      R            O           OH
  1   0.000       2.168-19    3.721-14
  2   5.196-04    2.168-19    3.721-14
  3   7.343-04    2.190-19    3.758-14
  4   8.983-04    2.212-19    3.796-14
  5   1.798-03    2.339-19    4.015-14
  6   4.590-03    2.737-19    4.697-14
  7   5.797-03    2.803-19    4.812-14
  8   7.029-03    2.821-19    4.843-14
  9   8.327-03    2.873-19    4.932-14
 10   9.999-03    2.873-19    4.932-14

-+-+-+-+-+              CHEMICAL-KINETICS SOLUTION              +-+-+-+-+-

  I      R            N           NO          NO2         N2O
  1   0.000       1.401-29    1.855-16    3.983-20    1.296-16
  2   5.196-04    1.401-29    1.855-16    3.983-20    1.296-16
  3   7.343-04    1.401-29    1.661-16    3.750-20    1.285-16
  4   8.983-04    1.401-29    1.372-16    3.351-20    1.278-16
  5   1.798-03    1.401-29    6.610-17    2.317-20    1.202-16
  6   4.590-03    1.401-29    3.122-17    2.010-20    1.276-16
  7   5.797-03    1.401-29    2.161-17    1.880-20    1.315-16
  8   7.029-03    1.401-29    1.502-17    1.654-20    1.304-16
  9   8.327-03    1.401-29    1.040-17    1.362-20    1.247-16
 10   9.999-03    1.401-29    1.040-17    1.362-20    1.247-16

***  X=  6.300-01  IX=    13      DX=  5.000-03
     PRESSD= -2.563-05
                           J =      1            2            3
UFLUX=  1.293-03 FLUX(J)=   2.564+02    1.048-05    9.958-06
DA1= -2.121-03 DA2=  2.951-04

  I      R           U VEL        TEMP         FUEL        OXYG          F
  1   0.000       2.883+00    9.298+02    2.166-02    2.226-01    2.270-02
  2   8.024-04    2.883+00    9.298+02    2.166-02    2.226-01    2.270-02
  3   1.135-03    2.883+00    9.298+02    2.166-02    2.226-01    2.269-02
  4   1.390-03    2.882+00    9.299+02    2.166-02    2.226-01    2.269-02
  5   2.807-03    2.877+00    9.304+02    2.165-02    2.226-01    2.269-02
  6   7.244-03    2.830+00    9.347+02    2.157-02    2.224-01    2.266-02
  7   9.146-03    2.805+00    9.371+02    2.153-02    2.223-01    2.264-02
  8   1.104-02    2.777+00    9.401+02    2.149-02    2.222-01    2.263-02
  9   1.295-02    2.747+00    9.435+02    2.145-02    2.220-01    2.263-02
 10   1.600-02    0.000       1.110+03    2.145-02    2.220-01    2.263-02

  I      R            N2          RHO         VISC        ENTLPY
  1    0.000        7.506-01    1.485+00    2.049-02    5.478+05
  2    8.024-04     7.506-01    1.485+00    2.049-02    5.478+05
  3    1.135-03     7.506-01    1.485+00    2.049-02    5.478+05
  4    1.390-03     7.506-01    1.485+00    2.049-02    5.479+05
  5    2.807-03     7.506-01    1.484+00    2.049-02    5.482+05
  6    7.244-03     7.506-01    1.478+00    2.049-02    5.513+05
  7    9.146-03     7.506-01    1.474+00    2.049-02    5.530+05
  8    1.104-02     7.506-01    1.469+00    2.049-02    5.551+05
  9    1.295-02     7.506-01    1.464+00    2.049-02    5.575+05
 10    1.600-02     7.506-01    1.464+00    3.332-05    7.621+05

-+-+-+-+-+              CHEMICAL-EQUILIBRIUM SOLUTION             +-+-+-+-+-

  I      R             CO          CO2          H           H2          H2O
  1    0.000        3.082-11    2.845-03    6.164-17    5.660-12    2.329-03
  2    8.024-04     3.082-11    2.845-03    6.164-17    5.660-12    2.329-03
  3    1.135-03     3.086-11    2.846-03    6.174-17    5.666-12    2.330-03
  4    1.390-03     3.090-11    2.847-03    6.187-17    5.673-12    2.331-03
  5    2.807-03     3.145-11    2.861-03    6.332-17    5.763-12    2.342-03
  6    7.244-03     3.641-11    2.984-03    7.673-17    6.563-12    2.443-03
  7    9.146-03     3.959-11    3.056-03    8.565-17    7.070-12    2.502-03
  8    1.104-02     4.373-11    3.143-03    9.761-17    7.722-12    2.573-03
  9    1.295-02     4.903-11    3.245-03    1.135-16    8.547-12    2.656-03
 10    1.600-02     4.903-11    3.245-03    1.135-16    8.547-12    2.656-03

  I      R              O          OH
  1    0.000        3.244-15    1.345-10
  2    8.024-04     3.244-15    1.345-10
  3    1.135-03     3.250-15    1.347-10
  4    1.390-03     3.256-15    1.348-10
  5    2.807-03     3.333-15    1.371-10
  6    7.244-03     4.042-15    1.560-10
  7    9.146-03     4.514-15    1.694-10
  8    1.104-02     5.148-15    1.856-10
  9    1.295-02     5.990-15    2.063-10
 10    1.600-02     5.990-15    2.063-10

-+-+-+-+-+               CHEMICAL-KINETICS SOLUTION              +-+-+-+-+-

  I      R              N          NO          NO2         N2O
  1    0.000        1.401-29    8.584-13    6.686-14    1.523-12
  2    8.024-04     1.401-29    8.584-13    6.686-14    1.523-12
  3    1.135-03     1.401-29    1.557-12    1.214-13    1.917-12
  4    1.390-03     1.401-29    3.290-12    2.583-13    2.640-12
  5    2.807-03     1.401-29    1.334-11    1.059-12    5.738-12
  6    7.244-03     1.401-29    2.948-11    2.282-12    9.742-12
  7    9.146-03     1.543-29    4.394-11    3.152-12    1.151-11
  8    1.104-02     1.973-29    6.165-11    4.764-12    1.383-11
  9    1.295-02     2.620-29    9.429-11    7.364-12    1.667-11
 10    1.600-02     2.670-29    9.429-11    7.364-12    1.667-11

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*** X=  6.350-01  IX=   14      DX=  5.000-03
    PRESSD= -2.305-05
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                              J =       1          2          3
UFLUX=  1.193-03 FLUX(J)=   2.562+02   1.047-05   9.567-06
DA1= -5.078-03 DA2=  8.276-04

  I      R           U VEL      TEMP       FUEL       OXYG       F
  1   0.000        2.650+00   9.613+02   2.086-02   2.196-01   2.266-02
  2   8.510-04     2.650+00   9.613+02   2.086-02   2.196-01   2.266-02
  3   1.204-03     2.650+00   9.613+02   2.086-02   2.196-01   2.266-02
  4   1.474-03     2.650+00   9.614+02   2.086-02   2.196-01   2.266-02
  5   2.977-03     2.645+00   9.620+02   2.085-02   2.195-01   2.266-02
  6   7.680-03     2.607+00   9.671+02   2.075-02   2.192-01   2.264-02
  7   9.694-03     2.587+00   9.701+02   2.070-02   2.190-01   2.263-02
  8   1.170-02     2.564+00   9.737+02   2.064-02   2.188-01   2.263-02
  9   1.372-02     2.539+00   9.779+02   2.056-02   2.185-01   2.262-02
 10   1.699-02     0.000      1.110+03   2.056-02   2.185-01   2.262-02

  I      R           N2         RHO        VISC       ENTLPY
  1   0.000        7.506-01   1.437+00   1.943-02   5.488+05
  2   8.510-04     7.506-01   1.437+00   1.943-02   5.488+05
  3   1.204-03     7.506-01   1.437+00   1.943-02   5.488+05
  4   1.474-03     7.506-01   1.437+00   1.943-02   5.489+05
  5   2.977-03     7.506-01   1.436+00   1.943-02   5.492+05
  6   7.680-03     7.506-01   1.428+00   1.943-02   5.515+05
  7   9.694-03     7.506-01   1.424+00   1.943-02   5.528+05
  8   1.170-02     7.506-01   1.418+00   1.943-02   5.543+05
  9   1.372-02     7.506-01   1.412+00   1.943-02   5.561+05
 10   1.699-02     7.506-01   1.412+00   3.332-05   7.189+05

-+-+-+-+-+                 CHEMICAL-EQUILIBRIUM SOLUTION              +-+-+-+-+-

  I      R           CO         CO2        H          H2         H2O
  1   0.000        1.124-10   4.931-03   3.119-16   1.838-11   4.037-03
  2   8.510-04     1.124-10   4.931-03   3.119-16   1.838-11   4.037-03
  3   1.204-03     1.126-10   4.932-03   3.124-16   1.840-11   4.038-03
  4   1.474-03     1.127-10   4.934-03   3.130-16   1.842-11   4.039-03
  5   2.977-03     1.149-10   4.959-03   3.208-16   1.873-11   4.060-03
  6   7.680-03     1.345-10   5.180-03   3.952-16   2.155-11   4.241-03
  7   9.694-03     1.474-10   5.311-03   4.457-16   2.336-11   4.349-03
  8   1.170-02     1.642-10   5.470-03   5.143-16   2.572-11   4.479-03
  9   1.372-02     1.861-10   5.656-03   6.067-16   2.873-11   4.631-03
 10   1.699-02     1.861-10   5.656-03   6.067-16   2.873-11   4.631-03

  I      R           O          OH
  1   0.000        1.652-14   4.522-10
  2   8.510-04     1.652-14   4.522-10
  3   1.204-03     1.655-14   4.527-10
  4   1.474-03     1.658-14   4.533-10
  5   2.977-03     1.700-14   4.612-10
  6   7.680-03     2.097-14   5.335-10
  7   9.694-03     2.366-14   5.802-10
  8   1.170-02     2.733-14   6.412-10
  9   1.372-02     3.227-14   7.193-10
 10   1.699-02     3.227-14   7.193-10

-+-+-+-+-+                  CHEMICAL-KINETICS SOLUTION              +-+-+-+-+-

  I      R           N          NO         NO2        N2O
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     1    0.000        1.413-28    7.282-12    5.937-13    7.136-12
     2    8.510-04     1.413-28    7.282-12    5.937-13    7.136-12
     3    1.204-03     1.418-28    1.151-11    9.420-13    8.359-12
     4    1.474-03     1.423-28    2.086-11    1.722-12    1.047-11
     5    2.977-03     1.493-28    6.957-11    5.809-12    1.688-11
     6    7.680-03     2.219-28    1.420-10    1.129-11    2.898-11
     7    9.694-03     2.790-28    1.831-10    1.459-11    3.307-11
     8    1.170-02     3.668-28    2.553-10    2.023-11    3.814-11
     9    1.372-02     5.034-28    3.625-10    2.882-11    4.414-11
    10    1.699-02     5.034-28    3.625-10    2.882-11    4.414-11

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  ***  X=  6.400-01  IX=   15     DX=  5.000-03
       PRESSD=  -2.101-05
                               J =      1           2           3
  UFLUX=  1.125-03 FLUX(J)=    2.540+02    1.047-05    8.923-06
  DA1=  1.371-03 DA2=  5.798-04

     I     R            U VEL       TEMP        FUEL        OXYG        F
     1    0.000        2.489+00    1.010+03    1.958-02    2.146-01    2.263-02
     2    9.000-04     2.489+00    1.010+03    1.958-02    2.146-01    2.263-02
     3    1.273-03     2.489+00    1.010+03    1.958-02    2.146-01    2.263-02
     4    1.559-03     2.489+00    1.010+03    1.958-02    2.146-01    2.263-02
     5    3.148-03     2.485+00    1.011+03    1.957-02    2.145-01    2.263-02
     6    8.119-03     2.455+00    1.017+03    1.942-02    2.139-01    2.262-02
     7    1.025-02     2.439+00    1.021+03    1.933-02    2.136-01    2.262-02
     8    1.237-02     2.421+00    1.026+03    1.923-02    2.132-01    2.261-02
     9    1.450-02     2.401+00    1.031+03    1.910-02    2.127-01    2.261-02
    10    1.799-02     0.000       1.110+03    1.910-02    2.127-01    2.261-02

     I     R            N2          RHO         VISC        ENTLPY
     1    0.000        7.506-01    1.368+00    1.849-02    5.464+05
     2    9.000-04     7.506-01    1.368+00    1.849-02    5.464+05
     3    1.273-03     7.506-01    1.368+00    1.849-02    5.464+05
     4    1.559-03     7.506-01    1.368+00    1.849-02    5.464+05
     5    3.148-03     7.506-01    1.367+00    1.849-02    5.466+05
     6    8.119-03     7.506-01    1.358+00    1.849-02    5.478+05
     7    1.025-02     7.506-01    1.353+00    1.849-02    5.484+05
     8    1.237-02     7.506-01    1.347+00    1.849-02    5.492+05
     9    1.450-02     7.506-01    1.340+00    1.849-02    5.500+05
    10    1.799-02     7.506-01    1.340+00    3.332-05    6.476+05

  -+-+-+-+-+               CHEMICAL-EQUILIBRIUM SOLUTION              +-+-+-+-+-

     I     R            CO          CO2         H           H2          H2O
     1    0.000        5.329-10    8.379-03    2.328-15    7.426-11    6.860-03
     2    9.000-04     5.329-10    8.379-03    2.328-15    7.426-11    6.860-03
     3    1.273-03     5.335-10    8.380-03    2.332-15    7.434-11    6.861-03
     4    1.559-03     5.343-10    8.383-03    2.337-15    7.444-11    6.864-03
     5    3.148-03     5.451-10    8.426-03    2.400-15    7.577-11    6.899-03
     6    8.119-03     6.474-10    8.807-03    3.017-15    8.822-11    7.211-03
     7    1.025-02     7.151-10    9.035-03    3.445-15    9.634-11    7.397-03
     8    1.237-02     8.052-10    9.312-03    4.035-15    1.070-10    7.624-03
     9    1.450-02     9.229-10    9.638-03    4.841-15    1.207-10    7.891-03
    10    1.799-02     9.229-10     9.638-03     4.841-15     1.207-10     7.891-03

     I      R            O            OH
     1    0.000        1.248-13     1.921-09
     2    9.000-04     1.248-13     1.921-09
     3    1.273-03     1.250-13     1.923-09
     4    1.559-03     1.253-13     1.926-09
     5    3.148-03     1.287-13     1.962-09
     6    8.119-03     1.621-13     2.300-09
     7    1.025-02     1.853-13     2.521-09
     8    1.237-02     2.173-13     2.812-09
     9    1.450-02     2.610-13     3.190-09
    10    1.799-02     2.610-13     3.190-09

  -+-+-+-+-+              CHEMICAL-KINETICS SOLUTION              +-+-+-+-+-

     I      R            N            NO           NO2          N2O
     1    0.000        5.875-27     4.783-11     4.152-12     2.886-11
     2    9.000-04     5.875-27     4.783-11     4.152-12     2.886-11
     3    1.273-03     5.892-27     6.788-11     5.900-12     3.170-11
     4    1.559-03     5.917-27     1.084-10     9.497-12     3.646-11
     5    3.148-03     6.236-27     3.019-10     2.660-11     5.428-11
     6    8.119-03     9.751-27     5.513-10     4.647-11     7.410-11
     7    1.025-02     1.264-26     6.848-10     5.659-11     8.202-11
     8    1.237-02     1.723-26     8.943-10     7.257-11     9.196-11
     9    1.450-02     2.465-26     1.192-09     9.560-11     1.040-10
    10    1.799-02     2.465-26     1.192-09     9.560-11     1.040-10

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  ***   X=   6.450-01   IX=    16        DX=   5.000-03
        PRESSD=  -1.939-05
                                  J =        1            2            3
  UFLUX=   1.094-03 FLUX(J)=      2.494+02     1.046-05     7.900-06
  DA1=   2.151-03 DA2=    9.039-04

     I      R           U VEL        TEMP         FUEL         OXYG          F
     1    0.000        2.406+00     1.085+03     1.755-02     2.065-01     2.261-02
     2    9.489-04     2.406+00     1.085+03     1.755-02     2.065-01     2.261-02
     3    1.342-03     2.405+00     1.085+03     1.755-02     2.065-01     2.261-02
     4    1.644-03     2.405+00     1.085+03     1.755-02     2.065-01     2.261-02
     5    3.319-03     2.403+00     1.086+03     1.752-02     2.064-01     2.261-02
     6    8.558-03     2.380+00     1.094+03     1.729-02     2.055-01     2.260-02
     7    1.080-02     2.368+00     1.100+03     1.716-02     2.050-01     2.260-02
     8    1.303-02     2.355+00     1.106+03     1.699-02     2.043-01     2.260-02
     9    1.527-02     2.341+00     1.113+03     1.679-02     2.035-01     2.259-02
    10    1.899-02     0.000        1.110+03     1.679-02     2.035-01     2.259-02

     I      R            N2           RHO          VISC         ENTLPY
     1    0.000        7.506-01     1.273+00     1.763-02     5.400+05
     2    9.489-04     7.506-01     1.273+00     1.763-02     5.400+05
     3    1.342-03     7.506-01     1.273+00     1.763-02     5.400+05
     4    1.644-03     7.506-01     1.273+00     1.763-02     5.400+05
     5    3.319-03     7.506-01     1.272+00     1.763-02     5.400+05
     6    8.558-03     7.506-01     1.262+00     1.763-02     5.396+05
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ORIGINAL PAGE IS
OF POOR QUALITY

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   7    1.080-02     7.506-01     1.256+00     1.763-02     5.392+05
   8    1.303-02     7.506-01     1.249+00     1.763-02     5.386+05
   9    1.527-02     7.506-01     1.241+00     1.763-02     5.378+05
  10    1.899-02     7.506-01     1.241+00     3.332-05     5.342+05

-+-+-+-+-+           CHEMICAL-EQUILIBRIUM SOLUTION                +-+-+-+-+-

   I      R           CO           CO2           H            H2          H2O
   1    0.000       3.421-09     1.390-02     2.745-14     3.870-10     1.138-02
   2    9.489-04    3.421-09     1.390-02     2.745-14     3.870-10     1.138-02
   3    1.342-03    3.424-09     1.390-02     2.748-14     3.873-10     1.138-02
   4    1.644-03    3.429-09     1.391-02     2.753-14     3.878-10     1.139-02
   5    3.319-03    3.501-09     1.398-02     2.831-14     3.950-10     1.144-02
   6    8.558-03    4.200-09     1.460-02     3.616-14     4.638-10     1.195-02
   7    1.080-02    4.670-09     1.497-02     4.172-14     5.094-10     1.226-02
   8    1.303-02    5.302-09     1.543-02     4.949-14     5.698-10     1.263-02
   9    1.527-02    6.137-09     1.597-02     6.028-14     6.485-10     1.308-02
  10    1.899-02    6.137-09     1.597-02     6.028-14     6.485-10     1.308-02

   I      R            O            OH
   1    0.000       1.503-12     1.076-08
   2    9.489-04    1.503-12     1.076-08
   3    1.342-03    1.505-12     1.077-08
   4    1.644-03    1.508-12     1.079-08
   5    3.319-03    1.551-12     1.099-08
   6    8.558-03    1.986-12     1.301-08
   7    1.080-02    2.294-12     1.436-08
   8    1.303-02    2.727-12     1.615-08
   9    1.527-02    3.328-12     1.849-08
  10    1.899-02    3.328-12     1.849-08

-+-+-+-+-+             CHEMICAL-KINETICS SOLUTION                +-+-+-+-+-

   I      R             N            NO          NO2          N2O
   1    0.000       7.368-25     2.555-10     2.453-11     1.034-10
   2    9.489-04    7.368-25     2.555-10     2.453-11     1.034-10
   3    1.342-03    7.387-25     3.332-10     3.158-11     1.076-10
   4    1.644-03    7.417-25     4.801-10     4.538-11     1.151-10
   5    3.319-03    7.849-25     1.134-09     1.040-10     1.427-10
   6    8.558-03    1.287-24     1.859-09     1.617-10     1.725-10
   7    1.080-02    1.718-24     2.200-09     1.869-10     1.654-10
   8    1.303-02    2.430-24     2.713-09     2.225-10     2.039-10
   9    1.527-02    3.627-24     3.425-09     2.697-10     2.298-10
  10    1.899-02    3.627-24     3.425-09     2.697-10     2.298-10

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      ***   X=  6.500-01   IX=    17     DX=  5.000-03
           PRESSD= -1.806-05
                                  J =      1             2             3
      UFLUX=  1.097-03 FLUX(J)=   7.421+02    1.045-05     6.350-06
      DA1=  1.326-03  DA2=  -2.162-04

         I      R             U VEL       TEMP         FUEL          OXYG          F
         1    0.000        2.401+00    1.199+03     1.443-02     1.941-01     2.259-02
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    2   9.988-04    2.401+00    1.199+03    1.443-02    1.941-01    2.259-02
    3   1.413-03    2.400+00    1.199+03    1.443-02    1.941-01    2.259-02
    4   1.730-03    2.400+00    1.199+03    1.443-02    1.941-01    2.259-02
    5   3.494-03    2.398+00    1.201+03    1.439-02    1.940-01    2.259-02
    6   9.004-03    2.382+00    1.212+03    1.406-02    1.927-01    2.258-02
    7   1.136-02    2.374+00    1.218+03    1.385-02    1.919-01    2.258-02
    8   1.370-02    2.365+00    1.226+03    1.360-02    1.908-01    2.258-02
    9   1.605-02    2.357+00    1.236+03    1.329-02    1.896-01    2.258-02
   10   2.000-02    0.000       1.110+03    1.329-02    1.896-01    2.258-02

    I   R              N2       RHO         VISC        ENTLPY
    1   0.000       7.507-01    1.151+00    1.686-02    5.295+05
    2   9.988-04    7.507-01    1.151+00    1.686-02    5.295+05
    3   1.413-03    7.507-01    1.151+00    1.686-02    5.295+05
    4   1.730-03    7.507-01    1.151+00    1.686-02    5.294+05
    5   3.494-03    7.507-01    1.150+00    1.686-02    5.291+05
    6   9.004-03    7.507-01    1.140+00    1.686-02    5.265+05
    7   1.136-02    7.507-01    1.134+00    1.686-02    5.246+05
    8   1.370-02    7.507-01    1.126+00    1.686-02    5.221+05
    9   1.605-02    7.507-01    1.117+00    1.686-02    5.190+05
   10   2.000-02    7.507-01    1.117+00    3.332-05    3.630+05

  -+-+-+-+-+             CHEMICAL-EQUILIBRIUM SOLUTION           +-+-+-+-+-

    I   R              CO         CO2          H           H2          H2O
    1   0.000       2.870-08    2.242-02    4.904-13    2.527-09    1.836-02
    2   9.988-04    2.870-08    2.242-02    4.904-13    2.527-09    1.836-02
    3   1.413-03    2.872-08    2.242-02    4.907-13    2.528-09    1.836-02
    4   1.730-03    2.875-08    2.243-02    4.915-13    2.531-09    1.836-02
    5   3.494-03    2.931-08    2.253-02    5.045-13    2.574-09    1.844-02
    6   9.004-03    3.494-08    2.343-02    6.407-13    3.006-09    1.919-02
    7   1.136-02    3.879-08    2.399-02    7.388-13    3.297-09    1.964-02
    8   1.370-02    4.403-08    2.469-02    8.778-13    3.688-09    2.022-02
    9   1.605-02    5.104-08    2.553-02    1.074-12    4.203-09    2.090-02
   10   2.000-02    5.104-08    2.553-02    1.074-12    4.203-09    2.090-02

    I   R              O          OH
    1   0.000       2.782-11    7.752-08
    2   9.988-04    2.782-11    7.752-08
    3   1.413-03    2.783-11    7.756-08
    4   1.730-03    2.788-11    7.764-08
    5   3.494-03    2.863-11    7.905-08
    6   9.004-03    3.649-11    9.312-08
    7   1.136-02    4.216-11    1.027-07
    8   1.370-02    5.023-11    1.156-07
    9   1.605-02    6.161-11    1.327-07
   10   2.000-02    6.161-11    1.327-07

  -+-+-+-+-+              CHEMICAL-KINETICS SOLUTION            +-+-+-+-+-

    I   R              N          NO          NO2         N2O
    1   0.000       2.782-22    1.168-09    1.214-10    3.396-10
    2   9.988-04    2.782-22    1.168-09    1.214-10    3.396-10
    3   1.413-03    2.786-22    1.427-09    1.433-10    3.412-10
    4   1.730-03    2.795-22    1.895-09    1.839-10    3.489-10
    5   3.494-03    2.953-22    3.851-09    3.327-10    3.758-10
    6   9.004-03    4.870-22    5.548-09    4.531-10    4.169-10
   7   1.136-02   6.565-22   6.247-09   5.007-10   4.384-10
   8   1.370-02   9.426-22   7.294-09   5.569-10   4.724-10
   9   1.605-02   1.439-21   8.771-09   6.153-10   5.269-10
  10   2.000-02   1.439-21   8.771-09   6.153-10   5.269-10

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  ***  X=  6.550-01  IX=   18     DX=  5.000-03
       PRESSD= -1.714-05
                         J =      1          2          3
UFLUX=  1.134-03 FLUX(J)=   2.324+02   1.044-05   4.226-06
DA1=  2.054-03 DA2= -3.446-04

   I     R          U VEL       TEMP       FUEL       OXYG       F
   1   0.000      2.471+00   1.363+03   9.997-03   1.765-01   2.257-02
   2   1.049-03   2.471+00   1.363+03   9.997-03   1.765-01   2.257-02
   3   1.484-03   2.471+00   1.363+03   9.997-03   1.765-01   2.257-02
   4   1.818-03   2.471+00   1.363+03   9.994-03   1.765-01   2.257-02
   5   3.670-03   2.469+00   1.364+03   9.954-03   1.763-01   2.257-02
   6   9.452-03   2.457+00   1.375+03   9.561-03   1.748-01   2.256-02
   7   1.192-02   2.451+00   1.382+03   9.310-03   1.738-01   2.256-02
   8   1.437-02   2.445+00   1.391+03   8.989-03   1.725-01   2.256-02
   9   1.683-02   2.439+00   1.402+03   8.586-03   1.709-01   2.256-02
  10   2.100-02   0.000      1.110+03   8.586-03   1.709-01   2.256-02

   I     R            N2        RHO        VISC       ENTLPY
   1   0.000      7.507-01   1.013+00   1.615-02   5.150+05
   2   1.049-03   7.507-01   1.013+00   1.615-02   5.150+05
   3   1.484-03   7.507-01   1.013+00   1.615-02   5.149+05
   4   1.818-03   7.507-01   1.013+00   1.615-02   5.149+05
   5   3.670-03   7.507-01   1.012+00   1.615-02   5.142+05
   6   9.452-03   7.507-01   1.004+00   1.615-02   5.088+05
   7   1.192-02   7.507-01   9.992-01   1.615-02   5.051+05
   8   1.437-02   7.507-01   9.929-01   1.615-02   5.003+05
   9   1.683-02   7.507-01   9.852-01   1.615-02   4.940+05
  10   2.100-02   7.507-01   9.852-01   3.332-05   1.324+05

-+-+-+-+-+       CHEMICAL-EQUILIBRIUM SOLUTION           +-+-+-+-+-

   I     R          CO          CO2        H          H2         H2O
   1   0.000      2.645-07   3.456-02   1.052-11   1.785-08   2.830-02
   2   1.049-03   2.645-07   3.456-02   1.052-11   1.785-08   2.830-02
   3   1.484-03   2.644-07   3.456-02   1.052-11   1.785-08   2.830-02
   4   1.818-03   2.645-07   3.457-02   1.052-11   1.786-08   2.830-02
   5   3.670-03   2.681-07   3.468-02   1.072-11   1.807-08   2.839-02
   6   9.452-03   3.069-07   3.575-02   1.291-11   2.038-08   2.927-02
   7   1.192-02   3.339-07   3.643-02   1.449-11   2.196-08   2.983-02
   8   1.437-02   3.708-07   3.731-02   1.674-11   2.410-08   3.055-02
   9   1.683-02   4.212-07   3.841-02   1.995-11   2.699-08   3.144-02
  10   2.100-02   4.212-07   3.841-02   1.995-11   2.699-08   3.144-02

   I     R           O          OH
   1   0.000      6.298-10   6.194-07
   2   1.049-03   6.298-10   6.194-07
   3   1.484-03   6.295-10   6.192-07
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       4     1.818-03    6.299-10    6.195-07
       5     3.670-03    6.419-10    6.275-07
       6     9.452-03    7.760-10    7.130-07
       7     1.192-02    8.731-10    7.720-07
       8     1.437-02    1.012-09    8.525-07
       9     1.683-02    1.210-09    9.620-07
      10     2.100-02    1.210-09    9.620-07

  -+-+-+-+-+                  CHEMICAL-KINETICS SOLUTION                  +-+-+-+-+-

       I      R              N           NO           NO2          N2O
       1     0.000       1.963-19    5.037-09    2.658-10    1.065-09
       2     1.049-03    1.963-19    5.037-09    2.658-10    1.065-09
       3     1.484-03    1.960-19    5.803-09    3.067-10    1.063-09
       4     1.818-03    1.963-19    7.170-09    3.745-10    1.068-09
       5     3.670-03    2.042-19    1.241-08    6.279-10    1.081-09
       6     9.452-03    3.035-19    1.525-08    7.306-10    1.160-09
       7     1.192-02    3.882-19    1.627-08    7.551-10    1.212-09
       8     1.437-02    5.278-19    1.793-08    7.941-10    1.281-09
       9     1.683-02    7.670-19    2.046-08    8.472-10    1.375-09
      10     2.100-02    7.670-19    2.046-08    8.472-10    1.375-09

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  ***   X=  6.600-01   IX=    19      DX=  5.030-03
        PRESSD= -1.641-05
                               J =      1            2            3
  UFLUX=  1.159-03 FLUX(J)=    2.212+02    1.043-05    2.068-06
  DA1=  2.389-03 DA2= -4.098-04

       I      R            U VEL        TEMP         FUEL         OXYG          F
       1     0.000       2.530+00    1.543+03    5.088-03    1.569-01    2.255-02
       2     1.104-03    2.530+00    1.543+03    5.088-03    1.569-01    2.255-02
       3     1.561-03    2.530+00    1.543+03    5.090-03    1.569-01    2.255-02
       4     1.911-03    2.529+00    1.543+03    5.090-03    1.569-01    2.255-02
       5     3.858-03    2.528+00    1.543+03    5.067-03    1.569-01    2.255-02
       6     9.922-03    2.516+00    1.547+03    4.804-03    1.558-01    2.254-02
       7     1.250-02    2.509+00    1.550+03    4.622-03    1.551-01    2.254-02
       8     1.506-02    2.501+00    1.554+03    4.377-03    1.541-01    2.254-02
       9     1.762-02    2.491+00    1.559+03    4.044-03    1.528-01    2.254-02
      10     2.200-02    0.000       1.110+03    4.044-03    1.528-01    2.254-02

       I      R              N2          RHO          VISC        ENTLPY
       1     0.000       7.507-01    8.952-01    1.551-02    4.973+05
       2     1.104-03    7.507-01    8.952-01    1.551-02    4.973+05
       3     1.561-03    7.507-01    8.953-01    1.551-02    4.972+05
       4     1.911-03    7.507-01    8.953-01    1.551-02    4.971+05
       5     3.858-03    7.507-01    8.952-01    1.551-02    4.961+05
       6     9.972-03    7.507-01    8.931-01    1.551-02    4.878+05
       7     1.250-02    7.507-01    8.915-01    1.551-02    4.823+05
       8     1.506-02    7.507-01    8.892-01    1.551-02    4.750+05
       9     1.762-02    7.507-01    8.860-01    1.551-02    4.656+05
      10     2.200-02    7.507-01    8.860-01    3.332-05   -9.028+04

  -+-+-+-+-+                CHEMICAL-EQUILIBRIUM SOLUTION                +-+-+-+-+-
  I        R            CO           CO2           H            H2           H2O
  1    0.000        1.711-06     4.800-02     1.450-10     9.265-08     3.930-02
  2    1.104-03     1.711-06     4.800-02     1.450-10     9.265-08     3.930-02
  3    1.561-03     1.709-06     4.799-02     1.447-10     9.253-08     3.929-02
  4    1.911-03     1.708-06     4.799-02     1.445-10     9.248-08     3.929-02
  5    3.858-03     1.711-06     4.805-02     1.449-10     9.266-08     3.934-02
  6    9.922-03     1.789-06     4.877-02     1.537-10     9.646-08     3.993-02
  7    1.250-02     1.846-06     4.926-02     1.604-10     9.926-08     4.033-02
  8    1.506-02     1.929-06     4.993-02     1.701-10     1.033-07     4.088-02
  9    1.762-02     2.053-06     5.084-02     1.851-10     1.092-07     4.162-02
 10    2.200-02     2.053-06     5.084-02     1.851-10     1.092-07     4.162-02

  I        R            O            OH
  1    0.000        9.228-09     3.630-06
  2    1.104-03     9.228-09     3.630-06
  3    1.561-03     9.208-09     3.625-06
  4    1.911-03     9.199-09     3.623-06
  5    3.858-03     9.222-09     3.630-06
  6    9.922-03     9.796-09     3.788-06
  7    1.250-02     1.023-08     3.905-06
  8    1.506-02     1.087-08     4.073-06
  9    1.762-02     1.185-08     4.324-06
 10    2.200-02     1.185-08     4.324-06

-+-+-+-+-+                 CHEMICAL-KINETICS SOLUTION                 +-+-+-+-+-

  I        R            N            NO           NO2          N2O
  1    0.000        5.588-17     2.184-08     4.730-10     2.813-09
  2    1.104-03     5.588-17     2.184-08     4.730-10     2.813-09
  3    1.561-03     5.562-17     2.362-08     5.120-10     2.810-09
  4    1.911-03     5.550-17     2.707-08     5.867-10     2.810-09
  5    3.858-03     5.576-17     3.795-08     8.214-10     2.814-09
  6    9.922-03     6.285-17     3.853-08     8.172-10     2.895-09
  7    1.250-02     6.852-17     3.872-08     8.090-10     2.954-09
  8    1.506-02     7.731-17     4.005-08     8.197-10     3.037-09
  9    1.762-02     9.195-17     4.302-08     8.548-10     3.156-09
 10    2.200-02     9.195-17     4.302-08     8.548-10     3.156-09

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***   X=   6.650-01   IX=    20        DX=  5.000-03
      PRESSD= -1.550-05
                               J =      1             2            3
UFLUX=  1.125-03 FLUX(J)=   2.095+02     1.042-05     7.905-07
DA1=  1.977-03 DA2= -3.457-04

  I        R            U VEL        TEMP         FUEL         OXYG          F
  1    0.000        2.465+00     1.652+03     1.937-03     1.444-01     2.253-02
  2    1.156-03     2.465+00     1.652+03     1.937-03     1.444-01     2.253-02
  3    1.635-03     2.465+00     1.652+03     1.940-03     1.444-01     2.253-02
  4    2.003-03     2.465+00     1.652+03     1.941-03     1.444-01     2.253-02
  5    4.042-03     2.464+00     1.651+03     1.938-03     1.444-01     2.253-02
  6    1.038-02     2.448+00     1.645+03     1.858-03     1.441-01     2.252-02
  7    1.307-02     2.439+00     1.642+03     1.788-03     1.438-01     2.252-02
  8    1.574-02     2.425+00     1.639+03     1.683-03     1.434-01     2.252-02
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   9   1.840-02   2.408+00    1.636+03   1.521-03   1.428-01   2.252-02
  10   2.300-02   0.000       1.110+03   1.521-03   1.428-01   2.252-02

   I   R          N2          RHO        VISC       ENTLPY
   1   0.000      7.507-01    8.365-01   1.492-02   4.776+05
   2   1.156-03   7.507-01    8.365-01   1.492-02   4.776+05
   3   1.635-03   7.507-01    8.366-01   1.492-02   4.774+05
   4   2.003-03   7.507-01    8.367-01   1.492-02   4.773+05
   5   4.042-03   7.507-01    8.372-01   1.492-02   4.760+05
   6   1.038-02   7.507-01    8.399-01   1.492-02   4.651+05
   7   1.307-02   7.507-01    8.414-01   1.492-02   4.580+05
   8   1.574-02   7.507-01    8.430-01   1.492-02   4.488+05
   9   1.840-02   7.507-01    8.444-01   1.492-02   4.371+05
  10   2.300-02   7.507-01    8.444-01   3.332-05  -2.135+05

 -+-+-+-+-+              CHEMICAL-EQUILIBRIUM SOLUTION              +-+-+-+-+-

   I   R          CO          CO2        H          H2         H2O
   1   0.000      4.573-06    5.660-02   5.857-10   2.210-07   4.634-02
   2   1.156-03   4.573-06    5.660-02   5.857-10   2.210-07   4.634-02
   3   1.635-03   4.565-06    5.659-02   5.842-10   2.207-07   4.633-02
   4   2.003-03   4.559-06    5.658-02   5.832-10   2.205-07   4.633-02
   5   4.042-03   4.527-06    5.659-02   5.770-10   2.191-07   4.633-02
   6   1.038-02   4.367-06    5.681-02   5.454-10   2.125-07   4.651-02
   7   1.307-02   4.289-06    5.699-02   5.300-10   2.094-07   4.666-02
   8   1.574-02   4.213-06    5.728-02   5.146-10   2.063-07   4.689-02
   9   1.840-02   4.159-06    5.772-02   5.026-10   2.042-07   4.725-02
  10   2.300-02   4.159-06    5.772-02   5.026-10   2.042-07   4.725-02

   I   R          O           OH
   1   0.000      3.868-08    9.281-06
   2   1.156-03   3.868-08    9.281-06
   3   1.635-03   3.858-08    9.265-06
   4   2.003-03   3.851-08    9.255-06
   5   4.042-03   3.809-08    9.194-06
   6   1.038-02   3.594-08    8.867-06
   7   1.307-02   3.489-08    8.738-06
   8   1.574-02   3.384-08    8.594-06
   9   1.840-02   3.302-08    8.491-06
  10   2.300-02   3.302-08    8.491-06

 -+-+-+-+-+              CHEMICAL-KINETICS SOLUTION              +-+-+-+-+-

   I   R          N           NO         NO2        N2O
   1   0.000      1.044-15    9.673-08   1.311-09   5.024-09
   2   1.156-03   1.044-15    9.673-08   1.311-09   5.024-09
   3   1.635-03   1.038-15    9.738-08   1.321-09   5.019-09
   4   2.003-03   1.034-15    1.016-07   1.379-09   5.016-09
   5   4.042-03   1.011-15    1.043-07   1.420-09   4.995-09
   6   1.038-02   8.961-16    8.683-08   1.201-09   4.904-09
   7   1.307-02   8.404-16    8.234-08   1.148-09   4.864-09
   8   1.574-02   7.869-16    7.964-08   1.118-09   4.827-09
   9   1.840-02   7.450-16    7.949-08   1.122-09   4.808-09
  10   2.300-02   7.450-16    7.949-08   1.122-09   4.808-09
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*** X=  6.700-01  IX=   21     DX=  5.000-03
    PRESSD= -1.448-05
                               J =      1           2          3
UFLUX=  1.052-03 FLUX(J)=   1.981+02   1.091-05   2.755-07
DA1=  1.179-03 DA2= -2.109-04

  I      R           U VEL       TEMP        FUEL        OXYG        F
  1    0.000       2.318+00    1.686+03    6.541-04    1.394-01    2.251-02
  2    1.204-03    2.318+00    1.686+03    6.561-04    1.394-01    2.251-02
  3    1.703-03    2.318+00    1.686+03    6.576-04    1.394-01    2.251-02
  4    2.086-03    2.318+00    1.685+03    6.585-04    1.394-01    2.251-02
  5    4.211-03    2.316+00    1.684+03    6.600-04    1.394-01    2.251-02
  6    1.082-02    2.297+00    1.674+03    6.475-04    1.394-01    2.250-02
  7    1.362-02    2.284+00    1.669+03    6.281-04    1.393-01    2.250-02
  8    1.639-02    2.267+00    1.662+03    5.927-04    1.392-01    2.250-02
  9    1.916-02    2.244+00    1.654+03    5.313-04    1.389-01    2.250-02
 10    2.400-02    0.000       1.110+03    5.313-04    1.389-01    2.250-02

  I      R           N2          RHO         VISC        ENTLPY
  1    0.000       7.507-01    8.199-01    1.437-02    4.569+05
  2    1.204-03    7.507-01    8.199-01    1.437-02    4.569+05
  3    1.703-03    7.507-01    8.200-01    1.437-02    4.567+05
  4    2.086-03    7.507-01    8.200-01    1.437-02    4.566+05
  5    4.211-03    7.507-01    8.207-01    1.437-02    4.550+05
  6    1.082-02    7.507-01    8.254-01    1.437-02    4.421+05
  7    1.362-02    7.507-01    8.282-01    1.437-02    4.338+05
  8    1.639-02    7.507-01    8.316-01    1.437-02    4.233+05
  9    1.916-02    7.507-01    8.356-01    1.437-02    4.103+05
 10    2.400-02    7.507-01    8.356-01    3.332-05   -2.612+05

-+-+-+-+-+             CHEMICAL-EQUILIBRIUM SOLUTION             +-+-+-+-+-

  I      R           CO          CO2         H           H2          H2O
  1    0.000       6.208-06    6.006-02    9.015-10    2.901-07    4.917-02
  2    1.204-03    6.208-06    6.006-02    9.015-10    2.901-07    4.917-02
  3    1.703-03    6.199-06    6.005-02    8.996-10    2.898-07    4.917-02
  4    2.086-03    6.192-06    6.005-02    8.981-10    2.895-07    4.917-02
  5    4.211-03    6.132-06    6.305-02    8.851-10    2.871-07    4.916-02
  6    1.082-02    5.718-06    6.007-02    7.962-10    2.703-07    4.918-02
  7    1.362-02    5.489-06    6.012-02    7.482-10    2.609-07    4.972-02
  8    1.639-02    5.228-06    6.022-02    6.947-10    2.502-07    4.930-02
  9    1.916-02    4.949-06    6.038-02    6.386-10    2.388-07    4.943-02
 10    2.400-02    4.949-06    6.038-02    6.386-10    2.388-07    4.943-02

  I      R           O           OH
  1    0.000       6.020-08    1.244-05
  2    1.204-03    6.020-08    1.244-05
  3    1.703-03    6.007-08    1.242-05
  4    2.086-03    5.996-08    1.241-05
  5    4.211-03    5.908-08    1.230-05
  6    1.082-02    5.297-08    1.151-05
  7    1.362-02    4.968-08    1.107-05
  8    1.639-02    4.602-08    1.057-05
  9    1.916-02    4.220-08    1.004-05
 10    2.400-02    4.220-08    1.004-05
 -+-+-+-+-+            CHEMICAL-KINCTICS SOLUTION                +-+-+-+-+-
  I      R           N           NO          NO2         N2O
  1  0.000       2.512-15    2.282-07    2.675-09    6.143-09
  2  1.204-03    2.512-15    2.282-07    2.675-09    6.143-09
  3  1.703-03    2.501-15    2.242-07    2.629-09    6.138-09
  4  2.086-03    2.492-15    2.242-07    2.631-09    6.133-09
  5  4.211-03    2.418-15    1.989-07    2.344-09    6.098-09
  6  1.082-02    1.936-15    1.486-07    1.806-09    5.854-09
  7  1.362-02    1.698-15    1.360-07    1.683-09    5.719-09
  8  1.639-02    1.451-15    1.263-07    1.597-09    5.566-09
  9  1.916-02    1.213-15    1.207-07    1.563-09    5.403-09
 10  2.400-02    1.213-15    1.207-07    1.563-09    5.403-09
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 ***  X=  6.750-01  IX=    22       DX=  5.000-03
      PRESSD= -1.355-05
                          J =      1           2           3
 UFLUX=  9.724-04 FLUX(J)=   1.874+02    1.040-05    9.499-08
 DA1=  1.841-03 DA2=   7.502-04

  I      R           U VEL       TEMP        FUEL        OXYG        F
  1  0.000       2.153+00    1.686+03    2.186-04    1.377-01    2.249-02
  2  1.250-03    2.153+00    1.686+03    2.186-04    1.377-01    2.249-02
  3  1.768-03    2.153+00    1.686+03    2.193-04    1.377-01    2.249-02
  4  2.165-03    2.153+00    1.686+03    2.197-04    1.377-01    2.249-02
  5  4.370-03    2.151+00    1.684+03    2.211-04    1.377-01    2.249-02
  6  1.123-02    2.128+00    1.673+03    2.223-04    1.377-01    2.248-02
  7  1.414-02    2.112+00    1.666+03    2.175-04    1.377-01    2.248-02
  8  1.703-02    2.093+00    1.658+03    2.063-04    1.377-01    2.248-02
  9  1.991-02    2.066+00    1.648+03    1.847-04    1.376-01    2.248-02
 10  2.499-02    0.000       1.110+03    1.847-04    1.376-01    2.248-02

  I      R           N2          RHO         VISC        ENTLPY
  1  0.000       7.507-01    8.197-01    1.387-02    4.362+05
  2  1.250-03    7.507-01    8.197-01    1.387-02    4.362+05
  3  1.768-03    7.507-01    8.197-01    1.387-02    4.361+05
  4  2.165-03    7.507-01    8.198-01    1.387-02    4.359+05
  5  4.370-03    7.507-01    8.205-01    1.387-02    4.341+05
  6  1.123-02    7.507-01    8.260-01    1.387-02    4.198+05
  7  1.414-02    7.507-01    8.294-01    1.387-02    4.109+05
  8  1.703-02    7.507-01    8.336-01    1.387-02    3.997+05
  9  1.991-02    7.507-01    8.387-01    1.387-02    3.859+05
 10  2.499-02    7.507-01    8.387-01    3.332-05   -2.772+05

 -+-+-+-+-+            CHEMICAL-EQUILIBRIUM SOLUTION             +-+-+-+-+-
  I      R           CO          CO2         H           H2          H2O
  1  0.000       6.347-06    6.121-02    9.234-10    2.965-07    5.011-02
  2  1.250-03    6.347-06    6.121-02    9.234-10    2.965-07    5.011-02
  3  1.768-03    6.340-06    6.121-02    9.217-10    2.962-07    5.011-02
  4  2.165-03    6.333-06    6.120-02    9.202-10    2.959-07    5.011-02
  5  4.370-03    6.266-06    6.120-02    9.056-10    2.932-07    5.011-02
  6  1.123-02    5.771-06    6.119-02    7.998-10    2.731-07    5.010-02
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   7    1.414-02    5.490-06    6.120-02    7.417-10    2.616-07    5.011-02
   8    1.703-02    5.164-06    6.123-02    6.761-10    2.481-07    5.013-02
   9    1.991-02    4.803-06    6.128-02    6.057-10    2.331-07    5.017-02
  10    2.499-02    4.803-06    6.128-02    6.057-10    2.331-07    5.017-02

   I      R            O           OH
   1    0.000       6.167-08    1.272-05
   2    1.250-03    6.167-08    1.272-05
   3    1.768-03    6.156-08    1.270-05
   4    2.165-03    6.145-08    1.269-05
   5    4.370-03    6.045-08    1.256-05
   6    1.123-02    5.319-08    1.162-05
   7    1.414-02    4.922-08    1.108-05
   8    1.703-02    4.474-08    1.046-05
   9    1.991-02    3.995-08    9.763-06
  10    2.499-02    3.995-08    9.763-06

 -+-+-+-+-+              CHEMICAL-KINETICS SOLUTION              +-+-+-+-+-

   I      R            N           NO          NO2         N2O
   1    0.000       2.619-15    3.088-07    3.571-09    6.273-09
   2    1.250-03    2.619-15    3.088-07    3.571-09    6.273-09
   3    1.768-03    2.609-15    3.032-07    3.508-09    6.269-09
   4    2.165-03    2.600-15    3.017-07    3.492-09    6.264-09
   5    4.370-03    2.515-15    2.667-07    3.101-09    6.225-09
   6    1.123-02    1.938-15    1.962-07    2.366-09    5.931-09
   7    1.414-02    1.654-15    1.779-07    2.193-09    5.764-09
   8    1.703-02    1.360-15    1.639-07    2.076-09    5.568-09
   9    1.991-02    1.076-15    1.554-07    2.033-09    5.350-09
  10    2.499-02    1.076-15    1.554-07    2.033-09    5.350-09

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 ***   X=   6.800-01   IX=    23      DX=  5.000-03
       PRESSD= -1.276-05
                           J =      1           2           3
 UFLUX=   8.955-04 FLUX(J)=   1.776+02    1.040-05    3.328-08
 DA1=   1.359-03 DA2=   5.509-04

   I      R          U VEL        TEMP        FUEL        OXYG         F
   1    0.000       1.991+00    1.676+03    7.416-05    1.372-01    2.247-02
   2    1.296-03    1.991+00    1.676+03    7.416-05    1.372-01    2.247-02
   3    1.832-03    1.991+00    1.676+03    7.442-05    1.372-01    2.247-02
   4    2.244-03    1.991+00    1.675+03    7.458-05    1.372-01    2.247-02
   5    4.530-03    1.988+00    1.674+03    7.530-05    1.372-01    2.247-02
   6    1.165-02    1.963+00    1.662+03    7.752-05    1.372-01    2.247-02
   7    1.467-02    1.946+00    1.655+03    7.643-05    1.372-01    2.246-02
   8    1.767-02    1.926+00    1.646+03    7.289-05    1.372-01    2.246-02
   9    2.067-02    1.900+00    1.635+03    6.537-05    1.372-01    2.246-02
  10    2.599-02    0.000       1.110+03    6.537-05    1.372-01    2.246-02

   I      R            N2          RHO         VISC.       ENTLPY
   1    0.000       7.507-01    8.248-01    1.340-02    4.162+05
   2    1.296-03    7.507-01    8.248-01    1.340-02    4.162+05
   3    1.832-03    7.507-01    8.249-01    1.340-02    4.160+05
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     4   2.244-03    7.507-01    8.250-01    1.340-02    4.159+05
     5   4.530-03    7.507-01    8.257-01    1.340-02    4.140+05
     6   1.165-02    7.507-01    8.316-01    1.340-02    3.991+05
     7   1.467-02    7.507-01    8.352-01    1.340-02    3.899+05
     8   1.767-02    7.507-01    8.397-01    1.340-02    3.784+05
     9   2.067-02    7.507-01    8.452-01    1.340-02    3.645+05
    10   2.599-02    7.507-01    8.452-01    3.332-05   -2.822+05

  -+-+-+-+-+             CHEMICAL-EQUILIBRIUM SOLUTION             +-+-+-+-+-

     I     R           CO          CO2           H           H2          H2O
     1   0.000       5.910-06    6.156-02    8.267-10    2.790-07    5.040-02
     2   1.296-03    5.910-06    6.156-02    8.267-10    2.790-07    5.040-02
     3   1.832-03    5.903-06    6.156-02    8.252-10    2.787-07    5.040-02
     4   2.244-03    5.897-06    6.155-02    8.239-10    2.785-07    5.040-02
     5   4.530-03    5.833-06    6.155-02    8.105-10    2.759-07    5.039-02
     6   1.165-02    5.349-06    6.154-02    7.112-10    2.560-07    5.038-02
     7   1.467-02    5.074-06    6.154-02    6.566-10    2.446-07    5.038-02
     8   1.767-02    4.752-06    6.155-02    5.946-10    2.311-07    5.039-02
     9   2.067-02    4.392-06    6.156-02    5.280-10    2.159-07    5.040-02
    10   2.599-02    4.392-06    6.156-02    5.280-10    2.159-07    5.040-02

     I     R            O           OH
     1   0.000       5.502-08    1.189-05
     2   1.296-03    5.502-08    1.189-05
     3   1.832-03    5.492-08    1.188-05
     4   2.244-03    5.483-08    1.186-05
     5   4.530-03    5.391-08    1.174-05
     6   1.165-02    4.712-08    1.082-05
     7   1.467-02    4.340-08    1.029-05
     8   1.767-02    3.920-08    9.668-06
     9   2.067-02    3.467-08    8.972-06
    10   2.599-02    3.467-08    8.972-06

  -+-+-+-+-+              CHEMICAL-KINETICS SOLUTION              +-+-+-+-+-

     I     R            N           NO          NO2          N2O
     1   0.000       2.073-15    3.295-07    3.926-09    6.030-09
     2   1.296-03    2.073-15    3.295-07    3.926-09    6.030-09
     3   1.832-03    2.065-15    3.252-07    3.877-09    6.026-09
     4   2.244-03    2.058-15    3.249-07    3.876-09    6.022-09
     5   4.530-03    1.988-15    2.969-07    3.558-09    5.984-09
     6   1.165-02    1.510-15    2.241-07    2.791-09    5.693-09
     7   1.467-02    1.275-15    2.045-07    2.608-09    5.526-09
     8   1.767-02    1.033-15    1.898-07    2.493-09    5.329-09
     9   2.067-02    8.010-16    1.813-07    2.468-09    5.106-09
    10   2.599-02    8.010-16    1.813-07    2.468-09    5.106-09

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