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COMOC: THREE DIMENSIONAL BOUNDARY REGION VARIANT

PROGRAMMER'S MANUAL

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### TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>SUMMARY</td>
<td>1</td>
</tr>
<tr>
<td>INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>PROBLEM TASK DESCRIPTION</td>
<td>4</td>
</tr>
<tr>
<td>METHOD OF SOLUTION</td>
<td>7</td>
</tr>
<tr>
<td>PROGRAM DESCRIPTION</td>
<td>16</td>
</tr>
<tr>
<td>Subroutine Descriptions</td>
<td>19</td>
</tr>
<tr>
<td>Macro Flow Charts</td>
<td>31</td>
</tr>
<tr>
<td>OPERATING INSTRUCTIONS</td>
<td>150</td>
</tr>
<tr>
<td>General</td>
<td>150</td>
</tr>
<tr>
<td>Editing and Diagnostics</td>
<td>152</td>
</tr>
<tr>
<td>Test Case</td>
<td>165</td>
</tr>
<tr>
<td>SYMBOLS</td>
<td>172</td>
</tr>
<tr>
<td>REFERENCES</td>
<td>181</td>
</tr>
<tr>
<td>APPENDIX A Mach 5.0 Data Deck</td>
<td>182</td>
</tr>
<tr>
<td>APPENDIX B Virtual Source Data Deck</td>
<td>185</td>
</tr>
<tr>
<td>APPENDIX C Mach 5.0 Sample Output</td>
<td>188</td>
</tr>
<tr>
<td>APPENDIX D Virtual Source Sample Output</td>
<td>203</td>
</tr>
<tr>
<td>APPENDIX E Listings of Diffusion Coefficient Subroutines</td>
<td>216</td>
</tr>
</tbody>
</table>
FIGURES

1. COMOC Macro Structure .................. 3
2. IBM 360/65 Deck Set-Up for Program ........ 151

TABLES

1. Standard Finite Element Matrix Forms For
   Simplex Functionals in One- and Two-Dimensional
   Space ............................... 12
2. MAIN Link of COMOC ...................... 17
3. Overlay Structure of COMOC for IBM 360/65 .... 18
4. Data Deck Changes to Produce Virtual Source
   Simulation ............................ 170
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

\[ u_i = u_1 \hat{i} + u_2 \hat{j} + u_3 \hat{k} \]  \hspace{1cm} (1)

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

\[ (\ )_1 \hat{i} + (\ )_2 \hat{j} + (\ )_3 \hat{k} \]  \hspace{1cm} (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

\[ 0 = (\rho u_1),_i + (\rho u_1),_1 \]  

\[ \rho u_1 v^1 = \left[ \frac{\mu_e}{Sc \cdot Re} \gamma^1 \right],_k - \rho u_k v^1, - s^1 \]  

\[ \rho u_1 u^1, = \left[ \frac{\mu_e}{Re} u^1, \right],_k - \rho u_k u^1, - p^1 \]  

\[ \rho u_1 u^3, = \left[ \frac{\mu_e}{Re} u^3, \right],_k - \rho u_k u^3, - p^3 \]  

\[ \rho u_1 H^1 = \left[ \frac{\mu_e}{Re \cdot Pr} H^1 \right],_k - \rho u_k H^1, \]  

\[ - M^2 \left[ \frac{1}{Pr} \frac{\mu_e}{2Re} \left( u^1 u^1 \right),_k \right] \]  

\[ - \left[ \frac{Sc-Pr}{Sc-Pr} \frac{\mu_e}{Re} \gamma^1 \right],_k \]  

The variables appearing in Eq. (3)-(7) are non-dimensionalized with respect to \( \rho \infty, U \infty, c \infty, T \infty, \) 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

\[ \frac{\mu_e}{Pr} = \frac{\mu_e}{Pr} + \frac{Pe}{PrT} \]  

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
\[ H = \sum_{\alpha} h_{\alpha} y_{\alpha} + \frac{1}{2} u_{k} u_{k} \]  

(9)

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

\[ h_{\alpha}^{0} \equiv \int_{T_{0}}^{T} c_{p} \, dT + h_{\alpha}^{0} \]  

(10)

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

\[ p = \rho R T \sum_{\alpha} \frac{y_{\alpha}}{M_{\alpha}} \]  

(11)

where \( R \) is the universal gas constant and \( M_{\alpha} \) 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.

\[ 2H + O \leftrightarrow H_{2}O \]

\[ 2H \leftrightarrow H_{2} \]

\[ 2O \leftrightarrow O_{2} \]

\[ H + O \leftrightarrow OH \]

\[ N_{2} + O \leftrightarrow 2NO \]  

(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 \( nA + mB \leftrightarrow \lambda C \), are expressed in terms of species mole fraction, \( \chi_{\alpha} \), 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.

\[ [N^B \alpha] [X^\alpha] = \{\text{const.}\} \]  

(14)

In Eq. (14), the elements of the matrix \([N^B \alpha]\) 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

\[ L(q) = \kappa[K(q)q, k] + f(q, q, x, x^i) - g(q, x) = 0 \]  

(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, \(\chi\) 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 \(\Omega\), with closure \(\partial\Omega\), where

\[ \Omega = R \times [x_0, x) \]  

(16)

and \(x_0 < x < \infty\). For Eq. (15) uniformly parabolic, unique solutions for \(q\) are obtained pending specification of boundary
constraints on \( \partial R \) and an initial condition on \( R \cup \partial R \). For the former, the general form relates the function and its normal derivative everywhere on the closure, \( \partial R \), as

\[
\varepsilon(q) \equiv a(1)q(x_i^\varepsilon, x) + a(2)kq(x_i^\varepsilon, x), k\eta - a(3) = 0 \tag{17}
\]

In Eq. (17), the \( a(i)(x_i^\varepsilon, x) \) are user specified coefficients, the superscript \( \varepsilon \) notation constrains \( x_i \) to \( \partial R \), and \( \eta \) is the local outward-pointing unit normal vector. For an initial distribution, assume given throughout \( R \cup \partial R \times x_o \),

\[
\phi(x_i, x_0) \equiv q_0(x_i) \tag{18}
\]

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 sub-domains, \( R_m \), described by \( (x_i^\varepsilon, x) \in R_m \times [x_0, x] \) called "finite elements," wherein \( \bigcup R_m = R \). 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

\[
q_m^*(x_i, x) \equiv \{\phi(x_i)\}^T \{q(x)\}_m \tag{19}
\]

wherein the functionals \( \phi_k(x_i) \) are members of a function set complete in \( R_m \), and the unknown expansion coefficients, \( Q_k(x) \), 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, \( \ell(a_m^*) \), 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

\[
\int_{R_m} \{\phi(x_i)\} L(q_m^*) d\tau - \lambda \int_{\partial R_m \cap \partial R} \{\phi(x_i)\} \ell(q_m^*) d\sigma \equiv 0 \tag{20}
\]
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

$$\int_{\Omega_m} \left\{ \phi(x_i) \right\} K q^*_m \kappa \tau \left( \sum_{k} \kappa \left\{ \phi(x_i) \right\} K q^*_m \kappa \right) \kappa d\tau = \kappa \int_{\Omega_m} \left\{ \phi(x_i) \right\} K q^*_m \kappa n_k \kappa d\sigma$$

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

$$\int_{\Omega_m} \left[ -\kappa \int_{\Omega_m} \left\{ \phi \right\} K q^*_m \kappa d\tau + \int_{\Omega_m} \left\{ \phi \right\} (f^*_m - g^*_m) d\tau \right] = \int_{\Omega_m} \left\{ \phi \right\} \left( \bar{a}^{(1)}_m q^* - a^{(3)}_m \right) d\sigma = \{0\}$$

The rank of the global equation system, Eq. (22), is identical to the total number of node points on $\partial \Omega \cap \partial R$ 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

\[
q^* = \{\phi(x_2)\}^T \{q(x_1, x_3)\}_m \tag{23}
\]

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 to a constant. The solution algorithm for Eq. (3) is directly specified as

\[
\int_{R_m} \{\phi\} L (\rho u_2) d\sigma = 0 \tag{24}
\]

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. 3DBR Variant of COMOC employs simplex (linear) functionals scanning 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 non-linear. All matrix expressions are determined in terms 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

\[
\int \{ \phi \} \rho u_k q_{*k} d\tau = \int \{ \phi \}^T \{ \rho u_k \}_m \{ \phi \}^T \{ Q \}_m d\tau
\]

\[
= [B200S]\{ \rho U^{-} \}_m[B11]^T\{ Q \}_m
\]  \hspace{1cm} (26)

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

\[
\int \{ \phi \} \rho u_l q_{*l} d\tau = \int \{ \phi \}^T \{ \rho u_l \}_m \{ L \}^T \{ Q \}_m d\tau
\]

\[
= \{ \rho U \}_m^T[B300OS]\{ Q \}_m^-
\]  \hspace{1cm} (27)

where the matrix elements of \( [B300OS] \) 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 1

Standard Finite Element Matrix Forms for Simplex Functionals in One- and Two-Dimensional Space

<table>
<thead>
<tr>
<th>Matrix Name</th>
<th>Matrix Function</th>
<th>Matrix Evaluation</th>
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<tbody>
<tr>
<td>(B10)</td>
<td>( \int \phi d\tau ) on ( R_m )</td>
<td>( \frac{3}{2} )</td>
</tr>
<tr>
<td>(B115)</td>
<td>( (\alpha)_k^{(0)} (\alpha)_k^T ) on ( (X_2P)^2 )</td>
<td>( \begin{pmatrix} 1 &amp; -1 &amp; 0 \ 1 &amp; 0 &amp; 0 \end{pmatrix} )</td>
</tr>
<tr>
<td>(B2005)</td>
<td>( \int (\alpha)(\alpha)^T d\tau ) on ( R_n )</td>
<td>( \begin{pmatrix} 2 &amp; 1 &amp; 1 \ 2 &amp; 1 &amp; 1 \ 2 &amp; 1 &amp; 1 \end{pmatrix} )</td>
</tr>
<tr>
<td>(B30005)</td>
<td>( \int (\alpha)(\alpha)^T d\tau ) on ( R_n )</td>
<td>( \begin{pmatrix} 2 &amp; 1 &amp; 1 \ 2 &amp; 1 &amp; 1 \ 2 &amp; 1 &amp; 1 \end{pmatrix} )</td>
</tr>
<tr>
<td>(A11)</td>
<td>( \left{ \epsilon_1^{(0)} \right} ) on ( R_m )</td>
<td>( \left{ \epsilon_1^{(0)} \right} )</td>
</tr>
<tr>
<td>(A2005)</td>
<td>( \int (\alpha)(\alpha)^T d\tau ) on ( R_n )</td>
<td>( \begin{pmatrix} 2 &amp; 1 \ 2 &amp; 1 \end{pmatrix} )</td>
</tr>
<tr>
<td>(A10)</td>
<td>( \int \phi d\tau ) on ( R_m )</td>
<td>( \frac{3}{2} )</td>
</tr>
</tbody>
</table>

1. Matrix names are a 5-digit code covering dimensionality, nonlinearity, degree of differentiation and special matrix properties, as \([a, b, c, d, e, f]\) where:
   - \(a = A, B, C\) 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,
   - \(f = S, A, A\) for matrix symmetric, antisymmetric or general.

2. Symmetric matrices are written in upper triangular form.

3. \(N^n = \frac{1}{2} (X_2P)^2 (X_3P)^2\), the plane area of the triangular finite element.

4. \(X_2P\) = the \(x_2\) prime coordinate of node 2.

5. \(X_3P\) = the \(x_3\) prime coordinate of node 3.

6. \(2^n\) = 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
\[
\int \{\phi\} S_{\alpha} \, d\tau = [B200S] \{S_{\alpha}\}_m
\]
\[R_m\] (29)

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
\[
\int \{\phi\} \left[ \frac{M^2}{2Re} \left( \frac{1}{Pr} \right) \mu e(u_j u_j),_k \right] \, d\tau
\]
\[R_m\]

\[= - \frac{M^2}{Re} \int \{\phi\},_k \left( 1 - Pr \right)^{\ast} \mu e^{\ast} u_j^\ast u_j^\ast,_k \, d\tau
\]
\[R_m\]

\[= - \frac{M^2}{Re} \left\{ X_{J1} \right\}_m^T \{PR\}_m \left[ B3000S \right] \sum_{j=1}^{3} \{U_j\}_m [B211S] \{U_j\}_m \] (30)

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 \(p_{n+1}^\ast\) as the sequentially predicted values of the dependent variable \(q_{n+1}\) at the \(n+1\)st \(x_1\) station, the integration algorithm is
\[
p_{n+1} = a_1 q_n + h b_1 q_n^-
\]
\[
p_{n+1}^2 = a_2 q_n + h [b_2^2 p_{n+1}^2 + b_2^2 q_n^2]
\]
\[
q_{n+1} = a_3 q_n + h [b_3^3 p_{n+1}^3 + b_2^3 q_n^3]
\]  \hspace{1cm} (31)

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 upon internal error control. An estimation of relative truncation error is used of the form

\[
|\text{RTE}| \approx \frac{|p_{n+1}^2 - q_n^2|}{|q_{n+1}|^2}
\]  \hspace{1cm} (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, \(\text{H}_2, \text{O}_2, \text{N}_2, \text{Ar}\) [Ref. 9]. The species considered are \(\text{H}_2\text{O}, \text{O}_2, \text{H}_2, \text{N}_2, \text{Ar}, \text{O}, \text{H}, \text{NO}, \text{and OH}\). 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, \( x_\alpha \). The computed composition, \( \bar{x}_\alpha \), 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 \( \text{H, O, OH, and NO} \) are negligibly small in comparison to \( \text{H}_2, \text{O}_2, \text{N}_2, \text{and H}_2\text{O} \).

The next parameter evaluation is solution of the continuity equation for \( u_2 \). An evaluation of \( (\rho u_1)_j \) 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 \( \{\rho U\} \); the following second-order accurate finite difference formula is employed.

\[
\{\rho U\}_{n+1}^j = \frac{1}{h_j h_{n+1}} \left[ h_n (2h_{n+1} + h_n) \{\rho U\}_{n+1} - (h_n + h_{n+1})^2 \{\rho U\}_n + h_n^2 \{\rho U\}_{n-1} \right] \tag{33}
\]

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

\[
\Delta(\rho u_2^x) = \sum_{k=0}^{2} a_k(x_3) \frac{x_2^{k+1}}{k+1} \tag{34}
\]
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**

<table>
<thead>
<tr>
<th>MAIN LINK OF COMOC</th>
</tr>
</thead>
<tbody>
<tr>
<td>BDINPT</td>
</tr>
<tr>
<td>SCHPRN</td>
</tr>
<tr>
<td>SUTHLD</td>
</tr>
<tr>
<td>SETDIF</td>
</tr>
<tr>
<td>LINK2</td>
</tr>
<tr>
<td>RITE</td>
</tr>
<tr>
<td>LINK5</td>
</tr>
<tr>
<td>LINK7</td>
</tr>
<tr>
<td>READER</td>
</tr>
</tbody>
</table>
### TABLE 3

**OVERLAY STRUCTURE OF COMOC FOR IBM 360/65 COMPUTER**

<table>
<thead>
<tr>
<th>OVERLAY</th>
<th>ALPH</th>
<th>INSERT</th>
<th>DEFDEL</th>
<th>PENDOR</th>
</tr>
</thead>
<tbody>
<tr>
<td>OVERLAY A</td>
<td>DEFDEL</td>
<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
</tr>
<tr>
<td>OVERLAY B</td>
<td>SETUP</td>
<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
</tr>
<tr>
<td>OVERLAY C</td>
<td>SETUP</td>
<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
</tr>
<tr>
<td>OVERLAY D</td>
<td>SETUP</td>
<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
</tr>
<tr>
<td>OVERLAY E</td>
<td>SETUP</td>
<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
</tr>
<tr>
<td>OVERLAY F</td>
<td>SETUP</td>
<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
</tr>
<tr>
<td>OVERLAY G</td>
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<td>INSERT</td>
<td>DEFDEL</td>
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<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
</tr>
<tr>
<td>OVERLAY I</td>
<td>SETUP</td>
<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
</tr>
<tr>
<td>OVERLAY J</td>
<td>SETUP</td>
<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
</tr>
<tr>
<td>OVERLAY K</td>
<td>SETUP</td>
<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
</tr>
<tr>
<td>OVERLAY L</td>
<td>SETUP</td>
<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
</tr>
<tr>
<td>OVERLAY M</td>
<td>SETUP</td>
<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
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<tr>
<td>OVERLAY N</td>
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<td>PENDOR</td>
</tr>
<tr>
<td>OVERLAY O</td>
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<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
</tr>
<tr>
<td>OVERLAY P</td>
<td>SETUP</td>
<td>INSERT</td>
<td>DEFDEL</td>
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</tr>
<tr>
<td>OVERLAY Q</td>
<td>SETUP</td>
<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
</tr>
<tr>
<td>OVERLAY R</td>
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<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
</tr>
<tr>
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<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
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<td>PENDOR</td>
</tr>
<tr>
<td>OVERLAY U</td>
<td>SETUP</td>
<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
</tr>
<tr>
<td>OVERLAY V</td>
<td>SETUP</td>
<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
</tr>
<tr>
<td>OVERLAY W</td>
<td>SETUP</td>
<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
</tr>
<tr>
<td>OVERLAY X</td>
<td>SETUP</td>
<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
</tr>
<tr>
<td>OVERLAY Y</td>
<td>SETUP</td>
<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
</tr>
<tr>
<td>OVERLAY Z</td>
<td>SETUP</td>
<td>INSERT</td>
<td>DEFDEL</td>
<td>PENDOR</td>
</tr>
</tbody>
</table>

**ENTRY**

**MAIN**
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 -

<table>
<thead>
<tr>
<th>PARAMETER FORMAT</th>
<th>CARD COLS.</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>V1 A8</td>
<td>1 – 8</td>
<td>CONTROL VARIABLE.</td>
</tr>
<tr>
<td>NX 12</td>
<td>9 – 10</td>
<td>INDEX FOR ROUTINE OR CALL LIST.</td>
</tr>
<tr>
<td>NPCD 15</td>
<td>11 – 15</td>
<td>START POS. FOR PDUMP.</td>
</tr>
<tr>
<td>NREPET 15</td>
<td>16 – 20</td>
<td>END POS. FOR PDUMP.</td>
</tr>
</tbody>
</table>
| 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 LINK8. 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 -

BBB88 (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 BDINPT.
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.

PDUMP 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.

VYEND NX - DFINES END OF INPUT FOR DEP. VAR. NX.
VYYRDF 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>BORDER</th>
<th>IPLACE</th>
<th>LOC</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>THICK</td>
<td>268</td>
<td>93</td>
<td>ELEMENT THICKNESS VECTOR.</td>
</tr>
<tr>
<td>IPINT</td>
<td>205</td>
<td>31</td>
<td>SOLUTION SEQUENCE VECTOR.</td>
</tr>
<tr>
<td>PLOTS</td>
<td>311</td>
<td>113</td>
<td>PLOT VARIABLE AVCTOR.</td>
</tr>
<tr>
<td>NMAT</td>
<td>315</td>
<td>98</td>
<td>MATERIAL NUMBER VECTOR.</td>
</tr>
<tr>
<td>MELEM</td>
<td>316</td>
<td>14</td>
<td>MATERIAL TYPE/ELEMENT VECTOR.</td>
</tr>
<tr>
<td>PLOTYP</td>
<td>312</td>
<td>113</td>
<td>TYPE OF PLOT/VARIABLE VECTOR.</td>
</tr>
<tr>
<td>ICALL</td>
<td>321</td>
<td>125</td>
<td>LINK NOS. TO BE CALLED AT END OF QKNUIN.</td>
</tr>
<tr>
<td>ICALLS</td>
<td>322</td>
<td>125</td>
<td>ENTRY IN LINK TO BE CALLED.</td>
</tr>
<tr>
<td>IOMULT</td>
<td>323</td>
<td>60</td>
<td>OUTPUT VARIABLE MULTIPLIER FROM RARRAY.</td>
</tr>
<tr>
<td>IOSAVE</td>
<td>324</td>
<td>60</td>
<td>VARIABLE LIST TO BE DISPLAYED AT OUTPUT.</td>
</tr>
<tr>
<td>CNTPTS</td>
<td>327</td>
<td>47</td>
<td>CONTOURS NODES TO BE USED IN CONTES AND DFCFBL.</td>
</tr>
<tr>
<td>CNTNDS</td>
<td>328</td>
<td>128</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(INPLACE(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>VTTAB</td>
<td>219</td>
</tr>
<tr>
<td>VCPTAB</td>
<td>218</td>
</tr>
<tr>
<td>VX1COR</td>
<td>289</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

VYYY 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 = 0.1163E-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

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

LINK 2
PLACE CALLS TO THE FOLLOWING ROUTINES.
1. DFCPNS
2. DFCFRL
3. WLFLXS
4. CONTEX
5. REDOUTP
6. PEOUP

IF RESTART CODE 'NRTAPE' IS GREATER THAN 0, WRITE RESTART
CONDITIONS ON TAPE 'NRTAPE'.

10. DRHOLB

22
PLACE CALLS TO THE FOLLOWING ROUTINES.
1. NBDNYR
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. SETDIFF

ABSAVE (CEVBL)
COMPUTE THE SUM OF ABSOLUTE VALUES OF A SEQUENCE OF NUMBERS.
ADODEL (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.
BNOSER (GETBND)
DETERMINE NODES TO BE INSERTED INTO BOUNDARY ARRAY.
COS (DSGRT2)
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 CP INF AT TSINF.
THE VECTOR CP IS RESET TO CPINF.
DELADD (ADDEL)
ADD ENTRIES TO AN INTEGER ARRAY 'NSIDE' AT A TIME.
DELELM (DELNOD)
DELETE ENTRIES IN AN INTEGER ARRAY 'NSIDE' AT A TIME.
DELETE (DSGRT2)
DELETE NODES THAT ARE NOT CONNECTED TO ANY ELEMENTS.

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

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

DERVBL (LINK1(8))
FORM THE DERIVATIVE OF THE ORDINARY DIFFERENTIAL EQUATION FIRST ON U-VELOCITY (GLOBAL CONTINUITY) AND THEN ON OTHER DEPENDENT VARIABLES INCLUDING SPECIES CONTINUITY, ENERGY, LARGITUDINAL 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 IMAX IS REACHED AND THEN THE LAMINAR FLOW CURVE E2 IS USED.

DFCFNS (LINK2(11))
SET THE TEMPERATURE AND DENSITY IF NOT INITIALIZED.
CALL DFCOFO TO COMPUTE VISCOITY (AMU VECTOR).

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

DIMEN (LINK3(4))
COMPUTE 'ALC' IF NOT INITIALIZED IN 'NAME02',
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.

DRHGS (LINK2(11))
CALLED IF IGAS = 1 IN NAME01.
COMPUTES THE TEMPERATURE, DENSITY AND SPECIFIC HEAT ON A RADIAL 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 THE NODES.

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

**ELEM (DSERZ)**
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 OVER FLOWS 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.

**FEPLPOT (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.
           IGNORE COL. 9 - 20.
  DELETE A8 1 - 8  CALL ADDDEL TO DELETE ENTRIES.
           IGNORE 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
GPAAHFT (THFRM0)
  IF NGETH = 1, COMPUTE ENTHALPY DISTRIBUTION.
  IF NGETH = 0, COMPUTE CPOINF 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(I))
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 'M' 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) + COEF * 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.
HII - 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(I))
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.

NDECRO (DSCRTZ)
GENERATE NODE COORDINATES, IF NNODE = 0 IN NAMEO1.

NMELST (FENAME, BDINPT)
READ NAMELIST DATA INPUT.
NAME01 = INTEGER INPUT.
NAME02 = REAL INPUT.
NCDELM (LINKL(2))
SET UP THE ARRAY IELS TO BE USED IN DRHONS.
IELS = NO. OF ELEMENTS CONNECTED TO NODE N.
ORDER (CULS, ROWS, XYSCL)
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 (GFOMFL)
PRINT THE ELEMENT NO. AND NODE CONNECTIONS AND NODE COORDINATES
FROM THE GEOMETRY ROUTINE 'GFCMHT'.
OUTVEC
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(1) IN Y = C(1) * 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 STORED 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 'QKNUIN' AND TRANSFER CALL TO 'FFCUTP' AT PROPER TIMES.
QKNUIN (LINK4(2))
INITIALIZE INTEGRATION CONSTANTS ON FIRST PASS.
COMPUTE STEP SIZE AND NEW VALUE OF DEPENDENT VARIABLES.
COMPUTE NEW DENSITIES, DIFFUSION COEFFICIENTS, VISCOITY
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 ZTEST 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 X45DF = ROUALC * (AREA-XSUM)
WHERE XSUM = AMOUNT OF H2 PRESENT AND ROUALC = ROINF * ALC * UINF**2
ROATE (COMOC, RITF)
ASSEMBLER ROUTINE TO GET MACHINE DATF AND STORE IN 2A4 FORMAT.
RECIP (DECPNS, STOUT1)
  COMPUTE THE RECIPROCAL OF AN ARRAY AND STORE IT INTO ITSELF.

REDRL (BDINPT, ADDOEL)
  SCAN AN 80 CHARACTER CARD IMAGE AND CONVERT THE INFORMATION THEREIN
  INTO REAL OR INTEGER NUMBERS ACCORDING TO THE FORMAT PRESCRIBED.

REORD (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.

(FEOOUTP) (LINK2(6)) FEOOUTP 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 'NN1' 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 (FEOOUTP)
  CALL SCALE ROUTINE FOR 10 OUTPUT VARIABLES.

SCHPRN (LINK5(5))
  COMPUTE THE SCHMIDT AND PRANDTL NUMBERS ON A NODE BASIS.

ROWS (DSCRZ)
  COMPUTE THE NUMBER OF ROWS, 'KROW', IN THE OUTPUT DISPLAY
  AND SET UP THE FOLLOWING ARRAYS,
  INROW - NO. OF NODES IN ROW I.
  INDRM - COLUMN NUMBERS OF NODES IN ROW I.
  INDEX - ROW NUMBERS OF NODES IN COLUMN J.
  NOCOL - STARTING COLUMN NO. FOR ROW I.

SETSC1 (SCALEV)
  SET SCALE FACTOR FOR AN ARRAY OF REAL NUMBERS, THUS NORMALIZING

SETUP (LINK1(1))
  IF NELEM .GE. 0,
    READ ELEMENT CONNECTIONS AND COUNT ELEMENTS ('NELEM').
  IF NNODE .GE. 0,
    READ NODE GEOMETRY AND COUNT NODES ('NNODE').
    CALL 'DSCRZ' 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 NAMEOL EQUAL TO OR GREATER THAN THE
    NUMBER OF CARDS TO BE READ.

SETVAL
COMPUTE $A(i) = B(i) \times C + D$

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

SOURCE (LINK1(6))
COMPUTE SOURCE TERMS FOR RIGHT HAND SIDE OF DIFFERENTIAL EQUATIONS.

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

STOUT1 (FEOUTP)
DIMENSIONALIZE OUTPUT VARIABLES FOR DISPLAY PURPOSES.
CALL PLOT ROUTINE AT APPROPRIATE TIME, IF REQUESTED.

SOUTHLD (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 (DRHOOS)
INITIATE CALL TO GPAHFT.

VARMAX (FEPLAT)
IF $N^k > 0$, FIND MAXIMUM ENTRY IN ARRAY.
IF $N^k < 0$, FIND MINIMUM ENTRY IN ARRAY.

VECMAT (PRESUR)
MULTIPLY A SYMMETRIC MATRIX OF VECTORS BY A VECTOR OF LENGTH NN.

VECTA
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 $X_1$ BY SCALE FACTOR $SCFT$.
FIND $XYD = MAX(X_1) - MIN(X_1) \times SCFT$.
IF TWO ADJACENT POINTS IF ARRAY $X_1$ ARE WITHIN $XYD$ OF EACH
OTHER, SET THE UPPER VALUE EQUAL TO THE LOWER VALUE.
MAIN

IRUN = 1

100

RESET

RESET

RESET

BDINPT

IRUN = IRUN + 1

100
READ ADDITIONAL ENTRIES INTO BORDER IPLACE AND LOC

READ ADDITIONAL ENTRIES INTO VALUE AND NPLACE

J=0

J=J+1

J: 50 >

V 1: BORDER (J) ≠

GETBND

STORE INTEGER DATA IN PROPER IZ LOCATIONS

KDUMP: 1 ≠

PRINT INTEGER INPUT

D
MAKE SURE BORDER NODES END WHERE THEY BEGIN

J = 0

J = J + 1

J : 50

J : VALUE(J)

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

400

500

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

400

510

PRINT START COND.

QKNINT

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

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

<=

RITE (TITLE)

RETURN

<=

KK: 3

RETURN

<=

KK: 4

DIMEN

RETURN

RETURN

CALLED BY:
MANY
ROUTINES
Called by:
BDINPT
LINK5
QKNINT
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
KTYP = If 1
KTYP = ( 2
ADDDEL--1
ADDDEL
SET INTEGERS
500
REDREL
KTY p = 1
DELNOD
KODE: NEND
= 600
KTY p = 2
DELADD
KODE: NEND
= 600
RETURN

Called By:
ELEM
GETBND
SETUP
BDINPT
DSCTRLZ
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
COLS

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

STORE COL. COORD IN 'COL' VECTOR

STORE NO. OF COLS. IN 'LCOL'

RETURN

CALLED BY: DSCRTZ
CALLED BY:
   BDMINPT
CONTES

NT : 0

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

IWRIT : 0

PRINT VSIN AND WCOS

TF : VSTART

RETURN

STORE RHO^2U

COMPUTE COEFFICIENTS FOR U PRIME COMPUTATION

A
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.

IF IWRITE \leq 0

PRINT RHO^V RHO^W

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

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

RESERUENCE VECTOR ELIMINATING DELETED ENTRIES

RETURN

CALLED BY:
ADDDEL
DERSET

LOCATE

NP: 0

\[ \neq \] RETURN

LINK3

DETERMINE Q#RHO

RETURN

CALLED BY:
DERVBL
DERVBL

RESET COMPUTATIONAL VECTORS

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
THIS IS A DUMMY SUBROUTINE TO SET THE TURBULENT VISCOSITIES TO 0.

IF NON-ZERO TURB. VISCOSITIES ARE DESIRED, USER MUST CODE ROUTINE.

RETURN

CALLED BY:
LINK2
DFCFNS

ND:1 ≠ 200

RHO(1) = 0.0

TEMP(1) = 0.0

DFCOPO

SET VISOSITY

SET DIFFUSION COEFFICIENTS EQUAL TO VISCOSITY

RETURN

CALLED BY: LINK2
DFCOFO

I=0

200

I=I+1

I: NNODE

SUTHLD

RETURN

200

CALLED BY:
DFCFNS
A

\( ALC \leq 0 \)

SET ALC

NON-DIMENSIONALIZE \( x_{1\text{COR}}, x_{2\text{COR}} \)

CONVERT COL, ROW TO OUTPUT UNITS

\( U_{\text{INF}} \leq 0 \)

\( U_{\text{INF}} \leq 0 \)

\( A_{\text{INF}} \times X_{\text{MACHS}} \)

COMPUTE SCALE FACTORS AND NON-DIMENSIONALIZE INTEGRATION PARAMETERS

RETURN

CALLED BY:
BDINPT
DPDXTB

CALCULATE PRESSURE GRADIENT TO BE CONSTANT BETWEEN X3 STATIONS.

RETURN

CALLED BY: LINK1
DRHOBL

LINK3
(1, u_yy)

LINK3
(1, H2, y)

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

RETURN

CALLED BY:
LINK2 67
DRHOGS - 1

- 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

\[ \text{NNO}DE : 0 \]

\[ \neq \]

\[ 400 \]

\[ \text{SCALE COORDS.} \]
\[ \text{BY XSCALE, YSCALE} \]

\[ \text{APPLY COMPRESSION FACTORS FOR OUTPUT} \]

\[ \text{NELEM} : 0 \]

\[ \leq \]

\[ \text{ELEM} \]

\[ \text{SET UP NODE NO. INDEX ARRAYS} \]

\[ \text{DELETE} \]

\[ \text{RETURN} \]

\[ \text{SET UP NODE COORDINATES AS FUNCTION OF INPUT} \]
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.
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
FEPL0T

WRITE STATION AND VAR. DATA ON KOUT

RETURN

CALLED BY: STOUT1
FINDBE

NS: 0

600

CONVERT NODE VECTOR ALONG BOUNDARY INTO CORRESPONDING ELEMENT VECTOR

RETURN

CALLED BY:
EDINPT
GAS

INTERPOLATE TABLES TO FIND: \( C_p, H/R, S/R, G/RT \) AT GIVEN TEMP. FOR ALL SPECIES

IF \( R \neq 1 \)

= 52

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

52

COMPUTE PROPERTIES \( H, S, C_p, \mu, \gamma, V_{sound} \) 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
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
GETPPR

TIMX = TIME * FACT

LOOK PRESSURE

LOOK DP/DX

RETURN

CALLED BY:
LINK1
GETBND

150

READ BOUNDARY INFO.

BNDSET

'DONE'

No

150

Yes

RETURN

CALLED BY:
BDINPT
GMADD

ADD TWO MATRICES ELEMENT BY ELEMENT

RETURN

CALLED BY:
DERVBL
GPAHFT

COMPUTE AND STORE
MASS FRACTIONS
AND
MOLE FRACTIONS

NGETH
= 1
≠

STORE INITIAL
DISTRIBUTION OF
ENTHALPY, DENSITY
AND SPECIFIC HEAT

IBUG1
= 0
≠

GAS

GAS

GASBUG

YES

TEMPERATURE
RIGHT

NO

ITERATE UP TO 100
TIMES TO FIND
CORRECT TEMP.
A

NO

RIGHT
TEMPERATURE

YES

PRINT
FAILURE
AND
CONDITIONS

GAS

IBUG1 : 0

PRINT
NO. OF
INTER.

GASBUG

24

NONC : 0

PRINT
NON-
CONVERGENCE
IN GAS

 COMPUTE AND CHECK
FOR EXIT
CONDITIONS

NBUG : 2

EXIT

RETURN

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
INITBL

INITIALIZE
DEP.
VARIABLES

IBL:1

DRHOBL

= 

DRHOBS

RETURN

CALLED BY:
LINK4
LOC-1

GENERAL MATRIX

MS: 0
≠ 

SYMmetric MATRIX

MS: 1
≠ 

DIAGONAL MATRIX

COMPUTE SUBSCRIPT (N*ELEM.)

IR=0

36

IR = IRX

RETURN

COMPUTE SUBSCRIPT (N*ELEM.)

COMPUTE SUBSCRIPT OF UPPER TRIANGLE

Called by: MFRD
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
GETPFP
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
MISSDIV

POLY FIT THRU 'NPT'
TO MTH ORDER

RETURN

CALLED BY: CONTES
LOCATE MINIMUM AND MAXIMUM ENTRIES IN A VECTOR AND STORE IN MN AND MX RESPECTIVELY. STORE THEIR LOCATIONS IN LOW AND LHI.
MPRD

MULTIPLIES TWO MATRICES

RETURN

CALLED BY:
DERVEL
GEOMFL
H2MIX
VECMAT
ENERSC
MTRA

TRANSPOSES
A
MATRIX

RETURN

CALLED BY:
GEOMFL
NBNDRY

SET UP 'NWN'
INTEGRATION
NODE ARRAY

185

STORE DEP.
VARIABLE VECTOR
U INTO YY
VECTOR

STORE YY
VECTOR INTO
DEP. VARIABLE
VECTOR U

RETURN

WRITE
INTEG
NODE
VECTOR

185

NBSET:
= 0

< 

CALLED BY:
LINK3
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
GEOMPL
DERVBL
GPAHFT
RESET LINE OF OUTPUT ARRAY TO BLANKS

PBLANK

RETURN

CALLED BY:
REOUTP
(FEOUTP)
CONVERT FLOATING POINT NO. TO 'A' FORMAT FOR OUTPUT

RETURN

CALLED BY:
REOUTP
(FEOUTP)
POLY

COMPUTE POLYNOMIAL COEFFICIENTS

RETURN
Q3CONC

COMPUTE THE MASS DEFECT OF H2 FOR LAMINAR FLOW

RETURN

CALLED BY:
DFCFBL
QIN(NP)

INITIALIZE DEPENDENT VARIABLE 'NP'

RETURN

CALLED BY: QINIT
QKNINT

DO 105 NS=1,NEQ

DERIV

105

FEOUTP

NRSTRT : 0

> 120

<

NROW = -1
PTIM = TIME + DELP

120

NROW = -NROW
IROW = IROW + NROW

A
QKNINT-2

A

TIME: PTIM < 190

\[ PTIM = \text{TIME} + \text{DELP} \]
\[ KPNT = 1 \]

190

KPNT: 0 > FEOUTP

<

NSTST: 0 ≠ TIME = TPTEST

TIME: TPTEST < 120

≥

FEOUTP

RETURN

CALLED BY:
BDINPT
QKNUIN

INIT: O

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

INITIALIZE INTEGRATION COEFFICIENTS
READER

REDREL

ANY NUMBERS READ

STORE IOS. IN RETURN VECTOR

RETURN
RECIP

STORE RECIPROCAL OF VECTOR INTO ITSELF

RETURN

CALLED BY:
STOUT1
SETDIF
DFCFNS
READ 80 CHARACTER CARD IMAGE

CONVERT DATA ON CARD INTO REAL OR INTEGER NUMBERS.

RETURN

CALLED BY:
ADDDEL
BDINPT
READER
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 : 1

LINK3(2)
RITE(0,0)

PRINT OUTPUT HEADING

NOUTPR : 0

GENERATE AND PRINT SCALAR HEADING

INITIALIZE LINE COUNT LIMITS

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

PRINT VARIABLES IN PATTERN SIMILAR TO DISCRETIZATION

LSET :-1

PRINT NODE DISCRETIZATION = LSET :-1

800

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?

WRITE APPROPRIATE FORMAT

WRITE DATE, TITLE

RETURN

CALLED BY:
LINK3
SETUP
ROWS

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

RETURN

CALLED BY: DS CRTZ
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
SETUP

NELEM = 0

\text{\#} \rightarrow 130

\text{\#} \rightarrow 130

IFORCE = 0

\leq \rightarrow \text{READ ELEMENTS IN 315 FORMAT}

\rightarrow \text{ADDDEL}

\rightarrow 130

NNODE = 0

\rightarrow 250

\rightarrow 130

\rightarrow \text{READ NCI, PT}

\rightarrow \text{PRINT NCI, PT}

\rightarrow \text{PT(999999)=0.0}

\rightarrow \text{EXIT}

A

NC1 = 0, 1, 2

\rightarrow 130

\rightarrow 130
250
DSCRTZ

LG := 0

LG = LCOL

300
READ TITLE CARD

TITLEC19 != :DONE

RETURN

CALLED BY:
LINK1
SET
A(I) = B(I) \times C + D
RETURN
SIMQ

OBTAIN 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

CALLED BY:
SOURCE
STOUT1

DO 400
L=1,NVOUT

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

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

KRECIPI = 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.

NP:=0

LSV=MOD(LOGG,1000)
LND+(NP-1)*NODE

LSV:=247
STORE DIFFUSION COEF. FOR NP IN OUTPUT ARRAY

LSV:=248
STORE DEP. VARIABLE FOR NP IN OUTPUT ARRAY

LSV:=249
STORE DERIV. FOR NP IN OUTPUT ARRAY

B
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 I LOGS ≠

KOUT ≤ 0 >

RETURN

CALLED BY:
FEOUTP.
SUTHLD-1

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: WLFLXS
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
FEPLDT
QKNUIN
LINK2
VECMAT

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

RETURN

CALLED BY:
ENERSC
VECTA

ASSEMBLE ELEMENT DATA INTO GLOBAL VECTOR

RETURN
DIMENSIONALIZE PRESSURE AND ENTHALPY

NGBUG := 1

NGBUG := 1

GPAHFT

NGBUG := 1

PRINT DEBUG INFO

NBYP := 1

PRINT DEBUG INFO

NBYP := 1
A

\[ \text{NBYP} : 1 \neq \]

\[ \text{NBYP} = 2 \]

\[ \text{NBYP} : 1 \]

\[ \leq 100 \]

\[ \text{SET DEBUG FLAGS} \]

\[ \text{NBYP} : 0 \neq \]

\[ \text{100} \]

\[ \text{NBUG} = 1 \]

\[ \text{RESUME DEBUG FLAGS} \]

\[ \text{NON-DIMENSIONALIZE VARIABLES} \]

\[ \text{NGBUG} : 1 \neq \]

\[ \text{PRINT DEBUG INFO} \]

\[ \text{RETURN} \]

\[ \text{CALLED BY:} \]

\[ \text{DRHOCS} \]

147
COMPUTE SKIN FRICTION AND STANTON NUMBER ALONG SURFACE FOLLOWING PATANKER AND SPALDING.
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

XYSCAL

CALLED BY:
DSCRTZ
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 NAME01, node coordinates and element connections are punched on unit 7. If KOUT.gt.0 and KPLVAR ,gt. 0 in NAME01, then data generated for the variables defined by the PLOTS card will be output from the FEPLTOT 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

```
// INPUT DATA DECK (S)
// GO.FT05F001 DD *
// GO.FT10F001 DD
// GO.FT08F001 DD
ENTRY MAIN

OVERLAY STRUCTURE
INCLUDE OLDLIB
// LKED.SYSIN DD *
// LKED.OLDLIB DD

FORTRAN SOURCE DECKS
// FORT.SYSIN DD *
// PARM.LKED=(LIST,LET,OVLY)
// STEP1 EXEC FORTHCLG,
// NAME JOB
```
Symbols | Interpretation
--- | ---
5*I3 12 | 12, 15, 18, 21, 24
3*I- .5 3.1E3 | 3100.0, 3099.5, 3099.0
6*23.2 | 23.2, 23.2, 23.2, 23.2, 23.2, 23.2

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
blank card

stores 42 temperatures of 533.0 in the TEMP vector.

Output

Output for 3DRR 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, NBUG1, NBUG2, INRIT, IDIFRT, KODG and KODS. In the following, each of these is discussed with respect to sample representative output from COMOC.
The table contains data with values and calculations. The values are presented in a tabular format with columns for variables and corresponding data points. The data includes factors and entries that vary across the table. The calculations seem to be related to some form of equation or analysis, but without further context, the specific purpose or application of the data is unclear. The table appears to be part of a larger report or analysis, and it is marked as a printout from a file named "RDINPT."
120 ELEMENTS.

<table>
<thead>
<tr>
<th>ELEMENTS</th>
<th>3 ARRAYS / ELEMENT</th>
<th>5 ELEMTNS / ROW</th>
</tr>
</thead>
<tbody>
<tr>
<td>55 62</td>
<td>61 55 56 62 58</td>
<td>63 62 56 57 63</td>
</tr>
<tr>
<td>57 58</td>
<td>64 58 65 59 65</td>
<td>66 59 66 65 59</td>
</tr>
<tr>
<td>49 56</td>
<td>59 56 57 56 57</td>
<td>59 56 57 57 51</td>
</tr>
<tr>
<td>52 58</td>
<td>52 58 59 58 59</td>
<td>53 59 60 59 53</td>
</tr>
<tr>
<td>45 59</td>
<td>60 44 44 51 50</td>
<td>51 44 65 51 45</td>
</tr>
<tr>
<td>45 52</td>
<td>52 46 46 47 47</td>
<td>46 47 47 47 47</td>
</tr>
<tr>
<td>57 44</td>
<td>43 37 34 36 37</td>
<td>38 45 30 39 45</td>
</tr>
<tr>
<td>50 56</td>
<td>56 47 48 40 41</td>
<td>41 47 41 47 41</td>
</tr>
<tr>
<td>31 56</td>
<td>11 32 32 32 32</td>
<td>32 33 33 33 33</td>
</tr>
<tr>
<td>73 51</td>
<td>84 41 21 34 35</td>
<td>36 41 35 41 36</td>
</tr>
<tr>
<td>42 32</td>
<td>31 26 20 32 20</td>
<td>20 26 20 21 27</td>
</tr>
<tr>
<td>68 34</td>
<td>24 24 41 29 29</td>
<td>29 35 29 35 29</td>
</tr>
<tr>
<td>21 23</td>
<td>20 12 22 22 22</td>
<td>22 23 23 23 23</td>
</tr>
<tr>
<td>13 20</td>
<td>19 13 22 14 21</td>
<td>21 20 14 15 21</td>
</tr>
<tr>
<td>15 45</td>
<td>22 22 16 17 23</td>
<td>23 21 17 18 24</td>
</tr>
<tr>
<td>7 14</td>
<td>13 7 14 15 15</td>
<td>15 15 15 16 15</td>
</tr>
<tr>
<td>4 14</td>
<td>13 17 17 11 17</td>
<td>17 11 1.1 11 12</td>
</tr>
<tr>
<td>1 3</td>
<td>7 1 2 3 19</td>
<td>19 23 2 3 19</td>
</tr>
<tr>
<td>3 4</td>
<td>10 4 11 10 4</td>
<td>5 11 5 12 11</td>
</tr>
<tr>
<td>INPUT NODE</td>
<td>INPUT NODE</td>
<td>INPUT NODE</td>
</tr>
<tr>
<td>------------</td>
<td>------------</td>
<td>------------</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>0.1045</td>
<td>0.2050</td>
<td>0.3050</td>
</tr>
<tr>
<td>0.4045</td>
<td>0.5050</td>
<td>0.6050</td>
</tr>
<tr>
<td>0.7045</td>
<td>0.8050</td>
<td>0.9050</td>
</tr>
</tbody>
</table>

If certain conditions are met, the program will continue to run. Otherwise, it will terminate.


<table>
<thead>
<tr>
<th>Input Node</th>
<th>T (°C)</th>
<th>P (MPa)</th>
<th>H2</th>
<th>O2</th>
<th>N2</th>
<th>CO2</th>
<th>CH4</th>
<th>C2H6</th>
<th>C3H8</th>
<th>C4H10</th>
<th>CO</th>
<th>C3H6</th>
<th>C2H4</th>
<th>C2H2</th>
<th>C3H4</th>
<th>C5H10</th>
<th>C6H12</th>
<th>C7H16</th>
<th>C8H18</th>
<th>C9H20</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
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<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

First and last input nodes are connected through pipes. All intermediate phases are shown.
**INTRT**, integer, debugging output from CONTEST.
INTRT is decremented by 1 for each pass thru CONTEST; when INTRT = 0, debugging print stops.

If INTRT is still > 0 when VSTART is passed, then more debugging information containing the RN1Vs is printed out.

The vectors VSIN and WCOS are printed on the first pass thru CONTEST.

<table>
<thead>
<tr>
<th>VSIN (SITE of angle between lowest and highest node in column)</th>
<th>WCOS (SITE of angle between lowest and highest node in column)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 0.1009E 01</td>
<td>2 0.1009E 01</td>
</tr>
</tbody>
</table>

The vectors VSIN and WCOS are printed on the first pass thru CONTEST.

<table>
<thead>
<tr>
<th>Present value of RN1U</th>
<th>Last value of RN1U</th>
<th>Last change in RN1U</th>
<th>Downstream derivative</th>
<th>Correct of normal node</th>
<th>Node number having processed</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Data for Column no. 1</th>
<th>Data for Column no. 2</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>X1</th>
<th>X2</th>
<th>X3</th>
<th>X4</th>
<th>X5</th>
<th>X6</th>
<th>X7</th>
<th>X8</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>0.2507E 03</td>
<td>0.2507E 03</td>
<td>0.2507E 03</td>
<td>0.2507E 03</td>
<td>0.2507E 03</td>
<td>0.2507E 03</td>
<td>0.2507E 03</td>
<td>0.2507E 03</td>
</tr>
<tr>
<td>0.1000E 01</td>
<td>0.1000E 01</td>
<td>0.1000E 01</td>
<td>0.1000E 01</td>
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**INERTIAL**: 
Inertial forces are calculated as follows:

- **INERTIAL**:
  - **RST**: Relative Static Test
  - **LST**: Local Static Test
  - **FST**: Forward Static Test
  - **NTR**: Normal Test Range
  - **VST**: Vertical Static Test
  - **UST**: Upward Static Test
  - **CTR**: Center Test Range
  - **LTR**: Lower Test Range
  - **DTR**: Downward Test Range

**Example Calculation**:

- **PRT**: Primary Rate Test
- **RST**: Relative Static Test
- **LST**: Local Static Test
- **FST**: Forward Static Test
- **NTR**: Normal Test Range
- **VST**: Vertical Static Test
- **UST**: Upward Static Test
- **CTR**: Center Test Range
- **LTR**: Lower Test Range
- **DTR**: Downward Test Range

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**Data Table**

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**Note**: The table above represents a simplified example of how inertial forces are calculated in a test scenario. Each column and row corresponds to specific parameters and test conditions.
IDIPRT .GT. 0 Debug output.

IDIPRT is documented by 1 for each pass thru WLPLNS. When IDIPRT .LE. 0 debug print stops.

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**GF2051** (1st part of B2001 matrix)

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| 6          | -0.77778E-01 7               | 0.27778E-00 8               | 0.27778E-01 9               | 0.0                     10              | 0.0 |
| 11         | 0.19444E-01 12              | 0.69444E-00 13              | 0.69444E-01 14              | 0.0                     15              | 0.0 |
| 16         | 0.33333E-01 17              | 0.13889E-00 18              | 0.13889E-01 19              | 0.0                     20              | 0.0 |
| 21         | 0.33333E-01 22              | 0.13889E-00 23              | 0.13889E-01 24              | 0.0                     25              | 0.0 |
| 26         | 0.50505E-01 27              | 0.12500E-00 28              | 0.12500E-01 29              | 0.0                     30              | 0.0 |

**GE202** (2nd part of B2001 matrix)

| 1          | -0.18826E-07 2               | 0.13889E-00 3               | -0.13889E-00 4               | -0.13889E-00 5               | 0.13889E-00 |
| 6          | 0.0                     7               | 0.23333E-00 8               | 0.23333E-01 9               | 0.13889E-01 10              | 0.13889E-00 |
| 11         | 0.13889E-00 12              | 0.0                     13               | -0.37253E-00 14              | 0.13889E-01 15              | 0.13889E-00 |
| 16         | 0.37253E-00 17              | 0.13889E-00 18              | 0.13889E-01 19              | 0.0                     20              | 0.13889E-00 |
| 21         | 0.69444E-00 22              | 0.13889E-00 23              | 0.13889E-01 24              | 0.0                     25              | 0.13889E-00 |
| 26         | 0.13889E-00 27              | -0.13889E-00 28              | 0.13889E-01 29              | 0.0                     30              | 0.0 |

**X12** (base of transformed triangle)

| 1          | 0.26281E-01 2               | 0.16667E-01 3               | 0.33333E-01 4               | 0.65555E-00 5               | 0.27778E-01 |
| 6          | 0.16667E-01 7               | 0.33333E-01 8               | 0.20000E-00 9               | 0.44444E-00 10              | 0.30000E-00 |
| 11         | 0.33333E-01 12              | 0.16667E-01 13              | 0.23333E-01 14              | 0.66667E-00 15              | 0.28674E-00 |
| 16         | 0.66666E-01 17              | 0.16667E-01 18              | 0.23333E-01 19              | 0.30000E-00 20              | 0.28674E-00 |
| 21         | 0.33333E-01 22              | 0.16667E-01 23              | 0.23333E-01 24              | 0.66667E-00 25              | 0.23570E-00 |
| 26         | 0.16667E-01 27              | 0.16667E-01 28              | 0.16667E-01 29              | 0.15455E-01 30              | 0.16667E-01 |

**X13** (height of transformed triangle)
...
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>NAME01</td>
<td>Initialization</td>
</tr>
<tr>
<td></td>
<td>&amp;NAME01</td>
<td>Integer parameter input</td>
</tr>
<tr>
<td>NEQKNN</td>
<td></td>
<td>Number of dependent variables to be integrated in X1 direction</td>
</tr>
<tr>
<td>IGAS</td>
<td>0</td>
<td>Isoenergetic flow with constant cp</td>
</tr>
<tr>
<td>IFR</td>
<td>0</td>
<td>General flows</td>
</tr>
<tr>
<td>KDUMP</td>
<td>0</td>
<td>Suppress debug output</td>
</tr>
<tr>
<td>NPVSX</td>
<td></td>
<td>No. of entries in pressure table</td>
</tr>
<tr>
<td>NSCX</td>
<td>0</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>&amp;NAME02</td>
<td></td>
<td>Floating point parameter input</td>
</tr>
<tr>
<td>UINF</td>
<td></td>
<td>Reference (freestream) velocity (F/S)</td>
</tr>
<tr>
<td>T0FINF</td>
<td></td>
<td>Reference stagnation temperature (°R)</td>
</tr>
<tr>
<td>REFL</td>
<td></td>
<td>Reference length (F)</td>
</tr>
<tr>
<td>T0</td>
<td></td>
<td>Initial X1 station (F)</td>
</tr>
</tbody>
</table>

165
<table>
<thead>
<tr>
<th>Call</th>
<th>Parameter Code</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<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>T0A,T0H</td>
<td></td>
<td></td>
</tr>
<tr>
<td>XMA,XMH</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

FEDIMN

Generate vector lengths and array entry points.

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
1 1 600, 7 1 600, 8 7 1200,...
T
1 11, 1 4,...
This generates a finite element discretization of 11 node rows x 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>KENO</td>
<td>KENO (N) establishes fixed boundary conditions for dependent variables N through NN.</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>
<tr>
<td>Call</td>
<td>Function</td>
</tr>
<tr>
<td>------------</td>
<td>--------------------------------------------------------------------------</td>
</tr>
<tr>
<td>ICALL -1</td>
<td>Fixed calling sequence for internal evaluations, not to be changed.</td>
</tr>
<tr>
<td>ICALLS -1</td>
<td></td>
</tr>
<tr>
<td>LINK3 4</td>
<td></td>
</tr>
<tr>
<td>LINK1 3</td>
<td></td>
</tr>
<tr>
<td>VTEMP -58</td>
<td>Read initial nodal total temperature distribution. Non-dimensionalize entries by number in location 58 (TREF).</td>
</tr>
<tr>
<td>e.g. VTEMP</td>
<td></td>
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</tr>
<tr>
<td>VYY - (X)</td>
<td>Reads initial conditions for dependent variable N. Non-dimensionalize entries by number in</td>
</tr>
<tr>
<td>VYYEND (N)</td>
<td></td>
</tr>
<tr>
<td>e.g. VYY</td>
<td>Initial U2 distribution is all zeros. Non-dimensionalize entries by number</td>
</tr>
<tr>
<td>-27</td>
<td>in location 27 (UREF)</td>
</tr>
<tr>
<td>42*0.0</td>
<td></td>
</tr>
<tr>
<td>T</td>
<td></td>
</tr>
<tr>
<td>VYYEND 2</td>
<td></td>
</tr>
<tr>
<td>e.g. VYY</td>
<td>Initial U1 distribution is zero at first two nodes, 1654 F/S at second</td>
</tr>
<tr>
<td>-27</td>
<td>two,..., last 72 nodes have 4004.8 F/S. Non-dimensionalize entries by</td>
</tr>
<tr>
<td>2*0.0</td>
<td>number in location 27 (UREF).</td>
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<tr>
<td>2*1654...</td>
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</table>
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</td>
<td>1</td>
<td>Title card for output cover page</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>Reference condition and control parameters for combustion calculations using five dependent variables</td>
</tr>
<tr>
<td></td>
<td>7</td>
<td></td>
</tr>
<tr>
<td>II</td>
<td>8</td>
<td>Form non-uniform discretization, using 11 node rows \times 6 node columns, producing 100 finite elements</td>
</tr>
<tr>
<td></td>
<td>13</td>
<td></td>
</tr>
<tr>
<td>III</td>
<td>14</td>
<td>Title card to head each output call</td>
</tr>
<tr>
<td></td>
<td>15</td>
<td>Detailed problem description</td>
</tr>
<tr>
<td></td>
<td>22</td>
<td></td>
</tr>
<tr>
<td>IV</td>
<td>23</td>
<td>Entry locations of longitudinal pressure distribution (constant)</td>
</tr>
<tr>
<td></td>
<td>24</td>
<td>66 nodes have uniform stagnation temperature</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>Initial (U_1) distribution</td>
</tr>
<tr>
<td></td>
<td>26</td>
<td></td>
</tr>
<tr>
<td></td>
<td>36</td>
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<tr>
<td></td>
<td>37</td>
<td>Initial (U_2) distribution is zero</td>
</tr>
<tr>
<td></td>
<td>38</td>
<td>Initial (O_2) distribution reflects location of virtual source</td>
</tr>
<tr>
<td></td>
<td>39</td>
<td>Initial (N_2) distribution</td>
</tr>
<tr>
<td></td>
<td>40</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>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>01</td>
<td>COMOC CHECK CASE FOR THREE DIMENSIONAL REACTING BOUNDARY REGION FLOW</td>
</tr>
<tr>
<td>02</td>
<td>NFORNN=5, IGAS=1, IFR=0, KDUMP=0,</td>
</tr>
<tr>
<td>03</td>
<td>MPVX=2, NSC=1, NSCY=1,</td>
</tr>
<tr>
<td>04</td>
<td>NCEF=2,</td>
</tr>
<tr>
<td>05</td>
<td>UINF=2272.0, TDINF=533.0, REFL=.003333333,</td>
</tr>
<tr>
<td>06</td>
<td>TD=0.0, TD=0.10, DELP=5.0,</td>
</tr>
<tr>
<td>07</td>
<td>XSCALE=0.003333333, YSCALE=0.003333333, VSTAR=101.0,</td>
</tr>
<tr>
<td>08</td>
<td>1 75 100, 2 5C 100, 3 125 100, 4 150 100, 5 225 100,</td>
</tr>
<tr>
<td>09</td>
<td>T INCREMENTS BETWEEN X3, NODE-NUMERATOR-DENOMINATOR</td>
</tr>
<tr>
<td>10</td>
<td>1 5, 10, 15 LC, 8 125 LC, 9 175 100, 10 250 100,</td>
</tr>
<tr>
<td>11</td>
<td>T INCREMENTS BETWEEN X2</td>
</tr>
<tr>
<td>12</td>
<td>1 11, 1 6,</td>
</tr>
<tr>
<td>13</td>
<td>11 ROWS AND 6 COLUMNS NORMALIZED BY LREF, HENCE X-Y SCALES = LREF</td>
</tr>
<tr>
<td>14</td>
<td>COMOC CHECK CASE, THREE DIMENSIONAL REACTING BOUNDARY REGION — VIRTUAL SOURCE</td>
</tr>
<tr>
<td>15</td>
<td>COMOC CHECK CASE, THREE DIMENSIONAL REACTING BOUNDARY REGION — VIRTUAL SOURCE</td>
</tr>
<tr>
<td>16</td>
<td>(H2/O2/AIR SYSTEM WITH EQUILIBRUM CHEMISTRY). PROBLEM CONSIDERED</td>
</tr>
<tr>
<td>17</td>
<td>REPRESENTS TRANSVERSE H2 INJECTION INTO A SUPersonic AIR STREAM</td>
</tr>
<tr>
<td>18</td>
<td>CHARACTERISTIC OF SCRAMJET FUEL INJECTION, SEE ROGERS NASA TNC-6114,</td>
</tr>
<tr>
<td>19</td>
<td>1971 AND NASA TMD-6476, 1971 PFR EXPERIMENTAL STUDY OF THIS PROBLEM.</td>
</tr>
<tr>
<td>21</td>
<td>CALCULATIONS ARE STARTED USING VIRTUAL SOURCE CONCEPT TO REPLACE</td>
</tr>
<tr>
<td>22</td>
<td>COMPLEX NEAR INJECTION FLOW FIELD.</td>
</tr>
<tr>
<td>23</td>
<td>0.0 100. 1 X1 TABLE PFR PRESSURE</td>
</tr>
<tr>
<td>24</td>
<td>193. 153. 1 PFR PRESSURE TABLE PSF</td>
</tr>
<tr>
<td>25</td>
<td>66*533.</td>
</tr>
<tr>
<td>26</td>
<td>6*3.0</td>
</tr>
<tr>
<td>27</td>
<td>6*1503.</td>
</tr>
<tr>
<td>28</td>
<td>6*1660.</td>
</tr>
<tr>
<td>29</td>
<td>2<em>1550. 4</em>1759.</td>
</tr>
<tr>
<td>30</td>
<td>2<em>1550. 4</em>1852.</td>
</tr>
<tr>
<td>31</td>
<td>2<em>1550. 4</em>1852.</td>
</tr>
<tr>
<td>32</td>
<td>2<em>2272. 4</em>1942.</td>
</tr>
<tr>
<td>33</td>
<td>2<em>2272. 4</em>1952.</td>
</tr>
<tr>
<td>34</td>
<td>2<em>2272. 4</em>2074.</td>
</tr>
<tr>
<td>35</td>
<td>2<em>2272. 4</em>2169.</td>
</tr>
<tr>
<td>36</td>
<td>6*2272.</td>
</tr>
<tr>
<td>37</td>
<td>66*533.</td>
</tr>
<tr>
<td>38</td>
<td>18.233 2<em>0.0 4</em>233 2<em>0.0 4</em>233 2<em>0.0 34</em>233</td>
</tr>
<tr>
<td>39</td>
<td>18.767 2<em>0.0 4</em>233 2<em>0.0 4</em>233 2<em>0.0 34</em>233</td>
</tr>
<tr>
<td>40</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 I0MULT -1, change entry to 15*2. Finally, in DEScript2, on third card headed EFF.MU/MUREF, add U3/UREF in columns 65-80.
SYMBOLS

CROSS REFERENCE LIST FOR EQUIVALENCED VARIABLES

17) RUN - CONTROL PAR. TO START END GENERATING OUTPUT.
18) IBL - I = BOUNDARY LAYER PROGRAM.
19) G - GASTER-STOKES PROGRAM.
11) FOPL - PRINT TAPES AND OUTPUT FOR CASE IN GRAPH.
13) IPGE - PRINT INTERMEDIATE STEPS IN GRAPH.
16) TCM - NO. OF TIMES FOR AXIS-SYM. COORD.
17) ITPLT - NO. OF TIMES TO PRINT LATER OUTPUT IN WELLS.
18) LED - READ DATA, WRITE TO .EIGS FORMAT IN SETUP.
22) ITAC - 1 = FROZEN CALCULATION IN TEMPO.
23) ICAS - 1 = CALL PROGRAM.
24) ICAT - INITIALIZE PARAMETERS IN TEMPO.
25) IMA = NO. OF MATERIALS IN PROG.
12) INAT - NO. OF TAPES IN MATERIAL TABLE.
10) TUK - TAPES IN CELL AT WHICH TO USE T CURVE.
15) INAS - STARTED PARADOX IN G.
28) PIP - WRITE CALL TO DRY.
29) ICPT - COUNTED TO OUTPUT FOR LATER OUTPUT.
15) ICA - FIRST POSITION IN LIGHT ARRAY.
21) IPM - I = index of present or past value of RELATIVE ANGULAR DENSITY. (SET IN GAROUT) 
26) IPM - PROBLEM AREA (USUALLY ONLY 1).
12) ISPED - 1 = COMPUTER CODED OUTPUT CATEGORIZING OUTPUT TYPE.
23) ISIS - NOT USED.
16) IT - TEMPERATURE CYCLATION COUNT IN GRAPH.
19) ITDI - WRITE HISTORY FOR WHICH TO PRINT IN PREP.
18) KALLEC - CODE TO REFRACTION OF SPECIES AREA OR HEIGHT IN EI.
24) KRAL - PRINT INPUT CODES AND DATA GENERATED IN PREP.
25) KRED - INTRODUCTION TECHNIQUE.
26) KRED - 1 = MAXIMUM ABSOLUTE STABILITY.
27) KRED - 2 = MAXIMUM RELATIVE STABILITY.
28) KRED - 3 = MAXIMUM ABSOLUTE STABILITY.
29) KRED - 4 = MAXIMUM RELATIVE STABILITY.
31) KRED - 5 = MAXIMUM ABSOLUTE STABILITY.
17) KRED - 6 = MAXIMUM RELATIVE STABILITY.
18) KRED - 7 = MAXIMUM ABSOLUTE STABILITY.
19) KRED - 8 = MAXIMUM RELATIVE STABILITY.
20) KRED - 9 = MAXIMUM ABSOLUTE STABILITY.
21) KRED - 10 = MAXIMUM RELATIVE STABILITY.
22) KRED - 11 = MAXIMUM ABSOLUTE STABILITY.
23) KRED - 12 = MAXIMUM RELATIVE STABILITY.
17 NS - LINEAR APPROX., INDEX  DEF. = 6
55 NODE - 2D ARRAY STARTING LOC. PARAMETER. MIN.=NAODE+3
150 NODEM - NODE NO. AT WHICH DRAGS IS COMPUTING.
19 NOF - NO. OF EQUATIONS BEING SOLVED FOR DEP. VAR. 'NP'.
5 NUMEB - NO. OF BOUNDARY NODES TO BE SOLVED FOR IN 'CMERGE'.
143 NONC - NON-CONVERGENCE CODE IN GAS.
142 NOUUT - NO. OF SCALARS TO PRINT IN OUTPUT.
30 NP - DEP. VARIABLE BEING SOLVED.
18 NPRT - 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
135 NPSEL - NO. OF BOUNDARY NODES TO COMPUTE PSI, PSIC.
134 NPSIC - NO. OF NODES READ IN FOR PSI, PSIC.
2 NPSLOC - NO. OF FIXED ST LOC. (USED IN 'STRF').
11 NPSTIF - NO. OF POINTS / DEG. OF FREEDOM. (JACUNG PAR.)
24 NPTE - NO. OF POINTS / ELEMENT. 'LTH'. DEF. = 3
153 NPUMT - SET = 1 IF ELEMENTS AND NODES ARE TO BE PRINTED.
161 NPUSX - NO. OF PRESSURES IN P VS X TABLE.
46 NPXL - NO. OF POINTS / ELEMENT. 'LTH'. DEF. = 3
66 NPXS - STEADY STATE PARAMETER IN 'DERIV'.
21 NROW - DEP. VAR. AND DERIVATIVE ALTERNATIVE IN JACINT.
6 NUNSTOT - LOGICAL TABLE NO. TO READ RESTART 'C', IN 'PRINT'.
17 NUTAPE - LOGICAL TABLE NO. TO STORE RESTART 'C', IN 'LINK2'.
67 NUS - PRINT OUT COUNT PARAMETER.
151 NVCX - SET = 1 IF INTERVAL IMPLT IS TO BE READ FOR YC00 IN DESCRT.
152 NVCY - SET = 1 IF INTERVAL IMPLT IS TO BE READ FOR YC00 IN DESCRT.
144 NVDIF - RESET SWITCH TO CHANGE NELF2 IN DECREL.
144 NVDEF - RESET CONDITION FLAG IN FINDF.
27 NXL - NO. OF POLYG. LOCATIONS / DEP. VARIABLE.
DEF. = NACOE / 3
54 ASW - STOP PROGRAM IF OUTPLT EXP. GT NSX. DEF. = 10
156 NXCDEF - SET = 1 IF SOURCE DATA IS TO BE USED ON RIGHT HAND SIDE IN CERVAL.
171 NXC - NO. OF SPECIES IN EQUATION. DEFAULT = 9.
160 NXCDEF - C = NO SOURCE COMPUTATION FOR ENTHALPY.
1 = USE PH1 SOURCE COMPUTATION.
2 = USE PH1 + PH2 SOURCE COMPUTATION. (ACT. USEC.)
146 NXC2 - RESET SWITCH TO CHANGE PH2 IN DECREL.
146 XCMTS - STARTUP PARAMETER IN CONTS.
142 XCMER - STARTUP PARAMETER IN DECREL.
143 XCMERP - STARTUP PARAMETER IN DECREL.
42 NTITL - NO. OF TITLE CARDS TO BE READ IN 'SETUP' AND PRINTED AT THE BEGINNING OF EACH OUTPUT SET.
23 NFR - NO. OF ELEMENTS HAVING NON-CONSTANT THICKNESS.
94 NUP SPA - NO. OF L-PARALLEL ELEMENTS IN STRE.
74 AHP - DEP. VARIABLE NO. FOR ENTHALPY.
70 AHP - DEP. VARIABLE NO. FOR PSI.
71 AHP - DEP. VARIABLE NO. FOR OMEGA.
72 AHP - DEP. VARIABLE NO. FOR VELOCITY 1.
73 AHP - DEP. VARIABLE NO. FOR VELOCITY 2.
91 AHP - NO. OF TIME INTERVALS TO STORE YY.
91 AHP - NO. OF TIME INTERVALS TO STORE 77.
ENTRIES

156 AINF - REFERENCE SPEED OF SOUND.
   IF LINF  LE  C, AINF = SQRT(G*GAMMA*PINF/RHOTAF);
   IF LINF  GT  C, AINF = SQRT(G*GAMMA*RUNIV*TCFINF/XMA)

* AJ - JOULES CONSTANT. DEF. = 77E.29

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

115 BSTART - NOT USED

176 CFTOKJ - SPECIFIC HEAT BRITISH TO MKS 4.184

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

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

124 CON - CONSTANT USED IN DFCFBL. DEFAULT = 0.4

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

62 CONV - OUTPUT SCALE FACTOR = 1.0 / REFL

77 CON1 - ALC / (RP*CP1*PINF*XMLINF)

78 CON2 - CON1 / TOFINF

158 CPA - SPECIFIC HEAT OF AIR. DEFAULT = 0.24

159 CPP - SPECIFIC HEAT OF HYDROGEN. DEFAULT = 3.445

160 CPINF - SPECIFIC HEAT COMPLETED IN CPINIT.

30 CPDINF - REFERENCE SPECIFIC HEAT.

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

148 CVM - ENTHALPY CONVERSION LSED IN THERMC. DEFAULT = 1.0

151 CVP - PRESSURE CONV. LSED IN THERMC. DEF. = 4725 E-3

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

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

149 CVU - VELOCITY CONVERSION LSED IN THERMC. DEF. = 0.3048

130 C4ED - CONSTANT USED IN DFCFAL. DEFAULT = 0.00023

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

144 C4FACT - MULTIPLIER FOR NEW C4ED AFTER C4EDSW OCCURS.

13 DEPL - PERCENT INTERVAL FOR PRINTOUT. DEFAULT = 2.0

13 DEPLT - PERCENT OF TO TO BE USED FOR PLOTTING STATIONS.

111 DELX3 - TIME STEP LSED IN CONTS.

113 DELAST - TIME STEP LSED IN CONTS.

114 MLXM1 - TIME STEP LSED IN CONTS.

161 DPINF - RP11N1F * LINF**2

165 DRTOKK - DEGREES RANKINE TO DEGREES KELVIN 5.0/9.0

175 FBTOKK - ENTHALPY BRITISH TO MKS 2.3244

137 FLIPS - NOT USED

138 FLIPSR - VFT LSFC

135 FLIPSH - NOT USED

136 FLIPSX - NOT USED

14 EPS - ACCURACY TEST BETWEEN PREDICTOR-CORRECTOR FORMULAS

145 F1F2SW - PERCENT OF TO AT WHICH TO SWITCH FROM F1 TO F2

1 FACT - NON-DIM FACTOR = ALC / UINF

80 FACTH - 1.0 / (CP11NF*TOFINF)

59 FACTMU - RP11N1F * LINF * ALC
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>FACTP</td>
<td>1.0 / FACTUL</td>
<td>30.41</td>
</tr>
<tr>
<td>FTFCM</td>
<td>FEET IN CENTIMETERS</td>
<td>12.0</td>
</tr>
<tr>
<td>FTTCN</td>
<td>FEET TO INCHES</td>
<td>0.3344</td>
</tr>
<tr>
<td>G</td>
<td>GRAVITATION CONSTANT</td>
<td>32.174</td>
</tr>
<tr>
<td>GAMMAF</td>
<td>FACTOR 1.01 IN GAS LAWS</td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>CURRENT TOTAL STEP SIZE</td>
<td></td>
</tr>
<tr>
<td>K</td>
<td>OUTPUT VARIABLE FOR TIME STEP = HS * FACT / FEET</td>
<td></td>
</tr>
<tr>
<td>H2FT</td>
<td>H2 MASS FLOW COMPUTED IN H2MIX</td>
<td></td>
</tr>
<tr>
<td>HRMIX</td>
<td>USED IN GKMIX FOR TIME STEP DETERMINATION</td>
<td></td>
</tr>
<tr>
<td>HINE</td>
<td>REFERENCE ENTHALPY COMPUTED IN H2MIX</td>
<td></td>
</tr>
<tr>
<td>HMAX</td>
<td>MAX. STEP SIZE ALLOWED</td>
<td></td>
</tr>
<tr>
<td>HKIN</td>
<td>MINIMUM INTEGRATION STEP SIZE</td>
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</tr>
<tr>
<td>HINTT</td>
<td>NOT USED</td>
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</tr>
<tr>
<td>FRCM</td>
<td>CONSTANT LED IN H2MIX</td>
<td>DEFAULT = 0.24126</td>
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<tr>
<td>HSMOT</td>
<td>MIXING EFFICIENCY COMPUTED IN H2MIX</td>
<td></td>
</tr>
<tr>
<td>HS</td>
<td>CURRENT STEP SIZE</td>
<td></td>
</tr>
<tr>
<td>I</td>
<td>START INTEGRATION STEP SIZE AT THIS VALUE</td>
<td>DEFAULT = 1.0</td>
</tr>
<tr>
<td>KCF</td>
<td>FLOATING POINT 1.0. SCALE FACTOR IN STHW</td>
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</tr>
<tr>
<td>ICUMS</td>
<td>ACCURACY TEST PARAMETER IN GKMIX</td>
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</tr>
<tr>
<td>ICUM</td>
<td>PRESENT IF H2 AT WHICH THE LIMIT CURVE IN GCM</td>
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</tr>
<tr>
<td>ICOTN</td>
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</tr>
<tr>
<td>IFR</td>
<td>INTEGRAL OVER PRESS</td>
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</tr>
<tr>
<td>PRESMOT</td>
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</tr>
<tr>
<td>IPR</td>
<td>PRESENT IN RUSC</td>
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</tr>
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<td>IPRSN</td>
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<tr>
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</tr>
<tr>
<td>PSMOT</td>
<td>PRESENT IN RUSC</td>
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</tr>
<tr>
<td>PSTMAT</td>
<td></td>
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<tr>
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<tr>
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</tr>
<tr>
<td>RPSM</td>
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</tr>
</tbody>
</table>

**ORIGINAL PAGE IS OF POOR QUALITY.**
56  RTCON5 = UNINF**2 / (RTCON1*CPCINF*TCFINF)
57  RTCON6 = 2.0 * RTCON4
117  RTON1 = PP * ( PON/TOA - 1.0 )
28  RUNIV = UNIVERSAL GAS CONSTANT, DEFAULT = 1545.33
129  SCX = CONSTANT SCHMIDT NUMBER DEFAULT = 0.7
108  SCXIIN = NOT USED
107  SCXILT = NOT USED
131  SPLT = CUTOFF LSDO IN H2MTX DEFAULT = 0.02835
44  SQ2 = SQRT(2.0)
51  STHMN = NOT USED
73  STLCRR = REF. CON. TEMP. IN SUTHERLAND. DEFAULT = 204.0
74  STLDFX = EXPONENT IN SUTHERLAND. DEFAULT = 1.5
77  STLDTR = REF. TEMP. IN SUTHERLAND. DEFAULT = 492.0
71  STLVR = VISCOSITY LSDO IN SUTHERLAND. DEFAULT = 1163 E-4
57  SSINIT = SSINIT / FACT
35  TP = TOTAL SOLUTION TIME FROM TC.
47  TFCGE = MINIMUM TEMPERATURE.
22  TF = FINAL TIME = TO + TO
47  TKH = DEFAULT NON-DIM. THICKNESS OF ELEMENTS. (1.0)
22  TIME = CURRENT TIME.
24  TO = STARTING TIME.
146  TNA = AIR TEMPERATURE FOR COMPUTATIONS IN DIMEN.
59  TOFINF = REFERENCE TEMPERATURE.
147  TTH = HYDROGEN TEMPERATURE FOR COMPUTATIONS IN DIMEN.
40  TRATIT = 1.0 + (GAMMAF-1.0) * XMACHS**2 / 2.0
25  TRNC = INTEGRATION PARAMETER IN 'CKNUNP'.
155  TSINF = STATIC TEMPERATURE COMPUTED IN COINIT.
26  TVDPI = PI * 2.0
46  VECCE = MAXIMUM L VELOCITY.
27  UN = VELOCITY (FREESTREAM).
141  VA = MAJOR AXIS OF ELLIPSE FOR VIRTUAL SOURCE.
142  VR = MINOR AXIS OF ELLIPSE FOR VIRTUAL SOURCE.
104  VELCST = UNINF**2 / (2.0*G*AJ*CPA*TOA)
139  VH = CENTER OF H2 ELLIPSE FOR VIRTUAL SOURCE.
140  VK = CENTER OF H2 ELLIPSE FOR VIRTUAL SOURCE.
177  VLBTON = VISCOSITY BRITISH TC MKS 1.488
178  VLBTOP = VISCOSITY BRITISH TC CGS 14.88
172  VSTART = PERCENT OF TO AT WHICH TC STARTV COMP. IN PNTES
81  XI = INITIAL MACH ON XI AXIS. DEFAULT = 0.0
125  XMAM = CONSTANT LSDO IN CFCFRL DEFAULT = 0.09
37  XLE = LEWIS NUMBER. DEFAULT = 1.0
109  XMA = MOLECULAR WEIGHT OF AIR. DEFAULT = 0.97
61  XMACHO = LOCAL MACH NUMBER.
154  XMACHS = INITIAL MACH NO. LSDO IN DIMEN.
66  XM = MASS FRACTION OF FLUID.
172  XMFACT = UNINF * SQRT(XMA/(TCFING*GAMMAF*G*RUNIV))
110  XMH = MOLECULAR WEIGHT OF HYDROGEN. DEFAULT = 2.016
118  XMSDF = MASS DENSITY COMPUTED IN Q3CNC.
126  XMUAP = VISCOSITY OF AIR. 0.00000115
127  XMUN2 = NOT LSDO
38  XMUNF = VISCOSITY (FREE STREAM)
128  XMUP5 = NOT LSDO
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 - OUTPLT STATICA = TIME * FACT / REF
112 X3LAST - LAST TIME STEP USED IN CONFS.
82 Y1 - INITIAL Coord. ON X2 AXIS. DEFAULT = 0.0
53 YSCALE - YICOR SCALE FACTOR. DEFAULT = 1.0
42 YSHIFT - SHIFT Y-COORDINATE. DEFAULT = 0.0
101 YUP - UPPER Y IN DECFNL.
173 ZMAX - MAX. DEPRIVATIVE COMPLETED IN QKNUK.
26 ZT - DIMENSIONAL CLRFAT TIME.
65 ZTTEST - STOP PROGRAM WHEN MAX.(Z?) LE ZTTEST. DEF. = 1.0E-4
IZARRAY

DEFINITION ENTRY POINTS IN IZ ARRAY.

IZARRAY ENTRY

201 ICOL --- OUTPUT COLUMN VECTOR USED IN FEOUTP.
202 IRW --- OUTPUT ROW VECTOR USED IN FEOUTP.
203 IEMTHD --- HEADINGS FOR OUTPUT VARIABLES.
204 ITITLE --- TITLE FOR START OF EACH OUTPUT PHASE.
205 IPRINT --- LIST OF DEPENDENT VARIABLES.
206 IESNO --- NO. OF BOUNDARY NODES / DEP. VARIABLE.
210 IINCOL --- NO. OF NODES PER COLUMN.
211 IINROW --- NO. OF NODES PER ROW.
218 ICPTAB --- SPECIFIC HEAT TABLE ENTRIES
219 IITAB --- TEMPERATURE TABLE ENTRIES.
220 ITUSED --- COUNTER USED FOR OUTPUT IN FEOUTP.
223 IXIPS --- TEMPORARY STORAGE FOR XCOORD COORDINATES.
224 IXPSDS --- TEMPORARY STORAGE FOR XCOORD COORDINATES.
225 IIND --- ARRAY OF BOUNDARY NODES FOR DEPENDENT VARIABLES.
226 IINDOF --- LIST OF ELEMENT CONNECTIONS (ELEM).
232 INWH --- SOLUTION ORDER OF NODES F/ DEP. VAR. IN DERIV.
233 INDEX --- ORDER OF NODES BY COLUMNS FROM LEFT TO RIGHT.
234 INDRA --- ORDER OF NODES BY ROWS FROM TOP TO BOTTOM.
235 INDCH --- OUTPUT COLUMN POSITION OF NODES.
236 ITELS --- NO. OF ELEMENTS CONNECTED TO NODES.
237 IETEM --- NOT USED.
238 IIORD --- LIST OF BORDER NODES IN CCW ORDER.
241 IB211 --- B211 MATRIX COMPUTED IN GEOMFL.
242 IB211S --- B211S MATRIX COMPUTED IN GEOMFL.
245 IB211A --- B211A ANTI-SYMMETRIC MATRIX.
247 IDIF --- FIRST HALF USED TO STORE DIFFUSION COEFFICIENTS.
2ND HALF USED TO STORE SOURCE TERMS.
248 IYY --- STORAGE FOR 2 VALUES OF DEPENDENT VARIABLES.
249 IIZZ --- STORAGE FOR 2 VALUES OF DERIVATIVES FOR DEP. VAR.
250 IXIP2 --- ELEMENT LENGTHS COMPUTED IN GEOMFL.
271 ISUM1 --- TEMPORARY STORAGE.
276 IOUT6 --- TEMPORARY STORAGE.
277 IAREA --- AREA OF ELEMENTS TIMES THICKNESS COMPUTED IN GEOMFL.
278 ICP --- VJOAL VALUES OF SPECIFIC HEAT.
279 TV --- NODAL VALUES OF ENTHALPY.
292 TD --- TEMPORARY STORAGE FOR DEPENDENT VARIABLE.
283 TQP --- TEMPORARY STORAGE FOR DERIVATIVE OF DEP. VAR.
284 TIRH --- NODAL VALUES OF DENSITY.
285 T1MP --- NODAL VALUES OF TEMPERATURE.
288 T1K --- ELEMENT THICKNESS DISTRIBUTION.
289 TVC0R --- NODAL VALUES OF TRANSVERSE COORDINATES.
290 TVC20R --- NODAL VALUES OF NORMAL COORDINATES.
291 TPS --- NODAL VALUES OF PRESSURE.
292 TVA --- NODAL VALUES OF VISCOSITY.
301 T0L --- RH0\*ULAST STORAGE FOR CONTES.
302 T0PL --- DELU STORAGE FOR CONTES.
303 TVEL --- RH0\*V STORAGE IN CONTES.

304 TV --- RH0\*W STORAGE IN CONTES.
306 TV12 --- TRANSFORMED X-AXIS OF ELEMENTS.
307 TV23 --- TRANSFORMED Y-AXIS OF ELEMENTS.
308 TVND --- Y-COORD. USED IN CONTES AND DFCFBL.
309 TVGM1 --- 1ST TERM OF R2001 ELEMENT MATRIX.
310 TVGM2 --- 2ND TERM OF R2001 ELEMENT MATRIX.
311 TIPLOTS --- LIST OF VARIABLES TO BE PLOTTED.
312 TPLTYP --- TYPE OF PLOT TO BE GENERATED.
313 TPLSCL --- SCALE FACTORS TO BE USED FOR PLOT.
314 TSCMT --- NODAL VALUES OF SCHMIDT NUMBERS.
315 TINMAT --- LIST OF MATERIALS IN REGION.
316 TIMAT --- ELEMENT VALUE OF MATERIAL.
319 TSCRE --- NOT USED.
320 T1INST --- NODAL VALUES OF STATIC ENTHALPY.
321 T1CALL --- LIST OF LINK NOS. TO CALL AT END OF QKNJT.
322 TICALLS --- LIST OF ROUTINE NOS. IN ASSOC. LINK TO BE CALLED.
323 TCMULT --- LIST OF MULTIPLIERS FOR OUTPUT VARIABLES.
324 TDSAVE --- LIST OF VARIABLES TO BE PRINTED IN OUTPUT.
325 T1NDOUT --- TEMPORARY STORAGE FOR OUTPUT VAR. AND SOURCE DATA.
327 TIENCL --- LIST OF NODES / COL. IN AXI-SYM. CONTES.
328 T1ENOX --- LIST OF NODES TO BE USED IN SOLVING AXI-S. CONTES.
329 T1CSTS --- COSTE OF ANGLE / COL. IN AXI-SYM. CONTES.
330 TVSIN --- SINE OF ANGLE / COL. IN AXI-SYM. CONTES.
331 T1PAR --- LIST OF PARAMETERS TO PRINT AT START OF OUTPUT.
332 T1PAR2 --- HOLLERITH DESC. OF PAR. AT START OF OUTPUT.
333 T1SUJT --- LIST OF CONSTANTS TO BE USED IN SUTHLO.
334 T1PR --- NODAL VALUES OF PRANDTL NUMBER.
335 T1MPAR --- LIST OF MULT. FOR PARAM. AT START OF OUTPUT.
336 T1FPS --- NODAL VALUES OF TURB. VISC. COMPUTED IN DFCFBL.
337 T1SKNFR --- LIST OF SKIN FRICTION PARA. COMP. IN WLFIX.
338 T1STM --- LIST OF STANTON NOS. COMPUTED IN WLFIX.
339 T1PST --- LIST OF DOWNSTREAM STATIONS IN PRESSURE TABLE.
340 T1PVX --- LIST OF DOWNSTREAM PRESSURES IN PRESSURE TABLE.
341 T1PX3 --- LIST OF DOWNSTREAM STATIONS IN PRESS. GRAD. TABLE.
342 T1PWX --- LIST OF DOWNSTREAM PRESS. GRAD. IN PR. GR. TABLE.
REFERENCES


APPENDIX A

DATA DECK LISTING FOR MACH 5
THREE-DIMENSIONAL FLOW CHECK CASE

FEAL  
COMTITL  
CHECK CASE, THREE-DIMENSIONAL SUPERSONIC FLOW WITH PRESSURE GRADIENT  
FNAME  
ENAME01  
KEND  
SNAMFO?  
\[ \text{UNF}=4004.8, \quad \text{TDFUNF}=1800, \quad \text{RFNL}=0.0132 \]  
\[ \text{TDF}=0.1, \quad \text{ODEP}=5.0, \quad \text{EPS}=0.01 \]  
\[ \text{VSTRT}=1.0, \quad \text{CPA}=0.24, \quad \text{CPI}=3.440 \]  
\[ \text{XDF}=1.0, \quad \text{XMA}=28.97, \quad \text{XHN}=2.016 \]  

FEND  
FEDINN  
L NK1  
\[ 1 \quad 2 \quad 1000, \quad 2 \quad 2 \quad 1000, \quad \text{SETUP} \]  
\[ 2 \quad 1000, \quad 21 \quad 2 \quad 1000, \]  
\[ 1 \quad 21, \quad 12, \]  
CHECK CASE, THREE-DIMENSIONAL SUPERSONIC FLOW WITH PRESSURE GRADIENT

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HOLIST  
LENGTH   | FT         | IN         | M     | CM     |
VELOCITY | FT/S       | NA         | M/S   | CM/S   |
DENSITY  | LBM/FT^3   | NA         | KG/M3 | G/CC   |
TEMPERATURE| RANKINF  | NA         | KELVIN| NA     |
ENTHALPY | LTL/LBM    | NA         | KJ/KG | NA     |
FROZEN   | RT/LBM     | NA         | KJ/KG | NA     |
HEAT     | LBM/LBM-R  | NA         | NA    |        |
VISCOSITY| LBM/FT-S   | NA         | NT/M2 | POISEF |
LOCAL PRESSURE| PSI        | PSI        | NT/M2 | TORR   |

182
LOCAL SOLUTION  MACH NC.  DPDXY(LREF/FT3) MAX. H2 CONC.  MIX EFF.(ETA)  
X1/LREF  DX1/LREF  EPSILON  GXMIN/LREF  

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<td>HSTATE/HREF</td>
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<tr>
<td>RHO/RHOREF</td>
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<tr>
<td>ELEM.N2 MAS.FRAC</td>
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<tr>
<td>U2/UREF</td>
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<td>CPF/CPFREF</td>
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<tr>
<td>HTOT/HREF</td>
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<tr>
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<td>ELEM.O2 MAS.FRAC</td>
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<td>EFF.PRANOTL NO.MU/MUREF</td>
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<td>EFF.SCHMIDT NO.</td>
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<tr>
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**COMOC 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 (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**

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<td>PINT 1 1 4 8 10 9 3 2</td>
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<td>KNO Bottom 1 DONE</td>
</tr>
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<td></td>
<td>KNO Bottom 2 DONE</td>
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<td></td>
<td>KNO Bottom 4 DONE</td>
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**183**
FIXES H (VARIABLE NO. 4) ALONG WALL TO INITIAL VALUE

ICALL   -1
    2    5    2    1    1    2    1
ICALLS  -1
    10    6    4    12    6    3    1
LINK3   4
LINK1   3
VFEND   -58

T INITIAL TOTAL TEMPERATURE PROFILE
VYY   -27
 2*0.0 2*865. 2*1654. 2*2373. 2*3004. 2*3550. 2*3879.
 2*3992. 2*4474. 2*4920. 2*5382. 2*6320. 2*7560. 2*9300.

T INITIAL U1 PROFILE
VYY   -27
 2*0.0 2*2.12 2*20.14 2*53.52 2*83.2 2*109.3 2*165.
 2*253. 2*447. 2*4920. 2*5382. 2*6320. 2*7560. 2*9300.

T INITIAL U2 PROFILE
VYY   -27
 2*0.0 2*2.12 2*20.14 2*53.52 2*83.2 2*109.3 2*165.
 2*253. 2*447. 2*4920. 2*5382. 2*6320. 2*7560. 2*9300.

T INITIAL N2 MASS FRACTION PROFILE
VYY   -27
 2*0.0 2*2.12 2*20.14 2*53.52 2*83.2 2*109.3 2*165.
 2*253. 2*447. 2*4920. 2*5382. 2*6320. 2*7560. 2*9300.

T INITIAL O2 MASS FRACTION PROFILE
VYY   -27
 2*0.0 2*2.12 2*20.14 2*53.52 2*83.2 2*109.3 2*165.
 2*253. 2*447. 2*4920. 2*5382. 2*6320. 2*7560. 2*9300.

T INITIAL H2 MASS FRACTION PROFILE
VYY   -27
 2*0.0 2*2.12 2*20.14 2*53.52 2*83.2 2*109.3 2*165.
 2*253. 2*447. 2*4920. 2*5382. 2*6320. 2*7560. 2*9300.

DIMEN

3KINT
DESCRIPT
COME
DESCRIPT 3
REFERENCE LENGTH LREF
REFERENCE VISCOSITY, LAMINAR VALUE
EVALUATED AT REF. TEMPERATURE
FREE STREAM VELOCITY AT X0=LREF
STAGNATION TEMPERATURE (CONSTANT = TREF)
FREE STREAM DENSITY AT X0=RHOREF
FREE STREAM MACH NUMBER AT X0
STATIC PRESSURE AT X
NUMBER OF NODES
NUMBER OF FINITE ELEMENTS

NONE
COMMON
END
EXIT
APPENDIX B
DATA DECK LISTING FOR VIRTUAL SOURCE
THREE-DIMENSIONAL CHECK CASE

FEAL
CONTILE
CHECK CASE FOR THREE DIMENSIONAL REACTING BOUNDARY REGION FLOW
FENAME
&NAMED1
NEQ=6,
IGAS=1,
IF=0,
KDUMP=0,
NPVSX=2,
NSC=1,
NSY=1,
&END
&NAMED2
UNF=2272.,
TCFINF=533.0,
REFL=.003333333,
TD=0.0,
TD=0.10,
DELP=50.0,
VSCALE=.003333333,
VSCALE=.003333333,
VSTART=101.0,
&END
FEDIMN
LINK1 1
1 75 100, 2 50 100, 3 125 100, 4 150 100, 5 225 100,
T INCREMENTS BETWEEN X3, NODE-NUMERATOR-DENOMINATOR
5 10, 5 10, 8 125 100, 9 175 100, 10 250 100,
T INCREMENTS BETWEEN X2
1 11, 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

PARA -1
2 2 2 162 164 163
2 2 2 164 163
2 2 2 170 174
2 2 2 165 2
2 2 2 165 2
2 2 2 176 2
2 2 2 177 178
2 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......... LB/FT^3........ NA............ KG/M^3............ G/CC............
TEMPERATURE...... RANKINE........ NA............ KELVIN............ NA............
ENTHALPY......... BTU/LBM........ NA............ B/J/KG............ NA............
FROZ SPEC HEAT... BTU/LBM-RT.. NA............ KJ/KG-RT........ NA............
VISOSITY......... LB/FT-S........ NA............ NT-S/HZ............ MSF............
LOCAL PRESSURE... PSI............ NA............ NT/HZ............ TORR............
LOCAL SOLUTION... MACH NO. DPDX1(LBF/FT3) MAX. H2 CONC. MIX EFF.(ETA)
<table>
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<tr>
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**TOSAVE -1**
1048 285 320 284 10248
2248 278 4248 9248 8248
1247 334 252 314

**TUMULT -1**
1492

**DESCRIP 2**

**CONEC**

**DESCRIP**

**CHECK CASE**

**THREE DIMENSIONAL REACTING BOUNDARY REGION - VIRTUAL SOURCE**

**(+H/0/2/AIR SYSTEM WITH EQUILIBRIUM CHEMISTRY)**

**PROBLEM CONSIDERED**

**REPRESENTS TRANSVERSE H2 INJECTION INTO A SUPERSONIC AIR STREAM**

**CHARACTERISTIC OF SCRAMJET FUEL INJECTION, SEE ROGERS NASA TN 6-114, 1971 AND NASA TN 5-1476, 1971 FOR EXPERIMENTAL STUDY OF THIS PROBLEM.**

**TURBULENCE MODEL EMPLOYED IS DESCRIBED IN USER'S MANUAL NASA CR-132450, 1974.**

**CALCULATIONS ARE STARTED USING VIRTUAL SOURCE CONCEPT TO REPLACE COMPLEX NEAR INJECTION FLOW FIELD.**

**NONE**

**VX3ST**
0.0 100 T X1 TABLE FOR PRESSURE

**VPPSX**
193, 193 T PRESSURE TABLE PSF

**PINT**
-1

1 4 8 10 5 3 2 T INTEGRATE U1, FATH, C2, N2, H2, U3, U2

**KEND**

**PITTIM**

**DCNE**

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

**KEND**

**BOTTOM**

**DCNE**

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

**KEND**

**BOTTOM**

**DCNE**

**FIXES H (VARIABLE NO. 4) ALONG WALL TO INITIAL VALUE**
$K:\text{M}$

**NOT**

$3CONE$ FINE

'SH (VARIABLE NO: 81 ALONG WALL TO INITIAL VALUE

$K:\text{ON}$

$3\text{DONE}$

$ICALL - 1$

$ICALLS - 1$

$LINK 3 4$

$LINK 1 3$

$VTMP - 58$

$T$ INITIAL TOTAL TEMPERATURE PROFILE

$\overline{VYY}$

$T$ INITIAL $U1$ PROFILE

$\overline{VYY}$

$T$ INITIAL $U2$ PROFILE

$\overline{VYY}$

$T$ INITIAL $O2$ MASS FRACTION PROFILE

$\overline{VYY}$

$T$ INITIAL $N2$ MASS FRACTION PROFILE

$\overline{VYY}$

$T$ INITIAL $H2$ MASS FRACTION PROFILE

$\overline{VYY}$

**DESCRIPTION 3**

**NUMBER OF NODES**

**NUMBER OF FINITE ELEMENTS**
APPENDIX C

SAMPLE OUTPUT FOR MACH 5
TWO-DIMENSIONAL FLOW CHECK CASE
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2 VARIABLES OF POG INTEGRATED.

7 VARIABLES IN SOLUTION.

Link 1 = DREM USE.

ORDER OF CALLS AT END OF DESIGN:

LINK1 61  LINK2 62  LINK3 41  LINK4 12  LINK5 31

Link 6 41  LINK2 31  LINK
## THREE-DIMENSIONAL SUPERSONIC FLOW WITH PRESSURE GRADIENT

### REFERENCE

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### LOCAL SOLUTION

- Mach No.: 0.79145
- Density:
- Pressure:
- Temperature:
- Viscosity:

### LOCAL PRESSURE

- PDE:
- NT/99:
- TNR:
- N/A:

### E

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**Skin Friction Distribution**: (CF/2)

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### Three-Dimensional Boundary Region Variant

#### Check Case, Two Dimensional Supersonic Flow with Pressure Gradient

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*IN FRICKER DISTRIBUTION 1/27*
APPENDIX D

SAMPLE OUTPUT FOR VIRTUAL SOURCE
THREE-DIMENSIONAL FLOW CHECK CASE
CONE CHECK CASE FOR THREE-DIMENSIONAL REACTING BOUNDARY REGION FLOW

CHARACTERISTIC OF SCRAMJET FUEL INJECTION INTO A SUPersonic AIR STREAM

COMPUTED TRANSVERSE H2 INJECTION INTO A SUPERSONIC AIR STREAM

CHARACTERISTIC OF SCRAMJET FUEL INJECTION INTO A SUPERSONIC AIR STREAM

THE VELOCITY MODEL EMPLOYED IS DESCRIBED IN USER'S MANUAL NASA CR-

CALCULATIONS ARE STARTED USING VIRTUAL SOURCE CONCEPT TO REPLACE

CONVEX WALL INJECTION FLOW FIELD.

| VN, INT. NODES FOR VARIABLE 1 | 1 | 2 | 3 | 4 | 5 | 6 |
| VN, INT. NODES FOR VARIABLE 2 | 1 | 2 | 3 | 4 | 5 | 6 |
| VN, INT. NODES FOR VARIABLE 3 | 1 | 2 | 3 | 4 | 5 | 6 |
| VN, INT. NODES FOR VARIABLE 4 | 1 | 2 | 3 | 4 | 5 | 6 |
| VN, INT. NODES FOR VARIABLE 5 | 1 | 2 | 3 | 4 | 5 | 6 |
| VN, INT. NODES FOR VARIABLE 6 | 1 | 2 | 3 | 4 | 5 | 6 |
| VN, INT. NODES FOR VARIABLE 7 | 1 | 2 | 3 | 4 | 5 | 6 |
| VN, INT. NODES FOR VARIABLE 8 | 1 | 2 | 3 | 4 | 5 | 6 |
| VN, INT. NODES FOR VARIABLE 9 | 1 | 2 | 3 | 4 | 5 | 6 |
| VN, INT. NODES FOR VARIABLE 10 | 1 | 2 | 3 | 4 | 5 | 6 |
| VN, INT. NODES FOR VARIABLE 11 | 1 | 2 | 3 | 4 | 5 | 6 |
| VN, INT. NODES FOR VARIABLE 12 | 1 | 2 | 3 | 4 | 5 | 6 |

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**Note:** The table represents a portion of a larger dataset, where each row corresponds to a different percentage of T/F, with CPF/CPF/REF and E 1/E 2/E 3 values for each row. The table is likely part of a scientific or technical report, indicating measurements or calculations across different conditions.
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THREE-DIMENSIONAL BOUNDARY REGION VARIANT

CHECK CASE THREE-DIMENSIONAL REACTING BOUNDARY REGION - VIRTUAL SOURCE

LENGTH

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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 CFCFR

E1 = MIXING LENGTH MODEL
E2 = MASS DEFECT MODEL

COMPUTE EDDY VISCOSITY IN TERMS OF NON-DIMENSIONAL PARAMETERS BEFORE LEAVING SUBROUTINE, DIMENSIONALIZE BY

FACTMU = ALC * RHOJREF * UREF
Y(I(U1)) = NON-DIMENSIONALIZED BY ALC
U(U1) = NON-DIMENSIONALIZED BY UREF
RHO = NON-DIMENSIONALIZED BY RHOS

CON = MIXING LENGTH CONSTANT
C4ED = MASS DEFECT CONSTANT
OMEGA = VAN DRIEST DAMPING FACTOR
GAMMA = INTERMITTENCY FACTOR
XMSDF = MASS DEFECT IN REGIONS CONTAINING ONE PERCENT OR MORE H2 (NOT THE USUAL DEFINITION OF MASS DEFECT).
ARR = AREA OF FLOW ContAINING ONE PERCENT OR MORE H2.
ELE2SW IS LOCATION DOWNSTREAM (FT) WHERE THE TURBULENCE MODEL SWITCHES FROM COMPLETELY MIXING LENGTH TO THE TWO LAYER MODEL.
FLE2SW USED ONLY FOR VIRTUAL SOURCE SIMULATION
PCNT IS THE PERCENT OF H2 DEFINING THE OUTER EDGE OF THE MIXING ZONE.

NOTE - SPECIAL SUBSCRIPTING TECHNIQUE USED TO LOCATE Y(I(U2),U(U1)) AND RHO RUNNING UP COLUMNS OF NODES. THIS WAS REQUIRED FOR COMPUTING MIXING LENGTHS AND DERIVATIVES OF U1 WITH RESPECT TO THE NORMAL TO THE WALL, (X2). NOTE - CONSTANTS WERE DETERMINED BY FITTING PREDICTIONS TO DATA OF ROGERS, NASA TND - 6114, 1971.

IF DEBUG PRINT OUT FOR E1 AND E2 COMPUTATIONS IS REQUESTED, SET IWRIT = 1

DIMENSION Y(1), RHO(1), U(1), ALF(1), TEMP(1)
DIMENSION INCOL(1), INDEX(1), AREA(1), INODE(1)
DIMENSION XICOR(1), X2COR(1), RHOUI(1), W(1), YY(I), EPSLNI(1)
DIMENSION FI(1), EZ(1), AL(1), GAMMA(1), CFUV2(I)
DIMENSION SCHMT(1)
COMMON / VARIF / IRAYAR(00200), IARRAY(0400)
EQUIVALENCE ( IARRAY(00016), NNODE )
EQUIVALENCE ( IARRAY(00030), NP )
EQUIVALENCE ( IARRAY(00041), LG )
EQUIVALENCE ( IARRAY(00070), NVQ3 )
EQUIVALENCE ( IARRAY(00071), NVQ )
EQUIVALENCE ( IARRAY(00086), KPNT )
EQUIVALENCE ( IARRAY(00107), NE1F2 )
EQUIVALENCE ( IARRAY(00108), NUQ3 )
EQUIVALENCE ( IARRAY(00111), IMAX )
EQUIVALENCE ( IARRAY(00122), IWPIT )
EQUIVALENCE ( IARRAY(00141), KALLQ3 )
EQUIVALENCE ( IARRAY(00143), NT )
EQUIVALENCE ( IARRAY(00144), NS )
EQUIVALENCE ( IARRAY(00145), NS2 )
EQUIVALENCE ( IARRAY(00030), ALC )
EQUIVALENCE ( IARRAY(00021), PE )
EQUIVALENCE ( IARRAY(00023), TIME )
EQUIVALENCE ( IARRAY(00038), XMUNINF )
EQUIVALENCE ( IARRAY(00059), FACTMU )
EQUIVALENCE ( RARRAY(00101), YUP )
EQUIVALENCE ( RARRAY(00118), XMSDF )
EQUIVALENCE ( RARRAY(00124), CON )
EQUIVALENCE ( RARRAY(00125), XLAM )
EQUIVALENCE ( RARRAY(00126), XMXAIR )
EQUIVALENCE ( RARRAY(00127), XMUH2 )
EQUIVALENCE ( RARRAY(00128), XMUP5 )
EQUIVALENCE ( RARRAY(00129), SCT )
EQUIVALENCE ( RARRAY(00130), C4ED )
EQUIVALENCE ( RARRAY(00133), PCNT )
EQUIVALENCE ( RARRAY(00134), QMAX )
EQUIVALENCE ( RARRAY(00143), C4EDSW )
EQUIVALENCE ( RARRAY(00144), C4FACT )
EQUIVALENCE ( RARRAY(00145), FL1E2SW )
EQUIVALENCE ( RARRAY(00010), RHOREF )
EQUIVALENCE ( RARRAY(00027), UREF )
EQUIVALENCE ( RARRAY(00046), UE )
EQUIVALENCE ( RARRAY(00048), RHOE )

SET CONSTANTS FOR TURBULENCE MODEL

AVD = 25.3
CN=0.135
C4ED=0.0007
F1E2SW=0.02
PCNT=1.0
USR4 = FACTMU
XLAM=0.0753
XMUW = AVD / XMUAI
19AX=2
FRAC = XLAM / CN*7

DEBUG OUTPUT HEADINGS

IF ( NT .EQ. 0.AND.IWRT.GT.0) WRITE(6,9600)
9600 FORMAT (1H1, 9X,6HE11(LL), 9X,6HAI1(LL), 6X,9HGAMMA(LL), 10X,
*5H(I1),22X,8HY(KTIl),5X,10HY(KT(l)-1), 9X,6HRH0(I1) / )
9610 FORMAT ( 1H0, 8115 / 8F15.5 )
9620 FORMAT ( 1H1, 5I( 4H E2(, 13, 3H) =, E13.5) )

INIZITALIZE ARRAY COUNTERS

XT = TIME * ALC
IF ( NS .GT. 0 ) GO TO 30
IF ( XT .LT. E1E2SW ) GO TO 30
NEIE2 = 3 - NEIE2
KPNT = 1
NS = 1
CONTINUE

IF ( NS2 .GT. 0 ) GO TO 40
IF ( XT .LT. C4EDSW ) GO TO 40
KPNT = 1
NS2 = 1
CONTINUE

SET UP ARRAY INDICES.

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

CALL CS3CONC ( INDOF, 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&M-1)

VAN DRIEST DAMPING FACTOR
RHODED = RHOD * RHODEF
UED = UE * UREF
TAUW = CF0V2(KK) * RHODED * UED * UED
OMEGA = 1.0
GAMMA(I) = 1.0
E1(I) = 0.0
AL(1) = CON * Y(KT)
DD 200 LL = 2, M
II = LL - 1
I = INDEX(KT&II-1)
IP1 = INDEX(KT&II)
YUP = Y(KT&M-1)
MM2 = M - 2
IU = INDEX(KT&M-1)
DD 160 IJ = 1, MM2
IL = INDEX(KT&M-IJ-1)
VAL = ABS ( U(I) / U(IU) - 1.0 )

DETERMINE UPPER BOUNDARY OF HYDROGEN CONCENTRATION
IF ( N103 .GE. 3 )
   *VAL = ABS ( W(IL) / Q3MAX )
   IF ( VAL .GT. PCNT ) YUP = Y(KT&M-IJ-1)
   IF ( VAL .GE. PCNT ) IMAX = M - IJ
   IF ( VAL .GE. PCNT ) GO TO 170

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

190 CONTINUE
   GAMMA(LL) = 1. / ( 1. & XI **9)
   RHOO = RHOD(IP1) * RHODEF
   YVD = Y(KT&LL-1) * ALC
   IF ( TAUW .GT. 0.0 )
   *OMEGA = OMEGA - EXP ( - YVD * X*UW * ( TAUW * RHOO )**.5 )

COMPUTE FL AND E2, BOTH ARE VECTORS WHICH WILL BE FILLED.
   VISCOSITY 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)) * RHOD(IP1)
   KTP1 = KT & II

219
KTPM = KT & II - 1
IF ( NT .NE. 0 ) GO TO 250
IF ( IWRIT .LE. 0 ) GO TO 250
WRITE ( 6, 9610 ) LL, LL, LL, IPI, I, KTP, KTM, IPI,
* E1(II), AL(II), GAMMA(II), U(II), U(I), Y(KTP), Y(KTM), RHO(IPI)
250 CONTINUE
200 CONTINUE
IF ( KALL03 .EQ. 0 ) ARR = Y(KTM-1)
TEMP1 = C4ED * XMSDF / ARR
DO 400 J = I, 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 IF E1 IS LESS THAN E2, USE E1, WHEN E1 BECOMES GREATER THAN E2 USE E2 FOR THE REMAINDER OF THE COEFFICIENTS.
C
KODE = 0
DO 500 K = I, M
J = K
I = INDEX(KTEK-1)
IF ( KODE .EQ. 1 ) GO TO 450
IF ( J .GT. IMAX ) GO TO 450
EPSLN(I) = E1(J) * USAR
GO TO 475
450 CONTINUE
KODE = 1
IF ( NE1E2 .NE. 2 ) EPSLN(II) = E1(J) * USAR
IF ( NE1F2 .EQ. 2 ) EPSLN(II) = E2(J) * USAR
475 CONTINUE
500 CONTINUE
KT = KT & M
600 CONTINUE
NT = 1
RETURN
END