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COMOC: THREE DIMENSIONAL BOUNDARY REGION VARIANT

PROGRAMMER'S MANUAL

by J. A. Orzechowski and A. J. Baker

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COMOC: THREE-DIMENSIONAL BOUNDARY REGION VARIANT
PROGRAMMER'S MANUAL

By

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SUMMARY

The Three-Dimensional Boundary Region Variant of the COMOC computer program system solves the partial differential equation system governing certain three-dimensional flows of a viscous, heat conducting, multiple-species, compressible fluid including combustion. The solution is established in physical variables, and employs a finite element solution algorithm for the boundary value portion of the problem description in combination with an explicit marching technique for the initial value character. The computational lattice may be arbitrarily non-regular, and boundary condition constraints are readily applied. The programmer's manual contains a brief capsule of the mathematical problem description and the theoretical foundation of the solution algorithm. It presents a detailed description on the construction and operational sequence of the program, and provides complete instructions on the utilization of the many optional features of the code. A more complete description of the theoretical foundation of the finite element solution algorithm, and a detailed discussion of computational results for several sample problems in fluid mechanics is contained in the theoretical guide and user's manual [Ref. 1].

INTRODUCTION

The finite element methodology for numerical solution of initial-boundary value problems in continuum mechanics is growing rapidly. Formerly constrained to solution of structural problems, or other linear field problems wherein an equivalent extremum principle exists, the theoretical support is now sufficiently generalized to render the method directly applicable to explicitly nonlinear problems, including viscous fluid mechanics [Ref. 1-3]. The COMOC computer program system is being developed to transmit this rapid theoretical progress into a viable numerical solution capability. On the way to generation of this general purpose concept, several Variants of COMOC have been developed for specific problem classes including transient thermal analysis [Ref. 4] and the two-dimensional Navier Stokes equations [Ref. 5].
The Three-Dimensional Boundary Region (3DBR) Variant of COMOC, to which this programmer's manual is addressed, solves the three-dimensional boundary region equations for flow of a viscous, heat conducting, multiple-species, compressible fluid including combustion. The flow may be external or confined, subsonic or supersonic, laminar and/or turbulent, and can contain up to nine or more distinct species in frozen composition or undergoing equilibrium chemical reaction for a hydrogen/oxygen/air system. The finite element solution procedure marches the discretized equivalent of the governing equation system in the direction parallel to the predominant flow. It numerically establishes the complete three-dimensional distributions of the three scalar velocity components, enthalpy, temperature, density, viscosity, and all applicable species mass fractions. Initial distributions of all dependent variables may be arbitrarily specified, and boundary condition constraints for each dependent variable are user-specifiable on arbitrarily disjoint segments of the solution domain closure. The solutions for each dependent variable, and all computed parameters, are established at node points lying on a specifiably non-regular computational lattice formed by plane triangulation of the elliptic solution domain.

All Variants of the COMOC system are built upon the macro-structure illustrated in Fig. 1. The main executive routine allocates core, using a variable dimensioning scheme, based upon the total degrees of freedom of the problem. The size of the largest problem that can be solved is thus limited by the core size of the computer in use. The precise mix between number of dependent variables (and parameters), and fineness of the discretization, is user-specifiable and widely variable. The Input module serves its standard function for all dependent variable, parameter, and geometric coordinate arrays. The Discretization module forms the finite element discretization of the solution domain, and evaluates all required finite element non-standard matrices and standard-matrix multipliers. The Initialization module computes the remaining initial parametric data required to start the solution. The Integration Module constitutes the primary execution sequence of problem solution. It is based upon an explicit finite difference integration algorithm for the column vector of unknowns of the solution, for which the discretized description is initial-valued. Calls to auxiliary routines for parameter evaluation, e.g., viscosity, Prandtl number, source terms, combustion parameters, etc., as specified functions of dependent and/or independent variables are governed by the Integration Module. The user has considerable latitude to adapt COMOC to the specifics of his particular problem at this point, by directly inserting easily written subroutines into COMOC to compute special forms of these parameters. The Output module is similarly addressed from the integration sequence and serves...
Figure 1. COMOC Macro Structure
its standard function via a highly automated array display algorithm. COMOC can execute distinct problems in sequence and contains an automatic restart capability to continue solutions.

The 3DBR Variant of COMOC, as a direct consequence of the expansive problem class to which it may be addressed, is a fairly large and complex computer program. This programmer's manual presents a brief introduction to the partial differential equation system being solved, and summarizes the theoretical foundations for the combined finite element-finite difference procedures used to establish the desired numerical solution. This is followed by a complete description of 3DBR COMOC including environment, program specifications, link and subroutine structure, program comments and detailed flow charts. The instructions for machine set-up and execution of the code are included, and sample output for the standard test cases is fully discussed. A complete discussion on the technical aspect of solutions for the standard test cases is presented in the user's guide [Ref. 1].

PROBLEM TASK DESCRIPTION

The system of partial differential equations governing the three-dimensional boundary region flow of a compressible fluid is obtained from the parabolic approximation to the full Navier-Stokes equations. The parabolic approximation, i.e., "parabolic Navier-Stokes equations," describe steady, three-dimensional flows wherein, 1) a predominant flow direction is uniformly discernible, 2) in this direction (only), diffusion processes are negligible compared to convection, and 3) no disturbances are propagated upstream antiparallel to this direction. The boundary region equation system is obtained from parabolic Navier-Stokes with the single additional assumption that a known pressure distribution is superimposed upon the flow field. It is the numerical solution of this equation system to which 3DBR COMOC is addressed. Identify the three-dimensional velocity vector

\[ \mathbf{u}_i = u_1 \mathbf{i} + u_2 \mathbf{j} + u_3 \mathbf{k} \quad (1) \]

For development of the differential equation system, assume that \( \mathbf{i} \) is aligned parallel to the predominant flow direction. Identify a two-dimensional vector differential operator as

\[ (\mathbf{\hat{j}})_2 \cdot \mathbf{k} \quad (2) \]
where the comma identifies the gradient operator. Employing Cartesian tensor notation, with summation over 2 and 3 for repeated latin subscripts, the three-dimensional boundary region equation system for a multiple-species, compressible, reacting flow takes the form

\[
0 = (\rho u_i)_i + (\rho u_j)_j
\]  

\[
\rho u_1 v_{\alpha, l} = \left[ \frac{\mu e}{Sc \cdot Re} \right]_{\alpha, k} v_{\alpha, k} - \rho u_k v_{\alpha, k} + s_{\alpha}
\]  

\[
\rho u_1 u_{1, l} = \left[ \frac{\mu e}{Re} u_{1, k} \right]_{k} - \rho u_k u_{1, k} - p_{1}
\]  

\[
\rho u_1 u_{3, l} = \left[ \frac{\mu e}{Re} u_{3, k} \right]_{k} - \rho u_k u_{3, k} - p_{3}
\]  

\[
\rho u_1 H_{l} = \left[ \frac{\mu e}{Re \cdot Pr} H_{k} \right]_{k} - \rho u_k H_{k}
\]

\[
- M^2 \left[ \frac{1-Pr}{Pr} \frac{\mu e}{2Re} (u_j u_j)_{, k} \right]_{k}
\]

\[
- \left[ \frac{Sc-Pr}{Sc \cdot Pr} \frac{\mu e}{Re} \sum_{\alpha} \alpha v_{\alpha, k} \right]_{k}
\]

The variables appearing in Eq. (3)-(7) are non-dimensionalized with respect to \( \rho_\infty, U_\infty, c_\rho_\infty, T_\infty \), and a length constant \( L \), and have their usual interpretation in fluid mechanics. The Reynolds (Re), Prandtl (Pr), and Schmidt (Sc) numbers are defined with respect to the effective diffusion coefficient, \( \mu e \), in algebraic combination with the laminar and turbulent contributions as, for example

\[
\frac{\mu e}{Pr} = \frac{\mu}{Pr} + \frac{\rho e}{Pr T}
\]

In Eq. (8), \( \mu \) is the laminar viscosity, \( \varepsilon \) is the kinematic eddy viscosity, and subscript \( T \) denotes a turbulent reference parameter. The stagnation enthalpy is defined in terms of species static enthalpies as
\[ H = \sum_{\alpha} h_{\alpha}^\alpha + \frac{1}{2} u_k u_k \quad (9) \]

The static enthalpy includes the heat of formation, \( h_{0}^\alpha \), of the species in its definition as

\[ h_{\alpha} \equiv \int_{0}^{T} c_{p} dT + h_{0}^\alpha \quad (10) \]

An equation of state is required to close the system. Assuming perfect gas behavior for each species, from Dalton's law, obtain

\[ p = \rho R T \sum_{\alpha} \frac{y_{\alpha}}{W_{\alpha}} \quad (11) \]

where \( R \) is the universal gas constant and \( W_{\alpha} \) is the molecular weight of the \( \alpha \)-th species.

Equilibrium combustion of hydrogen/oxygen/air systems in three-dimensional boundary region flow is operational in 3DBR COMOC. The following reactions are assumed operative.

\[ \begin{align*}
2H + O & \rightleftharpoons H_2O \\
2H & \rightleftharpoons H_2 \\
2O & \rightleftharpoons O_2 \\
H & + O \rightleftharpoons OH \\
N_2 & + O \rightleftharpoons 2NO
\end{align*} \quad (12) \]

The equilibrium composition of the combustion by-products is determined by applying the Law of Mass Action [Ref. 6] to each reaction defined in Eq. (12). This yields definition of a set of equilibrium rate constants, \( k \), which, for the simple reaction \( nA + mB \rightleftharpoons \lambda C \), are expressed in terms of species mole fraction, \( x_{\alpha} \), as
Solution of Eq. (12) with (13), and coupled with conservation of total and elemental mass, yields an algebraic equation system for determination of the equilibrium composition of the system, of the form.

$$\begin{align*}
[N^B][X^\alpha] &= \{\text{const.}\} \\
(14)
\end{align*}$$

In Eq. (14), the elements of the matrix \([N^B]\) account for the particular species mole fraction distribution, \(\{X^\alpha\}\), containing the \(\alpha\)th elemental material, e.g., O, H, and N.

METHOD OF SOLUTION

The three-dimensional boundary region equation system, except for global continuity, Eq. (3), is uniformly an initial-boundary value problem of mathematical physics. Each of the partial differential equations, Eq. (4)-(7), is a special case of the general second-order, nonlinear partial differential equation

$$L(q) \equiv x[K(q)q_k]_k + f(q,q_i,x_i) - g(q,x) = 0 \quad (15)$$

where \(q\) is a generalized dependent variable identifiable with each computational dependent variable. In Eq. (15), \(f\) and \(g\) are specified functions of their arguments, \(x\) is identified with \(x_1\) for boundary region flows, and \(x_i\) are the coordinates for which second order derivatives exist in the lead term. The finite element solution algorithm is based upon the assumption that \(L(q)\) is uniformly parabolic within a bounded open domain \(\Omega\), i.e., the lead term in Eq. (15) is uniformly elliptic within its domain \(R\), with closure \(\partial R\), where

$$\begin{align*}
\Omega &= R \times [X_0, X] \\
(16)
\end{align*}$$

and \(X_0 < X < \infty\). For Eq. (15) uniformly parabolic, unique solutions for \(q\) are obtained pending specification of boundary conditions.
constraints on $\partial R$ and an initial condition on $RUaR$. For the former, the general form relates the function and its normal derivative everywhere on the closure, $\partial R$, as

$$\mathcal{R}(q) \equiv a(1)q(x_i',x) + a(2)kq(x_i',x), n_k - a(3) = 0 \quad (17)$$

In Eq. (17), the $a(i)(x_i',x)$ are user specified coefficients, the superscript bar notation constrains $x_i$ to $\partial R$, and $n_k$ is the local outward-pointing unit normal vector. For an initial distribution, assume given throughout $RUaR \times \chi_0$,

$$\alpha(x_i',x_0) \equiv q_0(x_i') \quad (18)$$

The finite element solution algorithm is established for the equation system (15)-(18), using the Method of Weighted Residuals (MWR) formulated on a local basis. Since Eq. (15) is valid throughout $R$, it is valid within disjoint interior subdomains, $R_m$, described by $(x_i',x) \in R_m \times [x_0,x)$ called "finite elements," wherein $\cup R_m = R$. Form an approximate solution for $q$ within $R_m \times [x_0,x)$, called $q_m(x_i',x)$, by expansion into a series solution of the form

$$q_m(x_i',x) \equiv \left\{ \phi(x_i') \right\}^T \{\Omega(x)\}_m \quad (19)$$

wherein the functionals $\phi_k(x_i')$ are members of a function set complete in $R_m$, and the unknown expansion coefficients, $\Omega_k(x)$, represent the $x$-dependent values of $q_m(x_i',x)$ at specific locations interior to $R_m$ and on the closure, $\partial R_m$, called "nodes."

To establish the values taken by the expansion coefficients in Eq. (19), require that the local error in the approximate solution to both the differential equation, $L(q_m)$, and the boundary condition statement, $\mathcal{B}(q_m)$, for $\partial R_m \cap \partial R$, be rendered orthogonal to the space of the approximation functions. Employing an unknown algebraic multiplier, $\lambda$, the resultant equation sets can be combined as

$$\int_{R_m} \left\{ \phi(x_i') \right\} L(q_m') d\tau - \lambda \int_{\partial R_m \cap \partial R} \left\{ \phi(x_i') \right\} \mathcal{B}(q_m') d\sigma \equiv 0 \quad (20)$$
The number of equations (20) is identical to the number of node points of the finite element, \( R_m \).

Equation (20) forms the basic operation of the finite element solution algorithm and of 3DBR COMOC. Establishment of the global solution algorithm, and determination of \( \lambda \), is accomplished by evaluating Eq. (20) in each of the \( M \) finite elements of the discretized solution domain, and assembly of these \( M \times n \) equations into a global matrix system using Boolean algebra. The lead term can be rearranged, using a Green-Gauss Theorem, to yield

\[
\int_{R_m} \{ \phi(x_i) \} \kappa [Kq_m^*]_k d\tau = \kappa \int_{R_m} \{ \phi(x_i) \} Kq_m^* n_k d\sigma
\]

For \( R \cap \partial R_m \) nonvanishing, Eq. (21), the corresponding segment of the closed surface integral will cancel the boundary condition contribution, Eq. (20), by identifying \( \lambda_A(2) \) with \( \kappa \) of Eq. (15). The contributions to the closed surface integral, Eq. (21), where \( \partial R_m \cap \partial R = 0 \) can be made to vanish. Hence, combining Eq. (17)-(21), the globally assembled finite element solution algorithm for the representative partial differential equation system description becomes

\[
\begin{bmatrix}
- \kappa \int_{R_m} \{ \phi \} Kq_m^* n_k d\tau + \int_{R_m} \{ \phi \} (f_m^* - g_m^*) d\tau \\
- \kappa \int_{\partial R_m} \{ \phi \} (a_m(1) q_m^* - a_m(3)) d\sigma
\end{bmatrix} = \{ 0 \}
\]

The rank of the global equation system, Eq. (22), is identical to the total number of node points on \( \partial R \cap \partial R_m \) for which the dependent variable requires solution. Equation (22) is a first-order, ordinary differential system, and the matrix structure is sparse and banded. Solution of the ordinary differential
The solution algorithm for the global continuity equation is similarly derived. Recognizing that Eq. (3) is an initial value problem on $\rho u_2$ as a function of $x_2$, with $x_1$ and $x_3$ appearing as parameters, the approximation function need span only the transverse coordinate direction as

$$q^*_m = \{\phi(x_2)\}^T \{Q(x_1, x_3)\}_m$$

(23)

The matrix elements $Q_k$ are nodal values of $\rho u_2^*$; their functional dependence requires solution of Eq. (3) along lines $(x_1, x_3)$ equal a constant. The solution algorithm for Eq. (3) is directly specified as

$$\int \{\phi\} L(\rho u_2^*) d\sigma = 0$$

(24)

where the matrix elements of $\{\phi\}$ are not coincidental with those of $\{\phi\}$, Eq. (23), and the segments $R_m$ correspond to lines of $(x_1, x_3)$ equal to a constant.

The functional flow chart for 3DDR COMOC is presented as Fig. 1. MAIN initializes execution of COMOC and allocates core using a variable dimensioning procedure for the problem at hand. The first steps within INPUT evaluate if a problem solution has been completed, and if so, whether execution of an additional problem is to be initiated. QKNINT is the calling routine that begins execution of a problem. The first step is INITIALIZATION which includes reading of title cards as well as integer and floating point NAMELIST input.

DISCRETIZATION is then called to establish a finite element gridwork of the elliptic solution domain as specified in INPUT. 3DDR Variant of COMOC employs simplex (linear) functionals spanning triangular shaped two-dimensional finite elements as approximation functions, Eq. (19). Using a natural coordinate function specification [Ref. 1, 7], accurate determination of the finite element matrices is achieved including those that are highly nonlinear. All matrix expressions are determined in term of standard matrices and/or standard matrix multipliers. For example, the first term in Eq. (22) is standard for all dependent variables. Assuming the generalized diffusion coefficient is distributed over the $m^{th}$ element as a dependent variable, obtain
In Eq. (25) and the following, matrices with B prefixes are standard two-dimensional forms defined in Table 1. For Eq. (22) identified with each dependent variable, \( f_m \) and \( g_m \) universally contain the nonlinear convection term and the initial-value operator as dominant terms. The finite element equivalent for convection is

\[
\int_{\Omega_k} \{\alpha\} \rho u_k \kappa q_{kk} \, d\tau = \int_{\Omega_k} \{\alpha\} \{\rho u_k\} \{\phi\}^T \{\kappa\} \{\phi\}^T \{Q\} \, d\tau
\]

\[
= \int_{\Omega_k} \{\rho u_k\} \{Q\} \, d\tau
\]

\[
= [B200S]\{\rho U_m\} [B11]^T \{Q\}_m
\]

where the elements of the vector, \( \{\rho u_k\} \), are nodal values of the planar mass flux transformed to a local coordinate system. The initial-value operator, which comprises the mainstream convection term, similarly becomes

\[
\int_{\Omega_k} \{\alpha\} \rho u_{\gamma \phi} \kappa q_{\gamma \phi} \, d\tau = \int_{\Omega_k} \{\alpha\} \{\rho u_{\gamma \phi}\} \{\phi\}^T \{\kappa\} \{\phi\}^T \{Q\} \, d\tau
\]

\[
= \{\rho U\}_m [B3000S] \{Q\}_m
\]

where the matrix elements of \([B3000S]\) are column matrices, see Table 1. The superscript prime exterior to a matrix denotes an ordinary derivative.

Computational entry to the INTEGRATION module, for each dependent variable, is made through the inhomogeneous term in the differential equation, Eq. (15). For mainstream momentum, Eq. (5), this is the specified longitudinal pressure gradient. Therefore, in finite element matrix form
<table>
<thead>
<tr>
<th>Matrix Name</th>
<th>Matrix Function</th>
<th>Matrix Evaluation</th>
</tr>
</thead>
</table>
| (B10)       | \[\phi \, d\tau\] | \[
\begin{bmatrix}
\frac{1}{2} \\
\frac{1}{2} \\
\end{bmatrix}
\] |
| (B2115)     | \[\phi_j \phi_k \phi_k^T \] | \[
\begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 0 \\
\end{bmatrix}
\] |
| (B2005)     | \[\phi \phi^T \, d\tau\] | \[
\begin{bmatrix}
\frac{1}{2} & 0 \\
\frac{1}{2} & 0 \\
\end{bmatrix}
\] |
| (B30015)    | \[\phi \phi^T \, d\tau\] | \[
\begin{bmatrix}
\phi_1 & \phi_2 \\
\phi_2 & \phi_3 \\
\end{bmatrix}
\] |
| (B11)       | \[\phi_j \] | \[
\begin{bmatrix}
\phi_1 \\
\phi_2 \\
\phi_3 \\
\end{bmatrix}
\] |
| (A2005)     | \[\phi \phi^T \, d\tau\] | \[
\begin{bmatrix}
\frac{1}{2} & 0 \\
\frac{1}{2} & 0 \\
\end{bmatrix}
\] |
| (A10)       | \[\phi \, d\tau\] | \[
\begin{bmatrix}
\frac{1}{2} \\
\frac{1}{2} \\
\end{bmatrix}
\] |

(1) Matrix names are a 6 digit code covering dimensionality, nonlinearity, degree of differentiation and special matrix properties, as [a, b, c, d, e, f] where:
- a = 1, 2, 3 for spaces of one-, two-, and three-dimensions,
- b = number of coordinate functions appearing in integral or matrix,
- c, d, e = 0, 1 Boolean counters indicating (no, yes) differentiation of each function,
- f = 5, 6, 7 for matrix symmetric, antisymmetric or general.

(2) Symmetric matrices are written in upper triangular form.

(3) \( \mathbf{A} \) = \( \frac{1}{2} \times (X_2 P_2)(X_3 P_3) \), the plane area of the triangular finite element.

(4) \( z^m \) = length of side for boundary condition (=X2P2).
\[
\int \{ \phi \} p_{1} d\tau = [B10] p_{1}
\]
\[R_{m}\]

For each species mass fraction, the equivalent expression involves the element distributed source term, \( S_{\alpha} \), as

\[
\int \{ \phi \} S_{\alpha} d\tau = [B200S]\{S_{\alpha}\}_{m}
\]
\[R_{m}\]

For non-constant, but equal Prandtl and Schmidt numbers, the energy equation, Eq. (7), has one source term. An integration using a Green-Gauss Theorem is appropriate; the generated surface integral vanishes yielding

\[
\int \{ \phi \} \left[ \frac{M_{\infty}^{2}}{2Re} \left( \frac{1-Pr} {Pr} \right) \mu e (u_{j}u_{j})_{k} \right] d\tau
\]
\[R_{m}\]

\[
= - \frac{M_{\infty}^{2}}{Re} \int \{ \phi \}_{k} \left( \frac{1-Pr} {Pr} \right)^{*} \mu^{*} u_{j}^{*} u_{j}^{*} d\tau
\]
\[R_{m}\]

\[
= - \frac{M_{\infty}^{2}}{Re} \{X_{m}^{T}\}^{T} \{PR\}^{T} [B3000S] \sum_{j=1}^{3} \{U_{j}\}_{m} [B211S] \{U_{j}\}_{m}
\]

Solution of the matrix equivalent of Eq. (22) occurs in the INTEGRATION module, and is achieved using an explicit finite difference integration algorithm for large systems of nonlinear, first-order ordinary differential equations. 3DBR COMOC employs a first order accurate, predictor-multiple corrector algorithm with an extended stability interval [Ref. 1, 8]. Identifying \( p_{n+1} \) and \( p_{n+2} \) as the sequentially predicted values of the dependent variable \( q_{n+1} \) at the \( n+1 \)th \( x_{1} \) station, the integration algorithm is
The $a_i$ and $b_i$ are fixed coefficients, and $h$ is the current integration step-size, $\Delta x$. The integration algorithm attempts to extremize integration step-size automatically, based on internal error control. An estimation of relative truncation error is used of the form

$$|\text{RTE}| \approx \frac{|p_{n+1}^2 - q_n|}{|q_{n+1}|}$$

(32)

If the relative truncation error associated with using the given integration step-size, $h$, to estimate the $(n+1)^{st}$ value of the dependent variable, is less than the user-supplied acceptable limit, the $(n+1)^{st}$ estimate for the dependent variable is accepted. If the computed relative error exceeds the limit, the predicted values are discarded, a smaller step-size selected, and the operations of Eq. (31) repeated.

Following an integration sequence, entrance into the PARAMETER module is made to evaluate the remaining solution parameters and functions in terms of the newest distribution of dependent variables. Evaluation of node point density and static temperature is made first; for binary, isoenergetic flows with temperature-independent specific heats, a simple quick running subroutine may be addressed. For the more complex case, COMOC can handle arbitrary frozen flow compositions, as well as the equilibrium composition of combustion of hydrogen/oxygen/air mixtures as a function of temperature, pressure, and relative concentrations of the elements, $H_2$, $O_2$, $N_2$, and Ar [Ref. 9]. The species considered are $H_2O$, $O_2$, $H_2$, $N_2$, Ar, O, H, NO, and OH. Since all thermophysical properties are temperature dependent, initialization is based upon a user input total temperature distribution. As a function of input pressure at initialization and the built-in tables of thermodynamic data, distributions of static temperature, frozen specific heat, and stagnation enthalpy corresponding to input total temperature are determined using an iteration algorithm based upon the method of false position. All solutions following initialization are based upon iteration to equilibrium composition using computed nodal static temperature.
as the convergence parameter. The iteration on temperature is assumed to have converged when the difference between successive iterates is less than 0.001 non-dimensional.

After convergence to a static temperature, the equilibrium constants for chemical reaction are calculated from the Gibbs' function. Composition is then determined using a modified Newton-Raphson iterative procedure for solution of a system of nonlinear algebraic equations. Once the nodal species equilibrium (or frozen) composition is determined, enthalpy, entropy, molecular weight, and specific heat are calculated for mixtures of ideal gases in terms of the computed species mole fractions, $X^a$. The computed composition, $X^a$, is based upon solution of the nonlinear equilibrium equations for mole fraction of hydrogen, atomic oxygen, and the square root of molecular nitrogen at nodes of the discretization, using a Newton-Raphson iteration algorithm. A maximum of thirty iterations are allowed for the solution to converge within $10^{-5}$. In only a few cases has non-convergence occurred, always within a few degrees of the threshold temperature for dissociation. For these solutions, the equations are resolved assuming that dissociation is negligible, i.e., the mole fractions of H, O, OH, and NO are negligibly small in comparison to $H_2$, $O_2$, $N_2$, and $H_2O$.

The next parameter evaluation is solution of the continuity equation for $u_2$. An evaluation of $(ho u^2)_1$ is first required, since no streamwise derivatives of a dependent variable can be formed before the distribution of all variables is known in a plane. In the discretized solution, the actual requirement is to establish $(\rho U)_1$; the following second-order accurate finite difference formula is employed.

$$\{\rho U\}_{n+1}^{-} = \frac{1}{h_n h_{n+1} (h_n + h_{n+1})} \left[ h_n (2h_{n+1} + h_n)\{\rho U\}_{n+1} - (h_n + h_{n+1})^2\{\rho U\}_n + h^2_{n+1}\{\rho U\}_{n-1} \right]$$

In Eq. (33), $h_{n+1}$ and $h_n$ are the $x_1$ integration step-sizes, respectively, between the current $x_1$ station, $x_{n+1}$, and the previous two stations. An analytic expression is then established for the $x_2$ distributions of mass flux derivative using a 2nd order running-smoothing polynomial generator over appropriate sequential panels of data. Using a unit step for the weighting function, $\phi$, Eq. (24) is integrated directly as

$$\Delta(\rho u^2_x) = \sum_{k=0}^{2} a_k(x_3) \frac{x_2^k}{k+1}$$

15
Evaluation of Eq. (34) is repeated along each node column at each $x_1$ station.

Several additional subroutine calls then complete the parameter evaluation phase. Included herein is evaluation of an integral mixing parameter, pertinent to cold flow hydrogen-air mixing problems, and the skin friction and wall Stanton number distributions. Additional calls are made to evaluate the two-dimensional distribution of Prandtl and Schmidt numbers. An input data table is interrogated to evaluate the local static pressure and the longitudinal pressure gradient. The nodal distribution of laminar viscosity, as well as turbulent eddy viscosity if being used, is then determined. The parametric sequence is terminated with a call to subroutine SOURCE which evaluates the dependent variable initialization arrays for the next integration step forward. The integration execution phase is then completed, Fig. 1, with a test to establish if the solution is complete and/or if an output call is required. Following these tests, execution is returned to INTEGRATION to repeat the same sequence of operations.

PROGRAM DESCRIPTION

The 3DBR Variant of COMOC is written to be readily executed on any large scale computer such as an IBM 360, 370, CDC 6600, or UNIVAC 1108. It is programmed in FORTRAN IV exclusively, except for certain machine-dependent routines, e.g., date, address, error handling, etc. With overlay, COMOC uses about 60K words on an IBM 360 for a solution region involving about 200 nodes and about twelve degrees of freedom per node. Output can be stored on tape or punched cards for future restarts.

Considerable effort has been devoted to construction of 3DBR COMOC in a uniform and consistent manner. A comprehensive subroutine substructure is utilized to allow functional processing in a consistent and readily followed sequence. Input formats are consistent and flexible, and program input controls are standardized. Consistent notation of variable names is employed in all subroutines, and only three major arrays are maintained. The common block /VARBLE/ contains the IARRAY and the RARRAY. The IARRAY contains a list of all the integers used in common throughout the program in locations 1 thru 200. Locations 201 thru 400 contain the entry locations in the I7 array where dimensioned variables are stored. The RARRAY contains a list of all the real scalers used in common throughout the program. The common block /ARRAYS/ contains the IZ array. This array contains all the variable dimensioned vectors, matrices and hollerith data which are used by the program. Shown in Table 2 is a listing of
the MAIN link of COMOC, and Table 3 presents the overlay structure of the program for the IBM 360/65 computer.

The source listing of 3DBR COMOC is not included in this document due to its excessive length. The following pages of this section contain descriptions of the subroutines of 3DBR COMOC, followed by macro-flow charts of their functional sequencing.

| TABLE 2 |
|---------|---------|---------|---------|
|         | MAIN LINK OF COMOC                   |         |
| BDINPT  | LINK3  | LOC     | OUTVEC  |
| SCHPRN  | MAIN   | LOCATE  | PSIBC   |
| SUTHLD  | LINK4  | LOOK    | RECIP   |
| SETDIF  | ABSAVE | MATSUM  | RESET   |
| LINK2   | ASMVEC | MINMAX  | SETVAL  |
| RITE    | AVRG   | MPRD    | TENDA   |
| LINK5   | GENDA  | MTRA    | VARMAX  |
| LINK1   | GMADD  | NBNDRY  | VECTA   |
| READER  | INITBL | OUTNOD  | XYSCLAL |

17
<table>
<thead>
<tr>
<th>OVERLAY</th>
<th>ALPHA</th>
<th>OVERLAY</th>
<th>ALPHA</th>
</tr>
</thead>
<tbody>
<tr>
<td>INSERT</td>
<td>REDOED</td>
<td>INSERT</td>
<td>RENDOR</td>
</tr>
<tr>
<td>INSERT</td>
<td>REDOED</td>
<td>INSERT</td>
<td>RENDOR</td>
</tr>
<tr>
<td>ENTRY</td>
<td>MAIN</td>
<td>ENTRY</td>
<td>MAIN</td>
</tr>
<tr>
<td>ENTRY</td>
<td>MAIN</td>
<td>ENTRY</td>
<td>MAIN</td>
</tr>
</tbody>
</table>

**TABLE 3**

**OVERLAY STRUCTURE OF COMOC FOR IBM 360/65 COMPUTER**
THE FOLLOWING PAGES CONTAIN A BRIEF DESCRIPTION OF THE SUBROUTINES
IN THE COMOC COMPUTER PROGRAM.

NAMES IN PARENTHESES INDICATE CALLING ROUTINES.
IF NO NAME IS ENTERED THEN SEVERAL ROUTINES PLACE CALL.

MAIN
THIS IS THE MAIN CONTROL PROGRAM TO INITIALIZE THE IZ ARRAY
THE RARRAY AND THE IARRAY TO ZEROES.
TO INCREASE THE CAPACITY OF THE PROGRAM TO HANDLE MORE NODES
IT IS ONLY NECESSARY TO INCREASE THE DIMENSION OF THE IZ ARRAY.
AFTER INITIALIZATION THE CONTROL ROUTINE BDINPT IS CALLED.
BDINPT (MAIN)
THIS IS THE CONTROL ROUTINE TO INITIALIZE VECTORS AND TO CONTROL
THE FLOW OF THE PROGRAM ACCORDING TO USER INPUT.
A CONTROL CARD WITH THE FOLLOWING PARAMETERS IS READ IN -

PARAMETER FORMAT CARD COLS. DESCRIPTION
  V1   A8  1 - 8   CONTROL VARIABLE.
  NX   12  9 - 10  INDEX FOR ROUTINE OR CALL LIST.
 NPOO  15  11 - 15 START POS. FOR PDUMP.
 NREPET 15  16 - 20 END POS. FOR PDUMP.
 NMUL 1015 21 - 70 A. NMUL(1) = RESTART TAPE.
            NMUL(2) = RESTART PRINT NO.
            NMUL(3) = NEW RESTART TAPE.
            B. NMUL(1) THRU NMUL(8) ARE
               SCANNED TO FORM A MULTIPLIER
               FOR REAL INPUT. IF ALL ZERO
               THEN 1.0 IS USED.
     RTNE  A8  71 - 78   ASSOC. WITH V1 = LINK1 THRU
                           LINK5. DENOTES NAME OF ROUTINE
                           TO BE CALLED.
                           (NOT USED BY PROGRAM)

IF KDUMP = 1 IN NAME01, THEN THE ENTIRE INPUT CARD IS PRINTED
IMMEDIATELY AFTER BEING READ FOLLOWED BY THE DATA THAT IS BEING
STORED ALONG WITH THE DATA'S ENTRY POSITION IN THE IZ ARRAY.

THIS ROUTINE LOOKS FIRST FOR A MATCH OF V1 WITH CERTAIN KEY WORDS
WHICH WILL EITHER CAUSE A SUBROUTINE TO BE CALLED OR PROGRAM
FLOW TO OCCUR.

THE KEY WORDS THAT ARE SCANNED ARE -

BBBBBB (BLANK) - RETURN TO SCAN ANOTHER CARD.
COMOC - PRINT THE COMOC TITLE PAGE TWO TIMES.
COMTITLE - READ A TITLE CARD WHICH WILL APPEAR ON COMOC.
DESCRIPT NX - CALL DSCRPT AND PROCESS ACCORDING TO NX.
END  - RETURN CONTROL TO MAIN PROGRAM, RESET ARRAYS AND RETURN TO BINPT.
EXIT  - CALL EXIT.
FEBL  ' SET IBL = 1.
FEDIMN - CALL DIMENSIONALIZATION ROUTINE FEDIMN.
FENAME - CALL FENAME TO SET DEFAULT SCALARS AND THEN CALL NMELST TO READ IN NAME01 AND NAME02 NAMELISTS.
FENS  - SET IBL = 0.
ICOND - CALL ICOND TO PRINT REAL AND INTEGER SCALARS.
INTEGER - ALLOWS NEW VALUES TO BE READ INTO A SEQUENCE OF LOCATIONS IN THE BORDER, IPLACE AND LOC VECTORS.
KENO NX - ENTER BOUNDARY NODES FOR DEP. VAR. NX.
LINK1 NX - CALL LINK1(NX)
LINK2 NX - CALL LINK2(NX)
LINK3 NX - CALL LINK3(NX)
LINK4 NX - CALL LINK4(NX)
LINK5 NX - CALL LINK5(NX)
NAMELIST - CALL NMELST TO READ IN NAME01 AND NAME02 NAMELISTS.
PBUMP NX - CALL PDUMP (IZ(NPCD), IZ(NREPET), NX)
QKNINT - CHECK FOR DRHOBL OR DRHOGS USAGE.
COMPUTE DIFFUSION COEFFICIENTS.
COMPUTE SKIN FRICTION AND STANTON NUMBER.
INITIALIZE GAS ROUTINES.
PRINT INITIALIZATION CONTROLS.
CALL QKNINT.
REAL  - ALLOWS NEW VALUES TO BE READ INTO A SEQUENCE OF LOCATIONS IN THE VALUE AND NPLACE VECTORS.
RESTART - ALLOWS USER TO USE OUTPUT FROM A PREVIOUS RUN FOR RESTARTING AND ALSO TO DEFINE A NEW DATA SET TO SAVE OUTPUT FOR A FUTURE RESTART.
HOLIST - READ IN A SEQUENCE OF TITLES TO COINCIDE WITH A SCALAR OUTPUT LIST WHICH WILL APPEAR AT THE BEGINNING OF EACH OUTPUT DISPLAY.
VYYEND NX - DEFONES END OF INPUT FOR DEP. VAR. NX.
VYVYRDF NX - ALLOWS USER TO REDEFINE SELECTED ENTRIES EITHER IN A DEPENDENT VARIABLE OR ONE OF THE OTHER REAL VECTORS.

IF NEITHER SITUATION OCCURS,
THE VECTORS BORDER AND VALUE ARE SCANNED UNTIL A MATCH IS FOUND AND THE LOCATION IS STORED IN THE PARAMETER 'K'.

BORDER IS A VECTOR OF CONTROL NAMES WHICH IS SCANNED WITH THE USER INPUT CONTROL FOR INTEGER INPUT.
IARRAY(IPLACE(K)) = LOCATION IN THE IZ ARRAY AT WHICH TO BEGIN
STORING INTEGER ENTRIES.
IARRAY(LOC(K)) = NUMBER OF ENTRIES STORED STARTING AT
IARRAY(IPLACE(K)).

IF NX .NE. -1, CALL GETBND TO ENTER INTEGER DATA.
IF NX .EQ. -1, CALL ADDDEL TO ENTER INTEGER DATA.
SEE GETBND FOR INPUT DESCRIPTION.

<table>
<thead>
<tr>
<th></th>
<th>IPLACE</th>
<th>LOC</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>BORDER</td>
<td></td>
<td></td>
<td>ELEMENT THICKNESS VECTOR.</td>
</tr>
<tr>
<td>THICK</td>
<td>268</td>
<td>93</td>
<td>SOLUTION SEQUENCE VECTOR.</td>
</tr>
<tr>
<td>IPRINT</td>
<td>205</td>
<td>31</td>
<td>PLOT VARIABLE AVETOR.</td>
</tr>
<tr>
<td>PLOTS</td>
<td>311</td>
<td>113</td>
<td>MATERIAL NUMBER VECTOR.</td>
</tr>
<tr>
<td>NMAT</td>
<td>315</td>
<td>98</td>
<td>MATERIAL TYPE/ELEMENT VECTOR.</td>
</tr>
<tr>
<td>MELEM</td>
<td>316</td>
<td>14</td>
<td>TYPE OF PLOT/VARIABLE VECTOR.</td>
</tr>
<tr>
<td>PLOTYP</td>
<td>312</td>
<td>113</td>
<td>LINK NOS. TO BE CALLED AT END OF QKNVIN.</td>
</tr>
<tr>
<td>ICALL</td>
<td>321</td>
<td>125</td>
<td>ENTRY IN LINK TO BE CALLED.</td>
</tr>
<tr>
<td>ICALLS</td>
<td>322</td>
<td>125</td>
<td>OUTPUT VARIABLE MULTIPLIER FROM RARRAY.</td>
</tr>
<tr>
<td>IOMULT</td>
<td>323</td>
<td>60</td>
<td>VARIABLE LIST TO BE DISPLAYED AT OUTPUT.</td>
</tr>
<tr>
<td>IOSAVE</td>
<td>324</td>
<td>60</td>
<td>CONTOURS NODES TO BE USED IN CONTES AND DFCFBL.</td>
</tr>
<tr>
<td>CNTNDS</td>
<td>327</td>
<td>47</td>
<td>NO. OF NODES IN EACH CONTOUR LINE.</td>
</tr>
<tr>
<td>IBORD</td>
<td>238</td>
<td>131</td>
<td>COUNTER-CLOCKWISE LIST OF BOUNDARY.</td>
</tr>
<tr>
<td>IONUMB</td>
<td>331</td>
<td>142</td>
<td>LIST OF ENTRIES IN RARRAY TO BE DISPLAYED AT START OF EACH OUTPUT.</td>
</tr>
<tr>
<td>MPARA</td>
<td>335</td>
<td>142</td>
<td>LIST OF MULTIPLIERS IN RARRAY USED TO MULTIPLY IONUMB ENTRIES.</td>
</tr>
</tbody>
</table>

VALUE IS A VECTOR OF CONTROL NAMES WHICH IS SCANNED WITH THE USER INPUT CONTROL FOR REAL INPUT.

IARRAY(IPLACE(K)) = LOCATION IN THE IZ ARRAY AT WHICH TO BEGIN STORING REAL ENTRIES.

ROUTINE REDREL IS CALLED AT THIS TIME TO ENTER DATA.

<table>
<thead>
<tr>
<th>VALUE</th>
<th>NPLACE</th>
</tr>
</thead>
<tbody>
<tr>
<td>VTHICK</td>
<td>270</td>
</tr>
<tr>
<td>VRHO</td>
<td>284</td>
</tr>
<tr>
<td>VTAB</td>
<td>219</td>
</tr>
<tr>
<td>VCPTAB</td>
<td>218</td>
</tr>
<tr>
<td>VK1COR</td>
<td>289</td>
</tr>
<tr>
<td>VX1COR</td>
<td>289</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>
VX2COR  290  X2-COORDINATES AT NODE POINTS.
          DEFAULT = 0.0

VH  279  ENTHALPY DISTRIBUTION AT NODE POINTS.
          DEFAULT = 0.0

VPSTAT  281  STATIC PRESSURE AT NODE POINTS.
          DEFAULT = PINF / (RHOINF * UINF**2)

VPLTSCL  313  SCALE FACTORS FOR PLOT VARIABLES.
          DEFAULT = 1.0

VAKTAB  317  DEFAULT = 1.0

VAK2TAB  318  DEFAULT = 1.0

VPRESS  291  PRESSURE VALUES AT NODE POINTS.
          DEFAULT = PINF

VSCHMIDT  314  SCHMIDT NO. DIST. AT NODE POINTS.
          DEFAULT = 0.7

VYY  282  DEPENDENT VAR. DIST. AT NODE POINTS.
          DEFAULT = 0.0

VTEMP  285  TEMPERATURE DIST. AT NODE POINTS.
          DEFAULT = TOFINF

VTK  288  THICKNESS OF ELEMENTS IN THICK VECTOR.
          DEFAULT = 1.0 / ALC

VSUTHLD  333  MURFF, TREF, TCON AND EXP ENTRIES FOR SUTHLD.
          DEFAULT = .1163F-4, 494.0, 204.0, 1.5

VPRANDTL  334  PRANDTL NO. DIST. AT NODE POINTS.
          DEFAULT = 0.7

VX3ST  339  DOWNSTREAM STATIONS AT WHICH PRESSURE IS DEFINED.

VPVSX  340  DOWNSTREAM PRESSURES AT VX3ST.

VEPSILON  336  TURBULENT VISCOSITY AT NODE POINTS.
          DEFAULT = 0.0

LINK1
PLACE CALLS TO THE FOLLOWING ROUTINES.
1. SETUP
2. NODELM
3. GEOMFL
4. DPDXTB
5. GETPPR
6. SOURCE
7. DERVBL

LINK2
PLACE CALLS TO THE FOLLOWING ROUTINES.
1. DFCFNS
2. DFCFRL
3. WLFLXS
4. CONTES
5. REDOUTP
6. FEOUTP

IF RESTART CODE 'NRTAPE' IS GREATER THAN 0, WRITE RESTART
CONDITIONS ON TAPE 'NRTAPE'.
PLACE CALLS TO THE FOLLOWING ROUTINES.
1. NBNDRY
2. RITE - PRINT OUTPUT HEADING
4. DIMEN

PLACE CALLS TO THE FOLLOWING ROUTINES.
2. QKNUIN
6. INITNS
7. INITBL

PLACE CALLS TO THE FOLLOWING ROUTINES.
2. CALL ROUTINES FROM ICALLS LIST IN LINK FROM ICALL LIST.
3. CPINIT
5. SCHPRN
6. SETDI F

ABSAVE (CERVBL)
COMPUTE THE SUM OF ABSOLUTE VALUES OF A SEQUENCE OF NUMBERS.

ADDDEL (ELEM, GETBND, SETUP)
ADD OR DELETE ENTRIES IN AN INTEGER ARRAY DEPENDING ON THE VALUE OF 'KODE'.
KODE = 1, DELETE
KODE = 2, ADD

AVRG
COMPUTE THE ARITHMETIC AVERAGE OF 'NUMB' ENTRIES IN AN ARRAY.

BNDSET (GETBND)
DETERMINE NODES TO BE INSERTED INTO BOUNDARY ARRAY.

COLS (DSGRZ)
COMPUTE THE NUMBER OF COLUMNS, 'LCOL', IN THE OUTPUT DISPLAY AND SET UP THE FOLLOWING ARRAY,
INCOL - NO. OF NODES IN COLUMN J.

COMOC (BDINPT)
THIS ROUTINE PRINTS TWO TITLE PAGES ALONG WITH THE DATE.

CONTES (LINK2(4))
RUNNING SMOOTH CONTINUITY EQUATION SOLVER TO COMPUTE V AND W UP A COLUMN OF NODES AFTER VSTART HAS BEEN REACHED. IF NCOORD EQUALS 1, INPUT NODES (READ IN AS CNTPTS AND CNTNDS) ARE USED INSTEAD.

CPINIT (DIMEN)
COMPUTE CPINF AT TSINF.
THE VECTOR CP IS RESET TO CPINF.

DELADD (ADDDEL)
ADD ENTRIES TO AN INTEGER ARRAY 'NSIDE' AT A TIME.

DELELM (DELMOD)
DELETE ENTRIES IN AN INTEGER ARRAY 'NSIDE' AT A TIME.

DELETE (DSCRTZ)
DELETE NODES THAT ARE NOT CONNECTED TO ANY ELEMENTS.

DELNOD (ADODEL)
SET UP CALL TO DELFLM AND SUPPRESS ZERO ENTRIES IN ARRAY.

DERSET (DERVBL)
COMPUTE Q*RHO FOR Q = U, V, OR W.

DERVBL (LINK1(1))
FORM THE DERIVATIVE OF THE ORDINARY DIFFERENTIAL EQUATION FIRST
ON U-VELOCITY (GLOBAL CONTINUITY) AND THEN ON OTHER DEPENDENT
VARIABLES INCLUDING SPECIES CONTINUITY, ENERGY, LONITUDINAL
AND LATERAL MOMENTUM, IF REQUIRED.

DESCRP(N) (BDINPT)
N = 0, 1 READ TITLE FOR OUTPUT.
N = 2 READ HEADINGS FOR OUTPUT VARIABLES.
N = 3 READ AND WRITE SELECTED VARIABLES FROM IARRAY OR RARRAY
FOR PROBLEM DESCRIPTION.
   IF ENTRY IS NEGATIVE - SELECT IARRAY ENTRY
   IF ENTRY IS POSITIVE - SELECT RARRAY ENTRY.

DFCFBL (LINK2(2))
COMPUTE MIXING LENGTH DIFFUSION COEFFICIENTS FOR DEPENDENT VARIABLES.
IF NE1E2 = 1 THE TURBULENT CURVE E1 IS USED.
IF NE1E2 = 2 THE TURBULENT CURVE E1 IS USED UNTIL ROW IMA
IS REACHED AND THEN THE LAMINAR FLOW CURVE E2 IS USED.

DFCNS (LINK2(1))
SET THE TEMPERATURE AND DENSITY IF NOT INITIALIZED.
CALL DFCOF0 TO COMPUTE VISCOSITY (AMU VECTOR).

DFCOFO (DFCFNS)
ESTABLISH THE NODAL VALUES OF VISCOSITY USING SUTHERLAND'S
EQUATION FOR AIR.

DIMEN (LINK3(4))
COMPUTE 'ALC' IF NOT INITIALIZED IN 'NAME021'.
PUNCH COORDINATE CARDS, IF DESIRED (NPUNCH = 7).
COL - X1 COORDINATE OF COLUMN J.
ROW - X2 COORDINATE OF ROW I.

DPDXTB (LINK1(4))
COMPUTE DPDX FROM PRESSURE TABLE, DPDX IS CONSTANT OVER INTERVALS.

DRHCBL (LINK2(10))
CALLED IF IGAS = 0 IN NAME01.
COMPUTES THE TEMPERATURE AND DENSITY USING A SIMPLIFIED
ENERGY EQUATION.

ORHGS (LINK2(11))
CALLED IF IGAS = 1 IN NAMEC1.
COMPUTES THE TEMPERATURE, DENSITY AND SPECIFIC HEAT ON A ACDAL
BASIS AS A FUNCTION OF ENTHALPY, VELOCITY AND SPECIES
COMPOSITION.
IF NGETH = 1 IN NAME01, THE FIRST PASS THROUGH THIS ROUTINE
WILL RETURN ENTHALPY WHEN GIVEN THE TOTAL TEMPERATURE AT
AT THE NODES.

DSCRTZ (SETUP)
SET UP REGION DISCRETIZATION.
GENERATE ARRAYS USED FOR FINDING OUTPUT LOCATIONS.

ELEM (DSGRZ)
IF NELEM = 0 IN NAME01, GENERATES ELEMENTS AS A FUNCTION OF
NODE COORDINATE INPUT. USED PRIMARILY FOR RECTANGULAR DOMAIN.

ENERSC (SOURCE)
COMPUTE SOURCE TERMS FOR ENERGY EQUATION.

ERRSET (MAIN)
IBM 360 ERROR HANDLING ROUTINE TO SUPPRESS OVERFLOWS ETC.

FEDIMN (BDINPT)
SET UP DIMENSIONS OF VARIABLE LENGTH ARRAYS USED IN THE
SYSTEM. FINDS LOCATIONS OF OUTPUT ARRAYS FOR *FEOUTP*.
PRINT LOCATION OF ENTRY POINTS IN 'IZ' ARRAY IF KDUMP = 1.

FENAME (BDINPT)
THIS ROUTINE CONTAINS A LIST OF ALL EQUIVALENCE VARIABLES ALONG
WITH AN ALPHABETICAL CROSS-REFERENCE.
CALL NAMEST TO READ IN NAME01 AND NAME02 NAMELISTS.
MOST DEFAULTED PARAMETERS ARE SET ALSO SET HERE.

FEPLT (STOUTI)
AT PRESENT, ALLOWS FOR PUNCHING DATA AT PLOT STATIONS.

FINDBE (BDINPT)
DETERMINE A SERIES OF BOUNDARY ELEMENTS AS A FUNCTION OF
INPUTTING BOUNDARY NODES IN COUNTER-CLOCKWISE ORDER.
ON FIRST PASS, FIND BORDER ELEMENTS IF READ INTO IBCRD VECTOR.

FSTAE (MAIN)
IBM 360 ROUTINE TO SUPPRESS FORTRAN ERRORS.

GAS (GPAHFT)
DETERMINE COMPOSITION AT SPECIFIC TEMPERATURE TO CREATE
ENTHALPY REQUIRED FOR CONVERGENCE.

GASBUG (GAS)
PRINT DEBUG INFORMATION FOR GAS ROUTINE.

GENDA
ASSEMBLE AN ELEMENT VECTOR WHEN GIVEN THE GLOBAL VECTOR AND
A LIST OF NODES PERTAINING TO THE ELEMENT VECTOR.

GEOMFL (LINK1(3))
SET UP THICKNESS ARRAY.
GENERATE THE TRANSFORMED LENGTH OF ELEMENT AND STORE IN X12 VECTOR.
GENERATE THE TRANSFORMED HEIGHT OF ELEMENT AND STORE IN X23 VECTOR.
GENERATE THE V PART OF THE B2001 MATRIX AND STORE IN GEOM1 MATRIX.
GENERATE THE W PART OF THE B2001 MATRIX AND STORE IN GEOM2 MATRIX.
GENERATE LENGTH * THICKNESS ARRAY.
GENERATE AREA * THICKNESS ARRAY.
GENERATE THE NON-STANDARD ELEMENT MATRICES B211 AND B211S.
IF KODG IS GREATER THAN 0, PRINT ELEMENT NO., NODES OF ELEMENT,
COORDINATES OF NODES AND B211S ENTRIES FOR ELEMENT. AFTER
THE ELEMENT LOOP IS COMPLETED, PRINT THE VECTORS AND MATRICES
THAT WERE GENERATED IN THE ELEMENT LOOP.

GETADD (FEDIMN)
360 ASSEMBLER ROUTINE TO GET MACHINE ADDRESS OF VARIABLE.
GETALC (DIMEN)
   COMPUTE 'ALC' AS THE SHORTEST SIDE OF ALL THE ELEMENTS IF
   IT IS NOT READ IN.
GETBND (BDINPT)
   BOUNDARY OR INTEGER GENERATION ROUTINE USING EITHER THE WORDS 'ADD'
   OR 'DELETE' OR SIMPLE GEOMETRY OF THE PROBLEM WITH THE FOLLOWING
   KEYWORDS AND CODES -

   EACH CARD IS DIVIDED INTO FOUR IDENTICAL BLOCKS OF 20 COLUMNS EACH.
   ALL BLOCKS ARE SCANNED FOR SIMILAR INFORMATION SO A DESCRIPTION
   OF ONE BLOCK WILL BE GIVEN. THE BLOCKS START IN COL. 1,
   COL. 21, COL. 41 AND COL. 61.

   KEYWORD FORMAT BLOCK COLS. DESCRIPTION
   (BLANK) A8 1 - 8 IGNORE BLOCK
   ADD A8 1 - 8 CALL ADDDEL TO INSERT ENTRIES.
       IGNOR COL. 9 - 20.
   DELETE A8 1 - 8 CALL ADDDEL TO DELETE ENTRIES.
       IGNOR COL. 9 - 20.

   FOR THE FOLLOWING KEYWORDS, THE THREE CODES (WE'LL CALL THEM
   KODE1, KODE2 AND KODE3 FOR CONVENIENCE) WILL DETERMINE WHICH
   NODES WILL BE SELECTED)
   KODE1 I4 9 - 12 ROW OR COLUMN DISPLACEMENT FROM
       EDGE BEING DESCRIBED.
   KODE2 I4 13 - 16 POS. IN LINE TO START (DEF. = FIRST).
   KODE3 I4 17 - 20 POS. IN LINE TO END (DEF. = LAST).

   KEYWORD FORMAT BLOCK COLS. DESCRIPTION
   TOP A8 1 - 8 ACROSS TOP FROM LEFT TO RIGHT.
   -TOP A8 1 - 8 ACROSS TOP FROM RIGHT TO LEFT.
   BOTTOM A8 1 - 8 ACROSS BOTTOM FROM LEFT TO RIGHT.
   -BOTTOM A8 1 - 8 ACROSS BOTTOM FROM RIGHT TO LEFT.
   RIGHT A8 1 - 8 UP RIGHT HAND SIDE.
   -RIGHT A8 1 - 8 DOWN RIGHT HAND SIDE.
   LEFT A8 1 - 8 UP LEFT HAND SIDE.
   -LEFT A8 1 - 8 DOWN LEFT HAND SIDE.

GETPPR (LINK1(5))
   TABLE LOOK-UP OF PRESSURE AND DPDX AS FUNCTION OF DOWNSTREAM STATION.

GMADD
   GENERAL MATRIX ADDITION. C = A + B

GPAHFT (THFRMO)
   IF NGETH = 1, COMPUTE ENTHALPY DISTRIBUTION.
   IF NGETH = 0, COMPUTE CPCINF AND RHOINF.
   IF NGETH < 0, DETERMINE NODAL TEMPERATURE GIVEN PRESSURE,
       COMPOSITION AND ENTHALPY.

H2MIX (LINK2(12))
   COMPUTE THE MIXING EFFICIENCY HKSDOT AND THE MASS FLOW HDOT.

ICOND (BDINPT)
PRINT INTEGER AND REAL INITIAL CONDITIONS.
IARRAY(1) - IARRAY(200)
RARRAY(1) - RARRAY(200)

INITNS (LINK4(6))
INITIALIZE DEPENDENT VARIABLES.
THIS ROUTINE GOES THROUGH AN ELEMENT LOOP IN CASE THE VALUES
OF THE DEPENDENT VARIABLES DEPEND ON THE GEOMETRY OF THE PROBLEM.

LOC (MPRO)
COMPUTE VECTOR SUBSCRIPT FOR AN ELEMENT IN A MATRIX OF
SPECIFIED STORAGE MODE.

LOCATE
FIND THE LOCATION OF 'I' IN THE ARRAY 'NA' AND STORE IT IN 'N'.

LOOK (CPINIT, DRHONS)
LINEAR INTERPOLATION ROUTINE (USED ONLY FOR 'CP' AT PRESENT).

LSFT (MISDIV)
GENERATE A LEAST SQUARES FIT THRU A SERIES OF POINTS.

MATSUM
COMPUTE A(I) = B(I) + COEFF * C(I), I = 1, N

MINMAX (DSCRTZ, ORDER, SETSCL)
COMPUTE THE MINIMUM 'MN' AND MAXIMUM 'MX' ENTRIES IN AN ARRAY
AT LOCATION 'IMN' AND 'IMX' IN THE ARRAY.

MISCIV (CONTES)
POLYNOMIAL FIT THRU NPT POINTS TO THE 'MTH ORDER.
NPT MUST BE AN ODD NUMBER.

MLTPLY (PRESUR)
INTERMEDIATE MULTIPLICATION FOR PRESUR ROUTINE.

MNMX (ELEM)
FROM A VECTOR 'INA' CONTAINING 'NN' ENTRIES, STORE THE FOLLOWING-
LOW - POSITION IN INA OF MINIMUM.
LHI - POSITION IN INA OF MAXIMUM.
MN - MINIMUM VALUE IN INA.
MX - MAXIMUM VALUE IN INA.

MPRO
MULTIPLY TWO MATRICES AND STORE IN RESULTANT MATRIX.
R = A * B

MTRA (GEOMFL)
FIND THE TRANSPOSE OF A GENERAL MATRIX.

NBNDRY (LINK3(1))
THE VALUE OF 'NBSET' DETERMINES THE OPERATION OF THIS ROUTINE,
-1 = SET UP INTEGRATION NODES AND STORE DEPENDENT VARIABLE
INTO 'YY' ARRAY.
+1 = SET UP AND PRINT INTEGRATION NODES AND STORE DEPENDENT
VARIABLE INTO 'YY' ARRAY.
0 = SET UP INTEGRATION NODES AND RETRIEVE DEPENDENT VARIABLE
FROM 'YY' ARRAY.

NDECRD (DSCRTZ)
GENERATE NODE COORDINATES, IF NNODE = 0 IN NAME01.
NMELST (FENAME, BOINPT)
READ NAMELIST DATA INPUT.
NAMEO1 = INTEGER INPUT.
NAMEO2 = REAL INPUT.
NCDLM (LINK(l2))
SET UP THE ARRAY IELS TO BE USED IN ORHONS.
IELS = NO. OF ELEMENTS CONNECTED TO NODE N.
CHDR (C,ULS, ROWS, XYSCAL)
ORDER 3 ARRAYS ACCORDING TO THEIR X1 AND X2 COORDINATES. THE
THIRD ARRAY WILL CONTAIN THEIR ARRAY LOCATIONS.
OUTNOD
PRINT AN INTEGER ARRAY ALONG WITH A 32 CHARACTER TITLE.
OUTPG (GEOMFL)
PRINT THE ELEMENT NO. AND NODE CONNECTIONS AND NODE COORDINATES
FROM THE GEOMETRY ROUTINE 'GFCMHT'.
OUTVFC
PRINT A REAL ARRAY ALONG WITH A 32 CHARACTER TITLE.
PBLANK (REOUTP)
INSERT BLANKS IN THE OUTPUT VECTOR 'P' (USED IN 'REOUTP')..
PLINK (REOUTP)
CONVERT A FLOATING POINT NUMBER INTO 'A' FORMAT.
POLY (MISDIV)
FUNCTION TO GENERATE COEFFICIENTS C(l) IN Y = C(l) * X**M
QINIT (INITBL)
CALL QINO1 THRU QIN(NEQ) DEPENDING ON VALUE OF 'NP'.
QINO1 (QINIT)
INITIALIZE DEPENDENT VARIABLE 1 (U-VELOCITY).
THE VALUES ARE EITHER STORRED IN A DATA STATEMENT OR COMPUTED
ON THE GEOMETRY AND THEN ENTERED INTO THE ELEMENT LOCATIONS.
QINO2 THRU QIN(NEQ) (QINIT)
SAME AS QINO1 BUT FOR DEPENDENT VARIABLE NP.
QKNINT (BDINPT)
PRINT DISCRETIZATION OF REGION ALONG WITH NODE NUMBER LOCATIONS.
CALL 'QKNUN' AND TRANSFER CALL TO 'FFCUTP' AT PROPER TIMES.
QKNUN (LINK(4))(2))
INITIALIZE INTEGRATION CONSTANTS ON FIRST PASS.
COMPUTE STEP SIZE AND NEW VALUE OF DEPENDENT VARIABLES.
COMPUTE NEW DENSITIES, DIFFUSION COEFFICIENTS, VISCOSITY
AND OTHER PARAMETERS DEPENDENT ON THE NEW VALUES OF THE
DEPENDENT VARIABLES.
FIND THE MAXIMUM VALUE OF THE DEPENDENT VARIABLES AND STORE IN ZMAX.
IF ZMAX IS LESS THAN ZTST THE TIME WILL BE SET TO TF AND THE
PROBLEM WILL TERMINATE AFTER THE NEXT PRINTOUT.

Q3CONC (DFCFBL)
COMPUTE A ROUGH APPROXIMATION OF THE AREA OF H2 CONCENTRATION AND
STORE IN AREA. COMPUTE THE MASS DEFECT XX5DF = ROUALC * {AREA-XXSUM)
WHERE XXSUM = AMOUNT OF H2 PRESENT AND ROUALC = RHOINF + ALC * UINF**2
RODATE (COMOC, RITF)
ASSEMBLER ROUTINE TO GET MACHINE DATE AND STORE IN 2A4 FORMAT.
RECIP (DFCNS, STOUT)
   COMPUTE THE RECIPROCAL OF AN ARRAY AND STORE IT INTO ITSELF.
REDFL (BDINPT, ANODEL)
   SCAN AN 80 CHARACTER CARD IMAGE AND CONVERT THE INFORMATION THEREIN
   INTO REAL OR INTEGER NUMBERS ACCORDING TO THE FORMAT PRESCRIBED.
REORDER (FINDBE)
   REORDER THE NODES OF AN ELEMENT SO THAT THE FIRST TWO WILL BE
   BOUNDARY NODES AND THEIR ORDER WILL BE COUNTER-CLOCKWISE.
   IN ORDER FOR THIS FEATURE TO OPERATE IT IS NECESSARY TO
   INPUT THE ORDER OF BOUNDARY NODES INTO THE IBORD VECTOR
   IN A COUNTER-CLOCKWISE ORDER.
REOUTP (LINK2(5))
   PRINT THE ARRAY GEOMETRY AND NODE NUMBERS IN A PATTERN THAT
   RESEMBLES PROBLEM GEOMETRY.
(FEOUP) (LINK2(6)) FEOUTP IS AN ENTRY POINT IN REOUTP.
   PRINT OUTPUT PARAMETERS IN A PATTERN THAT RESEMBLES PROBLEM GEOMETRY.
   IF MAXIMUM SCALE FACTOR EXCEEDS 'NSM' (DEFAULT = 10), TERMINATE
   THE PROBLEM.
   IF OUTPUT PRINT NO. 'KOUNT', EXCEEDS PRINT LIMIT 'LPRINT' (DEFAULT =100)
   TERMINATE THE PROBLEM.
RESET
   RESET 'NN' ENTRIES OF ARRAY 'A' TO THE VALUE 'V'.
RITE (LINK3(2))
   COMPUTE ' NUMBER = (KEY-1)*10 + NMB '
   Go TO STATEMENT ACCORDING TO VALUE OF 'NUMBER'.
   IF 'NUMBER' IS OUT OF RANGE, WRITE TITLE INFORMATION.
SCALEV (FEOUP)
   CALL SCALE ROUTINE FOR 10 OUTPUT VARIABLES.
SCHPRN (LINK5(5))
   COMPUTE THE SCHM IDT AND PRANDTL NUMBERS ON A NODE BASIS.
ROWS (DSCRIT)
   COMPUTE THE NUMBER OF ROWS, 'KROW', IN THE OUTPUT DISPLAY
   AND SET UP THE FOLLOWING ARRAYS,
   INROW — NO. OF NODES IN ROW I.
   INDRW — COLUMN NUMBERS OF NODES IN ROW I.
   INDEX — ROW NUMBERS OF NODES IN COLUMN J.
   NOCOL — STARTING COLUMN NO. FOR ROW I.
SETSCV (SCALEV)
   SET SCALE FACTOR FOR AN ARRAY OF REAL NUMBERS, THUS NORMALIZING
SETUP (LINK1(1))
   IF NELEM .GT. 0,
   READ ELEMENT CONNECTIONS AND COUNT ELEMENTS ('NELEM').
   IF NNODE .GT. 0,
   READ NODE GEOMETRY AND COUNT NODES ('NNODE').
   CALL 'DSCRIT' TO SET UP OUTPUT DISPLAY ARRAYS.
   READ TITLE CARDS UNTIL THE WORD 'DONE' APPEARS IN COL. 1-4.
   THE DEFAULT NO. OF CARDS TO BE ENTERED IS 10, IF MORE NEED TO
   BE READ THEN SET 'NTITL' IN NAME01 EQUAL TO OR GREATER THAN THE
   NUMBER OF CARDS TO BE READ.
COMPUTE \( A(I) = B(I) \times C + D \)

SIMQ (GAS)
SIMULTANEOUS LINEAR EQUATION SOLVER USED IN GAS.

SOURCE (LINK(6))
COMPUTE SOURCE TERMS FOR RIGHT HAND SIDE OF DIFFERENTIAL EQUATIONS.

STOREV (SOURCE)
STORE APPROPRIATE VARIABLES IN DUMMY ARRAY FOR SOURCE COMPUTATION.

STOUTI (FEOUTP)
DIMENSIONALIZE OUTPUT VARIABLES FOR DISPLAY PURPOSES.

SUTHLD (DIMEN, DFCOFO)
COMPUTE VISCOSITY USING SUTHERLAND'S VISCOSITY LAW FOR AIR.

TAUW (WLFLXS)
FIND TAU ALONG THE WALL FOR SKIN FRICTION COMPUTATIONS.

TENDA
ASSEMBLE GLOBAL VECTOR WHEN GIVE THE ELEMENT VECTOR AND
A LIST OF NODES PERTAINING TO THE ELEMENT VECTOR.

THERMO (DROGS)
INITIATE CALL TO GPAHFT.

VARMAX (FEPLT)
IF 'NK' .GT. 0, FIND MAXIMUM ENTRY IN ARRAY.
IF 'NK' .LT. 0, FIND MINIMUM ENTRY IN ARRAY.

VECMAI (PRESUI)
MULTIPLY A SYMMETRIC MATRIX OF VECTORS BY A VECTOR OF LENGTH NN.

VECMAJ (PRESUI)
BOOLEAN ASSEMBLY OF AN ELEMENT VECTOR INTO A GLOBAL VECTOR
USING INTEGRATION NODE SEQUENCE.

WLFLXS (LINK2(3))
COMPUTE THE SKIN FRICTION DISTRIBUTION AND HEAT TRANSFER DISTRIBUTION
ALONG THE WALL.

XYSCAL (DSCRTZ)
COMPRESS AN ARRAY OF NUMBERS 'XI' BY SCALE FACTOR 'SCFT'.
FIND 'XYD' = MAX('XI') - MIN('XI') * SCFT.
IF TWO ADJACENT POINTS IF ARRAY 'XI' ARE WITHIN 'XYD' OF EACH
OTHER, SET THE UPPER VALUE EQUAL TO THE LOWER VALUE.
C

INTEGER = READ ADDITIONAL ENTRIES INTO BORDER IPLACE AND LOC

REAL = READ ADDITIONAL ENTRIES INTO VALUE AND NPLACE

J=0

J=J+1

J:50 > 450

V1: BORDER (J) ≠ 410

GETBND

STORE INTEGER DATA IN PROPER IZ LOCATIONS

KDUMP = PRINT INTEGER INPUT

≠ D
D

V1: IBORD ≠ 400

MAKE SURE BORDER NODES END WHERE THEY BEGIN

750

450

J=0

460

J=J+1

J:50 ≤ 400

V1: VALUE(J) ≠ 460

E
COMPUTER NON-D FACTOR FOR VARIABLE TO BE READ

RÉDREL

STORE REAL NOS. INTO PROPER LOC. IN IZ ARRAY

KDUMP 1

PRINT REAL INPUT

NON-DIMEN. REAL VECTOR

PRINT START COND.

PDUMP (RZ(NPCD, RZ(NREPET,NZ))

510

QKNINT

400

500

400
STORE DEPENDENT VARIABLE INTO PRESENT AND PAST LOCATIONS OF SPECIFIED VARIABLE.

SET RESTART PARAMETERS

REDEFINITION OF VARIABLE. STORE OLD VALUES SO THAT ONLY OVERRIDDEN VALUES WILL BE ENTERED

CALLED BY: MAIN
LINK3

KK = |KA|

< KK:1

KA:0

LOCATE

≤

NBNDRY

> NP:0

RETURN

≤

RETURN

< KK:2

RITE (TITLE)

RETURN

RETURN

< KK:3

RETURN

RETURN

< KK:4

DIMEN

RETURN

RETURN

RETURN

CALLED BY:

MANY

ROUTINES
Called by:
BDINPT
LINK5
QKNINT
LINK5

A

KK:1 = H2MIN → RETURN

KK:2 ≠ DETERMINE NCL, NCLS

KK:3 ≠ CPINIT

NCL: ILNK1 ≠ LINK1

NCL: ILNK2 ≠ LINK2

NCL: ILNK3 ≠ LINK3

NCL: ILNK4 ≠ LINK4

NCL: ILNK5 ≠ LINK5

A

KK=NCLS ≠ NCLS : 2

RETURN

CALLED BY:
BDINPT
DIMEN
QKNUIN
ABSsave

\[ I = 0 \]
\[ AVE = 0.0 \]

100

\[ I = I + 1 \]

I:N

\[ AVE = AVE + \text{ABS}(A(I)) \]

ABSsave = AVE/N

return

called by:
dervbl
q3conc
ADDDEL

SET INTEGERS

500

REDREL

KTYP = 1

DELNOD

KODE: NEND

= 600

KTYP = 2

DELADD

KODE: NEND

= 600

RETURN

CALLED BY:
ELEM
GETBND
SETUP
BDINPT
DSCRTZ
AVRG

COMPUTE ARITHMETIC AVERAGE OF ENTRIES IN AN ARRAY

RETURN

CALLED BY:
GEOMFL
BNDSET

PICK OUT NODE NUMBERS ACCORDING TO BOUNDARY LOCATIONS

RETURN

CALLED BY:
GETBND
CALLED BY: DSCRTZ

STORE NODE NOS IN 'INDEX' VECTOR BY THEIR LOCATION IN COLUMNS

STORE COL. COORD. IN 'COL' VECTOR

STORE NO. OF COLS. IN 'LCOL'

RETURN
COMOC

RDATE

PRINT 2 COVER PAGES

RETURN

CALLED BY: BDINPT
GENERATE THE FOLLOWING VECTORS:
YNOD - NORMAL DISP. FROM WALL
VSIN - SINE OF ANGLE OF COL.
WCOS - COSINE OF ANGLE OF COL.

PRINT
IWRIT
VSIN
AND
WCOS

STORE RHO^U

COMPUTE COEFFICIENTS FOR U PRIME COMPUTATION
COMPUTE UPRIME ON A NODAL BASIS

STORE RHO^U AND RHO^W INTO TEMP. VECTORS

EXECUTE A COLUMN BY COLUMN ITERATION TO COMPUTE NEW RHO^V AND RHO^W USING MISDIV TO GENERATE COEFFICIENTS.

IWRIT > 0

PRINT RHO^V RHO^W

IWRIT ≤ 0

STORE NEW V AND W BACK INTO DEP. VAR. ARRAY

RETURN

CALLED BY:
LINK2
CPINIT

LOOK

ITERATE TO
FIND STATIC
REF. TEMP.
TSINF

RESET

SETVAL

RETURN

CALLED BY:
DIMEN
DELADD

ADD ENTRIES TO INTEGER ARRAY

RETURN

CALLED BY:
ADDDEL
DELELM

DELETE ENTRIES IN INTEGER ARRAY

RETURN

CALLED BY:
DELNOD
DELETE

RESET

STORE NO. OF NODES ATTACHED TO ELEMENTS

850

SCAN ATTACHMENTS

ALL NODES SCANNED

YES

RETURN

NO

NODE ATTACHED

YES

850

NO

PRINT 'NODE N DELETED - NO CONNECTIONS'

850

CALLED BY: DSCRTZ
DELNOD

DELEM

RESEQUENCE VECTOR ELIMINATING DELETED ENTRIES

RETURN

CALLED BY:
ADDDEL
DERSET

LOCATE

NP:0

= RETURN

\[\neq\]

LINK3

DETERMINE \(Q\neq\rho\)

RETURN

CALLED BY:
DERVBL
DERVBL

RESET COMPUTATIONAL VECTORS

\( \text{NSORCE} = 1 \)

STORE SOURCE TERMS INTO RIGHT HAND SIDE VECTOR

COMPUTE AND STORE RHO^U, RHO^V AND RHO^W

IN AN ELEMENT LOOP, COMPUTE THE CONDUCTION AND CONVECTION TERMS AND ASSEMBLE INTO RIGHT HAND SIDE VECTOR 'V'. COMPUTE CONDENSED LEFT HAND SIDE AND STORE IN 'C'.

COMPUTE DERIVATIVE FOR DEP. VAR. AS 'V'/'C' AND STORE IN 'ZZ' VECTOR

RETURN

CALLED BY:
QKNINT, QKNUIN

59
DESCRP

KA=1

PRINT 'PROBLEM DESC.'

READ RECORD

READ RECORD

RETURN

RETURN

KA=2

READ FORMAT

RETURN

RETURN

KA=3

READ PLINE

PLINE(1) = 'DONE'

PRINT FROM LARRAY

PRINT FROM RARRAY

SKIP LINE

RETURN

NTRY = 0

300

CALLED BY: BDINPT
This is a dummy sub-routine to set the turbulent viscosities to 0.

If non-zero turb. viscosities are desired, user must code routine.

RETURN

Called by: LINK2
DFCNS

ND:1 ≠ 200

RHO(1):0.0 ≠ RESET

TEMP(1):0.0 ≠ RESET

200

DFCOPO

SET VISOSITY

SET DIFFUSION COEFFICIENTS EQUAL TO VISCOSITY

RETURN

Called by: LINK2
DIMEN — 2

CALLED BY:
BDINPT
CALCULATE PRESSURE GRADIENT TO BE CONSTANT BETWEEN X3 STATIONS.

RETURN

CALLED BY:
LINK1
DRHOBL

LINK3
(1,U,YY)

LINK3
(1,H2,YY)

COMPUTE TEMP.
AND DENSITY
AS FUNCTION
OF U-VELOCITY
AND H2 MASS
FRACTION

RETURN

CALLED BY:
LINK2
DRHOGS - I

STORE MASS FRACTIONS IN TEMP. ARRAYS

STORE VELOCITY AND ENTHALPY IN TEMP. ARRAYS

CALL THERMO ON A NODE BASIS TO COMPUTE TEMP., DENSITY AND SPECIFIC HEAT

INITIALLY RUN 3 PASSES
PASS 1 - GET TOTAL ENTHALPY DIST.
SET HINF
PASS 2 - GET STATIC TEMP. DIST.
SET TOFINF, CPOINF, PRSCON
PASS 3 - GET DENSITY, SPECIFIC HEAT

RETURN

CALLED BY: LINK2
DSCRTZ

NNODE : 0 ≠

400

SCALE COORDS.
BY XSCALE, YSCALE

APPLY COMPRESSION
FACTORS FOR OUTPUT

NELEM : 0 ≤

SET UP NODE NO.
INDEX ARRAYS

DELETE

RETURN

SET UP NODE COORDINATES
AS FUNCTION OF INPUT

ELEM

CALLED BY:
SETUP
SET UP INITIALIZATION

SCAN PAIRS OF ROWS STARTING WITH TOP ROWS AND WORK DOWN. WHEN A RECTANGULAR MATCH IS FOUND, FORM TWO TRIANGLES WITH DIAGONAL FROM LOWER LEFT TO UPPER RIGHT. IF A TRIANGULAR MATCH IS FOUND, USE IT.

RETURN

CALLED BY:
DSCRTZ
ENERSC

VECMAT

IN A DEP. VAR. LOOP
COMPUTE SOURCE TERM
FOR ENTHALPY IN
AN ELEMENT.

RETURN

CALLED BY:
SOURCE
FEDIMN

INITIALIZE STARTING LOCATIONS FOR VARIABLES IN IZ ARRAY

KDUMP: 1

= PRINT IZ ENTRY POINTS

≠

RETURN

CALLED BY:
BDINPT
FENAME

SET SCALARS

NMELST

IRUN = IRUN + 1

RETURN

CALLED BY:
BDINPT
CONVERT NODE VECTOR ALONG BOUNDARY INTO CORRESPONDING ELEMENT VECTOR
GAS

INTERPOLATE TABLES TO FIND: \( c_p, \frac{H}{R}, \frac{S}{R}, \frac{G}{RT} \) AT GIVEN TEMP. FOR ALL SPECIES

IFR = 52

#

COMPUTE COMPOSITION USING A TRIAL AND ERROR ITERATION WHICH IS A MULTI-VARIABLE ANALOG OF NEWTON'S METHOD.

52

COMPUTE PROPERTIES \( H, S, c_p, u, v, v_{\text{sound}} \) AND MASS FRACTIONS AND STORE IN VEC.

RETURN

CALLED BY:
GPAHFT
GASBUG-1

PRINTS DEBUG INFORMATION ABOUT GAS

RETURN

CALLED BY:
GPAHFT
GENDA

ASSEMBLE ELEMENT VECTOR 'TEL'

RETURN

CALLED BY:
MANY Routines
GEOMFL

DO 200 MEL=1,NELEM

COMPUTE
TK
X12  X1P2*TK
X23  AREA*TK
GEOM1  B211s
GEOM2  B211

KODG : 0

200

PRINT
AL,AK
B211s
B211

KODG : 0

PRINT
GEOM2
X1P2*TK  X12
AREA*TK  X23
GEOM1

RETURN

CALLED BY:
LINK1
GETALC

FIND SHORTEST ELEMENT SIDE AND STORE IN 'ALC'

RETURN

CALLED BY:
DIMEN
GETBND

150

READ BOUNDARY INFO.

BNDSET

'DONE'

RETURN

CALLED BY:
BDINPT
GMADD

ADD TWO MATRICES ELEMENT BY ELEMENT

RETURN

CALLED BY: DERVBL

83
GPAHFT

COMPUTE AND STORE MASS FRACTIONS AND MOLE FRACTIONS

\( \text{NGETH} : 1 \)

\( \neq \)

\( \text{GAS} \)

\( \text{STORE INITIAL DISTRIBUTION OF ENTHALPY, DENSITY AND SPECIFIC HEAT} \)

\( \text{IBUG1} : 0 \)

\( \neq \)

\( \text{GAS} \)

\( \text{GASBUG} \)

\( \text{GAS} \)

\( \text{YES} \)

\( \text{TEMPERATURE RIGHT} \)

\( \text{NO} \)

\( \text{ITERATE UP TO 100 TIMES TO FIND CORRECT TEMP.} \)

99
Called by: Thermo
H2MIX

LINK3 (1,U,YY)

LINK3 (1,H2,YY)

COMPUTE MIXING EFFICIENCY AND H2 MASS FLOW

RETURN

CALLED BY:
LINK2
ICOND

PRINT
INTEGER
INITIAL
CONDITIONS

PRINT
REAL
INITIAL
CONDITIONS

RETURN

CALLED BY:
BDINPT
CALLED BY:
LINK4

INITNS-1

INITBL

INITIALIZE
DEP.
VARIABLES

IBL:1 = DRHOGS

DRHOBL

RETURN
LOC-1

GENERAL MATRIX

MS: 0 = COMPUTE SUBSCRIPT (N*M ELEM)

SYMMETRIC MATRIX

MS: 1 = COMPUTE SUBSCRIPT OF UPPER TRIANGLE

DIAGONAL MATRIX

COMPUTE SUBSCRIPT (N ELEM.)

IR = 0

36

IR = IRx

RETURN

CALLED BY: MFRD

89
LOCATE

FIND LOCATION OF VALUE M IN ARRAY NA AND STORE LOCATION IN N

RETURN

CALLED BY:
MANY ROUTINES
LOOK

TABLE LOOKUP AND INTERPOLATION

RETURN

CALLED BY:
CPINIT
GETFPR

91
POLYNOMIAL LEAST SQUARES FIT TO A CURVE

RETURN

CALLED BY: MISDIV
MATSUM

COMPUTE
A(I) = B(I) + C(I)*D

RETURN

CALLED BY:
GEOMPL
QKNUIN
ENERSC
SETDIF
MINMAX

FIND MINIMUM
= MN AT
LOCATION IMN
OF ARRAY

FIND MAXIMUM
= MX AT
LOCATION IMX
OF ARRAY

RETURN

CALLED BY:
DSORTZ
ORDER
SETSCL
MISDIV

POLY FIT
THRU 'NPT'
TO MTH
ORDER

RETURN

CALLED BY:
CONTES
MNMX

LOCATE MINIMUM AND MAXIMUM ENTRIES IN A VECTOR AND STORE IN MN AND MX RESPECTIVELY. STORE THEIR LOCATIONS IN LOW AND LHI.

RETURN

CALLED BY:
ELEM
MPRD

MULTIPLIES TWO MATRICES

RETURN

Called by:
- DERVEL
- GEOMFL
- H2MIX
- VECMAT
- ENERSC
MTRA

TRANSPOSES A MATRIX

RETURN

CALLED BY: GEOMFL
SET UP 'NWN' INTEGRATION NODE ARRAY

<

STORE DEP. VARIABLE VECTOR U INTO YY VECTOR

RETURN

= 0

STORE YY VECTOR INTO DEP. VARIABLE VECTOR U

WRITE INTEG NODE VECTOR

>
NDECRD

COMPUTE X1 AND X2 COORDINATES AS A FUNCTION OF INPUT WHEN NNODE=0.

RETURN

CALLED BY: DSCRTZ
NMELST

READS NAMELIST

CHECK VARIABLES

RETURN

CALLED BY:
BDINPT
FENAME
DETERMINE THE NUMBER OF ELEMENTS ATTACHED TO EACH NODE AND STORE DATA IN IELS VECTOR.

DETERMINE THE ELEMENT NOS. ATTACHED TO EACH NODE AND STORE EACH SERIES SEQUENTIALLY IN IELEM VECTOR.
(NOT USED AT PRESENT)

RETURN

CALLED BY:
LINK1
ORDER

ORDER COORDINATES AND INDEX VECTORS
BY: X1COR OR X2COR
KODE=1 + X1COR
KODE=2 + X2COR

RETURN

CALLED BY:
COLS
ROWS
XYSCAL
OUTNOD

DISPLAY VECTOR OF INTEGERS

RETURN

CALLED BY:
FEDIMN
OUTPG

WRITE NODES AND COORD. OF ELEMENT

RETURN

CALLED BY:
GEOMFL

105
OUTVEC

DISPLAY VECTOR OF REALS

RETURN

CALLED BY:
CONTES
LINK2
GEOMFL
DERVBL
GPAHFT
PBLANK

RESET LINE OF OUTPUT ARRAY TO BLANKS

RETURN

CALLED BY:
REOUTP
(PEOUTP)
PLILNK

CONVERT FLOATING POINT NO. TO 'A' FORMAT FOR OUTPUT

RETURN

CALLED BY:
REOUTP
(PEOUTP)
POLY

COMPUTE POLYNOMIAL COEFFICIENTS

RETURN
Q3CONC

COMPUTE THE MASS DECEPT OF H2 FOR LAMINAR FLOW

RETURN

CALLED BY:
DFCFBL
QIN(NP) - 1

QIN(NP)

INITIALIZE DEPENDENT VARIABLE 'NP'

RETURN

CALLED BY:
QINIT
QKNUIN

INIT:O

INITIALIZE INTEGRATION COEFFICIENTS

40

COMPUTE PREDICTOR VALUES OF DEP. VARIABLES

COMPUTE CORRECTOR VALUES OF DEP. VARIABLES

PASS EPSILON TEST

Yes

INCREASE STEP SIZE

DRHOBL OR DRHOGS DFCFNS CONTES H2MIX

DERVBL

RETURN

No

40

CALLED BY: LINK4
READER

REDREL

ANY NUMBERS READ

YES  STORE NUMS. IN
     RETURN VECTOR

NO

RETURN

CALLED BY:
DSCRTZ
STORE RECIPROCAL OF VECTOR INTO ITSELF

RETURN

CALLED BY:
STOUT1
SETDIF
DFCFNS
REPD $0
',,
CHARACTER
CARD
IMAGE

CONVERT DATA
ON CARD INTO
REAL OR
INTEGER
NUMBERS.

RETURN

CALLED BY:
ADDDEL
BDINPT
READER
REORDR

REORDER THE NODES
OF AN ELEMENT SO
THAT THE FIRST TWO
ARE BOUNDARY NODES
AND THE ORDER IS
COUNTERCLOCKWISE

RETURN

CALLED BY:
FINDBE
REOUTP

INITIALIZE CONSTANTS.
INITIALIZE FORMATS.
SCALE COORDINATES.

NSS = 1

FEOUTP

NSS

= 200

\[
\text{LINK3}(2) \text{ RITE}(0,0) \quad \text{PRINT OUTPUT HEADING}
\]

\[
\text{NOUTPR} \leq 280
\]

\[
\text{GENERATE AND PRINT SCALAR HEADING}
\]

\[
\text{INITIALIZE LINE COUNT LIMITS}
\]

\[
\text{PRINT COUNTERS}
\]

A
DO 800 MTM=1,NMBTIM

GENERATE OUTPUT FOR 10 VARIABLES AT A TIME

STOUT1

GENERATE OUTPUT VARIABLES

SCALEV

NORMALIZE OUTPUT AND SET SCALE FACTORS

200

PRINT NODE DISCRETIZATION = LSET 

#

PRINT VARIABLES IN PATTERN SIMILAR TO DISCRETIZATION

PRINT CODES

CHECK CODES

RETURN

Called by LINK2
RESET

SET
A(I) = V
FOR I=1, N

RETURN

CALLED BY: MANY ROUTINES
RITE

NUMBER = (KEY-1)*10+NMB

GO TO (101,102,...), NUMBER

NUMBER IN RANGE?

Yes

WRITE APPROPRIATE FORMAT

RETURN

No

RDATE

WRITE DATE, TITLE

CALLED BY:
LINK3
SETUP
ROWS

SET-UP INDRW, ROW, AND NOCOL VECTORS AND SET KROW = NO. OF ROWS IN PRINTOUT

RETURN

CALLED BY:
DSCR TZ
SCALEV

DO 600
   LL=1,10

KPOS = IZ(LL)

IF (KPOS .EQ. -1) THEN
   100
ELSE
   SETSCL
   NSC(LL) = IT
   100
ENDIF

600

RETURN

CALLED BY: REOUTP

125
SCHPRN

RESET

SET SCHMIDT NO.

RESET

SET PRANDTL NO.

RETURN

CALLED BY:
LINK1
SETSCL

MINMAX

DETERMINE LARGEST SCALE FACTOR FOR AN OUTPUT VARIABLE

RETURN

CALLED BY:
REOUTP
SCALEV
DSCRTZ

LG : 0

LG = LCOL

READ TITLE CARD

TITLEC19 : DONE ≠

RETURN

CALLED BY:
LINK1
SETVAL

SET
A(I) = B(I)*C+D

RETURN
SIMQ

OBTAINT SOLUTION OF A SET OF SIMULTANEOUS LINEAR EQUATIONS

RETURN

CALLED BY:
GAS
133
DO 900 NS=1, NEQKNN

COMPUTE SOURCE TERMS FOR DEPENDENT VARIABLES AND STORE IN UPPER REGION OF DIF ARRAY.

RETURN

CALLED BY:
LINK1
STOREV

STORE A STRING OF SEQUENTIAL DEP. VAR. WHICH ARE STORED IN INTEGRATION ORDER INTO TEMPORARY STORAGE BY NODE NUMBER.

RETURN
DO 400
L=1,NVOUT

FIND MULTIPLIER LOCATION IOMLT(L) IN RARRAY. IF NEGATIVE, USE RECIPROCAL. STORE VALUE IN AMULT.

FIND VARIABLE LOCATION IOSAVE(L) IN IZ ARRAY. STORE VALUE IN LOGG.

KRECIP = 0

LOGG : 0

LOGG= |LOGG|
LOGS=LOGG
NP=(LOGG/1000)+1

NP: 1

100
FIND THE POSITION OF NX IN THE IPINT VECTOR. STORE POS. IN NP. IF NX IS NOT AN ENTRY, THEN NP=0.

\[ \text{LSV} = \text{MOD}((\text{LOGG}, 1000)) \]
\[ \text{LND} + (\text{NP}-1) \times \text{NODE} \]

- If \( LSV = 247 \):
  - STORE DIFFUSION COEF. FOR NP IN OUTPUT ARRAY

- If \( LSV = 248 \):
  - STORE DEP. VARIABLE NP IN OUTPUT ARRAY

- If \( LSV = 249 \):
  - STORE DERIV. FOR NP IN OUTPUT ARRAY
MULTIPLY OUTPUT VECTOR BY AMULT

MULTIPLY VECTOR BY AMULT AND STORE IN OUTPUT ARRAY

STORE RECIPROCAL OF OUTPUT VECTOR INTO ITSELF

KRECIP : 1

KPNT : 0

KPLVAR : 0

C
SCAN IPlOTS VECTOR TO SEE IF THIS IS A VARIABLE TO BE PLOTTED.

IRPL : LOGS

KOUT : 0

FEPLLOT

RETURN

CALLED BY:
FEOUTP.
SUTHLD

COMPUTE VISCOSITY USING SUTHERLAND'S EQUATION

RETURN

CALLED BY:
DFCOFO DIMEN
TAUW

CALCULATE SKIN FRICTION FOR ZERO PRESSURE GRADIENT AND ZERO SURFACE MASS ADD.

RETURN

CALLED BY: WLFLX
TENDA

STORE ELEMENT DATA INTO A NODE NUMBER SEQUENCED ARRAY

RETURN

CALLED BY:
INITNS
VARMAX

FIND MINIMUM OR MAXIMUM ENTRY IN AN ARRAY

RETURN

CALLED BY:
DRHOGS
FEPLOT
QKNUIN
LINK2
VECMAT

MULTIPLY A MATRIX OF VECTORS BY A VECTOR TO PRODUCE A SYMMETRIC MATRIX

RETURN

CALLED BY:
ENERSC
DIMENSIONALIZE PRESSURE AND ENTHALPY

NGBUG : 1

NGBUG : 1

GPAHFT

NGBUG : 1

PRINT DEBUG INFO

PRINT DEBUG INFO

NBYP = 1

NBYP = 1

NBYP = 1

NBYP = 1

A
A

NBYP : 1 = 2

NBYP : 1 = 600

NBUG : 1 = SET DEBUG FLAGS

600

NBUG : 1 = RESET DEBUG FLAGS

NON-DIMENSIONALIZE VARIABLES

NGBUG : 1 = PRINT DEBUG INFO

RETURN

CALLED BY:
DRHOGS
147
COMPUTE SKIN FRICTION AND STANTON NUMBER ALONG SURFACE FOLLOWING PATANKER AND SPALDING.

RETURN

CALLED BY:
LINK2
XYSCAL

COMPRESS A VECTOR OF NUMBERS 'X1' BY SCALE FACTOR 'SCFT'.
FIND Xyd=(MAX(X1)-MIN(X1))/SCFT. IF TWO ADJACENT
ENTRIES ARE WITHIN Xyd OF EACH OTHER, SET THE HIGHER
VALUE EQUAL TO THE LOWER VALUE.

RETURN

CALLED BY:
DSCRTZ
149
OPERATING INSTRUCTIONS

The 3DBR Variant of COMOC constitutes approximately 10,000 cards. Considerable effort has been placed on minimizing input/output complexity and on providing the user with considerable latitude in data deck preparation. This section describes deck set-up, input procedures, output files and procedures, internal diagnostics that can be used to debug operating phases, and a description of the data decks for the test cases.

Deck Set-Up

Shown in Fig. 2 is an illustration of the deck set-up for 3DBR COMOC. Any user-written subroutines should be compiled first. The various machine requirements for the program are listed below.

Tape: RESTART defines an input and/or output tape which will be used for a restart condition or to store data for a future restart. The integer ending in column 25 defines a restart tape and the integer ending in column 30 defines the output print number that will be used for restarting. The integer ending in column 35 defines a tape that will be used to store outputs for future restarts. This number may be the same as in column 25.

Print: Printed output is sent to unit 6.

Punch: If NPUNCH = 7, in NAMEO1, node coordinates and element connections are punched on unit 7. If KOUT.gt.0 and KPLVAR .gt. 0 in NAMEO1, then data generated for the variables defined by the PLOTS card will be output from the FEPLLOT routine.

Reader: Card reading is executed from unit 5.

Disc: No internal requirements by program

Input

Unless a restart condition exists, all data are read on unit 5. All data which are strictly scalar information are read in free format style. Delimiters on these input cards can be either blanks, commas or column 80. Many features enable input data to be read in a simplified fashion.
Fig. 2 IBM/360 DECK SETUP FOR PROGRAM
e.g. | Symbols | Interpretation |
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>5*I3</td>
<td>12, 15, 18, 21, 24</td>
</tr>
<tr>
<td>3*I-.5</td>
<td>3.1E3, 3100.0, 3099.5, 3099.0</td>
</tr>
<tr>
<td>6*23.2</td>
<td>23.2, 23.2, 23.2, 23.2, 23.2, 23.2, 23.2</td>
</tr>
</tbody>
</table>

A T at the end of input or a blank card will terminate the read cycle for a particular input parameter.

e.g.

```
ICALLS -1
2 2 4 5 1 4 2 5 T
```

stores the numbers 2 2 4 5 1 4 2 5 in the CALLS vector.

```
VTEMP 42*533.0
```

stores 42 temperatures of 533.0 in the TEMP vector.

Output

Output for 3DBR COMOC is standardized to the format of the test cases. A highly adaptive output subroutine automatically scales data and allows for widely variable field size displays. Output formats are generated in the input deck by specification of which dependent variables, parameters, and scalars are to be printed during the output phase. Addition of an output array to the standard output is presented after the discussion of the data deck for the test case.

Restrictions and Limitations

Size of problem to be solved depends on the amount of storage available in core. The program contains a variable dimensioning scheme so that the total size can be specified by adjusting the dimension of the IZ array in MAIN.

Editing and Diagnostics

There are several flags that can be user set to provide detailed intermediate output for debug purposes, including KDUMP, NGBUG, IBUG1, IBUG2, IWRIT, IDIFRT, KODG and KOD5. In the following, each of these is discussed with respect to sample representative output from COMOC.
<table>
<thead>
<tr>
<th>VTE</th>
<th>0</th>
<th>0</th>
<th>0</th>
<th>0</th>
<th>0</th>
<th>0</th>
<th>0</th>
<th>0</th>
<th>0</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>VY</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>VY</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Non-D Factor

*Original Page Quality Poor*
Below is a hexadecimal dump of the vector entry points in the IX array.

\[ 
\begin{array}{cccccccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
07611 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 \\
07612 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 \\
07613 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 \\
07614 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 \\
07615 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 \\
07616 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 \\
07617 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 \\
07618 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 \\
07619 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 & 0077744 \\
\end{array} 
\]

Below is a printout of locations 201-206 of the IARRAY vector.

\[ 
\begin{array}{cccccccc}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\
10 & 11 & 12 & 13 & 14 & 15 & 16 & 17 \\
18 & 19 & 20 & 21 & 22 & 23 & 24 & 25 \\
26 & 27 & 28 & 29 & 30 & 31 & 32 & 33 \\
34 & 35 & 36 & 37 & 38 & 39 & 40 & 41 \\
42 & 43 & 44 & 45 & 46 & 47 & 48 & 49 \\
50 & 51 & 52 & 53 & 54 & 55 & 56 & 57 \\
58 & 59 & 60 & 61 & 62 & 63 & 64 & 65 \\
66 & 67 & 68 & 69 & 70 & 71 & 72 & 73 \\
74 & 75 & 76 & 77 & 78 & 79 & 80 & 81 \\
82 & 83 & 84 & 85 & 86 & 87 & 88 & 89 \\
90 & 91 & 92 & 93 & 94 & 95 & 96 & 97 \\
98 & 99 & 100 & 101 & 102 & 103 & 104 & 105 \\
106 & 107 & 108 & 109 & 110 & 111 & 112 & 113 \\
114 & 115 & 116 & 117 & 118 & 119 & 120 & 121 \\
122 & 123 & 124 & 125 & 126 & 127 & 128 & 129 \\
130 & 131 & 132 & 133 & 134 & 135 & 136 & 137 \\
138 & 139 & 140 & 141 & 142 & 143 & 144 & 145 \\
146 & 147 & 148 & 149 & 150 & 151 & 152 & 153 \\
154 & 155 & 156 & 157 & 158 & 159 & 160 & 161 \\
162 & 163 & 164 & 165 & 166 & 167 & 168 & 169 \\
170 & 171 & 172 & 173 & 174 & 175 & 176 & 177 \\
178 & 179 & 180 & 181 & 182 & 183 & 184 & 185 \\
186 & 187 & 188 & 189 & 190 & 191 & 192 & 193 \\
194 & 195 & 196 & 197 & 198 & 199 & 200 & 201 \\
\end{array} 
\]

\[ 
\text{SETUP} 
\]

\[ 
\text{ORIGINAL PAGE IS OF POOR QUALITY} 
\]
<table>
<thead>
<tr>
<th>NODE</th>
<th>XCOORD</th>
<th>YCOORD</th>
<th>ZCOORD</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>2</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>3</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
</tr>
<tr>
<td>4</td>
<td>3.0</td>
<td>3.0</td>
<td>3.0</td>
</tr>
</tbody>
</table>

Original Page Is Poor Quality
**Phasing printout from THERMO and GRAFRT.**

- If INCH1 .eq. 1, print out from THERMO.
- If INCH1 .eq. 2, print out from GRAFRT.

**PRINT out from THERMO:**

- All three flags are decremented by 1 with each pass thru PRINTS;
- Print stops when flags reduce to 0 or lower.

- If INCH1 .eq. 0, then certain failures in THERMO will turn on flags and printout.
- Thus ensuing printout at failure conditions. Some conditions will be fatal and create a node coordinate printout followed by a dependent variable printout.

---

### INPUT NODE 1

<table>
<thead>
<tr>
<th>Node</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### INPUT NODE 2

<table>
<thead>
<tr>
<th>Node</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

---

### MASS FRACTIONS

<table>
<thead>
<tr>
<th>Node</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

---

### POLE FRACTIONS

<table>
<thead>
<tr>
<th>Node</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

---

**PRINT out from GRAFRT.**

- If INCH2 .eq. 1, print out from GRAFRT.
- If INCH2 .eq. 2, print out from GRAFRT.

---

### INPUT NODE 1

<table>
<thead>
<tr>
<th>Node</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### INPUT NODE 2

<table>
<thead>
<tr>
<th>Node</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

---

### MASS FRACTIONS

<table>
<thead>
<tr>
<th>Node</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

---

### POLE FRACTIONS

<table>
<thead>
<tr>
<th>Node</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

---

**PRINT out from GRAFRT.**

- If INCH2 .eq. 1, print out from GRAFRT.
- If INCH2 .eq. 2, print out from GRAFRT.
### MASS FRACTIONS

<table>
<thead>
<tr>
<th>Node</th>
<th>H2</th>
<th>H2O</th>
<th>H</th>
<th>N2</th>
<th>O2</th>
<th>CO</th>
<th>CO2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.3</td>
<td>0.757</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>2</td>
<td>0.3</td>
<td>0.757</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>3</td>
<td>0.3</td>
<td>0.757</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

### MASS FRACTION-

- H2: 0.3
- H2O: 0.757
- H: 0.0
- N2: 0.0
- O2: 0.0
- CO: 0.0
- CO2: 0.0

### MASS FRACTION-

- H2: 0.3
- H2O: 0.757
- H: 0.0
- N2: 0.0
- O2: 0.0
- CO: 0.0
- CO2: 0.0

### MASS FRACTION-

- H2: 0.3
- H2O: 0.757
- H: 0.0
- N2: 0.0
- O2: 0.0
- CO: 0.0
- CO2: 0.0

### MASS FRACTION-

- H2: 0.3
- H2O: 0.757
- H: 0.0
- N2: 0.0
- O2: 0.0
- CO: 0.0
- CO2: 0.0

### MASS FRACTIONS-

- H2: 0.3
- H2O: 0.757
- H: 0.0
- N2: 0.0
- O2: 0.0
- CO: 0.0
- CO2: 0.0

### MASS FRACTIONS-

- H2: 0.3
- H2O: 0.757
- H: 0.0
- N2: 0.0
- O2: 0.0
- CO: 0.0
- CO2: 0.0

### MASS FRACTIONS-

- H2: 0.3
- H2O: 0.757
- H: 0.0
- N2: 0.0
- O2: 0.0
- CO: 0.0
- CO2: 0.0

### MASS FRACTIONS-

- H2: 0.3
- H2O: 0.757
- H: 0.0
- N2: 0.0
- O2: 0.0
- CO: 0.0
- CO2: 0.0

### MASS FRACTIONS-

- H2: 0.3
- H2O: 0.757
- H: 0.0
- N2: 0.0
- O2: 0.0
- CO: 0.0
- CO2: 0.0

Compute temperature, specific heat, and density as function of enthalpy, pressure and mass fractions.

1st and last passes are printed when INPUT=0.

When INPUT=0 all intermediate passes are shown.
IF IRIT is decremented by 1 for each pass thru C0NTER, when IRIT .le. 0 debug print stops.

If VSTART is passed, then more debug information containing the VOSVs is printed out.

The vectors VEIN and WCOS are printed on the first pass thru C0NTER.

**VEIN**: (SITE of angle between lowest and highest node in column)

<table>
<thead>
<tr>
<th>V</th>
<th>1</th>
<th>0.1000E 01</th>
<th>2</th>
<th>0.1000E 01</th>
<th>3</th>
<th>0.1000E 01</th>
<th>4</th>
<th>0.1000E 01</th>
<th>5</th>
<th>0.1000E 01</th>
</tr>
</thead>
</table>
| WCOS**: (COST of angle between lowest and highest node in column.)

| WCOS | 1 | 0.1000E 01 | 2 | 0.1000E 01 | 3 | 0.1000E 01 | 4 | 0.1000E 01 | 5 | 0.1000E 01 |

**Columns**

<table>
<thead>
<tr>
<th>Column no. 1</th>
<th>Column no. 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Data for</td>
<td>Data for</td>
</tr>
<tr>
<td>Node number</td>
<td>Node number</td>
</tr>
<tr>
<td>being</td>
<td>being</td>
</tr>
<tr>
<td>processed</td>
<td>processed</td>
</tr>
</tbody>
</table>

**Data for Column no. 1**

<table>
<thead>
<tr>
<th>X2</th>
<th>X1</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1</td>
</tr>
</tbody>
</table>

**Data for Column no. 2**

<table>
<thead>
<tr>
<th>X2</th>
<th>X1</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>6</td>
</tr>
</tbody>
</table>

**Partially printed lines**

<table>
<thead>
<tr>
<th>0</th>
<th>0</th>
<th>0</th>
<th>0</th>
<th>0</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2322E 03</td>
<td>0.2322E 03</td>
<td>0.2322E 03</td>
<td>0.2322E 03</td>
<td>0.2322E 03</td>
<td>0.2322E 03</td>
</tr>
<tr>
<td>0.2322E 03</td>
<td>0.2322E 03</td>
<td>0.2322E 03</td>
<td>0.2322E 03</td>
<td>0.2322E 03</td>
<td>0.2322E 03</td>
</tr>
</tbody>
</table>

**Partially printed lines**

<table>
<thead>
<tr>
<th>0</th>
<th>0</th>
<th>0</th>
<th>0</th>
<th>0</th>
<th>0</th>
</tr>
</thead>
<tbody>
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INERT .gt. 0 debug output from user's DFCBFL.
INERT is decremented by 1 in CONDES for each pass thru CONDES when INERT i.e. 0 debug print-stops.

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**Note:**
- P1111: Pseudo-viscosity
- B1111: Mixing length
- H1111: Interimanty factor
- V1111: Velocity at upper node
- V1111-1-11: Velocity at lower node
- P1111: Pressure at upper node
- V1111-1-11: Pressure at lower node

**Eddy visc.**
- B1111-1: Basu defect
- B1111-2: Outer region
IDIPRT is documented by 1 for each pass thru NLPINS, when IDIPRT is 0, debug print stops.

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|     | x2  | 0.0           | 0.0           | 0.66667E 00 (non-dim. normal coordinate) |
|     |     |               |               | (L-matrix) |
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| 6   | 0.15000E 01 |               |               |               |               |               |
|     | L-matrix (K-matrix) |
| 1   | 0.10000E 01 | -2 | 0.0 | 3 | 0.0 | 4 | 0.10000E 01 |
| .2115 | 0.11111E 00 | 2 | -0.11111E 00 | 3 | 0.23611E 01 | 4 | 0.0 | 5 | -0.22500E 01 |
| .211 | 2.11111E 00 | 2 | -0.11111E 00 | 3 | 0.0 | 4 | 0.11111E 00 | 5 | 0.23611E 01 |
| 6   | -0.22500E 01 | 7 | 0.0 | 8 | -0.22500E 01 | 9 | 0.22500E 01 |

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<tr>
<td>16</td>
<td>0.16667E 01</td>
<td>17</td>
<td>0.30000E 01</td>
<td>18</td>
<td>0.30000E 01</td>
</tr>
<tr>
<td>19</td>
<td>0.30000E 01</td>
<td>20</td>
<td>0.23500E 01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>0.12500E 00</td>
<td>22</td>
<td>0.10000E 01</td>
<td>23</td>
<td>0.11951E 01</td>
</tr>
<tr>
<td>24</td>
<td>0.66667E 00</td>
<td>25</td>
<td>0.23500E 01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>26</td>
<td>0.12500E 00</td>
<td>27</td>
<td>0.11951E 01</td>
<td>28</td>
<td>0.66667E 00</td>
</tr>
<tr>
<td>29</td>
<td>0.12500E 00</td>
<td>30</td>
<td>0.30000E 01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### X13 (height of transformed triangle)

<p>| | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.49314E 00</td>
<td>2</td>
<td>0.33333E 01</td>
<td>3</td>
<td>0.65518E 00</td>
</tr>
<tr>
<td>4</td>
<td>0.33333E 01</td>
<td>5</td>
<td>0.14907E 01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>0.23333E 01</td>
<td>7</td>
<td>0.17195E 01</td>
<td>8</td>
<td>0.33333E 01</td>
</tr>
<tr>
<td>9</td>
<td>0.22999E 01</td>
<td>10</td>
<td>0.33333E 01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>0.23333E 01</td>
<td>12</td>
<td>0.23333E 01</td>
<td>13</td>
<td>0.65518E 00</td>
</tr>
<tr>
<td>14</td>
<td>0.23333E 01</td>
<td>15</td>
<td>0.19444E 01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>0.23333E 01</td>
<td>17</td>
<td>0.19444E 01</td>
<td>18</td>
<td>0.33333E 01</td>
</tr>
<tr>
<td>19</td>
<td>0.19444E 01</td>
<td>20</td>
<td>0.23333E 01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>0.23333E 01</td>
<td>22</td>
<td>0.12904E 01</td>
<td>23</td>
<td>0.16667E 01</td>
</tr>
<tr>
<td>24</td>
<td>0.16667E 01</td>
<td>25</td>
<td>0.15000E 01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>26</td>
<td>0.10000E 01</td>
<td>27</td>
<td>0.12904E 01</td>
<td>28</td>
<td>0.16667E 01</td>
</tr>
<tr>
<td>29</td>
<td>0.14907E 01</td>
<td>30</td>
<td>0.16667E 01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
The document contains a table with columns labeled "GLOBAL VECTOR" and "Condim. nodal values of dependent variable being computed at this time." The table rows include numerical values. Additionally, there is a paragraph discussing the output from DERBVSL and the process of integrating nodes using the GSLN subroutine. The document also mentions the use of the GSLN subroutine to integrate nodes and the integration of dependent variables across boundaries.
Test Case

Two data decks, generating a nominal Mach 5 isoenergetic boundary layer flow and the three-dimensional virtual source simulation [Ref. 1], come as standard test cases for 3DBR COMOC. The listings of these data decks are included in Appendices A and B. Another problem specification can be readily adapted from these decks, since approximately one-third of a data deck is associated with standard call sequences and output format specification and arrangement instructions. Instructions for additions to these standard data outputs follows discussion of the data decks. This discussion covers details pertinent to the data deck for the Mach 5 test case. Comments and descriptions should be interpreted with reference to Appendix A. Subsequently, the alterations required to establish the non-uniformly discretized virtual source problem data deck from the Mach 5 test case are presented and discussed.

Preparation of the data deck is subdivided into four phases.

### Phase I. Reference Conditions and Control Parameter Specification

<table>
<thead>
<tr>
<th>Call</th>
<th>Parameter Code</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>FEBL</td>
<td></td>
<td>Starts execution of COMOC</td>
</tr>
<tr>
<td>COMTITLE</td>
<td></td>
<td>Reads one title card to appear on cover page of output</td>
</tr>
<tr>
<td>FENAME</td>
<td>&amp;NAME01</td>
<td>Initialization</td>
</tr>
<tr>
<td>NEQKNN</td>
<td></td>
<td>Integer parameter input</td>
</tr>
<tr>
<td>IGAS</td>
<td>0</td>
<td>Number of dependent variables to be integrated in X1 direction</td>
</tr>
<tr>
<td>IFR</td>
<td>0</td>
<td>Isoenergetic flow with constant cp</td>
</tr>
<tr>
<td>KDUMP</td>
<td>0</td>
<td>General flows</td>
</tr>
<tr>
<td>KDUMP</td>
<td>1</td>
<td>Equilibrium composition (IGAS=1)</td>
</tr>
<tr>
<td>KDUMP</td>
<td>1</td>
<td>Frozen composition</td>
</tr>
<tr>
<td>NPVSX</td>
<td></td>
<td>Suppress debug output</td>
</tr>
<tr>
<td>NSCX</td>
<td>0</td>
<td>Print debug output</td>
</tr>
<tr>
<td>NSCX</td>
<td>1</td>
<td>No. of entries in pressure table</td>
</tr>
<tr>
<td>NSCY</td>
<td>1</td>
<td>Uniform X3 interval in discretization</td>
</tr>
<tr>
<td>NSCY</td>
<td>1</td>
<td>Non-uniform X3 interval in discretization</td>
</tr>
<tr>
<td>UINF</td>
<td></td>
<td>Reference (freestream) velocity (F/S)</td>
</tr>
<tr>
<td>TØFINF</td>
<td></td>
<td>Reference stagnation temperature (°R)</td>
</tr>
<tr>
<td>REFLL</td>
<td></td>
<td>Reference length (F)</td>
</tr>
<tr>
<td>TØ</td>
<td>&amp;NAME02</td>
<td>Initial X1 station (F)</td>
</tr>
<tr>
<td>Call</td>
<td>Parameter Code</td>
<td>Function</td>
</tr>
<tr>
<td>-------</td>
<td>---------------</td>
<td>--------------------------------------------------------------------------</td>
</tr>
<tr>
<td>TD</td>
<td></td>
<td>Length of X1 solution, starting at T0 (F)</td>
</tr>
<tr>
<td>DELP</td>
<td></td>
<td>Percent of TD at which output is desired</td>
</tr>
<tr>
<td>EPS</td>
<td></td>
<td>Integration control parameter (.01 to .0001)</td>
</tr>
<tr>
<td>VSTART</td>
<td></td>
<td>Percent of TD at which transverse velocity (U2) computation starts</td>
</tr>
<tr>
<td>XSCALE</td>
<td></td>
<td>Multipliers to convert discretization to feet</td>
</tr>
<tr>
<td>YSCALE</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CPA,CPH</td>
<td></td>
<td>Specific heats, stagnation temperatures, and molecular weights for two- component, isoenergetic, frozen flow mixing (IGAS=0)</td>
</tr>
<tr>
<td>XMA,XMH</td>
<td></td>
<td></td>
</tr>
<tr>
<td>FEDIMN</td>
<td></td>
<td>Generate vector lengths and array entry points.</td>
</tr>
</tbody>
</table>

**Phase II. Finite Element Discretization**

**LINK1 1**  
This call generates the finite element discretization of the X2X3 plane. The data are read in free format fields. A "T" terminates any sequence.

A. Automatic Uniform Discretization  
Occurs for NSCX = NSCY = 0  
Set XSCALE = desired element width in the X3 direction  
Set YSCALE = desired element height in the X2 direction  
Read selection keys  
e.g. YSCALE = 0.004  
XSCALE = 0.002  
1 21, 1 2,  
T  
Generates discretization made up of 21 node rows x 2 node columns, or 40 elements (x 1 element). Elements are 0.004 F high by 0.002 F wide.

B. Automatic Non-Uniform Discretization  
Occurs for NSCX = 1 and NSCY = 1  
Set X3 discretization first, X2 discretization second.  
Data are used in sets of 3 integers at a time. First integer identifies finite element interval concerned, next two indicate element width (or height) as ratio in feet, e.g., 3/1200 = 3/1200(F).  
e.g. 1 3 1200, 2 1 600, 3 5 1200, ...  
T  
T 1 600, 7 1 600, 8 7 1200, ...  
T 1 11, 1 4,  
T
This generates a finite element discretization of 11 node rows × 4 node columns. The element widths (intervals between node columns) are respectively 3/1200 (F), 1/600 (F), ... . The height of the first 7 element rows is uniformly 1/600 (F), eighth is 7/1200 (F), etc.

Phase III. Output Specification

Following the discretization phase, the user can input up to 10 title cards to head each generated output sequence. The next -65 input cards specify output format, see Appendix A, and are typically not to be changed without reference to the programmer's manual. Up to 10 title cards can follow the standard output specification to fully describe the problem being solved. This output will occur once, directly after printing of the cover page.

DONE Calls end to output specification phase

Phase IV. Solution Parameters, Boundary Conditions, and Initial Distributions

<table>
<thead>
<tr>
<th>Call</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>VX3ST</td>
<td>Establishes NPVSX entries into static pressure table as function of X1</td>
</tr>
<tr>
<td>e.g. 11*10.05 0.1</td>
<td>Eleven pressure values at intervals ΔX1 of 0.05, starting at X1 = 0.1.</td>
</tr>
<tr>
<td>VPVSX</td>
<td>Read pressures in PSFA</td>
</tr>
<tr>
<td>e.g. 4.3494 3.41...</td>
<td></td>
</tr>
<tr>
<td>IPINT</td>
<td>Standard Input consisting of integer array of numbers corresponding to dependent variables. Program will integrate first NEQKNN of them, plus U2.</td>
</tr>
<tr>
<td>KBNO (N)</td>
<td>KBNO (N) establishes fixed boundary conditions for dependent variables N through NN.</td>
</tr>
<tr>
<td>KBNO (NN)</td>
<td></td>
</tr>
<tr>
<td>e.g. KBNO 4</td>
<td>Fixes variable 4 nodes on bottom of discretization at their initial input values.</td>
</tr>
</tbody>
</table>
ICALL -1
ICALLS -1
LINK3 4
LINK1 3

VTEMP -58
Read initial nodal total temperature distribution. Non-dimensionalize entries by number in location 58 (TREF).

VYY - (X)
Reads initial conditions for dependent variable N. Non-dimensionalize entries by number in |X|.

VYYEND (N)

QKNINT DESCRIPT
DONE
DESCRIPT 3

DONE COMOC

EXIT

If a second test case is desired, insert data deck starting with COMTITLE before EXIT card.

Standard completion of data deck
Listed in Table 9 are the changes to the Mach 5 test case data deck required to establish the three-dimensional virtual source data deck. The complete listing of the latter is included as Appendix B. The following explains the alterations with respect to input phase and the line numbers in Table 9.

<table>
<thead>
<tr>
<th>Input Phase</th>
<th>Line No.</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>I 1</td>
<td></td>
<td>Title card for output cover page</td>
</tr>
<tr>
<td>I 2</td>
<td></td>
<td>Reference condition and control parameters for combustion calculations using five dependent variables</td>
</tr>
<tr>
<td>I 7</td>
<td></td>
<td></td>
</tr>
<tr>
<td>II 8</td>
<td></td>
<td>Form non-uniform discretization, using 11 node rows × 6 node columns, producing 100 finite elements</td>
</tr>
<tr>
<td>III 13</td>
<td></td>
<td></td>
</tr>
<tr>
<td>III 14</td>
<td></td>
<td>Title card to head each output call</td>
</tr>
<tr>
<td>III 15</td>
<td></td>
<td>Detailed problem description</td>
</tr>
<tr>
<td>IV 22</td>
<td></td>
<td>Entry locations of longitudinal pressure distribution (constant)</td>
</tr>
<tr>
<td>IV 24</td>
<td></td>
<td>66 nodes have uniform stagnation temperature</td>
</tr>
<tr>
<td>IV 26</td>
<td></td>
<td>Initial ( U_1 ) distribution</td>
</tr>
<tr>
<td>IV 36</td>
<td></td>
<td></td>
</tr>
<tr>
<td>IV 37</td>
<td></td>
<td>Initial ( U_2 ) distribution is zero</td>
</tr>
<tr>
<td>IV 38</td>
<td></td>
<td>Initial ( O_2 ) distribution reflects location of virtual source</td>
</tr>
<tr>
<td>IV 39</td>
<td></td>
<td>Initial ( N_2 ) distribution</td>
</tr>
<tr>
<td>IV 40</td>
<td></td>
<td>Initial ( H_2 ) distribution</td>
</tr>
</tbody>
</table>

Hence, establishing the data deck for a multiple dependent variable, three-dimensional problem using a non-uniform finite element discretization is readily accomplished. In this case, only forty data card changes were required, using the two-dimensional Mach 5 data deck as a master deck.
**TABLE 4**

**DATA DECK CHANGES TO PRODUCE VIRTUAL SOURCE SIMULATION**

<table>
<thead>
<tr>
<th>Line</th>
<th>Line Content</th>
</tr>
</thead>
<tbody>
<tr>
<td>O1</td>
<td>CHECK CASE FOR THREE DIMENSIONAL REACTING BOUNDARY REGION FLOW</td>
</tr>
<tr>
<td>O2</td>
<td>NFOKNN=5, IGAS=1, IFR=0, KDUMP=0,</td>
</tr>
<tr>
<td>O3</td>
<td>NPSX=2, NSCX=1, NSCY=1,</td>
</tr>
<tr>
<td>O4</td>
<td>NEI2=1,</td>
</tr>
<tr>
<td>O5</td>
<td>UNIN=2272.0, TDFIN=533.0, REFL=0.033333333,</td>
</tr>
<tr>
<td>O6</td>
<td>TD=0.0, TD=0.10, DELP=5.0,</td>
</tr>
<tr>
<td>O7</td>
<td>XSCALE=C.003333333, YSCALE=0.003333333, VSTART=101.0,</td>
</tr>
<tr>
<td>O8</td>
<td>1 25 100, 2 50 100, 3 125 100, 4 150 100, 5 225 100,</td>
</tr>
<tr>
<td>O9</td>
<td>T INCREMENTS BETWEEN X3, NODE-NUMERATOR-DENOMINATOR</td>
</tr>
<tr>
<td>O10</td>
<td>1 5 10, 7 5 10, 8 125 100, 9 175 100, 10 250 100,</td>
</tr>
<tr>
<td>O11</td>
<td>T INCREMENTS BETWEEN X2</td>
</tr>
<tr>
<td>O12</td>
<td>1 11, 1 6,</td>
</tr>
<tr>
<td>O13</td>
<td>T 11 ROWS AND 6 COLUMNS NORMALIZED BY LREF, HENCE X-Y SCALES = LREF</td>
</tr>
<tr>
<td>O14</td>
<td>CHECK CASE, THREE DIMENSIONAL REACTING BOUNDARY REGION - VIRTUAL SOURCE</td>
</tr>
<tr>
<td>O15</td>
<td>CHECK CASE, THREE DIMENSIONAL REACTING BOUNDARY REGION - VIRTUAL SOURCE</td>
</tr>
<tr>
<td>O16</td>
<td>(H2/O2/AIR SYSTEM WITH EQUILIBRATED CHEMISTRY). PROBLEM CONSIDERED</td>
</tr>
<tr>
<td>O17</td>
<td>REPRESENTS TRANSVERSE H2 INJECTION INTO A SUPERSONIC AIR STREAM</td>
</tr>
<tr>
<td>O18</td>
<td>CHARACTERISTIC OF SCRAMJET FUEL INJECTION, SEE ROGERS NASA TNC-6114,</td>
</tr>
<tr>
<td>O19</td>
<td>1971 AND NASA TNO-6476, 1971 FOR EXPERIMENTAL STUDY OF THIS PROBLEM.</td>
</tr>
<tr>
<td>O20</td>
<td>TURBULENCE MODEL EMPLOYED IS DESCRIBED IN USER'S MANUAL NASA CR-13245091974.</td>
</tr>
<tr>
<td>O21</td>
<td>CALCULATIONS ARE STARTED USING VIRTUAL SOURCE CONCEPT TO REPLACE</td>
</tr>
<tr>
<td>O22</td>
<td>COMPLEX NEAR INJECTION FLOW FIELD.</td>
</tr>
<tr>
<td>O23</td>
<td>0.0 100. T XI TABLE FOR PRESSURE</td>
</tr>
<tr>
<td>O24</td>
<td>193. 193. T PRESSURE TABLE PSF</td>
</tr>
<tr>
<td>O25</td>
<td>6*533.0</td>
</tr>
<tr>
<td>O26</td>
<td>6*533.0</td>
</tr>
<tr>
<td>O27</td>
<td>6*1503.0</td>
</tr>
<tr>
<td>O28</td>
<td>6*1660.0</td>
</tr>
<tr>
<td>O29</td>
<td>2<em>1550.0 4</em>1759.0</td>
</tr>
<tr>
<td>O30</td>
<td>2<em>1550.0 4</em>1833.0</td>
</tr>
<tr>
<td>O31</td>
<td>2<em>1550.0 4</em>1852.0</td>
</tr>
<tr>
<td>O32</td>
<td>2<em>2272.0 4</em>1942.0</td>
</tr>
<tr>
<td>O33</td>
<td>2<em>2272.0 4</em>1985.0</td>
</tr>
<tr>
<td>O34</td>
<td>2<em>2272.0 4</em>2074.0</td>
</tr>
<tr>
<td>O35</td>
<td>2<em>2272.0 4</em>2169.0</td>
</tr>
<tr>
<td>O36</td>
<td>6*2272.0</td>
</tr>
<tr>
<td>O37</td>
<td>6*533.0</td>
</tr>
<tr>
<td>O38</td>
<td>18<em>233 2</em>0.0 4<em>233 2</em>0.0 4<em>233 2</em>0.0 34*233</td>
</tr>
<tr>
<td>O39</td>
<td>18<em>767 2</em>0.0 4<em>767 2</em>0.0 4<em>767 2</em>0.0 34*767</td>
</tr>
<tr>
<td>O40</td>
<td>18<em>0.0 2</em>1.0 4<em>0.0 2</em>1.0 4<em>0.0 2</em>1.0 34*0.0</td>
</tr>
</tbody>
</table>
Sample output for the three-dimensional virtual source test case is presented in Appendix D. The processing of pre-solution output is identical to the Mach 5 test case, and complete solution outputs are presented for the initial and final solution station. For the aspect ratio of this particular discretization, COMOC ascertained the six outputs could be placed on a page as illustrated. Appendix E contains listings of the specifically written subroutines for eddy viscosity, laminar viscosity, and effective Schmidt and Prandtl number for the virtual source simulation.

An additional output array can be readily provided by COMOC during the output phase of execution. For example, referring to Appendix A, suppose that the array U3/UREF is to be printed. Then, in I0SAVE -1, before the card headed by T, add 3248 to card headed by 1247. The "3" refers to dependent variable number three, which is U3 in the YY array, and 248 is the entry position in the YY matrix in the IZ array. Also, in IOMULT -1, change entry to 15*2. Finally, in DESCRIP2, on third card headed EFF.MU/MUREF, add U3/UREF in columns 65-80.
SYMBOLS

CROSS REFERENCE LIST FOR EQUIVALENCED VARIABLES

7 ITOT - CONTROL PAR. INSTEAD FOR GENERATING OUTPUT.
60 IRL - 1 = BOUNDARY LAYERS PROGRAM,
- C = NAVIER-STOKES PROGRAM.
117 ITOT1 - PRINT TALLY AND OUTPUT FOR GAS IN GRANIT.
113 ITOT2 - PRINT INTERMEDIATE STEPS IN GRANIT.
122 ITEND - NO. OF TIMES FOR AXIS-SYM. CORES.
127 ITENDT - NO. OF TIMES TO PRINT TALLY, OUTPUT IN WELLS.
115 ITORD - READ YOUR WORK IN 2015-5 FORMAT IN SETUP.
120 ITED - 1 = FROZEN CALCULATION IN THEPO.
122 ICAS - 1 = CALI SAMPLES,
- C = CALL TRIG.
116 ITINIT - INITIALICATION PARAMETER IN THEPO.
65 IMAT - NO. OF MATERIALS IN PROGRAM.
128 IMATM - NO. OF MATERIALS IN MATERIAL TABLE.
111 INAV - HIGHEST NODE IN CELL AT WHICH TO USE F1 CURVE.
130 INGAS - STARTED VORTEX IN GAS.
158 INBIT - INITIATION IN CORES.
28 IPASS - NO. OF CALLS TO DERIV.
122 IPEMT - COUNTING NO. OF OUTPUTS FOR INTER. OUTPUT.
122 IPEMPE - F/R POSITION IN INDEX ARRAY.
A IPOS - 1 TO 2 = INDEX FOR PRESENT OR PAST VALUE OF CRI,
- VARIABLES AND DERIVATIVE (SET IN GRANIT)
122 ITPM - FRM CNL, ING, DNG (USUALLY ONLY 1)
126 ISPED - 1 = CONTROL SAVED BEFORE ENTERING OUTPUT STATE.
37 IIOA - I = OUTPUT.
146 ITP - TEMPERATURE INITIATION COUNT IN GRANIT.
133 ITOP - NO. OF TIMES FOR WHICH TO PRINT IN GRANIT.
141 KALPE - COUNT OF REQUIRED TO USE SPECIF. AREA OR HEIGHT IN 42.
41 KOPEN - PRINT OUTPUT CARDS AND DATA GENERATED IN PRINT.
4 KVAR - - INTEGRATION TECHNIQUE.
K = MAXIMUM ABSOLUTE STABILITY.
2 = MAXIMUM RELATIVE STABILITY.
97 KINV - K = INVERTED, USED IN 141) OFF = 4
17 KINV - 1 = INVERTED.
12 KINOF - PRINT OUTF. IF OUTPUT IF = 1.
7 KINOF - ORIGIN TALLY, PRINT OUTPUT KNOCK LIVES.
16 KINOF - PRINTING OUTPUT LIMIT (LIMITED BY LIMIT).
12 KINOF - ORIGIN TALLY, PRINT OUTPUT LIMIT.
113 KONVL - NO. OF VARIATION TO BE PLTTER OR PUNCH.
12 KONVT - PRINT OPTION (SET DURING EXECUTION).
- 1 = CALL "PRINT",
- 1 = CALL "FIND"
82 KONVT - 1 = PRINTS IN DISCRIMINATION. OFF = 120

172

ORIGIINAL PAGE A
OF POOR QUALITY
136 KS	AV - PLOT TAPE NO. SAVED IN QKNT.  
50 LCOL - NO. OF COLLUMNS IN DISCRETIZATION.  
156 LFIL - FILL PARAMETER USED IN ELM.  
47 LG - NO. OF COLS. USED IN COATES AND DFCFBL.  
34 LPRINT - LIMIT ON OUTPUT COLUMNS.  
137 LPS1A1 - PSIROC INPUT 1 = PRINT, 2 = SLOPE AT LOWER NODE  
13H LPS1A2 - PSIROC INPUT 1 = PRINT, 2 = SLOPE AT UPPER NODE  
157 LRS - DISCRETIZATION PARAMETER USED IN ELM.  
102 MTM - NO. OF PASSES IN FCSLTP.  
22 NR - NO. OF CHAR. IN EACH WORD OF OUTPUT VAR. TITLE.  
131 NBORD - NO. OF NODES AROUND BORDR OF DISCRETIZATION.  
69 NASET - 1 = STORE DEP. VARIABLE INTO YY ARRAY AND PRINT INTEGRATION NODES. (USED IN 'NBDRY')  
O = STORE YY ENTRY IN DEP. VARIABLE.  
-1 = STORE DEP. VARIABLE INTO YY ARRAY.  
22 NRUG - 1 = PRINT OUTPUT FROM 'LTH' ROUTINES.  
22 NC - NO. OF CHARACTER IN OUTPUT FORMAT.  
125 NCALLS - NO. OF ROUTINES TO CALL AT END OF QKNT.  
13 NCOORD - 0 = TWO DIMENSIONAL.  
1 NO = AXIS-SYMMETRIC (NOT OPERATIONAL)  
69 NCPTMP - NO. OF ENTRIES IN SPECIFIC HEAT TABLE.  
1 NO = INITIALIZATION PARAMETER IN DFCSN.  
51 NDCT - QKNT IA CODE TO DETERMINE MINIMUM STEP SIZE.  
124 NDERIV - 7 = CALL DERIVS. R = CALL DERRAL.  
48 NDEE - NO. OF DEGREES OF FREEDOM. (USED IN LTH)  
56 NDNUTZ = C = SET LP DOLTP VECTOR IN *STRE ONLY ENCE.  
92 NDOF = APPROX. LENGTH OF DOLTP VECTOR.  
162 NDPVSY - NO. OF DOPXY'S IN THENE TABLE.  
155 NFTPDC - SET = 1 IF ELEMENTS ARE TO BE ADDED IN FLEM.  
154 NLEDEL - SET = 1 IF ELEMENTS ARE TO BE DELETED IN FLEM.  
14 NLEEM - NUMBER OF ELEMENTS (TRIANGLES).  
95 NMIN - STARTING LOC. PAR. IN DIF ARRAY.  
31 NEQ = NO. OF DEP. VARIABLES TO BE SOLVED.  
58 NFKNN - NO. OF DEP. VARIABLES TO BE INTEGR. USING 'QKNT'.  
45 NFEX = NO. OF BOUNDARY NODES IN JACUN Array. (LTH)  
107 NFF2 - 1 = LSE F1 CURVE FOR EPSILCN.  
2 = LSE F1 AND FP CURVE FOR EPSILCN IN DFCFBL.  
46 NF = NO. OF 'NA' BYTE WORDS IN TITLE FOR EACH DEP. VAR.  
96 NFTRCL = CONTROL PAR. IN FANCHO FOR 1ST OR SUBS. PASSES.  
104 NFRCP = PLOT PARAMETER TO MIRROR OUTPUT. (2=MIRROR)  
119 NFUG = PRINT IMPLT AND OUTPLT IN THREMD.  
130 NGETH = COUNTER IN DPHOS TO INIT. VARIABLES IN GAS.  
95 NH = NO. OF ELEMENTS CONTAINING BOUNDARY GRACIFAT INFORMATION FOR 'LH', 'TRE' AND 'F'.  
53 NH2 = NO. OF INCREASES IN STEP SIZE IN QKNT.  
54 NHHALF = NO. OF DECREASES IN STEP SIZE IN QKNT.  
68 NI = STARTING LOC. IN YY ARRAY FOR DEP. VAR. NP.  
63 NIND = '171 ARRAY STARTING LOC. PAR. APPROX. = 5*NOCE  
65 NJ = STARTING LOC. IN 22 ARRAY FOR DEP. VAR. NP.  
88 NLINE = LINE COUNT FOR OUTPUT CONTROL.  
60 NNPNT = NO. OF VARIABLES TO BE PRINTED.  
15 NNP - LINEAR APPROX. INDEX.  
16 NNODE = NUMBER OF NODES.  

ORIGINAL PAGE: OF POOR QUALITY.
| 17 | MNS  | LINEAR APPROX. INDEX | DEF. = 6 |
| 55 | NODE  | **17** ARRAY STARTING LOC. PARAMETER. MIN. = NODE + 3 |
| 150 | NO MOD | NODE NO. AT WHICH DRAGS IS COMPUTING |
| 19 | NPF | NO. OF EQUATION HEING SCELLED FOR DEP. VAR. **NP** |
| 5 | NMEFP | NO. OF BOUNDARY NODES TC TC SOLVEX FOR IN **CMEOC** |
| 143 | NONC | NON-CONVERGENCE CODE IN GAS |
| 142 | NOUTPR | NO. OF SCALARS TO PRINT IN OUTPUT |
| 30 | NO | DEP. VARIABLE BEING SOLVED |
| 14 | NPART | NO. OF PARTITIONS (USED IN **LTH**) | DEF. = 2 |
| 101 | NPRESS | NO. OF NODES AT WHICH PRESSURE IS COMPUTED |
| 20 | NPRINT | NO. OF PRINT POSITIONS ON A LINE OF OUTPUT. C = 132 |
| 145 | NPSDEL | NO. OF BOUNDARIES TO COMPUTE PSIRC |
| 134 | NPSIQC | NO. OF NODES READ IN FOR PSIRC |
| 2 | NPSLOC | NO. OF FIXED ST. LOC. (USED IN **STREF** |
| 11 | NPTIME | NO. OF POINTS / DEG. OF FREEDOM (JHUCN.C PAR.) |
| 24 | NPTFL | NO. OF POINTS / ELEMENT. (LTH) | DEF. = 3 |
| 153 | NPUIF | SET = 1 IF ELEMENTS AND NODES ARE TO BE PRINTED |
| 161 | NPVEX | NO. OF PRESSURES IN P VS X TABLE |
| 45 | NPXL | NO. OF POINTS / ELEMENT. (LTH) | DEF. = 3 |
| 66 | NPXPS | STEADY STATE PARAMETER IN **DERIV** |
| 21 | NROW | DEP. VAR. AND DERIVATIVE ALTERNATOR IN CNMNAT |
| 6 | NRSN | LOGICAL TABLE NO. TO READ RESTART DATA IN **PRINT** |
| 37 | NRSTOP | LOGICAL TABLE NO. TO STORE RESTART COND. IN **LINK2** |
| 67 | AS | PRINTOUT CONTROL PARAMETER |
| 151 | NSVG | SET = 1 IF INTERVAL INPLT IS TO BE READ FOR YYYY IN INCRT. |
| 152 | ASCII | SET = 1 IF INTERVAL INPLT IS TO BE READ FOR YYYY IN INCRT. |
| 144 | ASCRIE | RESET SWITCH TO CHANGE ALEFZ IN DECEZ |
| 144 | ASCRIE | RESET CONDITION FLAG IN FINDE |
| 27 | ASKIP | NO. OF READ. LOCATIONS / DEP. VARIABLE |
| | | DEF. = NACCE / 3 |
| 64 | ASW | STOP PROGRAM IF OUTPUT EXP. GT. NSW. | DEF. = 10 |
| 156 | N$ | SET = 1 IF SOURCE DATA IS TO BE USEC ON RIGHT HAND SIDE IN CNRMAL |
| 17 | ASEC | V. OF SPECIES IN SOLUTION. DEFAULT = 9 |
| 160 | WSRSC | C = NO SOURCE COMPUTATION FOR ENTHALPY. |
| | | 1 = USE PHIL SOURCE COMPUTATION |
| | | 2 = USE PHIL + PSI2 SOURCE COMP. (ACT. USEC) |
| 145 | WSRSC | SET = 1 IF SOURCE CHANG IN DECEB |
| 140 | WSCNS | STARTUP PARAMETER IN CNRTNS |
| 142 | WSCNS | STARTUP PARAMETER IN DECEB |
| 20 | NTITL | V. OF TITLE CARDS TO BE READ IN **SETUP** AND PRINTED AT THE BEGINNING OF EACH OUTPUT SET |
| 93 | NK | V. OF ELEMENTS HAVING NON-CONSTANT THICKNESS |
| 94 | NUPW | V. OF L-PARALLEL ELEMENTS IN STREF |

| 74 | AVV | DEP. VARIABLE NO. FOR ENTHALPY | DEF. = 4 |
| 70 | AVV | DEP. VARIABLE NO. FOR PSI | DEF. = 5 |
| 71 | AVV | DEP. VARIABLE NO. FOR OMEGA |
| 72 | AVV | DEP. VARIABLE NO. FOR VELOCITY 1 |
| 73 | AVV | DEP. VARIABLE NO. FOR VELOCITY 2 |
| 90 | AVV | NO. OF TIME INTERVALS TO STORE YY |
| 77 | AVV | NO. OF TIME INTERVALS TO STORE 77 | MUST = 2 |
ENTRIES

156 AINF - REFERENCE SPEED OF SOUND.
   IF LINF .LE. C, AINF = SQRT(G*GAMMAF*PINF/RHCTAF)
   IF LINF .GT. C, AINF = SQRT(G*GAMMAF*RUNI*TCFINF/XMA)

* AJ - MOLES CONSTANT. 77E.2A

3 ALC - CHARACTERISTIC ELEMENT SIZE.  DEF. = MIN. SIDE

115 BSTART - NOT LSED

176 CRTOKJ - SPECIFIC HEAT BRITISH TO MKS 4.184

83 COMPX - COMPRESSION FACTOR FOR OUTPUT COL VECTOR.
   INDICATES PERCENT OF XL AXIS TO BE USED TO SHORTEN
   PRINT SPACING INTERVALS.  DEF. = 0.0

84 COMPY - COMPRESSION FACTOR FOR OUTPUT ROW VECTOR.
   SAME AS COMPC, ALT FOR X2 AXIS.

124 CON - CONSTANT LSED IN DFCFBL  DEF. = 0.4

70 CONRHO - IF GT C.0, SET ALL RHO = CONRHO.

62 CONV - OUTPUT SCALE FACTOR = 1.0 / REFL

77 CON1 - ALC / (RE*CP)*TINF*XMLINF

78 CON2 - CON1 / TOFINF

158 CPA - SPECIFIC HEAT OF AIR.  DEF. = 0.24

159 CPPH - SPECIFIC HEAT OF HYDROGEN.  DEF. = 3.445

160 CPINF - SPECIFIC HEAT COMPLETED IN CPINIT.

30 CPDINF - REFERENCE SPECIFIC HEAT.

153 CVCP - SPEC. HEAT CONV. LSED IN THERMC.  DEF. = 4186.0

148 CVH - ENTHALPY CONVERSION.LSED IN THERMC.  DEF. = 1.0

151 CVP - PRESSURE CONV. LSED IN THERMC.  DEF. = 5725 E-3

152 CVRHDO - DENSITY CONV. LSED IN THERMC.  DEF. = 16.02

150 CVT - TEMP. CONVERSION LSED IN THERMC.  DEF. = 1.0

149 CVU - VELOCITY CONVERSION LSED IN THERMC.  DEF. = 0.0408

130 C4ED - CONSTANT LSED IN DFCFBL  DEF. = 0.00023

143 C4EDSW - PERCENT OF TO AT WHICH TO SWITCH C4ED IN DFCFBL.

144 C4FACT - MULTIPLIER FOR NEW C4ED AFTER C4EDSW OCCURS.

13 DELP - PERCENT INTERVAL FOR PRINTOUT.  DEF. = 2.0

133 DEPLT - PERCENT OF TO TO BE LSED FOR PLOTTING STATIONS.

111 DELX3 - TIME STEP LSED IN CONTES.

113 DELAST - TIME STEP LSED IN CONTES.

114 DELXLX - TIME STEP LSED IN CONTES.

161 DPIINF - RPMINF * LININF

165 DRTOKK - DEGREES RANKINE TO DEGREES KELVIN 5.0/9.0

175 FBTOKJ - ENTHALPY BRITISH TO MKS 2.3244

137 FLIPSA - NOT LSED

138 FLIPSAR - NOT LSED

135 FLIPS - NOT LSED

136 FLIPSK - NOT LSED

14 EPS - ACCURACY TEST BETWEEN PREDICTOR-CORRECTOR FORMULAS

145 FLF2SW - PERCENT OF TO AT WHICH TO SWITCH: FROM E1 TO E2

1 FACT - NON-DIM FACTOR = ALC / XMA

80 FACTH - 1.0 / (CPINF*TOFINF)

59 FACTMU - RPMINF * LININF * ALC

175
56 RTCON5 = UINF**2 / (RTCON1*CPCINF*TCFINF)
57 RTCON6 = 2.6 * RTCON4
117 RTMIN = T0 * (T0/TCA - 1.0)
28 RUNIV = UNIVERSAL GAS CONSTANT. DEFAULT = 1545.33
129 SCT = CONSTANT SCHMIDT NUMBER DEFAULT = 0.7
108 SCTRMIN = NOT USED
107 SCTRMT = NOT USED
131 SPLIT = CUTOFF LSFED IN H2MTX DEFAULT = 0.02835
44 SQ2 = SQRT(2.0)
51 STHMIN = NOT USED
73 STLCCR = REF. CON. TEMP. IN SUTHERLAND. DEFAULT = 204.0
74 STLDFX = EXPONENT IN SUTHERLAND. DEFAULT = 1.5
77 STLDTTR = REF. TEMP. IN SUTHERLAND. DEFAULT = 492.0
71 SULVR = VISCOITY LSFED IN SUTHERLAND. DEFAULT = 1163 E-4
57 SSINIT = M SINIT / FACT
36 TP = TOTAL SOLUTION TIME FROM TC.
47 TFCGF = MINIMUM TEMPERATURE.
24 TF = FINAL TIME = TO + TD
4 THK = DEFAULT NON-DIM. THICKNESS OF ELEMENTS. (1.0)
22 TIME = CURRENT TIME.
24 TP = STARTING TIME.
146 TTA = AIR TEMPERATURE FOR COMPUTATIONS IN DIMEN.
59 TFINF = REFERENCE TEMPERATURE.
147 TTH = HYDROGEN TEMPERATURE FOR COOMPUTATIONS IN DIMEN.
40 TRATTH = 1.0 + (GAMMA-1.0) * XMACH**2 / 2.0
25 TRNC = INTEGRATION PARAMETER IN QCKNUIN.
155 TSINF = STATIC TEMPERATURE COMPUTED IN COINIT.
26 TVFR = PI * 2.0
46 UEFCOE = MAXIMUM L VELOCITY.
27 UINF = VELOCITY (FREESTRAEM)
141 VA = MAJOR AXIS OF ELLIPSE FOR VIRTUAL SOURCE.
142 VA = MINOR AXIS OF ELLIPSE FOR VIRTUAL SOURCE.
104 VELCSF = UINF**2 / (2.0*G*A/J*CPA*TOA)
139 VS = CENTER OF H2 ELLIPSE FOR VIRTUAL SOURCE.
140 VK = CENTER OF H2 ELLIPSE FOR VIRTUAL SOURCE.
177 VLBTON = VISCOITY BRITISH TO MKS 1.488
178 VLBTOP = VISCOITY BRITISH TO CGS 14.88
102 VSTART = PERCENT OF TO AT WHICH TO START V COMP. IN CONTES
81 XI = INITIAL MUM. ON XI AXIS. DEFAULT = 0.0
125 XLAM = CONSTANT LSFED IN DCFBR DEFAULT = 0.09
37 XLE = LEWIS NUMBER. DEFAULT = 1.0
109 XMA = MOLECULAR WEIGHT OF AIR. DEFAULT = 28.97
61 XMA = LOCAL MACH NUMBER.
154 XMACHS = INITIAL MACH NO. LSFED IN DIMEN.
66 XMF = MASS FRACTION OF FLUID.
172 XMFACT = UINF * SQRT((YMA/(TCFING*GAMMA*G*RUNIV)))
110 XMH = MOLECULAR WEIGHT OF HYDROGEN. DEFAULT = 2.016
118 XMWDF = MASS DEPOSIT COMPUTED IN G3CCNC.
126 XMUAP = VISCOITY OF AIR. 0.0000115
127 XMUH2 = NOT LSFED
38 XMUNF = VISCOITY (FREESTRAEM)
128 XMUP = NOT LSFED
98 XPRIME = NON-DIM. PRESSURE GRADIENT AT PRESENT STATION.
52 XSCALE - XICOR SCALE FACTOR. DEFAULT = 1.0
41 XSHIFT - SHIFT X-COORDINATE. DEFAULT = 0.0
76 XT - OUTPUT STATIC TIME = TIME + FACT / REFL
112 X3LAST - LAST TIME STEP USED IN CENIFS.
82 YI - INITIAL COORD. ON X2 AXIS. DEFAULT = 0.0
53 YSCALE - Y2COR SCALE FACTOR. DEFAULT = 1.0
42 YSHIFT - SHIFT Y-COORDINATE. DEFAULT = 0.0
101 YUP - UPPER Y IN DECR.
173 ZMAX - MAX. DERIVATIVE COMPLETED IN QKNUIN.
29 ZT - DIMENSIONAL CLRFAT TIME.
65 ZTFST - STOP PROGRAM WHEN MAX. (ZZ) LE ZTFST. DEF. = .1E-4
IZARRAY

**DEFINITION OF ENTRY POINTS IN IZ ARRAY.**

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<th>DESCRIPTION</th>
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<td>202 IRW</td>
<td>OUTPUT ROW VECTOR USED IN FEOUTP.</td>
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<tr>
<td>203 IEMTHD</td>
<td>HEADINGS FOR OUTPUT VARIABLES.</td>
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<td>204 ITITLE</td>
<td>TITLE FOR START OF EACH OUTPUT PHASE.</td>
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<td>205 IPRINT</td>
<td>LIST OF DEPENDENT VARIABLES.</td>
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<tr>
<td>206 IKBNO</td>
<td>NO. OF BOUNDARY NODES / DEP. VARIABLE.</td>
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<tr>
<td>210 IINCOL</td>
<td>NO. OF NODES PER COLUMN.</td>
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<td>211 IINROW</td>
<td>NO. OF NODES PER ROW.</td>
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<td>218 ICPTAB</td>
<td>SPECIFIC HEAT TABLE ENTRIES</td>
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<td>219 ITTAB</td>
<td>TEMPERATURE TABLE ENTRIES.</td>
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<td>220 ITUSED</td>
<td>COUNTER USED FOR OUTPUT IN FEOUTP.</td>
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<tr>
<td>223 IX1POS</td>
<td>TEMPORARY STORAGE FOR XCOR COORDINATES.</td>
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<td>224 IX2POS</td>
<td>TEMPORARY STORAGE FOR YCOR COORDINATES.</td>
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<td>225 I1INDV</td>
<td>ARRAY OF BOUNDARY NODES FOR DEPENDENT VARIABLES.</td>
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<td>226 IINDF</td>
<td>LIST OF ELEMENT CONNECTIONS (3/ELEMENT).</td>
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<td>SOLUTION ORDER OF NODES FOR DEP. VAR. IN DERIV.</td>
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<td>ORDER OF NODES BY COLUMNS FROM LEFT TO RIGHT.</td>
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<td>ORDER OF NODES BY ROWS FROM TOP TO BOTTOM.</td>
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<td>237 IIELEM</td>
<td>NO. OF ELEMENTS CONNECTED TO NODES.</td>
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<td>238 IIBORD</td>
<td>LIST OF BORDER NODES IN CCW ORDER.</td>
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<td>241 IB211</td>
<td>B211 MATRIX COMPUTED IN GEOMFL.</td>
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<td>242 IB211S</td>
<td>B211S MATRIX COMPUTED IN GEOMFL.</td>
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<tr>
<td>245 IB211A</td>
<td>B211A ANTI-SYMMETRIC MATRIX.</td>
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<td>247 IDIF</td>
<td>FIRST HALF USED TO STORE DIFFUSION COEFFICIENTS. 2ND HALF USED TO STORE SOURCE TERMS.</td>
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<td>248 IYY</td>
<td>STORAGE FOR 2 VALUES OF DEPENDENT VARIABLES.</td>
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<td>249 IZZ</td>
<td>STORAGE FOR 2 VALUES OF DERIVATIVES FOR DEP. VAR.</td>
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<td>ELEMENT LENGTHS COMPUTED IN GEOMFL.</td>
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<td>AREA OF ELEMENTS TIMES THICKNESS COMP. IN GEOMFL.</td>
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REFERENCES


APPENDIX A
DATA DECK LISTING FOR MACH 5
THO-DIMENSIONAL FLOW CHECK CASE

FEAL
COMTILE
CHECK CASE, TWO-DIMENSIONAL SUPERSONIC FLOW WITH PRESSURE GRADIENT
FNAME
GNAME01
END
GNAME02
END
FEDIMN
L INK 1
1 2 1000, 2 2 ICCC,
T
1 2 1000, 21 2 ICCC,
T
1 21, 1 2,
T
CHECK CASE, TWO-DIMENSIONAL SUPERSONIC FLOW WITH PRESSURE GRADIENT

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<th>REFERENCE</th>
<th>ENGLISH-FT</th>
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HOLIST
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VELOCITY............ FT/S............ NA............ M/S............ CM/S............
DENSITY............ LB/FT3............ NA............ KG/M3............ G/CC............
TEMPERATURE........ RAANING............ NA............ KELVIN............ NA............
ENTHALPY............ RT/LBH............ NA............ KJ/KG............ N.A............
PROPERTIES HEAT......... RT/LBM............ NA............ KJ/KC-K............ N.A............
VISCOSITY............ LM/FT-S............ NA............ NT-S/M2............ POISE............
LOCAL PRESSURE........ PSF............ PSI............ NT/M2............ TORR............

182
### LOCAL SOLUTION

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### TOSAVE -1

1248 284 204 10200
2248 278 4248 9248 8248
1247 334 252 114

### IOMULT -1

14*2

### DESCRIPT 2

**U1/UREF** T/TREF H/STAT/HREF RHO/RHOREF ELEM. N2 MAS.FRAC
**U2/UREF** CPF/CPRREF HTOT/HREF FLEM. H2 MAS.FRAC ELEM. O2 MAS.FRAC
**EFF. MU/MUREF EFF. PRANDTL NO. MU/MUREF EFF. SCHMIDT NO.**

**CCMOC**

**DESCRIP**

**CCMOC** CHECK CASE FOR TWO-DIMENSIONAL FLOW WITH PRESSURE GRADIENT. A COMPARABLE SIMILARITY SOLUTION HAS BEEN REPORTED BY CHRISTIAN ET AL., ARL 70-0023. SPECIFIC CASE CONSIDERED CORRESPONDS TO MACH NO. 5 BETA = 0.5, S 0 = 0 (ADIABATIC WALL). SOLUTION STARTED AT X = 0.10 FT. WITH SIMILAR SOLUTION PROFILE. LAMINAR FLOW WITH VISCOSITY FROM SUTHERLANDS LAW.

**DISCRETIZATION SPANS THREE TIMES INITIAL BOUNDARY LAYER THICKNESS. ISOENERGETIC FLOW WITH TOTAL TEMPERATURE = 1800 R.**

### DONE

**VXST**

11*10.05 0.1

**T X1 TABLE FOR PRESSURE**

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**FIXES U1 (VARIABLE NO. 1) ALONG WALL TO INITIAL VALUE**

**FIXES U2 (VARIABLE NO. 2) ALONG WALL TO INITIAL VALUE**

**DONE**
FIXES H (VARIABLE NO. 4) ALONG WALL TO INITIAL VALUE

ICALL -1
2 5 2 1 1 2
ICALLS -1
10 6 4 12 5 6 3

LINK3 4
LINK1 3

VFEND

62*1000.

T INITIAL TOTAL TEMPERATURE PROFILE

VYY -27
2*0.0 7*8.65, 2*16.54, 2*2373, 2*30.94, 2*3550, 2*3879,
2*3992, 2*4004, 2*4004, 2*4004, 2*4004.

T INITIAL U1 PROFILE

VYYEND

VYY -27
2*0.0 2*5.2, 2*20.14 2*53.52 2*83.2 2*109.3 2*165,
2*253, 2*447, 2*456.

T INITIAL U2 PROFILE

VYYEND 2

VYY

42*233C

T INITIAL O2 MASS FRACTION PROFILE

VYYEND 8

VYY

42*767C

T INITIAL N2 MASS FRACTION PROFILE

VYYEND 10

VYY

42*0.4C

T INITIAL w2 MASS FRACTION PROFILE

VYYEND 9

2XINT

DESCRIP'T

NONE

DESCRIPT 3
REFERENCE LENGTH LREF
REFERENCE VISCOSITY LAMINAR VALUE
EVALUATED AT REF. TEMPERATURE
FREE STREAM VELOCITY AT X0(LREF)
STAGNATION TEMPERATURE (CONSTANT = LREF)
FREE STREAM DENSITY AT X0(LREF)
FREE STREAM STATIC PRESSURE AT X0
NUMBER OF NODES
NUMBER OF FINITE ELEMENTS
NONE
CCMOD
END
EXIT
APPENDIX B
DATA DECK LISTING FOR VIRTUAL SOURCE
THREE-DIMENSIONAL CHECK CASE

FEAL
CONTILE
CONOC CHECK CASE FOR THREE DIMENSIONAL REACTING BOUNDARY REGION FLOW
FENANE
&NAMED1
NEQKN=5, IGAS=1, IFR=0, KDUMP=0,
NPVSS=2, NSCX=1, NSCY=1,
&END
&NAME2
UINF=2272., TCFINF=533.0, REFN=0.03333333,
TD=0.0, T=0.10, DELP=0.0,
YSCALE=0.03333333, YSCALE=0.03333333, VSTART=101.0,
&END
FEDNM
LINK1 1
1 75 100, 2 50 100, 3 125 100, 4 150 100, 5 225 100,
T INCREMENTS BETWEEN X3, NODE-NUMERATOR-DENOMINATOR
1 5 10, 7 5 10, 8 125 100, 9 175 100, 10 250 100,
T INCREMENTS BETWEEN X2
1 111, 1 11,
T 11 ROWS AND 6 COLUMNS NORMALIZED BY LREF,HENCE X-Y SCALES =LREF
CHECK CASE, THREE DIMENSIONAL REACTING BOUNDARY REGION - VIRTUAL SOURCE

REFERENCE ENGLISH-FT ENGLISH-IN M-K-S C-G-S
--------------- ------------- ------------- --------------

NONE

UPARA -1
2 2 162 164 163
2 2 2 164 163
2 2 2 170 174
2 2 2 165 2
2 -175 2 2 2
2 2 2 176 2
2 2 2 177 178
2 2 169 168 167
2 2 2 2 2
2 2 2 2

HOLIST
LENGTH.............. FT.............. IN.............. M.............. CM..............
VELOCITY.............. FT/S.............. NA.............. M/S.............. CM/S..............
DENSITY.............. LBM/FT3........... NA.............. KG/M3........... G/CC............
TEMPERATURE........... RANKINE........... K.............. KELVIN........... N/A..............
ENTHALPY.............. BTU/LBM........... NA.............. KJ/KG........... N/A..............
FROZ.*SPEC. HEAT ....... BTU/LBM-R........ NA.............. KJ/KG-R........ N/A..............
VISCOITY.............. LBM/FT-S........... NA.............. NT-S/H2........ POISE........
LOCAL PRESSURE ....... PSF.............. PSI.............. NT/H2........ TORR........
LOCAL SOLUTION ....... MACH NO. DPDX1(LBF/FT3) MAX. H2 CONC. MIX EFF.(ETA)
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10SAVF -1
1248 285 320 284 10248
2248 278 4248 9248 8248
1247 334 252 314

T U, T, HS, RH0, N0, V, CP, HTOT, H2, N2, DIFU, PR NO., LAM, VISC, SCT, NO.

10MUL -1
14*2
T U, T, HS, PH0, N0, V, CP, HTOT, H2, N2, DIFU, PR NO., LAM, VISC, SCT, NO.

DESCRIPT 2
V1/LREF | T/LREF | HSTAT/LREF | RHOC/RHOREF | ELEM, N0 | MAS, FRAC |
|---------|--------|------------|-------------|---------|-----------|
U2/LREF | CPF/CPFREF | HTOT/LREF | ELEM, H2 | MAS, FRAC | ELEM, N0 | MAS, FRAC |

DESCRIPT
CHECK CASE, THREE-DIMENSIONAL REACTING BOUNDARY REGION - VIRTUAL SOURCE
(2D/2A/AIR SYSTEM WITH EQUILIBRIUM CHEMISTRY), PROBLEM CONSIDERED
REPRESENTS TRANSVERSE H2 INJECTION INTO A SUPERSONIC AIR STREAM
CHARACTERISTIC OF SCRAMJET FUEL INJECTION, SEE ROGERS NASA TND-6114,
1971 AND NASA TND-476, 1971 FOR EXPERIMENTAL STUDY OF THIS PROBLEM.
CALCULATIONS ARE STARTED USING VIRTUAL SOURCE CONCEPT TO REPLACE
COMPLEX NEAR INJECTION FLOW FIELD.

NONE

VX3ST

0,0
100.

T X1 TABLE FOR PRESSURE

VPVSY

193.

T PRESSURE TABLE PSF

PRINT -1
1 4 8 10 4 3 2
T INTEGRATE U1, FATH, C2, N2, H2, U3, U2

NONE

KEND

1

DEFINES U1 (VARIABLE NO. 1) ALONG WALL TO INITIAL VALUE

KEND

2

DEFINES U2 (VARIABLE NO. 2) ALONG WALL TO INITIAL VALUE

KEND

4

DEFINES U (VARIABLE NO. 4) ALONG WALL TO INITIAL VALUE

RETURN

30CNE

186
KENDO 8
BOTTOM 3DONE
FIFER N0. 3 ALONG WALL TO INITIAL VALUE
KENDO 9
BOTTOM 3DONE
FIFER N0. 3 ALONG WALL TO INITIAL VALUE
KENDO 10
BOTTOM 3DONE
FIFER N0. 3 ALONG WALL TO INITIAL VALUE
ICALL 4
2 5 2 1 1 2
ICALLS I
10 6 4 12 5 6 3
LINK3 4
LINK1 3
VTENP 66.533.
T INITIAL TOTAL TEMPERATURE PROFILE
VYV -27
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VYV -27
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T INITIAL U2 PROFILE
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T INITIAL O2 MASS FRACTION PROFILE
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VYV
18.233 2.00. 4.233 2.00. 4.233 2.00. 34.233
T INITIAL N2 MASS FRACTION PROFILE
VYVEND 10
VYV -27
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T INITIAL N2 MASS FRACTION PROFILE
VYVEND 9
QMNINT
DESCRIPTION
NONE
DESCRIPTION 3
REFERENCE LENGTH, LREF 43 FT
REFERENCE VISCOITY, LAMINAR VALUE 38 LBM/FT-S
EVALUATED AT REF. TEMPERATURE
FREESTREAM VELOCITY AT X0(=UREF) 27 FT/S
STAGNATION TEMPERATURE=(CONSTANT,=UREF) 27 DEG R
FREESTREAM DENSITY AT X0(=URHREF) 10 LBM/FT3
FREESTREAM MACH NUMBER AT X0 154
STATIC PRESSURE AT X0 9 PSF
NUMBER OF NODES -16
NUMBER OF FINITE ELEMENTS -14
NONE
END
EXIT
APPENDIX C

SAMPLE OUTPUT FOR MACH 5
TWO-DIMENSIONAL FLOW CHECK CASE
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2 variables being integrated.

7 variables in solution.

Order of calls at end of iteration:
LINK1, LINK2, LINK3, LINK4, LINK5, LINK6, LINK7

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### Additional Notes

- All values are in scientific notation.
- The table represents a set of initial conditions for a system or process.
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#### CHECK CASE, TWO DIMENSIONAL, SUPERSONIC FLOW WITH PRESSURE GRADIENT

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APPENDIX D

SAMPLE OUTPUT FOR VIRTUAL SOURCE
THREE-DIMENSIONAL FLOW CHECK CASE
COMPUTATIONAL CONTINUUM MECHANICS
THREE-DIMENSIONAL BOUNDARY REGION VARIANT

CASE: THREE DIMENSIONAL BOUNDARY REGION - VIRTUAL SOURCE 04/26/74
PROBLEM DESCRIPTION

CUMULATIVE CASE FOR THREE DIMENSIONAL REACTING BOUNDARY REGION FLOW

CFL2D/3D1P SYSTEM WITH EQUILIBRIUM CHEMISTRY: "PROBLEM" CONSIDERED

REPRESNTS TRANSVERSE N2 INJECTION INTO A SUPERSONIC AIR STREAM


TURBULENT MODEL EXPONENTIAL DESCRIBED IN USER'S MANUAL NASA CR-34114.

CALCULATIONS ARE STARTED USING VIRTUAL SOURCE CONCEPT TO REPLACE

COMPOUND INJECTION FLOW FIELD.

6 NODES FOR VARIABLE 1

3 NODES FOR VARIABLE 2

3 NODES FOR VARIABLE 3

3 NODES FOR VARIABLE 4

3 NODES FOR VARIABLE 5

3 NODES FOR VARIABLE 6

60 INTEGRATION NODES FOR VARIABLE 1

60 INTEGRATION NODES FOR VARIABLE 2

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**CHECK CASE: THREE-DIMENSIONAL EXCITING BOUNDARY REGION - VIRTUAL SOURCE**

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**N + PASS**

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| EFF. ,PRANLIV NO. E  | 0.70000 0.70000 0.70000 0.70000 0.70000 0.70000 | 0.70000 0.70000 0.70000 0.70000 0.70000 0.70000 | 0.70000 0.70000 0.70000 0.70000 0.70000 0.70000 |

| SKIN, FRICTION DISTRIBUTION(E/F)  | 0.999100 | 0.999100 | 0.999100 | 0.999100 | 0.999100 | 0.999100 |

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APPENDIX E

LISTINGS OF AUXILIARY USER-WRITTEN SUBROUTINES FOR EDDY VISCOSITY, PRANDTL NUMBER, SCHMIDT NUMBER, AND LAMINAR VISCOSITY FOR VIRTUAL SOURCE SIMULATION.
SUBROUTINE FCFCFL
& ( INCOL, INDEX, INODE, IPINT, XICOR, X2COR, AREA, RHO, RHOU,
1 U, W, Y, EPSLN, YY, SCHMT, E1, E2, AL, GAMMA, CFV2 )
C C TWO LAYER EDDY VISCOSITY MODEL FOR COLD FLOW HYDROGEN MIXING
C E1 = MIXING LENGTH MODEL
C E2 = MASS DEFECT MODEL
C COMPUTE EDDY VISCOSITY IN TERMS OF NON-DIMENSIONAL PARAMETERS
C BEFORE LEAVING SUBROUTINE, DIMENSIONALIZE BY
C FACTMU = ALC * RHOR = RHOU
C Y(11) - NON-DIMENSIONALIZED BY ALC
C RHO - NON-DIMENSIONALIZED BY RHOU
C CON = MIXING LENGTH CONSTANT
C C4ED = MASS DEFECT CONSTANT
C OMEGA = VAN DRIEST DAMPING FACTOR
C GAMMA = INTERMITTENCY FACTOR
C XMSDF = MASS DEFECT IN REGIONS CONTAINING ONE PERCENT OR MORE H2
C (NOT THE USUAL DEFINITION OF MASS DEFECT).
C ARR = AREA OF FLOW CONTAINING ONE PERCENT OR MORE H2.
C E1E2SW IS LOCATION DOWNSTREAM (FT) WHERE THE TURBULENCE MODEL
C SWITCHES FROM COMPLETELY MIXING LENGTH TO THE TWO LAYER MODEL.
C F1E2SW USED ONLY FOR VIRTUAL SOURCE SIMULATION
C PCNT IS THE PERCENT OF H2 DEFINING THE OUTER EDGE OF
C THE MIXING ZONE.
C NOTE - SPECIAL SUBSCRIPTING TECHNIQUE USED TO LOCATE Y(X2), U(UJ)
C AND RHO RUNNING UP COLUMNS OF NODES, THIS WAS REQUIRED FOR
C COMPUTING MIXING LENGTHS AND DERIVATIVES OF UI WITH RESPECT TO THE
C NORMAL TO THE WALL (X2).
C NOTE - CONSTANTs WERE DETERMINED BY FITTING PREDICTIONS TO DATA OF
C IF DERUG PRINT OUT FOR E1 AND E2 COMPUTATIONS IS REQUESTED,
C SET IWHIT = 1
C
C DIMENSION Y(1), RH0(1), U(1), ALF(1), TEMP(1)
C DIMENSION INCOL(1), INDEX(1), AREA(1), INODE(1)
C DIMENSION XICOR(1), X2COR(1), RHOU(1), W(1), YY(1), EPSLN(1)
C DIMENSION FI(1), E2(1), AL(1), GAMMA(1), CFV2(1)
C DIMENSION SCHMT(1)
C COMMON / VARBLE / IARRAY(00200), IARRAY(0400)
C EQUIVALENCE ( IARRAY(00016), NNODE )
C EQUIVALENCE ( IARRAY(00030), NP )
C EQUIVALENCE ( IARRAY(00047), LG )
C EQUIVALENCE ( IARRAY(00070), NVQ3 )
C EQUIVALENCE ( IARRAY(00071), NVU )
C EQUIVALENCE ( IARRAY(00086), KPNT )
C EQUIVALENCE ( IARRAY(00107), NE1F2 )
C EQUIVALENCE ( IARRAY(00108), NVQ3 )
C EQUIVALENCE ( IARRAY(00111), IMAX )
C EQUIVALENCE ( IARRAY(00122), IWHIT )
C EQUIVALENCE ( IARRAY(00141), KALO3 )
C EQUIVALENCE ( IARRAY(00143), NT )
C EQUIVALENCE ( IARRAY(00144), NS )
C EQUIVALENCE ( IARRAY(00145), NS2 )
C EQUIVALENCE ( IARRAY(00030), ALC )
C EQUIVALENCE ( IARRAY(00021), PE )
C EQUIVALENCE ( IARRAY(00023), TIME )
C EQUIVALENCE ( IARRAY(00038), XmUNIF )
C EQUIVALENCE ( IARRAY(00059), FACTMU )
C
EQUIVALENCE ( RARRAY(00101), YUP )
EQUIVALENCE ( RARRAY(00118), XMSDF )
EQUIVALENCE ( RARRAY(00124), CON )
EQUIVALENCE ( RARRAY(00125), XLM )
EQUIVALENCE ( RARRAY(00126), XMUAI )
EQUIVALENCE ( RARRAY(00127), XMUH2 )
EQUIVALENCE ( RARRAY(00128), XMUP )
EQUIVALENCE ( RARRAY(00129), SCT )
EQUIVALENCE ( RARRAY(00130), C4ED )
EQUIVALENCE ( RARRAY(00133), PCNT )
EQUIVALENCE ( RARRAY(00134), Q3MAX )
EQUIVALENCE ( RARRAY(00143), C4EDSW )
EQUIVALENCE ( RARRAY(00144), C4FACT )
EQUIVALENCE ( RARRAY(00145), F1E2SW )
EQUIVALENCE ( RARRAY(00010), RHOREF )
EQUIVALENCE ( RARRAY(00027), UREF )
EQUIVALENCE ( RARRAY(00046), UE )
EQUIVALENCE ( RARRAY(00048), RHOE )

SET CONSTANTS FOR TURBULENCE MODEL

AVD = 25.3
CND=0.135
C4ED=0.0007
F1E2SW=0.02
PCNT=1.0
USAP = FACTMU
XLM=0.0753
XMUW = AVD / XMUAI
I4AX=2
FRAC = XLM / CND*.7

DEBUG OUTPUT HEADINGS

IF ( NT .EQ. 0 .AND. IWRIT.GT.0 ) WRITE(6,9600)
9600 FORMAT (1H1, 9X,6HE11(LL), 9X,6HAL(LL), 6X,9HGAMMA(LL), 10X, *5H(I), 22X,8HY(KTI), 5X,10HY(KTI-1), 9X,6HRH0(I) )
9610 FORMAT ( 1H0, 8E15.5 )
9620 FORMAT ( 1H1, 5I( 4H E2(, 13, 3H) =, E13.5) )

INITIALIZE ARRAY COUNTERS

XT = TIME * ALC
IF ( NS .GT. 0 ) GO TO 30
IF ( XT .LT. E1E2SW ) GO TO 30
NE1E2 = 3 - NE1E2
KPNT = 1
NS = 1
30 CONTINUE
IF ( NS2 .GT. 0 ) GO TO 40
IF ( XT .LT. C4EDSW ) GO TO 40
KPNT = 1
NS2 = 1
40 CONTINUE

SET UP ARRAY INDICES.

NP = NVU,
CALL LINK3 ( 1, U(1), YY(1) )
NP = NVQ3
CALL LINK3 ( 1, W(1), YY(1) )
DO 100 K = 1, NNODE
RHOU(K) = (HK) * RHO(K)
100
COMPUTE MAX. H2 MASS FRACTION. COMPUTE AREA CONTAINING H2 LEVELS
*GT.1.0 PERCENT
COMPUTE MASS DEFFCT.
CALL O3CONC ( INOF, AREA, W, RHOU, ARR )
ARR = SORT (ARR)
KT = 1

COMPUTE MIXING LENGTH MODEL
FL = L**2 * OMEGA * GAMMA * ABS(DU/DY).

DD 600 KK = 1, LG
M = INCOL(KK)
IF ( M .LT. 2 ) GO TO 600
N = INDEX(KT&I-1)

VAN ORNIST DAMPING FACTOR

RHOED = RHOE * RHOREF
UED = UE * UREF
TAUW = CDV2(KK) * RHOED * UED * UED

OMEGA = 1.0

GAMMA(1) = 1.0
E(1) = 0.0
AL(1) = CON * Y(KT)
DO 200 LL = 2, M
II = LL - 1
I = INDEX(KT&II-1)
JP1 = INDEX(KT&II)
YUP = Y(KT&M-1)
MM2 = MM - 2
IU = INDEX(KT&M-1)
DO 160 IU = 1, MM2
IL = INDEX(KT&M-IJ-1)

VAL = ABS ( U(II)L / U(IU) - 1.0 )

DTERMINE UPPER BOUNDARY OF HYDROGEN CONCENTRATION

IF ( NUO3 .GE. 3 )
*VAL = ABS ( W(II) / O3MAX )
IF ( VAL .GT. PCNT ) YUP = Y(KT&M-IJ-1)
IF ( VAL .GT. PCNT ) IMAX = M - IJ
IF ( VAL .GT. PCNT ) GO TO 170

160 CONTINUE
170 CONTINUE
X1 = Y(KT&L-1) / Y(KT&M-1)
AL(LL) = CON * Y(KT&L-1)
IF ( Y(KT&L-1) .LT. FRAC*YUP ) GO TO 190
AL(LL) = XLAM * YUP

190 CONTINUE
GAMMA(LL) = 1. / ( 1. & XI **9)
RHVO = RH0(IP1)* RHOREF
YVD = Y(KT&L-1)*ALC
IF ( TAUW .GT. 0.0 )
*OMEGA = OMEGA - EXP ( - YVD * XMTW / ( TAUW * RHVO )**.5 )

COMPUTE E1 AND E2. BOTH ARE VECTORS WHICH WILL BE FILLED.

VISOSITY SELECTED FROM E1 OR E2

E1(LL) = AL(LL)*AL(LL)*OMEGA*GAMMA(LL)*ABS( (U(IP1)-U(I))/
1 ( Y(KT&II) - Y(KT&II-1)) ) * RH0(IP1)
KTP1 = KT & II

219
KTPM = KT & II - 1 
IF ( NT .LE. 0 ) GO TO 250 
IF ( IWRIT .NE. 0 ) GO TO 250 
WRITE ( 6, 9610 ) LL, LL, LL, [PI, I, KTPM, IPI, 
* E(I), AL(LL), GAMMA(LL), U(I), Y(KTPM), Y(KTPM), RHO(I) ) 
250 CONTINUE 
200 CONTINUE 
IF ( KALL03 .EQ. 0 ) ARR = Y(KTSM-1) 
TEMP1 = C4ED * XMSDF / ARR 
DO 400 J = 1, M 
E2(J) = GAMMA(J) * TEMP1 
400 CONTINUE 
IF ( IWRIT .GT. 0 .AND. NT .EQ. 0 ) 
WRITE ( 6, 9620 ) ( K, E2(K), K = 1, M ) 
C C IF E1 IS LESS THAN E2, USE E1. WHEN E1 BECOMES GREATER THAN E2 US 
C E2 FOR THE REMAINDER OF THE COEFFICIENTS. 
C 
KODE = 0 
DO 500 K = 1, M 
J = K 
I = INDEX(KTKM) 
IF ( KODE .EQ. 1 ) GO TO 450 
IF ( K .GT. IMAX ) GO TO 450 
EPSLN(I) = E1(J) * USR 
GO TO 475 
450 CONTINUE 
KODE = 1 
IF ( NE1E2 .NE. 2 ) EPSLN(I) = E1(J) * USR 
IF ( NE1E2 .EQ. 2 ) EPSLN(I) = E2(J) * USR 
475 CONTINUE 
500 CONTINUE 
K = KT & M 
600 CONTINUE 
NT = 1 
RETURN 
FNO