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A THEORETICAL STUDY OF A LAMINAR DIFFUSION FLAME

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I. ABSTRACT

Theoretical models of an axisymmetric laminar diffusion flame are discussed, with an emphasis on the behavior of such flames at increasing pressures. The flame-sheet or Burke-Schumann model (in terms of Bessel functions) and various boundary-layer numerical solutions are presented and their results compared with experimental data. The most promising theoretical model combines the numerical flow field solution of the Patankar-Spalding computer code with the Pratt-Wormeck chemical reaction subroutine. The flame shapes for pressures of 1, 5, 10, 20, and 50 atmospheres have been computed and agree remarkably well with experimental data. There is a noticeable shape change with pressure, believed to be a result of buoyancy effects. The chemical concentration profiles do not exhibit much dependence on pressure, a reflection of the fact that only one chemical mechanism was utilized at all pressures.

II. INTRODUCTION

The problem of pollutant formation in turbine combustors is currently receiving a great deal of warrented attention, especially the pollution associated with aircraft turbine engines in and around airports. Of the various pollutants discharged from these engines, two of the most harmful are nitric oxide and nitrogen dioxide, commonly referred to as NO_x. Since actual combustors may operate at pressures up to 30 atm, it is of special interest to consider the effect of pressure on the formation of NO_x during the combustion process, which has been done experimentally by Miller and Maahs [1] at NASA-Langley.

In their experimental investigation, an intentionally simplified combustion system--a laminar diffusion flame--was chosen to model the actual combustion process. The diffusion, or non-premixed, flame was selected over the premixed flame because it is an experimentally simpler system and because larger NO_x concentrations are expected with the diffusion flame. The laminar flow regime was selected in order to eliminate fluid flow effects as much as possible so as to concentrate on chemical effects.

The structure of laminar diffusion flames has been the subject of investigation for a great many years. The first analytical study of diffusion flames was made by Burke and Schumann [2] in 1928. They introduced the assumption that the zone of combustion might be approximated as a surface, i.e. infinitely thin. It would then follow that the associated reaction rates would be infinite. Burke and Schumann were concerned with a cylindrical laminar fuel jet discharging into an air stream moving with the same velocity as the fuel; they proceeded to calculate the flame shape for various initial conditions. The same assumption has been utilized to predict the length of both laminar and turbulent open flames. (Hottel and Hawthorne [3], Wohl, Gasley, and Knapp [4], Barr [5]).

Zeldovich [6] was among the first to consider the structure of a reaction zone of finite thickness and hence the effects of finite reaction rates. Similar studies have been done by Spalding [7] with an emphasis on the phenomenon of extinction. Linan [8] has also studied the effects of finite chemical reaction rates by means of a boundary-layer-type solution, while many have applied perturbation techniques to the problem (Fendell [9], Kassoy and Williams [10], Chung, Fendell, and Holt [11]).

The computer simulation and prediction of chemically reacting flows, an extremely difficult problem because one must describe the interaction of many reacting chemical species with fluctuating temperature and velocity fields, is nevertheless a method of solution that is being used to a greater and greater degree as computer software/hardware facilities become more advanced.

There exist at present two well-defined bodies of literature on the numerical (computer) solution to chemically reacting flows: 1) fluid flow with infinite-rate chemistry (chemical equilibrium), and 2) finite-rate chemically reacting flow without mixing or with infinite-rate mixing. Examples of such works are those by Patankar and Spalding [12] and Pratt [13], respectively. Pratt and Wormeck [14] have then attempted to combine aspects of both bodies of literature to achieve a scheme that could model the phenomena of a diffusion flame-a laminar finite-rate chemically reacting flow field.

It is the purpose of this study to construct an analytical model of the laminar diffusion flame described by Miller and Maahs [1] and to compare experimental and theoretical results concerning the effects of high pressure on flame shape, temperature distribution and NO_x formulation.

Sections III and IV describe the physical system and experimental results, Section V introduces the governing equations and Section VI describes various theoretical models and associated results.

III. DESCRIPTION OF THE PHYSICAL SYSTEM

For purposes of completeness a summarized description of the physical system employed at NASA-Langley is included. For a more detailed description, Reference [1] should be consulted.

A diagram of the burner and collection system is shown in Figure 1. Methane gas issues from a cylindrical tube into a concentric cylindrical tube through which air is flowing. The fuel tube has an inside diameter of 3.06 mm and the air tube has an inside diameter of 20.5 mm. Fuel and air flow rates are held constant at 41.8 standard cm^3/min (sccm) and 2450 sccm, respectively.

In order to obtain a flat velocity profile in the fuel and air streams as they exit from their respective ducts, porous disks of sintered stainless steel were installed near the duct exits. Ignition is accomplished by means of an electrical hot-wire igniter. During operation the igniter is positioned 10 to 20 mm above the burner; once ignition is attained the igniter is removed from the flow.

The combustion products exit from the top of the quartz chimney and are swept into a total-sample collector by the nitrogen pressurizing gas. The nitrogen flow rate is kept low enough so as not to excessively dilute the gases to be analyzed. The products are analyzed by a continuous infrared CO_2 monitor and a chemiluminescent NO-NO_x analyzer.

The measurement of flame temperature is the most difficult and most uncertain of any measurements made. The method of two-color pyrometry was employed (with the carbon in the flame as the radient emitter) to determine a spatial average temperature near the hottest point in the flame.

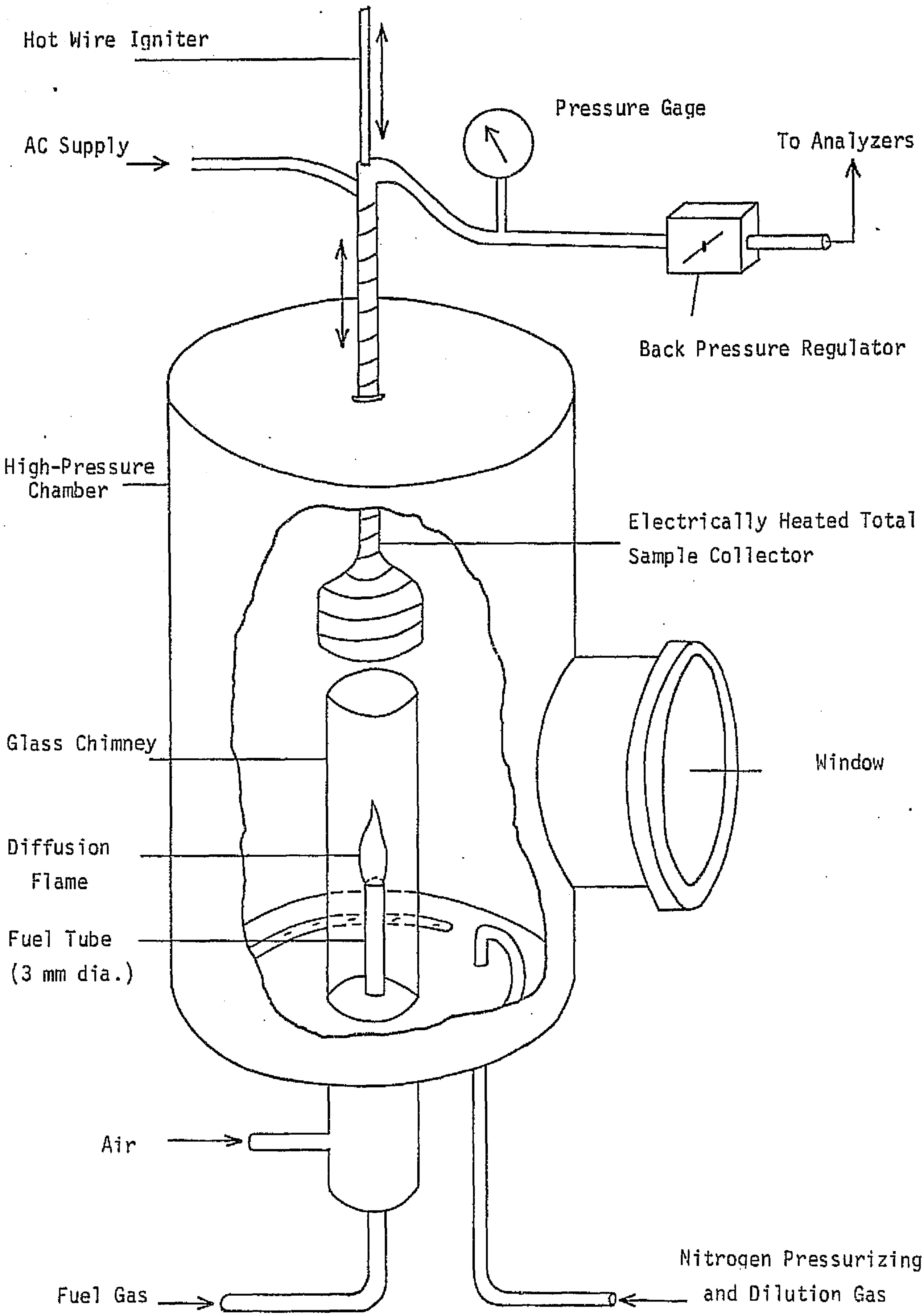

Figure 1 - Schematic diagram of burner and collection system

IV. EXPERIMENTAL RESULTS

A. Flame Shape

A definite change in the shape of the diffusion flame occurred as pressure was increased from 1 to 50 atm. This is shown in Figure 2, taken from Reference [1]. At 1 atm the sides of the flame bow outward, but this decreased as the pressure was increased above 1 atm. At about 10 atm the flame exhibited a slight concavity and the diameter decreased considerably. A further decrease in flame diameter occurred as the pressure increased, the maximum change associated with a pressure of approximately 20 atm.

An increase in the amount of carbon accompanied the change of flame shape and at pressures higher than 20 atm only minor changes occurred.

The height of the flame did not change drastically with pressure, as illustrated in Figure 3. The flames were typically 10 mm in height.

B. Nitrogen Oxide

The molar emission index of NO_x, Im, is defined as the number of moles of NO and NO_2 produced per mole of fuel burned. Figure 4 shows that this quantity increases rapidly as pressure increases, reaching a maximum at about 9 atm. Above this pressure the molar emission index decreases slowly and continuously until it returns to roughly its original value.

C. Flame Temperature

A plot of the optically-measured peak temperature as a function of pressure is shown in Figure 5, with data limits shown by vertical lines. There is a steady decrease of peak temperature with pressure.

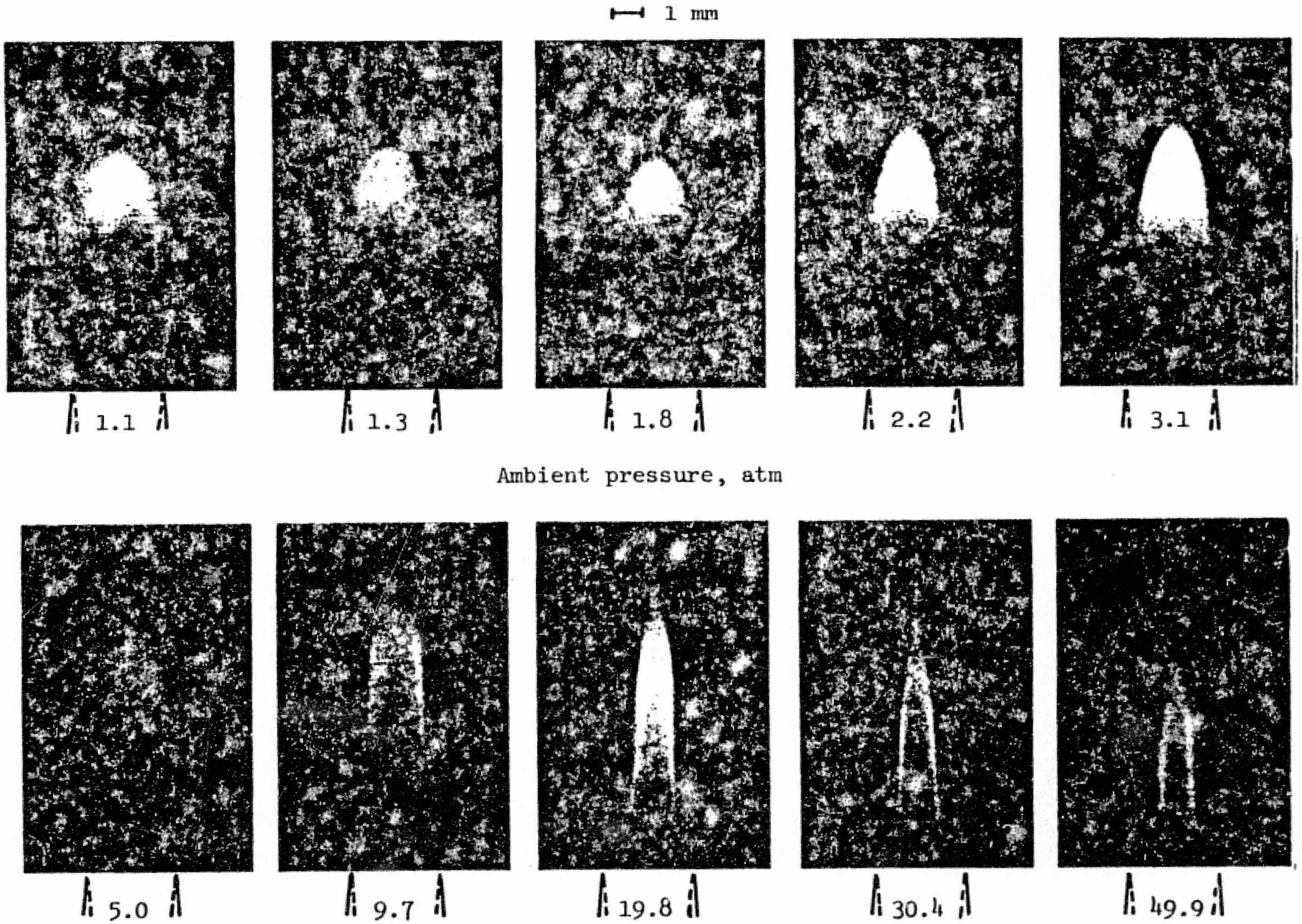

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Figure 2 - Photographs of methane-air diffusion flames for various ambient pressures. Methane flow rate, 41.8 sccm; air flow rate, 2450 sccm; burner diameter, 3.06 mm. See Ref. 1.

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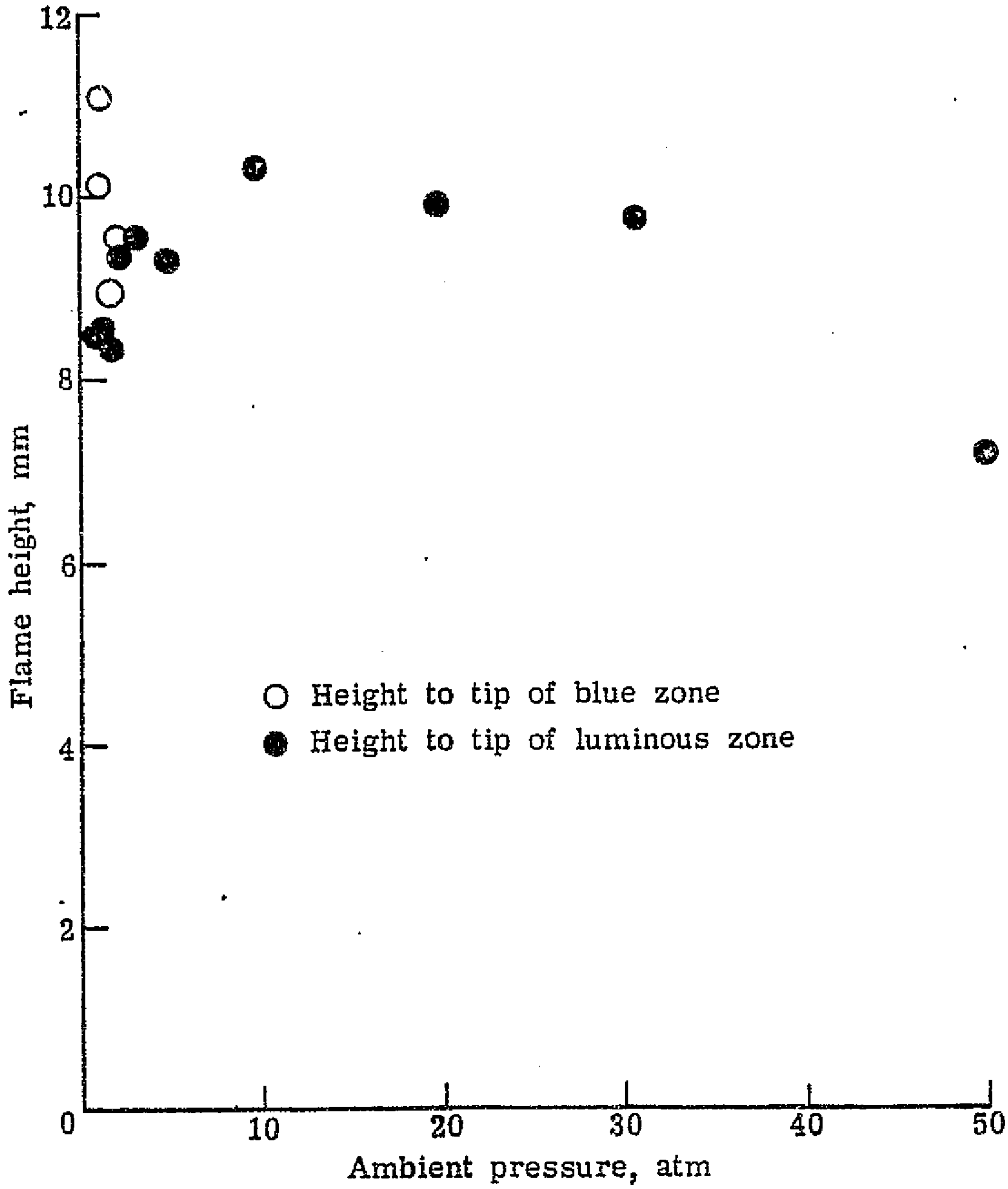

Figure 3 - Flame height as function of pressure. See Ref. 1

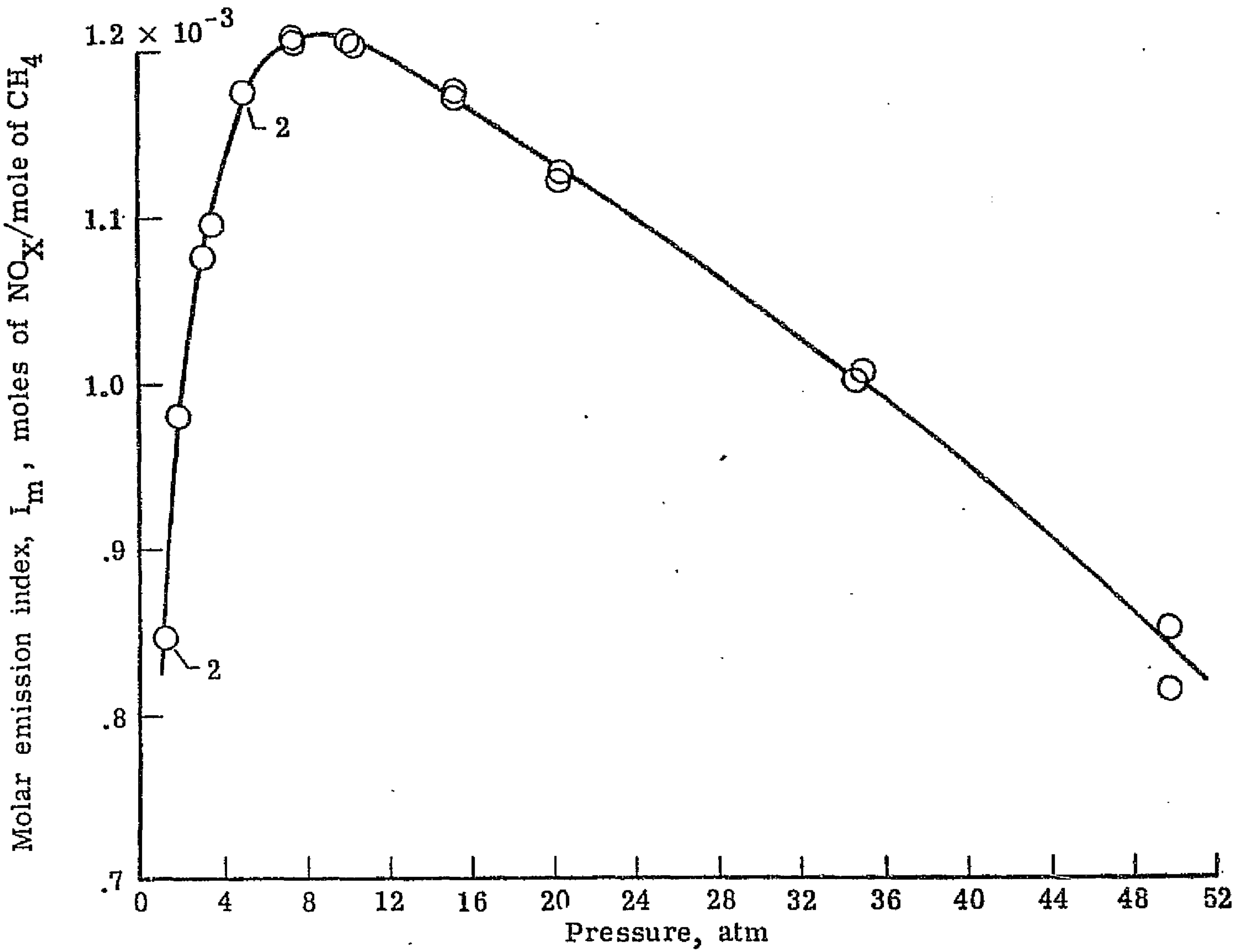

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Figure 4 - Molar emission index of NO_X as function of pressure. See Ref. 1

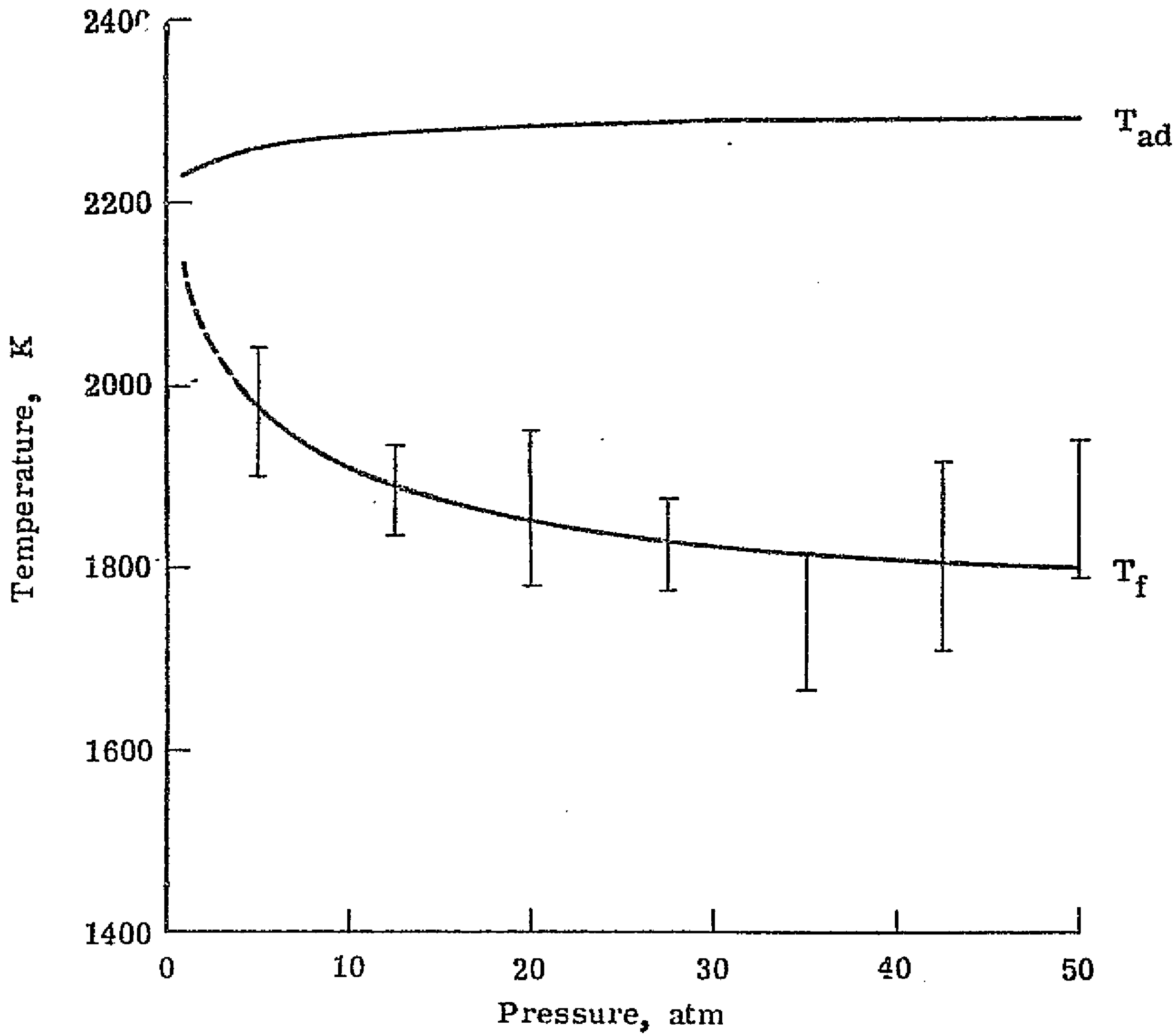

Figure 5 - Flame temperature as function of pressure. Dashed line indicates extrapolation. See Ref. 1

V. GOVERNING DIFFERENTIAL EQUATIONS

The equations of motion reflecting the conservation of mass, momentum, energy, and mass of each component for a chemically reacting gas mixture are:

Conservation of Mass

$$\frac{\partial \rho}{\partial t} + \text{div } \rho \overline{V} = 0$$

where ρ = density $\overline{V}$ = velocity vector

Newton's Second Law

$$\rho \frac{D\overline{V}}{Dt} = -\nabla p + \text{div } \tau$$

where $\frac{D}{Dt}$ = substantial derivative = $\frac{\partial}{\partial t} + \overline{V} \cdot \nabla$

p = pressure

τ = viscous stress tensor

Conservation of Energy

$$\rho \frac{Dh}{Dt} = \frac{Dp}{Dt} + \tau : \varepsilon - \text{div } \overline{q}$$

where

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h = enthalpy

ε = rate of strain tensor

$\overline{q}$ = heat flux vector

Species Conservation

$$\rho \frac{Dm_i}{Dt} = - \text{div } \overline{j}_i + R_i$$

where

m_i = mass fraction of species i = $\frac{\rho_i}{\rho}$

$\overline{j}_i$ = mass flux vector

R_i = rate of creation of species i by chemical reactions

In order to close the system the following constitutive relationships and equations of state are introduced:

$$\tau = 2\mu\varepsilon + \lambda \text{div}\, \overline{V}\, \Pi$$

where μ + λ are the 1st and 2nd coefficient of viscosity and Π is the unit tensor

$$\varepsilon = 1/2(\nabla\overline{V} + \nabla\overline{V}^T)$$

$$j_i = \rho\sum_j \tilde{D}_{ij}\nabla m_j$$

where $\overline{j}_i$ is the mass flux vector and $\tilde{D}_{ij}$'s are the diffusion coefficients

$\overline{q} = -k\nabla T + \Sigma h_i\overline{j}_i$ $\quad$ $\overline{q}$ is the heat flux vector $\quad$ T = temperature

k = coefficients of conductivity.

$p = \rho RT \sum_i \frac{m_i}{W_i}$ $\quad$ $h = \Sigma h_i m_i$ $\quad$ $h_i = h_i + \int_{T_0}^{T} C_{p_i}\, dT$

where W_i = molecular weight of species i.

The above equations are non-linear second order partial differential equations. The two main types of solutions are analytical and numerical.

Analytical methods are those that express the solution as algebraic formulae, power series, etc. Methodologies such as separation of variables, series expansions, and coordinate transformations are employed to obtain such solutions. These types of solutions are usually limited to linear or linearized differential equations.

Numerical methods are those that express the solution in the form of numbers related to the particular circumstances of the flow. The differential equations are transformed to algebraic "finite-difference" equations and the values of all dependent variables are calculated at the nodes of a grid covering the domain of interest.

The flow to be considered is in general governed by nonlinear equations with the rate of chemical production term (R_i) being highly complex. Simplifying assumptions may be made and various solutions obtained. A discussion of these solutions and associated assumptions follows in Section VI.

VI. THEORETICAL ANALYSES

A. Burke - Schumann Analytical Solution

If the following assumptions are made:

1. steady cylindrical flow
2. inviscid flow
3. negligible pressure and thermal diffusion
4. Ficks Diffusion Law
5. single step chemical reaction of fuel and oxidant → product
6. parallel and equal gas velocities
7. constant mass flux
8. axial diffusion <<< radial diffusion
9. entire chemical reaction occurs at the flame surface

then the governing equations may be combined into a single linear partial differential equation with appropriate boundary conditions. The solution is in terms of Bessel functions and a flame shape may be predicted from the analysis. Reference [15] presents a more detailed discussion of this solution.

The predicted flame shape agrees fairly well with the experimental evidence, although the predicted flame height at 1 atm (3.6 cm) is greater than the experimental. Furthermore, the Burke-Schumann model predicts absolutely no change of shape with pressure, hence it is evident that a more refined theoretical analysis is necessary.

B. Edelman - Fortune - Weilerstein Numerical Solution

The effects of inertia, viscosity, diffusion, gravity, and combustion on an axisymmetric laminar diffusion flame have been investigated via a boundary layer type formulation by Edelman, Fortune, and Weilerstein [16]. First a von Mises transformation is made in going from axisymmetric physical coordinates (x, r), where x is the axial distance and r the radial distance, to (x, ψ) coordinates. The stream function ψ is defined by

$$\int_{\psi_a}^{\psi_b} \psi d\psi = \int_{r_a}^{r_p} \rho u r dr$$

The governing equations are then non-dimensionalized by means of an emperical normalization parameter.

> "It is customary practice to do this (non-dimensionalization) by normalizing the variables directly in terms of the boundary conditions. However . . . the resulting dimensionless groups do not truly characterize the process and that is due to the large variation in flow properties throughout the domain of interest. Accordingly, the current approach involves the introduction of a set of characteristic quantities which are based upon some state within the flow that more accurately reflects the flame structure." [16]

The equations are then solved numerically by means of an explicit finite difference formulation.

The Burke-Schumann combustion model, or "flame sheet assumption", is that all the heat is released on the suface where the fuel-air ratio is stoichiometric. A more accurate combustion description is offered in this model in terms of a basic equilibrium theory for the combustion in either the fuel-lean or fuel-rich regime.

For a pressure of one atmosphere this program predicted a flame height of .8 cm and a flame shape that agrees remarkably well with experimental data. However, the results for pressures greater than one atmosphere could not be substantiated either qualitatively or quantitatively by experimental data. This was due to the fact that the analysis in Ref. [16] utilizes a normalization parameter obtained experimentally at one atmosphere of pressure. This does not affect the original work since the problem considered was buoyancy effects of diffusion flames, all at one atmosphere. The analysis, limited as it is to a pressure of one atmosphere, does not therefore lend itself to the problem at hand.

C. Patankar-Spalding Numerical Solution

Patankar and Spalding [12] likewise utilize a boundary layer formulation and a von Mises coordinate transformation so as to put the conservation equations in the general form

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

where

x and ω are the two independent coordinates

a and b are arbitrary functions of x

c and d are arbitrary functions of any dependent and independent variables

ϕ stands for any one of a set of variables, each possessing its own differential equation, e.g., fluid velocity, stagnation enthalpy, mass fraction, etc.

These differential equations are transformed into finite difference equations and solved by means of the tri-diagonal matrix algorithm (TDMA).

The chemistry incorporated into this numerical scheme is a very simple fuel-oxidant-product equilibrium model where the rate of generation of fuel by chemical reaction, R_{f_u}, is assumed to obey an "Arrhenius-type" relation.

For the case of negligible chemical reactions this program produces acceptable results in that the diffusional nature of the axial flow of fuel and air is well represented by means of velocity and concentration profiles. With the inclusion of limited equilibrium chemistry a flame shape can be obtained that agrees qualitatively with that obtained experimentally. The theoretical flame height at one atmosphere is 8 cm as opposed to an experimental height of .8 cm however. Since the chemistry of the flow field under consideration is of prime importance, the very simple chemistry incorporated into this model does indeed limit its ability to accurately describe the flame under investigation.

D. Patankar-Spalding and Pratt-Wormeck Numerical Solution

As stated previously, the hydrodynamic aspects of Spaldings code are well-developed and offer a valid model of the diffusional nature of the flow. A more realistic chemical model is provided by Pratt and Wormeck [14] in their subroutine for the calculation of chemically complex equilibrium or non-equilibrium stationary states.

The scheme employed by Pratt and Wormeck in their determination of chemical equilibrium states at prescribed temperature and pressure is essentially the same utilized by Gordon and McBride [17]: Gibbs function minimization.

A similiar procedure is employed for the case of non-equilibrium (kinetic) stationary states. A chemical-kinetic source term is included which takes into account the effects of forward and reverse reaction rates, and reaction contact indices.

A combination of the hydrodynamic code of Spalding and the chemical package of Pratt and Wormeck results in a computer code that is capable of producing a numerical solution to the hydrodynamic equations of motion while taking into account the effects of complex chemical reaction. This combination computer code was applied to the problem at hand for the two cases of equilibrium and kinetic chemistry. It was found that the kinetic solution proved much too costly in computer time (IBM 370) to even consider, so the following results are limited to the case of equilibrium chemistry.

The thermochemical data were taken from Gordon and McBride [17]. A reaction mechanism consisting of 19 species and 34 reactions was utilized, as given in the actual computer listing found in the Appendix. A cross-stream grid of 21 grid points was used. The results were found to be fairly sensitive to the input value for the temperature at the base of the burner. Since the computer solution is for a steady flow, the actual ignition phase is not considered, but a temperature is chosen that hopefully represents the physical situation after a steady state has been achieved. All the results discussed are for a base temperature of 1000°K.

Figure 6 demonstrates the change in theoretical flame height with pressure. As can be seen from a comparison of Figures 6 and 3, this agrees very well with the data obtained experimentally. The average computed flame height was 8.6 mm, as compared to the value of 10 mm for the emperical case.

Figures 7 and 8 demonstrate the theoretical flame shapes for pressures of one and five atmospheres of pressure and ten, twenty, and fifty atmospheres, respectively. The flame position at a particular height above the burner was assumed to be at the point of maximum temperature for that height.

As can be seen from a comparison of these Figures (7 and 8) with the actual flame shapes obtained (Figure 2), there is a remarkable agreement between the mathematical model and the emperical data. At one atmosphere the computed flame is fairly bulbous in nature, the sides of the flame bowing outward away from the burner. As pressure is increased the outward bowing of the sides of the flame decreases, and at 10 atmospheres there is almost no bowing at all. At 20 and 50 atmospheres the flame exhibits a concave appearance, which agrees extremely well with experimental results.

This shape change is believed to be a direct result of buoyancy effects. As the pressure increases, the difference between the densities

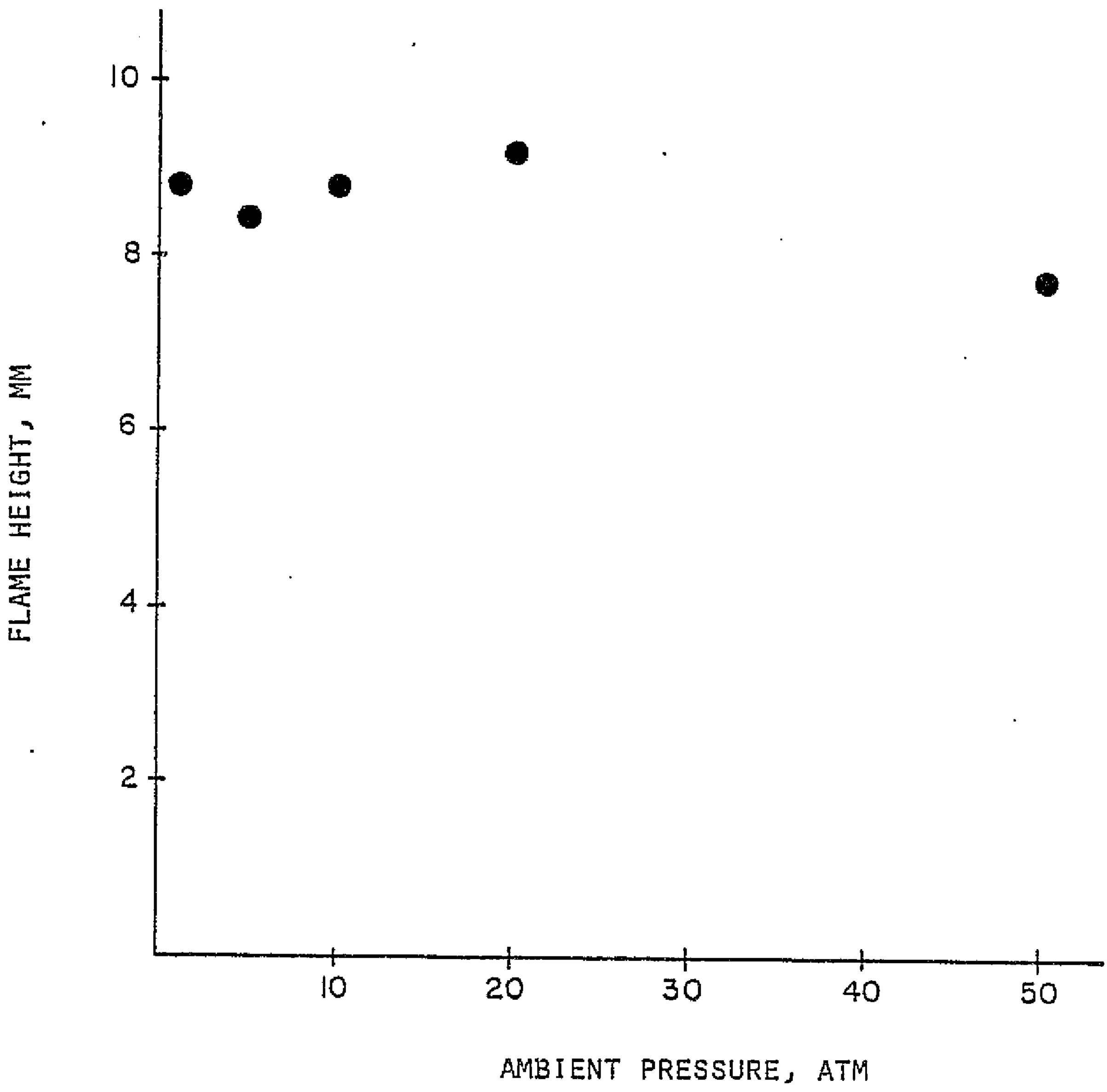

FIGURE 6 - THEORETICAL FLAME HEIGHT AS A FUNCTION OF PRESSURE

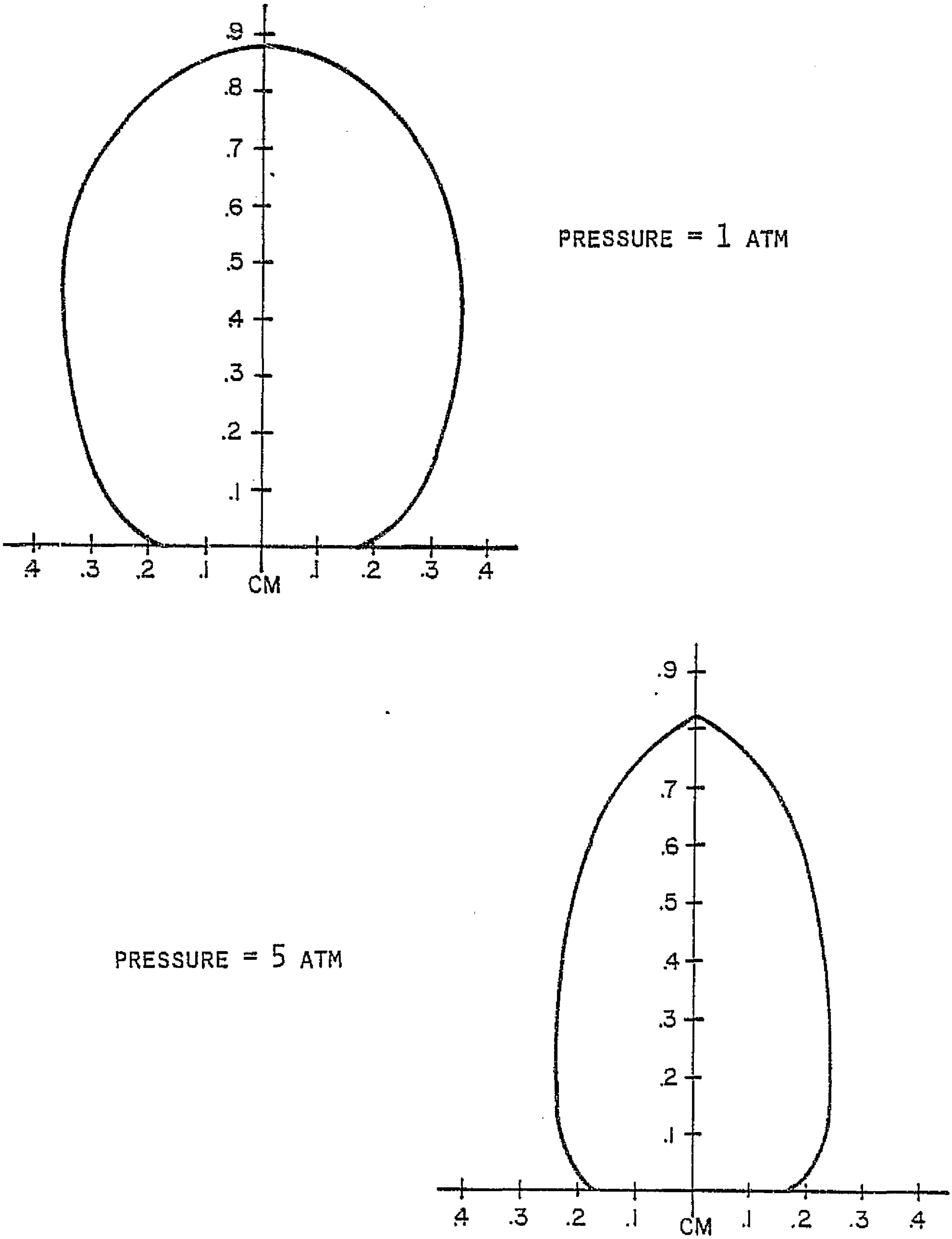

FIGURE 7 - THEORETICAL FLAME SHAPES

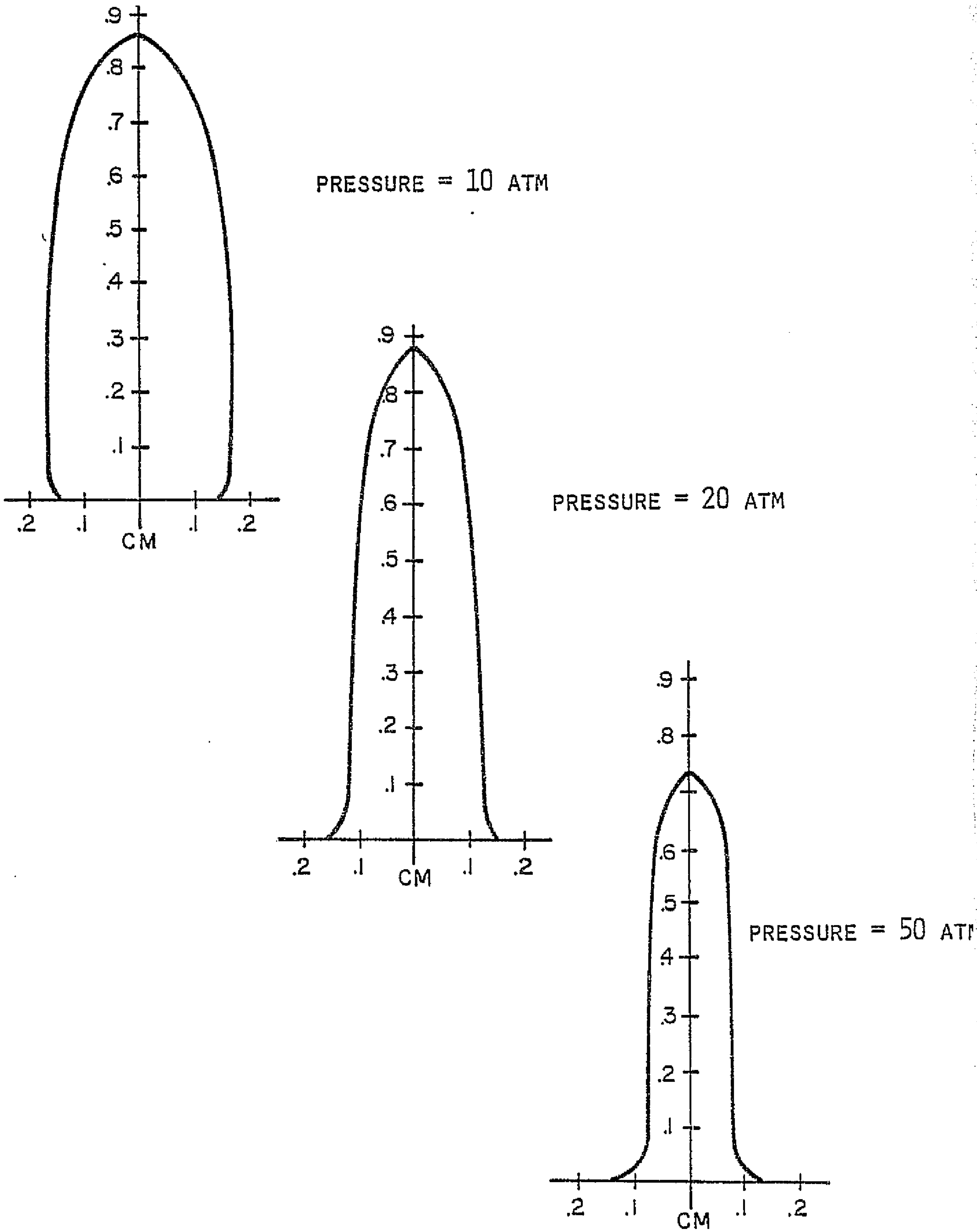

FIGURE 8 - THEORETICAL FLAME SHAPES

of methane and air become much more pronounced, hence the behavior of the two now very different gases under the action of gravity, i.e., buoyancy, affects the resulting flow field. In addition, the problem at hand is one of fairly low velocities. As the pressure is increased these velocities become even smaller and the fluid flow more sensitive to buoyancy effects. Prior to the inclusion of buoyancy effects in the computer program, all flames exhibited a somewhat bulbous shape similar to that found at one atmosphere.

Figure 9 is a plot of approximate maximum flame temperature as a function of pressure. Since these values are fairly sensitive to the input temperature at the base of the burner, it is difficult to make any general statement concerning this data except to say that in comparison with Figure 5, the computed flame temperature behaves in qualitatively the same manner as the adiabatic flame temperature shown there.

Figures 10-15 demonstrate various species mass fractions as a function of the radial distance outward from the center of the burner. Figure 10 is for a pressure of 1 atmosphere at a position of .15 cm above the inlet. Figures 11-15 are for a position of 0.5 cm above the burner, toward the top of the flame, and for pressures of 1, 5, 10, 20, and 50 atmospheres respectively.

At a vertical distance of .15 cm above the burner there still exists some unburned fuel close to the axis of the burner. The maximum NO_x concentration occurs closer to the flame position, as does the maximum concentration of CO_2.

At a vertical distance of .5 cm above the burner, there is no CH_4 present and once again the maximum NO_x production occurs near the flame front. There is essentially no change in the relative magnitude of this maximum concentration with pressure, only a change in where it occurs. This of course corresponds to the change of flame position with pressure.

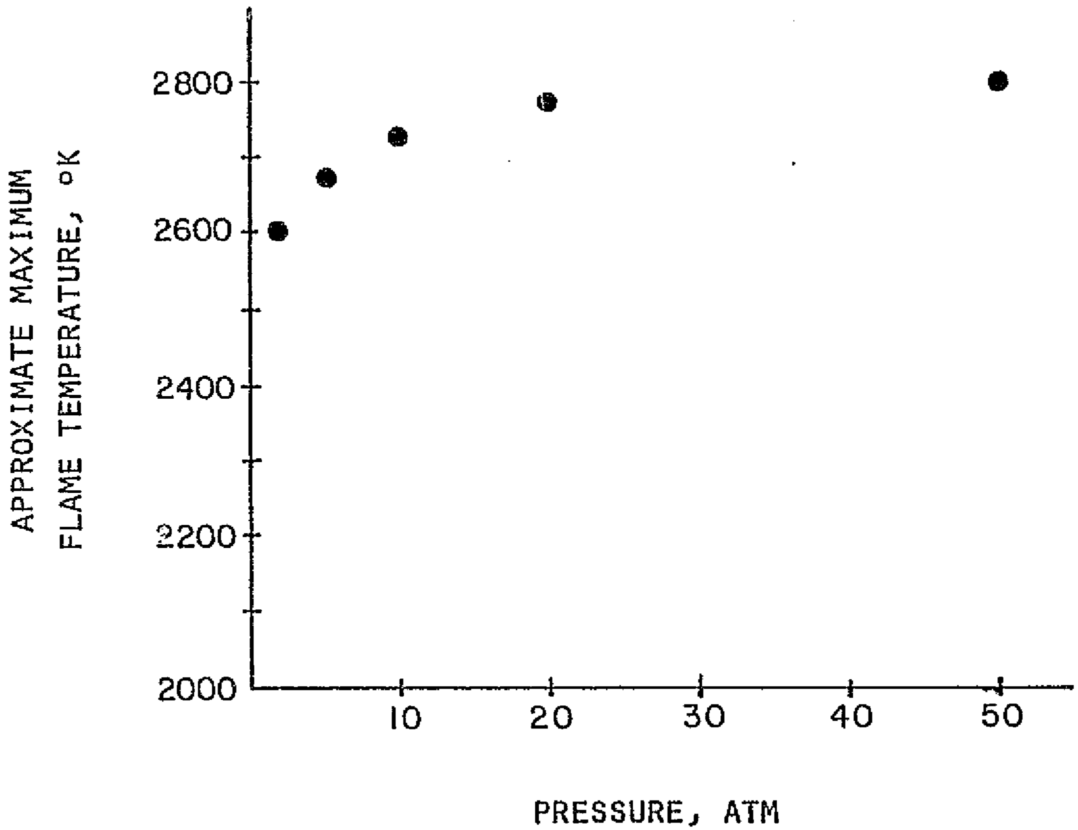

FIGURE 9 - MAXIMUM FLAME TEMPERATURE AS A FUNCTION OF PRESSURE

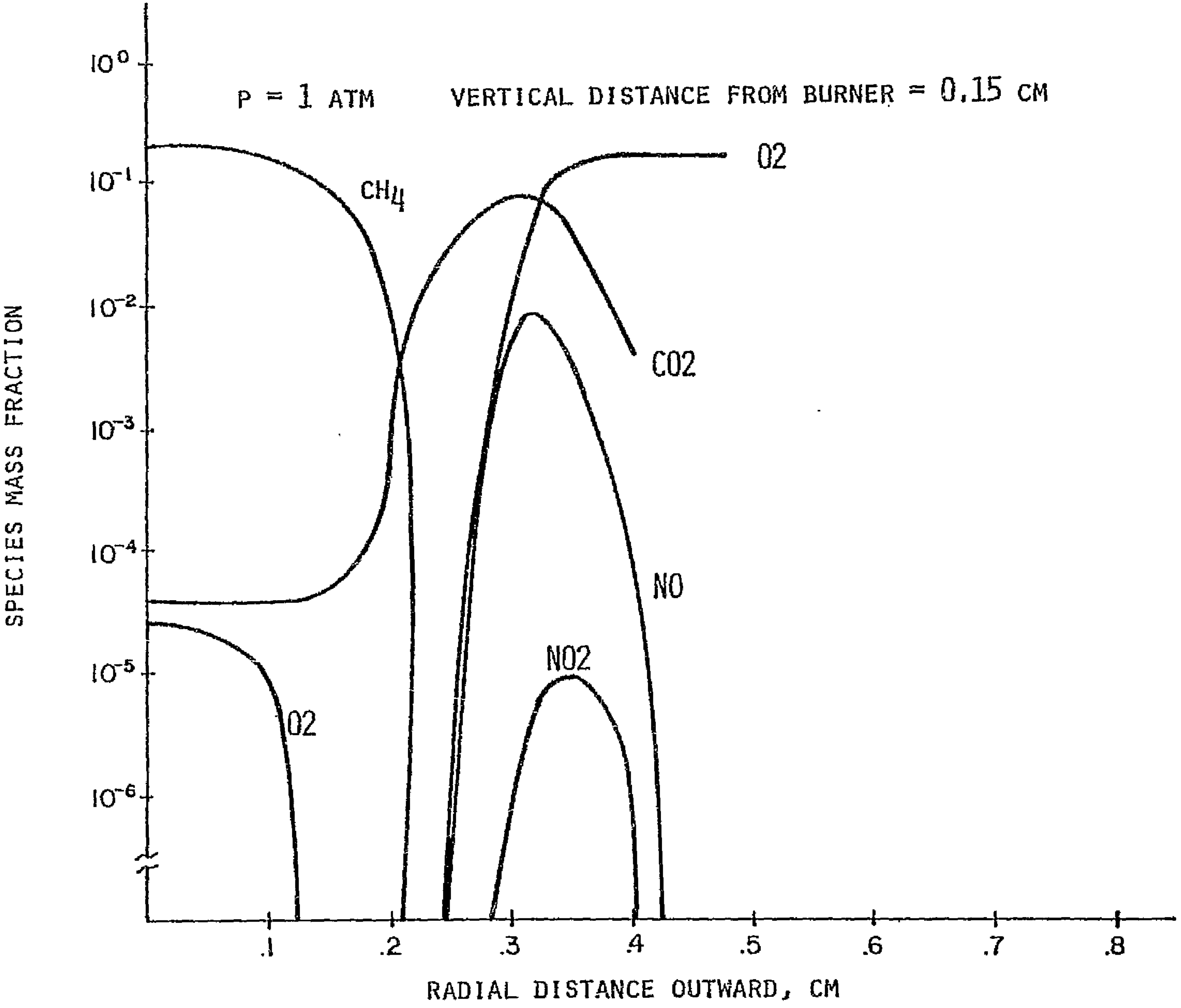

FIGURE 10 - SPECIES MASS FRACTION AS FUNCTION OF PRESSURE

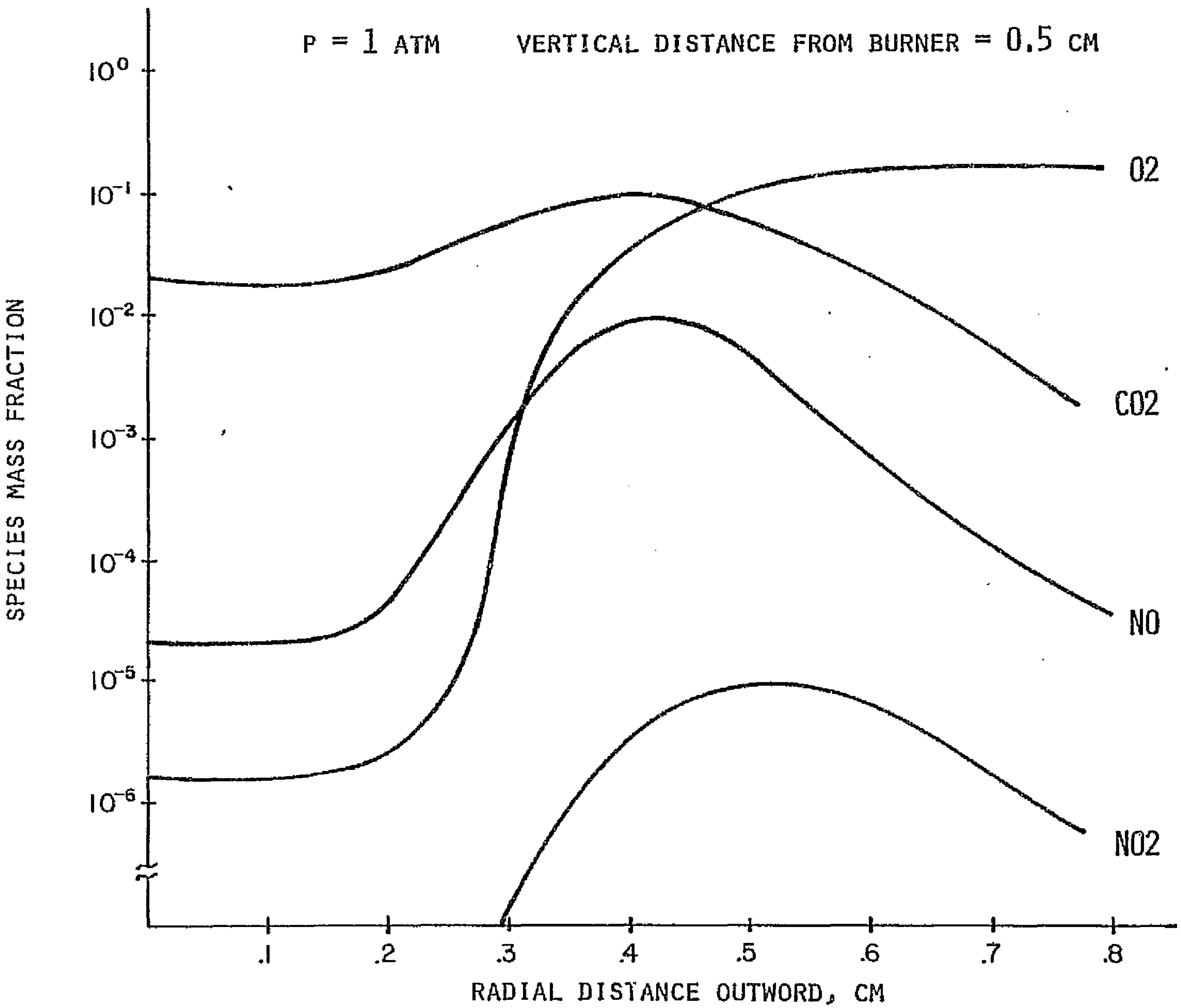

FIGURE 11 - SPECIES MASS FRACTION AS FUNCTION OF PRESSURE

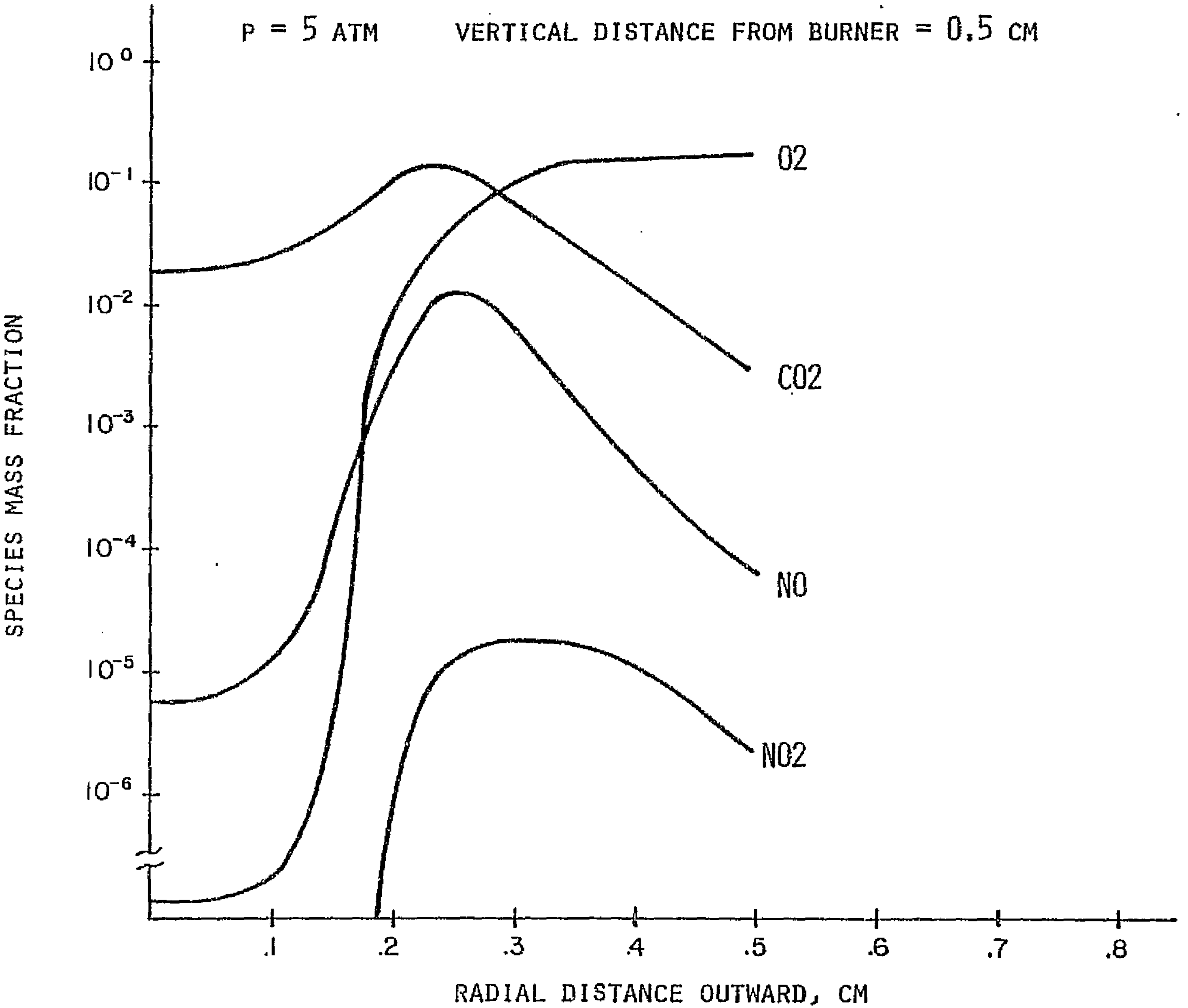

FIGURE 12 - SPECIES MASS FRACTION AS FUNCTION OF PRESSURE

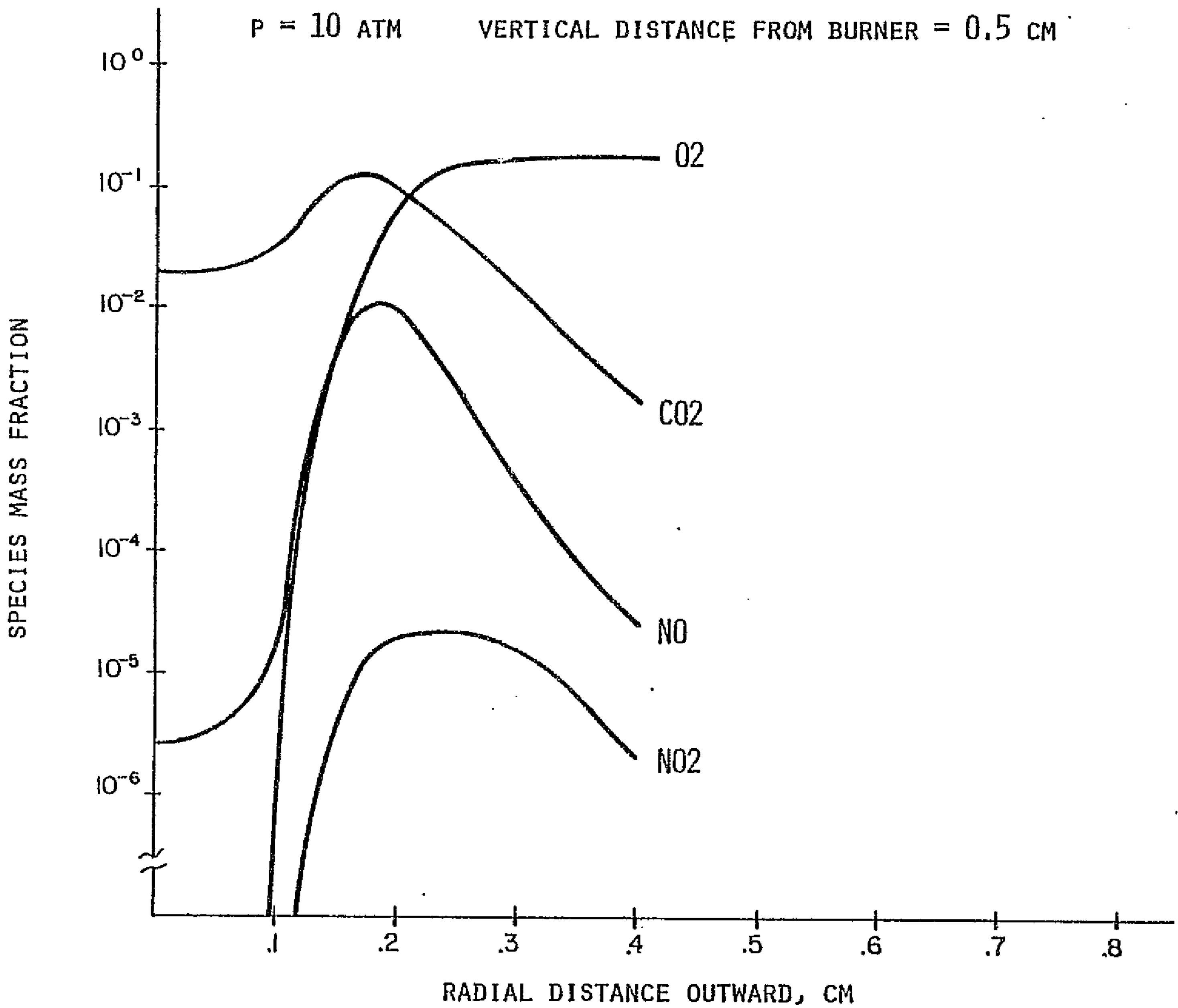

FIGURE 13 - SPECIES MASS FRACTION AS FUNCTION OF PRESSURE

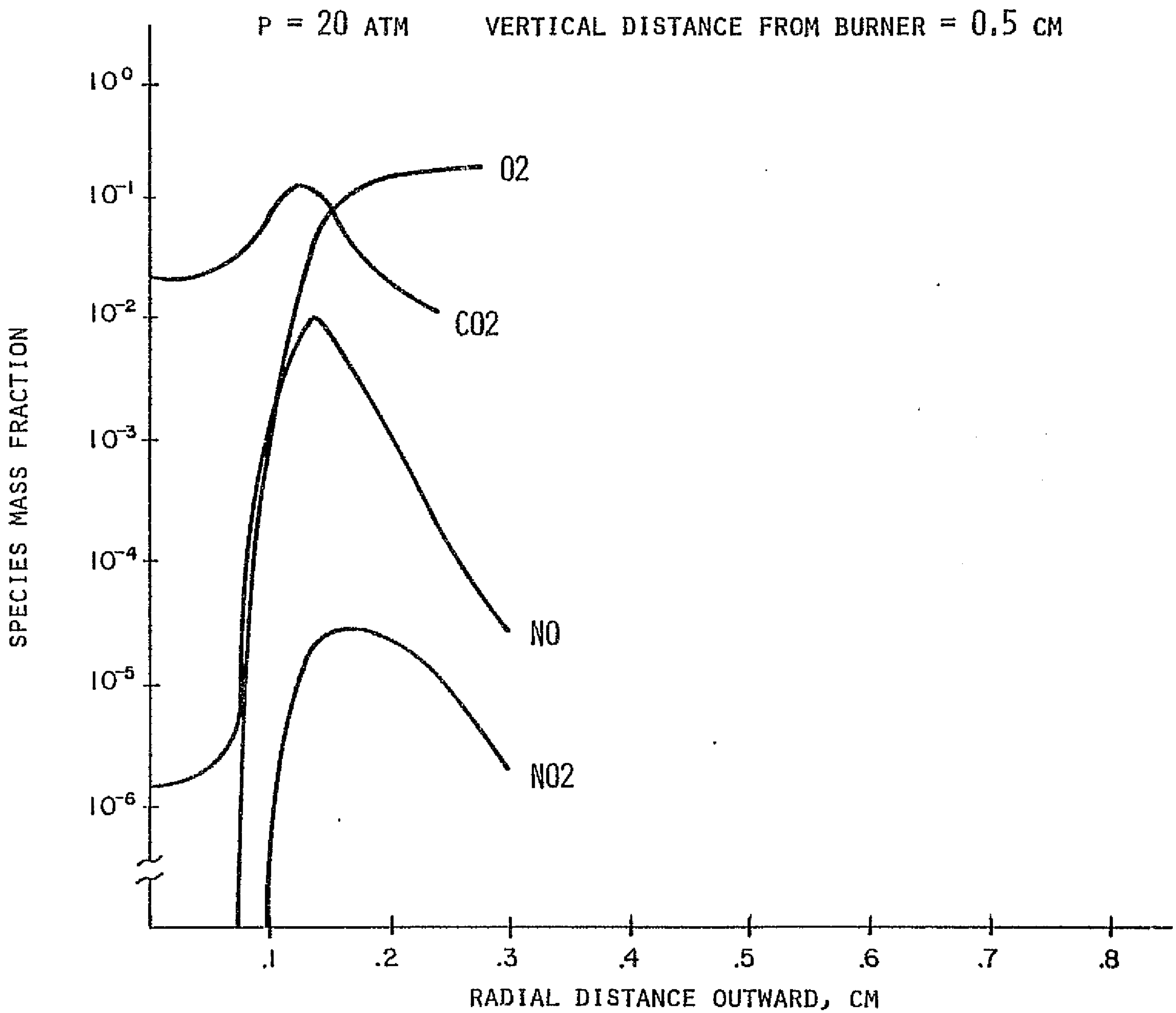

FIGURE 14 - SPECIES MASS FRACTION AS FUNCTION OF PRESSURE

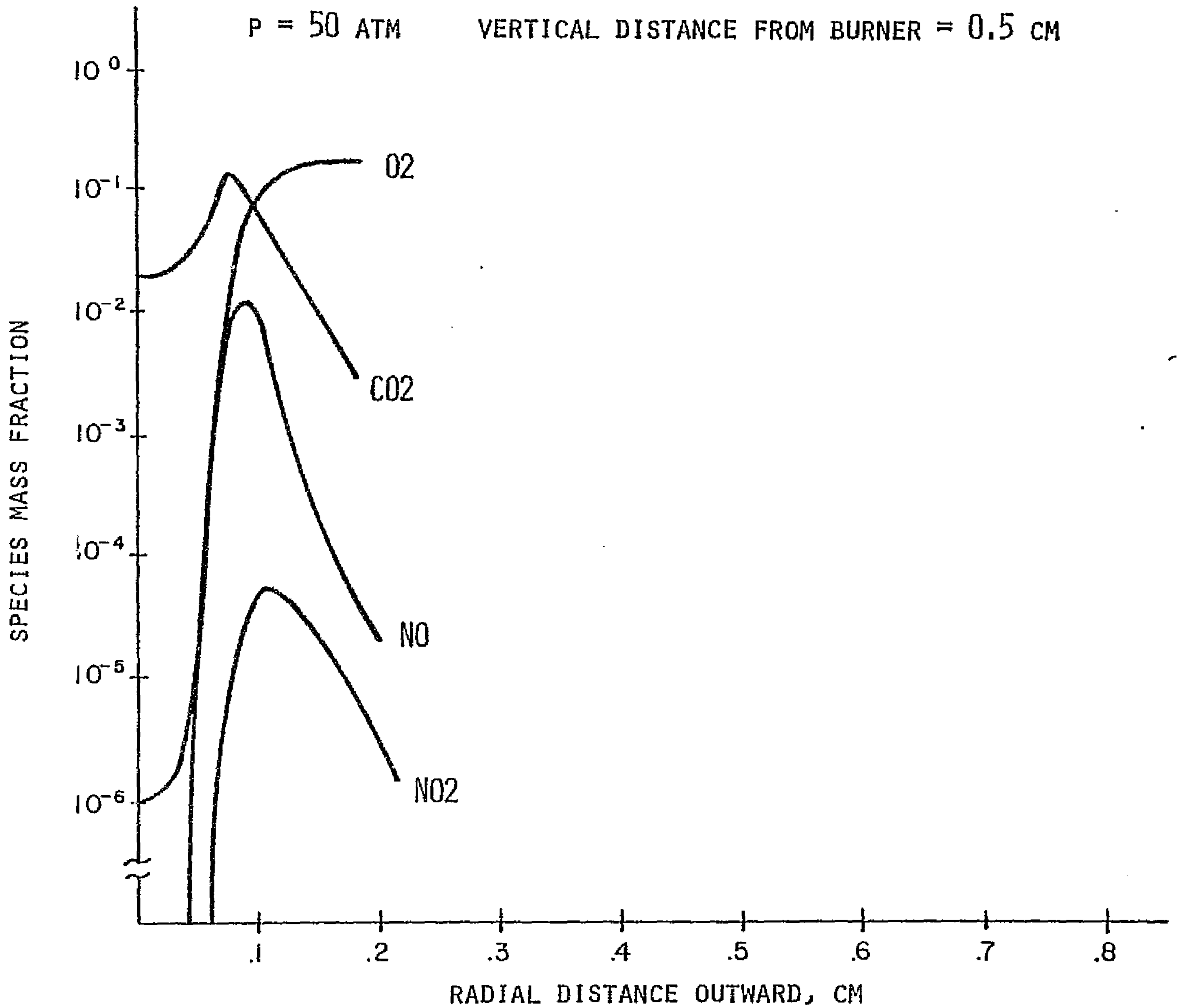

FIGURE 15 - SPECIES MASS FRACTION AS FUNCTION OF PRESSURE

VII. CONCLUSIONS

In order to reflect the physical system under consideration to an acceptable degree, the governing differential equations must be solved numerically. The algorithm utilized by the Patankar-Spalding computer code produces a solution that represents the hydrodynamic nature of the flow field extremely well. It has been found, however, that refinements must be made to the chemical reaction portion of the code in order to produce meaningful results. These refinements take the form of the Pratt-Wormeck chemical subroutine which has been incorporated into the Patankar-Spalding computer code.

The flame shapes for pressures of 1, 5, 10, 20, and 50 atm have been computed and agree remarkably well with experimental data. There is a noticeable shape change that occurs with increasing pressure and believed to be a result of buoyancy effects, which become increasingly important at higher pressures.

The species concentrations computed for the flow regime at hand seem to reflect the chemical aspect of combustion fairly well. The concentration profiles do not reflect much dependence on pressure, however, except in so far as position is concerned. Since the chemical mechanism incorporated into the program did not vary with pressure this is a somewhat expected result. It would be of considerable interest to change the input chemical mechanism with pressure and to note any resulting changes in the general shape of the concentration profiles.

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APPENDIX

Computer Listing and Sample Output

REQUESTED OPTIONS:

OPTIONS IN EFFECT: NAME(MAIN) NOOPTIMIZE LINECOUNT(57) SIZE(MAX) AUTODBL(NONE)
SOURCE EBCDIC NOLIST NODECK OBJECT NOMAP NOFORMAT NOGOSTMT NOXREF NOALC NOANSF TERM FL

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ISN 0002            IMPLICIT REAL*8 (A-H,O-Z)                                        GEN00002
ISN 0003            DIMENSION ASUB(20,3)                                             GEN00004
              C     ---------------------------------------------------------------GEN00006
              CHAPTER0000000000000000000  PRELIMINARIES  000000000000000000000000000000GEN00008
ISN 0004            LOGICAL LADIAB,LDEBUG,LEQUIL,LREACT                              GEN00010
ISN 0005            COMMON                                                           GEN00012
                   1/CCHEM1/CPSUM,EQ,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LCONVG,LNRG    GEN00014
                   1/CINDEX/IDCO,IDCO2,IDH2,IDH2O,IDN2,IDO2,IHCPS,ILC,ILM,IMAT,ITER,  GEN00016
                   2     JJ,NI,NZ,N3,NA,NGLOB,NGLOBP,NLM,NQ,NSM                      GEN00018
                   1/CPARAM/ASUB,NT,NE,EMV,ER,MSUBO,NDEBUG,NS,PA,Q0,Q1,Q2,Q3,Q4,RHOP, GEN00020
                   2        SM,S1(20),S2(20),TR,LADIAB,LDEBUG,LEQUIL,LREACT          GEN00022
                   1/CSPECE/HO(20),SO(20),SMW(20),SSAVE(20),Z(7,2,20)                GEN00024
ISN 0006            COMMON/COMA/A(43),AJE(22),AJI(22),B(43),C(43),CSALFA,D(43),DPDX(43GEN00026
                   1),DX,EMU(43),F(22,43),IAX,IEND,IFIN,INDE(22),INDI(22),IOUT,IDUMY, GEN00028
                   2 ISTEP,ITEST,IUTRAP,JS,JSW,JV,JY,KEX,KIN,KRAD,N,NDZ,NF,NOVEL,NP1, GEN00030
                   3 NP2,NP3,OM(43),OMD(43),P(43),PEI,PR(22),PREF(22,43),PSIE,PSII,R(4GEN00032
                   43),RHO(43),RME,RMI,RO(43),SD(5,43),TAUE,TAUI,U(43),XD,XU,SU(5,43),GEN00034
                   5 Y(43),YE,YI                                                     GEN00036
ISN 0007            COMMON/COMB/AK,ALMG,ARRCON,EWALL,FR,H,HFU,INERT,MASSTR,NDUMY,    GEN00038
                   1 MODEL,OXDFU,PREEXP,PRESS,UBAR,UFAC                              GEN00040
ISN 0008            DIMENSION TITLE(24),OUT(43)                                      GEN00042
ISN 0009            DIMENSION XPLOT(43),YPLOT(10,43),YAXES(10,2),SYMBOL(10)          GEN00044
ISN 0010            DIMENSION FLUX(22),DFI(22),DFE(22),AJIO(22),AJEO(22)             GEN00046
ISN 0011            DIMENSION FA(22),FB(22),FC(22),FD(22)                            GEN00048
ISN 0012            DIMENSION TSAVE(43),DATO(10)                                     GEN00050
              C                                                                      GEN00052
ISN 0013            DATA DATO/4HM (J,4HM/KG.,4HI (K,4H)    ,4HEQ R,4HATIO,4HKG/M,4H3-S ,GEN00054
                   1 4HREST,4HM (S)/                                                 GEN00056
ISN 0014            DATA TINY/1.D-20/                                                GEN00058
ISN 0015            EQUIVALENCE (ARRCON,SZFUEL)                                      GEN00060
ISN 0016            READ(5,1) TITLE                                                  GEN00062
ISN 0017          1 FORMAT (18A4)                                                    GEN00064
              C                                                                      GEN00066
              C  READ ELEMENT,THERMO,MECHANISM DATA CARDS, INITIALIZE PARAMETERS     GEN00068
ISN 0018            CALL CHEMC                                                       GEN00070
              C     ---------------------------------------------------------------GEN00072
              CHAPTER11111111111111111  PARAMETERS AND CONTROL INDICES  1111111111111GEN00074
ISN 0019            LAG=0                                                            GEN00076
ISN 0020            LESSON=0                                                         GEN00078
ISN 0021            KASE=1                                                           GEN00080
              C     ----- NSTAT= NO. OF STEPS BETWEEN OUTPUT OF SINGLE VARIABLES.    GEN00082
              C     ----- NPROF= NO. OF STEPS BETWEEN OUTPUT OF ARRAY VARIABLES.     GEN00084
ISN 0022            NSTAT=20                                                         GEN00086
ISN 0023            NPROF=20                                                         GEN00088
ISN 0024            NSTAT=1                                                          GEN00090
ISN 0025            NPROF=1                                                          GEN00092
              C    NPLOT= NO. OF STEPS BETWEEN OUTPUT OF PLOT                        GEN00094
              C    IN THIS EXAMPLE, PLOT IS CALLED AT END OF INTEGRATION ONLY        GEN00096
ISN 0026            NPLOT=10000                                                      GEN00098
              C     ----- ITEST.NE.0 GIVES EXTRA TEST OUTPUT.                        GEN00100
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                 C      ----- IOTRAP.GT.0 IS ACTIVE FOR NEGATIVE U'S, SEE STRIDE(3).       GEN00102
   ISN 0027             ITEST=0                                                            GEN00104
   ISN 0028             IOTRAP=2                                                           GEN00106
                 C                                                                         GEN00108
                 C   ESTABLISH THERMOCHEMICAL PROBLEM TYPE HERE, IF DIFFERENT FROM         GEN00110
                 C   INITIALIZED VALUES IN CHEMO.  EXAMPLES ARE INITIALIZED AS SUCH.       GEN00112
   ISN 0029             LREACT=.TRUE.                                                      GEN00114
   ISN 0030             LADIAB=.TRUE.                                                      GEN00116
                 C ------------------------------------------------------------------------GEN00118
                 CHAPTER2222222222222222222222222  GRID AND GEOMETRY  22222222222222222222GEN00120
   ISN 0031             N=19                                                               GEN00122
   ISN 0032             XULAST=2.                                                          GEN00124
   ISN 0033             LASTEP=500                                                         GEN00126
   ISN 0034             XOUT=0.                                                            GEN00128
   ISN 0035             XEND=0.                                                            GEN00130
   ISN 0036             FRA=0.1                                                            GEN00132
   ISN 0037             ULIM=.05                                                           GEN00134
   ISN 0038             TAN=0.01                                                           GEN00136
   ISN 0039             PEILIM=.01                                                         GEN00138
   ISN 0040             AFAC=.2                                                            GEN00140
   ISN 0041             AEXDLM=.02                                                         GEN00142
   ISN 0042             KRAD=1                                                             GEN00144
   ISN 0043             CSALFA=1.                                                          GEN00146
                 C      ----- R(I) ADJUSTMENT MADE JUST BEFORE CALL STRIDE(1).             GEN00148
                 C      ----------STRIDE4----------STRIDE4----------STRIDE4-------STRIDE4 GEN00150
   ISN 0044             CALL STRIDE(4)                                                     GEN00152
                 C      ------------------ CHANGE IEND, IAX AND IOUT, IF NECESSARY.        GEN00154
   ISN 0045             IF (XEND.EQ.0.) IEND=0                                             GEN00156
   ISN 0047             IF (XOUT.EQ.0.) IOUT=0                                             GEN00158
   ISN 0049             IAX=0                                                              GEN00160
   ISN 0050             POWER=1.                                                           GEN00162
   ISN 0051             DO 20 I=2,NP2                                                      GEN00164
   ISN 0052          20 OM(I)=(DFLOAT(I-2)/DFLOAT(N))**POWER                               GEN00166
                 C                                                                         GEN00168
                 C ------------------------------------------------------------------------GEN00170
                 CHAPTER3333333333333333333333333  DEPENDENT VARIABLES SELECTION  3333333GEN00172
                 C      U(I)=VELOCITY                                                      GEN00174
                 C   F(K,I)=MOLE NUMBERS OF SPECIES K AT STATION I  KG-MOLES I.KG          GEN00176
                 C   F(NH,I)=STATIC(CHEMICAL PLUS SENSIBLE) ENTHALPY OF MIXTURE            GEN00178
                 C              AT STATION I  J/KG                                         GEN00180
                 C   F(NT,I)=TEMPERATURE,  DEG K                                           GEN00182
                 C   F(NE,I)=FUEL/AIR EQUIVALENCE RATION AT STATION I                      GEN00184
                 C                                                                         GEN00186
                 C      ----- MASSTR=0= UNIFORM COMPOSITION, OTHERWISE MASSTR=1            GEN00188
                 C      ----- MASSTR=0= UNIFORM COMPOSITION, OTHERWISE MASSTR=1            GEN00190
   ISN 0053             MASSTR=1                                                           GEN00192
                 C                                                                         GEN00194
                 C ------------------------------------------------------------------------GEN00196
                 C     NOVEL=1 = NO VELOCITY, OTHERWISE NOVEL=2                            GEN00198
   ISN 0054             NOVEL=2                                                            GEN00200
                 C                                                                         GEN00202
   ISN 0055             NEQ=NS+2                                                           GEN00204
   ISN 0056             IF (MASSTR.EQ.0) NEQ=2                                             GEN00206
   ISN 0058             NF=NEQ+1                                                           GEN00208
   ISN 0059             NR=NF                                                              GEN00210
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ISN 0060         NT=NF+1                                                          GEN00212
ISN 0061         NE=NF+2                                                          GEN00214
           CHAPTER+++++++++++++++++++++++++++++  MATERIAL CONSTANTS  ++++++++++++++GEN00216
           C                                   S.I. UNITS                         GEN00218
           C  SPECIES MOLECULAR WEIGHT ARE STORED IN SMW(K)  K=1,NS               GEN00220
ISN 0062         GASCON=RGAS                                                      GEN00222
ISN 0063         WMIX=29.                                                         GEN00224
ISN 0064         GAMMA=1.3                                                        GEN00226
ISN 0065         VISMIX=1.D-6                                                     GEN00228
           C                                                                      GEN00230
           C     -----MODEL=1=LAMINAR, =2=TURBULENT.                              GEN00232
           C     ----- INERT=1= INERT FLUID, OTHERWISE INERT=2                    GEN00234
ISN 0066         MODEL=1                                                          GEN00236
ISN 0067         INERT=2                                                          GEN00238
           C                                                                      GEN00240
ISN 0068         PL=.7                                                            GEN00242
ISN 0069          PLEF=.86                                                        GEN00244
ISN 0070         DO 41 J=1,NF                                                     GEN00246
ISN 0071         PR(J)=PL                                                         GEN00248
ISN 0072         PREF(J,1)=PLEF                                                   GEN00250
ISN 0073         IF (MODEL.EQ.1) PREF(J,1)=PR(J)                                  GEN00252
ISN 0075      41 CONTINUE                                                         GEN00254
ISN 0076         H=.9                                                             GEN00256
ISN 0077         AK=.435                                                          GEN00258
ISN 0078         ALMG=.09                                                         GEN00260
ISN 0079         FK=.033                                                          GEN00262
ISN 0080         UFAC=.01                                                         GEN00264
           C                                                                      GEN00266
           C ---------------------------------------------------------------------GEN00268
           CHAPTER5555555555555555555555555555555  INITIAL CONDITIONS  5555555555GEN00270
ISN 0081         TKA=2000.                                                        GEN00272
ISN 0082         TKB=2000.                                                        GEN00274
ISN 0083         TKC=500.                                                         GEN00276
ISN 0084         TKD=500.                                                         GEN00278
ISN 0085         TWALL=500.                                                       GEN00280
ISN 0086         TKC=2000.
ISN 0087         TKD=2000.
ISN 0088         TWALL=2000.
ISN 0089         RA=0.                                                            GEN00282
ISN 0090         RB=0.                                                            GEN00284
ISN 0091         PRESS=20.E5                                                      GEN00286
ISN 0092         TKA=1000.
ISN 0093         TKB=1000.
ISN 0094         TKC=1000.
ISN 0095         TKD=1000.
ISN 0096         TWALL=1000.
ISN 0097         PRESS=1.E5
ISN 0098         RC=.155E-2                                                       GEN00288
ISN 0099         RD=.822E-2                                                       GEN00290
ISN 0100         RO=.1025E-1                                                      GEN00292
ISN 0101         PI=3.141592654                                                   GEN00294
ISN 0102         AFLOW=2450.                                                      GEN00296
ISN 0103         FFLOW=41.8                                                       GEN00298
ISN 0104         FAREA=PI*(RC*100.)**2                                            GEN00300
ISN 0105         AAREA=PI*(RD*100.)**2-FAREA                                      GEN00302
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ISN 0106          UB=FFLOW*(TKB/273.)*(1.E5/PRESS)*(1./FAREA)                     GEN00304
ISN 0107          UC=AFLOW*(TKC/273.)*(1.E5/PRESS)*(1./AAREA)                     GEN00306
ISN 0108          UB=UB/6000.                                                     GEN00308
ISN 0109          UC=UC/6000.                                                     GEN00310
ISN 0110          UA=UB                                                           GEN00312
ISN 0111          UD=UC                                                           GEN00314
ISN 0112          RD=RC                                                           GEN00316
ISN 0113          PA=PRESS                                                        GEN00318
ISN 0114          DPLDX=0.                                                        GEN00320
ISN 0115          R(1)=RB                                                         GEN00322
ISN 0116          ROUT=RD                                                         GEN00324
            C  ESTABLISH PROPERTIES OF FUEL STEAAM                                GEN00326
ISN 0117          TK=TKA                                                          GEN00328
ISN 0118          CALL CREKO                                                      GEN00330
ISN 0119          DO 551 K=1,NS                                                   GEN00332
            C$$$IDCO USED TO IDENTIFY CH4, THE FUEL                               GEN00334
ISN 0120          IF (S2(K).GT.0.) IDCO=K                                         GEN00336
ISN 0122          IF (S2(K).LT.TINY) S2(K)=TINY                                   GEN00338
ISN 0124          FA(K)=S2(K)                                                     GEN00340
ISN 0125          FB(K)=S2(K)                                                     GEN00342
ISN 0126      551 CONTINUE                                                        GEN00344
            C***ARRCON USED TO SAVE INLET STREAM FUEL MOLE NUMBER                 GEN00346
ISN 0127          S2FUEL=S2(IDCO)                                                 GEN00348
ISN 0128          FA(NF)=HSOLD                                                    GEN00350
ISN 0129          FB(NF)=HSOLD                                                    GEN00352
ISN 0130          FA(NT)=TK                                                       GEN00354
ISN 0131          FB(NT)=TK                                                       GEN00356
ISN 0132          FA(NE)=1000000.                                                 GEN00358
ISN 0133          FB(NE)=1000000.                                                 GEN00360
ISN 0134          ROA=RHOP                                                        GEN00362
ISN 0135          ROB=RHOP                                                        GEN00364
            C  ESTABLISH PROPERTIES OF AIR STREAM                                 GEN00366
ISN 0136          TK=TKD                                                          GEN00368
ISN 0137          CALL CREKO                                                      GEN00370
ISN 0138          DO 552 K=1,NS                                                   GEN00372
ISN 0139          IF (S2(K).LT.TINY) S2(K)=TINY                                   GEN00374
ISN 0141          FC(K)=S2(K)                                                     GEN00376
ISN 0142          FD(K)=S2(K)                                                     GEN00378
ISN 0143      552  CONTINUE                                                       GEN00380
ISN 0144          FC(NF)=HSOLD                                                    GEN00382
ISN 0145          FD(NF)=HSOLD                                                    GEN00384
ISN 0146          FC(NT)=TK                                                       GEN00386
ISN 0147          FD(NT)=TK                                                       GEN00388
ISN 0148          FC(NE)=0.                                                       GEN00390
ISN 0149          FD(NE)=0.                                                       GEN00392
ISN 0150          ROC=RHOP                                                        GEN00394
ISN 0151          ROD=RHOP                                                        GEN00396
ISN 0152          FLOA=ROA*UA*.5*RB**2                                            GEN00398
ISN 0153          FLOB=ROB*UB*.5*(RC**2-RB**2)                                    GEN00400
ISN 0154          FLOC=ROC*UC*.5*(RD**2-RC**2)                                    GEN00402
            C                                                                     GEN00404
ISN 0155          UMDIV=FLOB/(FLOB+FLOC)                                          GEN00406
            C     ------------------- SEQUENCE TO PUT CELL BOUNDARY AT UMDIV.     GEN00408
ISN 0156          IF(UMDIV.EQ.0..OR.UMDIV.EQ.1.) GO TO 53                         GEN00410
ISN 0158          DO 52 I=3,NP2                                                   GEN00412
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ISN 0159          IF(UM(I).LE.UMDIV) GO TO 52                                          GEN00414
ISN 0161          DIF=UMDIV-.5*(UM(I)+UM(I-1))                                         GEN00416
ISN 0162          UM(I-1)=DMAX1(UM(I-1)+DIF,UM(I-2)+1.D-7)                             GEN00418
ISN 0163          UM(I)=DMIN1(UM(I)+DIF,UM(I+1)-1.D-7)                                 GEN00420
ISN 0164          GO TO 53                                                             GEN00422
ISN 0165       52 CONTINUE                                                             GEN00424
ISN 0166       53 CONTINUE                                                             GEN00426
           C                                                                           GEN00428
           C      ------------------ INITIAL PROFILES ARE UNIFORM.                     GEN00430
ISN 0167          DO 50 I=1,NP3                                                        GEN00432
ISN 0168          IF(UM(I).GT.UMDIV) GO TO 51                                          GEN00434
ISN 0170          U(I)=UO                                                              GEN00436
ISN 0171          DO 501 K=1,NE                                                        GEN00438
ISN 0172          F(K,I)=FB(K)                                                         GEN00440
ISN 0173      501 CONTINUE                                                             GEN00442
ISN 0174          RHO(I)=ROB                                                           GEN00444
ISN 0175          GO TO 50                                                             GEN00446
ISN 0176       51 U(I)=UC                                                              GEN00448
ISN 0177          DO 511 K=1,NE                                                        GEN00450
ISN 0178          F(K,I)=FC(K)                                                         GEN00452
ISN 0179      511 CONTINUE                                                             GEN00454
ISN 0180          RHO(I)=ROC                                                           GEN00456
ISN 0181       50 CONTINUE                                                             GEN00458
ISN 0182          PSII=FLOA                                                            GEN00460
ISN 0183          PEI=FLOB+FLOC                                                        GEN00462
ISN 0184          PSIE=PSII+PEI                                                        GEN00464
ISN 0185          FLOTOT=PEI                                                           GEN00466
           C                                                                           GEN00468
           C      ---------------------------------------------------------------------GEN00470
           CHAPTER666666666666666666666666666666666   THERMODYNAMIC PROPERTIES   666666GEN00472
           C   ********************   START OF MAIN LOOP   *******************         GEN00474
ISN 0186       60 CONTINUE                                                             GEN00476
           C                                                                           GEN00478
ISN 0187          PRESS=PRESS+DPDDX*DX                                                 GEN00480
ISN 0188          PA=PRESS                                                             GEN00482
           C      ------------------------------- ADJUST R(1)                          GEN00484
ISN 0189          IF(KIN.EQ.2.AND.KRAD.EQ.1) R(1)=DSQRT(DABS(2.*PSII/(RHO(1)*U(1))))GEN00486
           C                                                                           GEN00488
           C      -----------STRIDE1-----------STRIDE1-----------STRIDE1--------STRIDE1 GEN00490
ISN 0191          CALL STRIDE(1)                                                       GEN00492
           C                                                                           GEN00494
           C      ---------------------------------------------------------------------GEN00496
           CHAPTER7777777777777777777777777777777777777   FORWARD STEP   77777777GEN00498
ISN 0192          DX=FRA*Y(NP3)                                                        GEN00500
           C                                                                           GEN00502
ISN 0193          IF(ISTEP.GE.IEND) GO TO 70                                           GEN00504
ISN 0195          IF(DX.LT.XEND-XU) GO TO 70                                           GEN00506
ISN 0197          DX=XEND-XU                                                           GEN00508
ISN 0198          IEND=ISTEP+1                                                         GEN00510
ISN 0199       70 IF(ISTEP.GE.IOUT) GO TO 71                                           GEN00512
ISN 0201          IF(DX.LT.XOUT-XU) GO TO 71                                           GEN00514
ISN 0203          DX=XOUT-XU                                                           GEN00516
ISN 0204          IOUT=ISTEP+1                                                         GEN00518
ISN 0205       71 IF(DX.GT.XULAST-XU) DX=XULAST-XU                                     GEN00520
ISN 0207          IF(DX.GT.0.) GO TO 75                                                GEN00522
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  ISN 0209             IFIN=1                                                          GEN00524
  ISN 0210             GO TO 1011                                                      GEN00526
                 C                                                                     GEN00528
  ISN 0211          75 XU=XU+DX                                                        GEN00530
                 C     ----- FURTHER ADJUSTMENTS TO DX ARE MADE IN CHAPTERS 8 AND 9.   GEN00532
                 C                                                                     GEN00534
                 CHAPTER8888888888888888888888  ADJUST LONGITUDINAL CONDITIONS  888888GEN00536
                 C ------------------------------------------------------------------GEN00538
                 C   CHAPTER 8A   BOUNDARY CONDITIONS                                  GEN00540
  ISN 0212             IF (ISTEP-IAX) 8000,80,84                                       GEN00542
  ISN 0213       8000  IF (ISTEP-IEND) 8002,83,84                                      GEN00544
                 C     ------    WALL                                                  GEN00546
  ISN 0214       8002  KIN=1                                                           GEN00548
  ISN 0215             U(1)=0.                                                         GEN00550
  ISN 0216             IF (ISTEP.EQ.0) TAUI=0.                                         GEN00552
  ISN 0218             EWALL=9.                                                        GEN00554
  ISN 0219             DO 81 J=1,NF                                                    GEN00556
  ISN 0220             INDI(J)=2                                                       GEN00558
  ISN 0221          81 AJI(J)=0.                                                       GEN00560
  ISN 0222             RMI=0.                                                          GEN00564
  ISN 0223             GO TO 84                                                        GEN00562
                 C     ------FREE                                                      GEN00566
  ISN 0224          83 KIN=2                                                           GEN00568
  ISN 0225             TAUI=0.                                                         GEN00570
  ISN 0226             U(1)=UA                                                         GEN00572
  ISN 0227             RU(1)=RHO(1)*U(1)                                               GEN00574
  ISN 0228             DO 831 K=1,NE                                                   GEN00576
  ISN 0229             F(K,1)=FA(K)                                                    GEN00578
  ISN 0230         831 CONTINUE                                                        GEN00580
  ISN 0231             GO TO 84                                                        GEN00582
                 C     -------------------- ADJUSTMENT WHEN PIPE AXIS IS REACHED.      GEN00584
  ISN 0232          80 KIN=3                                                           GEN00586
  ISN 0233             RMI=0.                                                          GEN00588
  ISN 0234             R(1)=0.                                                         GEN00590
  ISN 0235             PSII=0.                                                         GEN00592
  ISN 0236             TAUI=0.                                                         GEN00594
                 C    ----  E BOUNDARY                                                 GEN00596
  ISN 0237          84 IF (ISTEP-IOUT) 8004,85,85                                      GEN00598
                 C    ---   WALL                                                       GEN00600
  ISN 0238       8004  KEX=1                                                           GEN00602
  ISN 0239             U(NP3)=0.                                                       GEN00604
  ISN 0240             RME=0.                                                          GEN00606
  ISN 0241             IF (ISTEP.EQ.0) TAUE=0.                                         GEN00608
  ISN 0243             EWALL=9.                                                        GEN00610
  ISN 0244             DO 82 J=1,NF                                                    GEN00612
  ISN 0245             INDE(J)=2                                                       GEN00614
  ISN 0246          82 AJE(J)=0.                                                       GEN00616
  ISN 0247             INDE(1)=1                                                       GEN00618
  ISN 0248             F(NT,NP3)=TWALL                                                 GEN00620
  ISN 0249             TK=TWALL                                                        GEN00622
  ISN 0250             IHCPS=1                                                         GEN00624
  ISN 0251             HSUM=0.                                                         GEN00626
  ISN 0252             CALL HCPS                                                       GEN00628
  ISN 0253             DO 821 K=1,NS                                                   GEN00630
  ISN 0254             HSUM=HSUM+F(K,NP3)*HC(K)                                        GEN00632
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ISN 0255        821 CONTINUE
ISN 0256            HSUBO=HSUM*RGAS*TK
ISN 0257            F(NH,NP3)=HSUBO
ISN 0258            GO TO 86
              C --- FREE
ISN 0259         85 KEX=2
ISN 0260            TAUE=0.
ISN 0261            U(NP3)=UD
ISN 0262            RU(NP3)=RHO(NP3)*U(NP3)
ISN 0263            DO 851 K=1,NE
ISN 0264            F(K,NP3)=FD(K)
ISN 0265        851 CONTINUE
ISN 0266            RHO(NP3)=ROD
              C   CHAPTER 8B   DUCT GEOMETRY
ISN 0267         86 IF (ISTEP.GE.1001) GO TO 89
ISN 0269            IF (ISTEP.GT.0) GO TO 87
ISN 0271            ROUT=RD
ISN 0272            ADUD=(R(NP3)**2-R(1)**2)*.5
ISN 0273         87 YDUCT=ROUT-R(1)
ISN 0274            ADUO=ADUD
ISN 0275            AIN=R(1)**2*.5*DFLOAT(1/KIN)
ISN 0276            IF (ISTEP.EQ.IEND) ADUO=.5*ROUT**2
ISN 0278            AFLO=R(NP3)**2*.5-AIN
ISN 0279            AEX=AFLO-ADUO
ISN 0280            AEXD=AEX/AFLO
ISN 0281            IF(XD.EQ.XEND.OR.XD.EQ.XOUT.OR.XD.EQ.XOLAST.OR.IAX.EQ.ISTEP+1)
                1         GO TO 88
ISN 0283            IF(DABS(AEXD).GT.AEXDLM) DX=DX*AEXDLM/DABS(AEXD)
ISN 0285            XD=XD+DX
ISN 0286         88 ROUT=ROUT+TAN*DX
ISN 0287            ADUD=ROUT**2*.5-AIN
ISN 0288            DA=AFAC*(ADUD-AFLO)
              C
              C
              C   CHAPTER 8C   SUBSONIC PRESSURE GRADIENT
ISN 0289         89 UBAR=0.
ISN 0290            DO 820 I=2,NP1
ISN 0291        820 UBAR=UBAR+(U(I)+U(I+1))*UMD(I)
ISN 0292            UBAR=.5*UBAR
ISN 0293            IF(KIN.EQ.2) UBAR=(UBAR-UA)*PEI/PSIE+UA
              C     SUBSONIC FLOW
ISN 0295        803 IF (ISTEP-1001) 822,823,900
ISN 0296        823 DPDDX=0.
ISN 0297            GO TO 824
              C          CONFINED SUBSONIC FLOW
ISN 0298        822 FLUTOT=PSIE-PSII*FLOAT(1/KIN)
ISN 0299            DYNHED=UBAR*FLUTOT/AFLO
ISN 0300            DPDDX=(DYNHED*DA/DX-TAUI*R(1)-TAUE*R(NP3)+2.*RME*UBAR)/ADUO
ISN 0301        824 DP=DPDDX*DX
ISN 0302            DO 825 I=1,NP3
ISN 0303        825 DPDX(I)=DPDDX
              C    TESTS
ISN 0304            IF(ITEST) 802,801,802
ISN 0305        802 LAB=1
ISN 0306            WRITE(6,100) LAB,UBAR,DYNHED,DX,DA,DPDDX,AEXD,RMI
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ISN 0307          WRITE(6,101) LAB,ISTEP,KIN,KEX,IAX,IEND,IOUT                    GEN00744
ISN 0308          LAB=2                                                           GEN00746
ISN 0309          WRITE(6,100) LAB,(Y(I),I=1,NP3)                                 GEN00748
ISN 0310          LAB=3                                                           GEN00750
ISN 0311          WRITE(6,100) LAB,(R(I),I=1,NP3)                                 GEN00752
ISN 0312          LAB=4                                                           GEN00754
ISN 0313          WRITE(6,100) LAB,(RU(I),I=1,NP3)                                GEN00756
ISN 0314      801 CONTINUE                                                        GEN00758
            C                                                                     GEN00760
            C ----------------------------------------------------------------------GEN00762
            CHAPTER99999999999999999999999  TRANSPORT AND ENTRAINMENT PROPERTIES  9999GEN00764
            C     ---------- LAMINAR VISCOSITY ACCORDING TO SQUARE-ROOT FORMULA,   GEN00766
            C                     WITH WEIGHTING ACCORDING TO MASS FRACTION.      GEN00768
ISN 0315      900 IF (MASSTR.EQ.1) GO TO 90                                       GEN00770
ISN 0317          DO 98 I=1,NP3                                                   GEN00772
ISN 0318       98 EMU(I)=VISMIX*DSQRT(F(NT,I))                                    GEN00774
ISN 0319          GO TO 99                                                        GEN00776
ISN 0320       90 DO 92 I=1,NP3                                                   GEN00778
ISN 0321       92 EMU(I)=VISMIX*DSQRT(F(NT,I))                                    GEN00780
ISN 0322       99 CONTINUE                                                        GEN00782
ISN 0323          EMU(2)=EMU(1)                                                   GEN00784
ISN 0324          EMU(NP2)=EMU(NP3)                                               GEN00786
            C     ---------------------------------------------------- TEST 4     GEN00788
ISN 0325          IF(ITEST) 902,901,902                                           GEN00790
ISN 0326      902 LAB=5                                                           GEN00792
ISN 0327          WRITE(6,100) LAB,RMI,RME,PEI                                    GEN00794
ISN 0328          LAB=6                                                           GEN00796
ISN 0329          WRITE(6,100) LAB,(EMU(I),I=1,NP3)                               GEN00798
ISN 0330      901 CONTINUE                                                        GEN00800
            C                                                                     GEN00802
            C     ----------AUX----------AUX----------AUX----------AUX----------AUX GEN00804
ISN 0331          DO 987 I=1,NP3
ISN 0332          DPDX(I)=DPDX(I)+9.81*(RHO(I)-RHO(NP3))
ISN 0333    987   CONTINUE
ISN 0334          CALL AUX                                                        GEN00806
            C     ------------------------------ ENTRAINMENT CONTROL.             GEN00808
ISN 0335          IF(KIN.NE.2) GO TO 94                                           GEN00810
ISN 0337          RAT=DABS((U(3)-U(1))/(U(NP3)-U(1)+1.D-30))                      GEN00812
ISN 0338          IF(RAT.LT.ULIM) EM U(2)=EM U(2)*RAT/ULIM                        GEN00814
ISN 0340          RMI=2.*EM U(2)                                                  GEN00816
ISN 0341       94 CONTINUE                                                        GEN00818
ISN 0342          IF(KEX.NE.2) GO TO 97                                           GEN00820
ISN 0344          RAT=DABS((U(NP1)-U(NP3))/(U(NP3)-U(1)+1.D-30))                  GEN00822
ISN 0345          RME=-2.*EM U(NP1)                                               GEN00824
ISN 0346          IF(RAT.LT.ULIM) RME=RME*(RAT/ULIM)**2                           GEN00826
ISN 0348       97 IF(XD.EQ.XEND.OR.XD.EQ.XOUT.OR.XD.EQ.XULAST.OR.IAX.EQ.ISTEP+1)  GEN00828
                 1          GO TO 96                                              GEN00830
            C     ---------- LIMIT ON INCREMENT IN PEI.                           GEN00832
ISN 0350          IF ((DABS(RMI)+DABS(RME))*DX.LT.PEI*PEILIM) GO TO 96            GEN00834
ISN 0352          DX=PEI*PEILIM/(DABS(RMI)+DABS(RME))                             GEN00836
ISN 0353          XD=XU+DX                                                        GEN00838
ISN 0354       96 CONTINUE                                                        GEN00840
            C     ---------- ADJUSTMENT OF DX TO REACH AXIS.                      GEN00842
ISN 0355          IF(KIN.EQ.1) GO TO 95                                           GEN00844
ISN 0357          IF(ISTEP.GE.IAX) GO TO 95                                       GEN00846
```

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ISN 0359          IF(PSI1.GT.RM1*DX.OR.IAX.EQ.ISTEP+1) GO TO 95                    GEN00848
ISN 0361          RM1=PSI1/DX                                                      GEN00850
ISN 0362          IAX=ISTEP+1                                                      GEN00852
            C                                                                      GEN00854
            C     ----------STRIDE2----------STRIDE2----------STRIDE2-------STRIDE2 GEN00856
ISN 0363       95 CALL STRIDE(2)                                                   GEN00858
            C                                                                      GEN00860
            C -------------------------------------------------------------------GEN00862
            CHAPTER 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10   OUTPUT   10 10 10GEN00864
ISN 0364          IF(ISTEP.GT.0) GO TO 106                                         GEN00866
ISN 0366          ANSTAT=NSTAT                                                     GEN00868
ISN 0367          ANPROF=NPROF                                                     GEN00870
ISN 0368          ANPLOT=NPLOT                                                     GEN00872
            CHAPTER 10A ----------------------------------- HEADINGS               GEN00874
ISN 0369          REY=(FLOA+FLOB+FLOC)*4./EMU(1)/R(NP3)                            GEN00876
ISN 0370          ER=0.                                                            GEN00878
ISN 0371          IF (INERT.NE.1) CALL ERATIO                                      GEN00880
ISN 0373          EQRAT=ER                                                         GEN00882
            C                                                                      GEN00884
ISN 0374          WRITE(6,1013) TITLE,KASE,LESSON,MODEL,MASSTR,INERT               GEN00886
ISN 0375     1013 FORMAT(1H1,12A6/12A6/6H KASE=,I3,8H LESSON=,I3,7H MODEL=,I3,    GEN00888
                 1 8H MASSTR=,I3,7H INERT=,I3)                                     GEN00890
            C                                                                      GEN00892
ISN 0376          WRITE (6,1010) UA,UB,UC,UD,TKA,TKB,TKC,TKD,RA,RB,RC,RD,          GEN00894
                 1XEND,XOUT,XULAST,DTAN,PRESS,PREEXP,REY,EQRAT                     GEN00896
ISN 0377     1010 FORMAT(1H ,1X,2HUA,8X,2HUB,8X,2HUC,8X,2HUD,8X,2HTA,8X,2HTB,8X,   GEN00898
                 1 2HTC,8X,2HTD,8X,2HRA,8X,2HRB,8X,2HRC,8X,2HRD/1H ,  12D10.3/     GEN00900
                 2 1H ,1X,4HXEND,7X,4HXOUT,7X,6HXULAST,5X,3HTAN,8X,5HPRESS,6X,     GEN00902
                 3 6HPREEXP,5X,3HREY,8X,5HEQRAT,6X,5HAMACH/1H ,9D11.3)             GEN00904
            C                                                                      GEN00906
ISN 0378          LAB=7                                                            GEN00908
ISN 0379          WRITE(6,100) LAB,(UM(I),I=1,NP3)                                 GEN00910
ISN 0380          PRESS1=PRESS                                                     GEN00912
ISN 0381      106 CONTINUE                                                         GEN00914
            C     ---------------------------------------------------- TEST 5      GEN00916
ISN 0382          IF(ITEST) 1002,1001,1002                                         GEN00918
ISN 0383     1002 LAB=6                                                            GEN00920
ISN 0384          WRITE(6,100) LAB,RMI,RME,DX                                      GEN00922
ISN 0385     1001 CONTINUE                                                         GEN00924
            C                                                                      GEN00926
            CHAPTER 10B ----------------------------------- TESTS FOR PRINTOUT     GEN00928
            C     ----- IPRINT=0 GIVES NO OUTPUT,  =1 GIVES SINGLE VARIABLES ONLY, GEN00930
            C                     =2 GIVES BOTH SINGLE AND ARRAY (PROFILE) VARIABLES. GEN00932
ISN 0386     1011 IPRINT=0                                                         GEN00934
ISN 0387          IF(DFLOAT(ISTEP/NSTAT).EQ.DFLOAT(ISTEP)/ANSTAT) IPRINT=1         GEN00936
ISN 0389          IF(DFLOAT(ISTEP/NPROF).EQ.DFLOAT(ISTEP)/ANPROF) IPRINT=2         GEN00938
ISN 0391          IF(ISTEP.EQ.IEND.OR.ISTEP.EQ.IAX.OR.ISTEP.EQ.IOUT) IPRINT=2      GEN00940
ISN 0393          IF(ITEST.NE.0.OR.IFIN.NE.0) IPRINT=2                             GEN00942
            C     IF (FLOAT(ISTEP/NPLOT).EQ.FLOAT(ISTEP)/ANPLOT) IPRINT=3          GEN00944
ISN 0395          IF (XU.GE.XULAST.OR.IFIN.NE.0.OR.ISTEP.EQ.LASTEP) IPRINT=3       GEN00946
            C                                                                      GEN00948
            CHAPTER 10C     ---------------------------SINGLE STATION VARIABLES.   GEN00950
ISN 0397          IF(IPRINT.EQ.0) GO TO 110                                        GEN00952
ISN 0399          WRITE(6,1050) ISTEP,IAX,IEND,IOUT,KIN,KEX,DX,PSI1,PSIE,RMI,RME,PEIGEN00954
ISN 0400     1050 FORMAT(/H ISTEP=,I5,5H IAX=,I5,6H IEND=,I5,6H IOUT=,I5,5H KIN=,I2,GEN00956
```

```
                          1 5H KEX=,I2,4H UX=,  D11.3,6H PSII=,D11.3,6H PSIE=,D11.3/
                          2 5H RMI=,D11.3,5H RME=,D11.3,5H PEI=,D11.3)
                    C
                    C
ISN 0401                  UBAR=0.
ISN 0402                  DO 1020 J=1,NF
ISN 0403             1020 FLUX(J)=0.
ISN 0404                  DO 1021 I=2,NP1
ISN 0405                  UBAR=UBAR+UMD(I)*(U(I)+U(I+1))
ISN 0406                  DO 1021 J=1,NF
ISN 0407             1021 FLUX(J)=FLUX(J)+UMD(I)*(F(J,I)+F(J,I+1))
ISN 0408                  UBAR=.5*UBAR
ISN 0409                  UFLUX=PEI*UBAR
ISN 0410                  DO 1022 J=1,NF
ISN 0411             1022 FLUX(J)=.5*PEI*FLUX(J)
                    C
ISN 0412                  UREF=UBAR
ISN 0413                  RUREF=PEI/.5/(R(1)+R(NP3))/Y(NP3)
ISN 0414                  DO 1023 J=1,NF
ISN 0415                  DFI(J)=FLUX(J)/PEI-F(J,1)
ISN 0416             1023 DFE(J)=DFI(J)+F(J,1)-F(J,NP3)
ISN 0417                  UFLUX=UFLUX-PEI*U(NP3)    +U(1)*PSII
ISN 0418                  DO 1041 K=1,NF
ISN 0419                  FLUX(K)=FLUX(K)-PSIE*FD(K)+FA(K)*PSII
ISN 0420             1041 CONTINUE
ISN 0421                  PRESSD=PRESS/PRESS1-1.
                    C
ISN 0422                  WRITE(6,1031) XU,UFLUX,PRESSD,AEXD,(FLUX(J),J=1,NF)
ISN 0423             1031 FORMAT(4H XU=,  D11.3,7H UFLUX=,D11.3,8H PRESSD=,D11.3,
                          1 6H AEXD=,D11.3,9H FLUX(J)= /10D12.3/10D12.3/10D12.3/)
                    C
ISN 0424                  IF(KIN.NE.1) GO TO 1024
ISN 0426                  TAUID=TAUI/UREF/RUREF
ISN 0427                  DO 1025 J=1,NF
ISN 0428             1025 AJID(J)=AJI(J)/RUREF/DFI(J)
ISN 0429                  WRITE(6,1029) KIN,TAUID,(AJID(J),J=1,NF)
ISN 0430             1029 FORMAT(5H KIN=,I2,7H TAUID=,2PD11.3,9H AJID(J)=,/3(10D12.3/))
ISN 0431            1024   IF (KEX.NE.1) GO TO 1026
ISN 0433                  TAUED=TAUE/UREF/RUREF
ISN 0434                  DO 1027 J=1,NF
ISN 0435            1027  AJED(J)=AJE(J)/RUREF/DFE(J)
ISN 0436                  WRITE (6,1028) KEX,TAUED,(AJED(J),J=1,NF)
ISN 0437             1028 FORMAT(5H KEX=,I2,7H TAUED=,2PD11.3,9H AJED(J)=,/3(10D12.3/))
ISN 0438            1026   CONTINUE
                    CHAPTER 10D
ISN 0439                  IF (IPRINT.EQ.1) GO TO 110
ISN 0441                  LAB=9
ISN 0442                  DIV=1.
ISN 0443                  DO 1095 I=2,NP3
ISN 0444             1095 UUI(I)=Y(I)/DIV
ISN 0445                  WRITE(6,100) LAB,R(1),(UUI(I),I=2,NP2),Y(NP3)
                    C
ISN 0446                  LAB=10
ISN 0447                  SUB=0.
ISN 0448                  DIV=1.
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  ISN 0449          DO 1094 I=2,NP3                                               GEN01072
  ISN 0450     1094 OUT(I)=(U(I)-SUB)/DIV                                         GEN01074
  ISN 0451          IF (NLVEL.NE.1)                                               GEN01076
                   1WRITE(6,100) LAB,U(1),(OUT(I),I=2,NP2),U(NP3)                 GEN01078
  ISN 0453          NY=1                                                          GEN01080
                C                                                                 GEN01082
  ISN 0454          WRITE (6,997) (ASUB(K,1),ASUB(K,2),K=1,NS),(DATO(J),J=1,10)   GEN01084
  ISN 0455      997 FORMAT (1H0,6X,44HMASS FRACTIONS,ENTHALPY,TEMP,F/A EQUIV RATIO, GEN01086
                  1 42HCELL LOADING EMV (KG/M 3-S), CELL RES TIME/8H0  STA. ,     GEN01088
                  2 12(2A4,2X)/6X,12(2A4,2X)/)                                    GEN01090
  ISN 0456          DO 999 I=1,NP3                                                GEN01092
  ISN 0457          DO 300 J=1,NS                                                 GEN01094
  ISN 0458          OUT(J)=F(J,I)*SMW(J)                                          GEN01096
                C       SUPPRESS PRINTOUT OF MASS FRAC.LE.1.D-10                  GEN01098
  ISN 0459          IF (OUT(J).LT.1.D-10) OUT(J)=0.                               GEN01100
  ISN 0461      300 CONTINUE                                                      GEN01102
  ISN 0462          IF (ISTEP.EQ.0) GO TO 301                                     GEN01104
  ISN 0464          IF (I.EQ.1.OR.I.EQ.NP3) GO TO 301                             GEN01106
  ISN 0466          OUT(NF)=E(I)/S O(3,I)                                         GEN01108
  ISN 0467          OUT(NT)=RHO(I)/OUT(NF)                                        GEN01110
  ISN 0468          IF (.NOT.LREACT) GO TO 302                                    GEN01112
  ISN 0470          IF (LEQUIL) OUT(NF)=0.                                        GEN01114
  ISN 0472          IF (LEQUIL) OUT(NT)=1000000.                                  GEN01116
  ISN 0474          GO TO 302                                                     GEN01118
  ISN 0475      301 CONTINUE                                                      GEN01120
  ISN 0476          OUT(NF)=0.                                                    GEN01122
  ISN 0477          OUT(NT)=0.                                                    GEN01124
  ISN 0478      302 CONTINUE                                                      GEN01126
  ISN 0479          WRITE (6,998) I,(OUT(K),K=1,NS),(F(K,I),K=NH,NE),OUT (NF),OUT(NT) GEN01128
  ISN 0480      998 FORMAT (1H ,I5,1P12D10.2/6X,1P12D10.2/6X,1P12D10.2)           GEN01130
  ISN 0481      999 CONTINUE                                                      GEN01132
               CHAPTER 11  11  11  11  11  11  11  11  11  11  11  END OF MAIN LOOP GEN01134
  ISN 0482      110 IF(ISTEP.GE.LASTEP.OR.XU.GE.XULAST.OR.IFIN.NE.0) GO TO 111    GEN01136
                C                                                                 GEN01138
                C       ----------STRIDE3----------STRIDE3----------STRIDE3-------STRIDE3 GEN01140
  ISN 0484          CALL STRIDE(3)                                                GEN01142
  ISN 0485          IF(IFIN) 1011,60,111                                          GEN01144
                C                                                                 GEN01146
                C       ---------------------------------------- TERMINATION      GEN01148
  ISN 0486      111 WRITE(6,112) ISTEP,LASTEP,XU,XULAST,IFIN                      GEN01150
  ISN 0487      112 FORMAT(23H TERMINATED WITH ISTEP=,I5,8H LASTEP=,I5,           GEN01152
                  1 4H XU=,2PD11.3,8H XULAST=,D11.3,6H IFIN=,I3)                  GEN01154
                C ----------------------------------------------------------------GEN01156
  ISN 0488      120 CONTINUE                                                      GEN01158
  ISN 0489          STOP                                                          GEN01160
  ISN 0490      100 FORMAT(1H ,I6, 11D11.3/(9X,11D11.3))                          GEN01162
  ISN 0491      101 FORMAT(1H ,I8,11I11)                                          GEN01164
  ISN 0492          END                                                           GEN01166

*OPTIONS IN EFFECT*NAME(MAIN) NOOPTIMIZE LINECOUNT(57) SIZE(MAX) AUTODBL(NONE)
*OPTIONS IN EFFECT*SOURCE EBCDIC NOLIST NODECK OBJECT NOMAP NOFORMAT NOGOSTMT NOXREF NOALC NOANSF TERM FL/
*STATISTICS*     SOURCE STATEMENTS =      491, PROGRAM SIZE =     16176, SUBPROGRAM NAME =  MAIN
*STATISTICS*  NO  DIAGNOSTICS GENERATED
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REQUESTED OPTIONS:

OPTIONS IN EFFECT: NAME(MAIN) NOOPTIMIZE LINECOUNT(57) SIZE(MAX) AUTODBL(NONE)
SOURCE EBCDIC NOLIST NODECK OBJECT NOMAP NOFORMAT NOGOSTMT NOXREF NOALC NOANSF TERM FLA

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ISN 0002          SUBROUTINE AUX                                                  GEN01150
ISN 0003          IMPLICIT REAL*8 (A-H,O-Z)                                       GEN01152
ISN 0004          DIMENSION ASUB(20,3)                                            GEN01154
ISN 0005          COMMON/COMA/A(43),AJE(22),AJI(22),B(43),C(43),CSALFA,D(43),DPDX(43GEN01156
                 1),DX,EMU(43),F(22,43),IAX,IEND,IFIN,INDE(22),INDI(22),IOUT,IDUMY, GEN01158
                 2 ISTEP,ITEST,IUTRAP,JS,JSW,JV,JY,KEX,KIN,KRAD,N,NO2,NF,NOVEL,NP1, GEN01160
                 3 NP2,NP3,OM(43),OMD(43),P(43),PEI,PR(22),PREF(22,43),PSIE,PSII,R(43GEN01162
                 43),RHO(43),RME,RMI,RU(43),SD(5,43),TAUE,TAUI,U(43),XD,XU,SU(5,43),GEN01164
                 5 Y(43),YE,YI                                                      GEN01166
ISN 0006          COMMON/COMB/AK,ALMG,ARRCON,EWALL,FR,H,HFU,INERT,MASSTR,NDUMY,    GEN01168
                 1 MODEL,OXOFU,PREEXP,PRESS,UBAR,UFAC                               GEN01170
            C/-------- SUBROUTINE FOR PROGRAM GENMIX 4A                            GEN01172
ISN 0007          DIMENSION YEDGE(6),OS(43)                                       GEN01174
ISN 0008          EQUIVALENCE (DPDX(1),OS(1))                                     GEN01176
            C                                                                     GEN01178
            C  SU(1,I) IS USED FOR DUDY                                           GEN01180
            C  SU(2,I) INDICATES WHETHER DUDY EXCEEDS A MINIMUM VALUE             GEN01182
            C  SU(3,I) IS USED FOR MIXING LENGTH                                  GEN01184
            C                                                                     GEN01186
            C  1111111111111.111111111111111111111111111111111  MIXING LENGTH     GEN01188
ISN 0009          IF(MODEL.EQ.1) GO TO 200                                        GEN01190
ISN 0011          UMAX=0.                                                         GEN01192
ISN 0012          UMIN=0.                                                         GEN01194
ISN 0013          DO 1 I=1,NP3                                                    GEN01196
ISN 0014          UMAX=DMAX1(UMAX,U(I))                                           GEN01198
ISN 0015        1 UMIN=DMIN1(UMIN,U(I))                                           GEN01200
ISN 0016          UDMAX=UMAX-UMIN                                                 GEN01202
ISN 0017          DUDYMN=FR*UDMAX/Y(NP3)                                          GEN01204
ISN 0018          DO 10 I=2,NP1                                                   GEN01206
ISN 0019          S U(1,I)=(U(I+1)-U(I))/(Y(I+1)-Y(I))                            GEN01208
ISN 0020          IF(DABS(S U(1,I))-DUDYMN) 111,111,112                           GEN01210
ISN 0021      111 S U(2,I)=0.                                                     GEN01212
ISN 0022          GO TO 10                                                        GEN01214
ISN 0023      112 S U(2,I)=1.                                                     GEN01216
ISN 0024       10 CONTINUE                                                        GEN01218
ISN 0025          IF(KIN.EQ.1) S U(2,2)=1.                                        GEN01220
ISN 0027          IF(KEX.EQ.1) S U(2,NP1)=1.                                      GEN01222
ISN 0029          S U(2,1)=0.                                                     GEN01224
            C  ----------------------------------------  TEST 7                  GEN01226
ISN 0030          IF(ITEST) 17,16,17                                              GEN01228
ISN 0031      17  LAB=11                                                          GEN01230
ISN 0032          WRITE(6,100) LAB,DUDYMN,FR,AK,ALMG,UBAR                         GEN01232
ISN 0033          LAB=12                                                          GEN01234
ISN 0034          WRITE(6,100) LAB,(S U(1,2),I=1,NP3)                             GEN01236
ISN 0035          LAB=13                                                          GEN01238
ISN 0036          WRITE(6,100) LAB,(S U(2,I),I=1,NP3)                             GEN01240
ISN 0037       16 CONTINUE                                                        GEN01242
            C  ------------------------------------------------------            GEN01244
ISN 0038          K=1                                                             GEN01246
ISN 0039          DO 13 L=1,6                                                     GEN01248
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ISN 0040        13 YEDGE(L)=Y(NP3)                                              GEN01250
ISN 0041           DO 11 I=2,NP1                                                GEN01252
ISN 0042           IF(S U(2,I)-S U(2,I-1)) 110,11,110                           GEN01254
ISN 0043       110 YEDGE(K)=Y(I)                                                GEN01256
ISN 0044           K=K+1                                                        GEN01258
ISN 0045           IF(K.GT.6) GO TO 14                                          GEN01260
ISN 0047        11 CONTINUE                                                     GEN01262
ISN 0048        14 EL12=(YEDGE(2)-YEDGE(1))*ALMG                                GEN01264
ISN 0049           EL34=(YEDGE(4)-YEDGE(3))*ALMG                                GEN01266
ISN 0050           EL56=(YEDGE(6)-YEDGE(5))*ALMG                                GEN01268
ISN 0051           EL23=.5*(EL12+EL34)                                          GEN01270
ISN 0052           EL45=.5*(EL34+EL56)                                          GEN01272
         C    ---------------------------------------------------- TEST 8      GEN01274
ISN 0053           IF(ITEST) 19,18,19                                           GEN01276
ISN 0054      19   LAB=14                                                       GEN01278
ISN 0055           WRITE(6,100) LAB                                             GEN01280
ISN 0056           LAB=15                                                       GEN01282
ISN 0057           WRITE(6,100) LAB,EL12,EL23,EL34,EL45,EL56                    GEN01284
ISN 0058           LAB=16                                                       GEN01286
ISN 0059           WRITE(6,100) LAB,(YEDGE(I),I=1,6)                            GEN01288
ISN 0060        18 CONTINUE                                                     GEN01290
         C    --------------------------------------------------------------   GEN01292
ISN 0061           DO 12 I=2,NP1                                                GEN01294
ISN 0062           IF(Y(I)-YEDGE(1)) 120,121,121                                GEN01296
ISN 0063       121 IF(Y(I)-YEDGE(2)) 122,123,123                                GEN01298
ISN 0064       123 IF(Y(I)-YEDGE(3)) 124,125,125                                GEN01300
ISN 0065       125 IF(Y(I)-YEDGE(4)) 126,127,127                                GEN01302
ISN 0066       127 IF(Y(I)-YEDGE(5)) 128,129,129                                GEN01304
ISN 0067       120 S U(3,I)=0.                                                  GEN01306
ISN 0068           GO TO 130                                                    GEN01308
ISN 0069       122 S U(3,I)=EL12                                                GEN01310
ISN 0070           GO TO 130                                                    GEN01312
ISN 0071       124 S U(3,I)=EL23                                                GEN01314
ISN 0072           GO TO 130                                                    GEN01316
ISN 0073       126 S U(3,I)=EL34                                                GEN01318
ISN 0074           GO TO 130                                                    GEN01320
ISN 0075       128 S U(3,I)=EL45                                                GEN01322
ISN 0076           GO TO 130                                                    GEN01324
ISN 0077       129 S U(3,I)=EL56                                                GEN01326
         C    ------------------------------ UPPER LIMITS TO MIXING LENGTH     GEN01328
ISN 0078       130 S U(3,I)=DMIN1(S U(3,I),.5*UDMAX/(DABS(S U(1,I))+1.D-30))    GEN01330
ISN 0079           IF(KIN-1) 131,132,131                                        GEN01332
ISN 0080       132 S U(3,I)=DMIN1(S U(3,I),AK*.5*(Y(I)+Y(I+1)))                 GEN01334
ISN 0081       131 IF(KEX-1) 12,133,12                                          GEN01336
ISN 0082       133 S U(3,I)=DMIN1(S U(3,I),AK*(Y(NP3)-.5*(Y(I)+Y(I+1))))        GEN01338
ISN 0083        12 CONTINUE                                                     GEN01340
         C    ---------------------------------------- TEST 9                  GEN01342
ISN 0084           IF(ITEST) 109,108,109                                        GEN01344
ISN 0085     109   LAB=17                                                       GEN01346
ISN 0086           WRITE(6,100) LAB                                             GEN01348
ISN 0087           LAB=18                                                       GEN01350
ISN 0088           WRITE(6,100) LAB,(S U(3,I),I=1,NP3)                          GEN01352
ISN 0089       108 CONTINUE                                                     GEN01354
         C    --------------------------------------------------------------   GEN01356
         C    2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 VISCOSITIES    GEN01358
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            C      --------------------- LAMINAR VISCOSITIES FOR CELL BOUNDARIES      GEN01360
ISN 0090         200 DO 23 I=2,NP1                                                    GEN01362
ISN 0091          23 EMU(I)=.5*(EMU(I)+EMU(I+1))                                      GEN01364
ISN 0092             IF(MODEL.EQ.1) GO TO 29                                          GEN01366
            C      ------------------------------------- TURBULENT CONTRIBUTION       GEN01368
ISN 0094             DO 20 I=2,NP1                                                    GEN01370
ISN 0095             DUDYL=DABS(S U(1,I)*S U(3,I))                                    GEN01372
ISN 0096             UDMIN=UFAC*.5*(U(I)+U(I+1))                                      GEN01374
ISN 0097             DUDYL=DMAX1(DUDYL,UDMIN)                                         GEN01376
ISN 0098             RHM=.5*(RHO(I)+RHO(I+1))                                         GEN01378
ISN 0099             EMUT=RHM*S U(3,I)*DUDYL                                          GEN01380
            C      -------- IN THIS VERSION, THE TURBULENT AND LAMINAR CONTRIBUTIONS GEN01382
            C                ARE SIMPLY ADDED. AN ALTERNATIVE WOULD BE TO INTRODUCE   GEN01384
            C                THE VAN DRIEST DAMPING FUNCTION.                         GEN01386
ISN 0100             EMU(I)=EMU(I)+EMUT                                               GEN01388
ISN 0101          20 CONTINUE                                                         GEN01390
            C      ----------------------------------------- TEST IO                  GEN01392
ISN 0102             IF(ITEST) 202,201,202                                            GEN01394
ISN 0103         202 LAB=19                                                           GEN01396
ISN 0104             WRITE (6,100) LAB                                                GEN01398
ISN 0105             LAB=20                                                           GEN01400
ISN 0106             WRITE(6,100) LAB,(EMU(I),I=1,NP3)                                GEN01402
ISN 0107             LAB=21                                                           GEN01404
ISN 0108             WRITE(6,100) LAB,(S U(1,I),I=1,NP3)                              GEN01406
ISN 0109         201 CONTINUE                                                         GEN01408
            C      ---------------- MODIFICATION OF EMU ARRAY                         GEN01410
ISN 0110          29 DO 24 I=2,NP1                                                    GEN01412
ISN 0111          24 EM U(I)=EMU(I)/(Y(I+1)-Y(I))                                     GEN01414
ISN 0112             IF(KRAD.EQ.0) GO TO 25                                           GEN01416
ISN 0114             DO 26 I=2,NP1                                                    GEN01418
ISN 0115          26 EM U(I)=EM U(I)*.5*(R(I)+R(I+1))                                 GEN01420
ISN 0116          25 IF (ISTEP) 28,28,300                                             GEN01422
            C        INITIAL PREF S.                                                  GEN01424
ISN 0117          28 DO 27 J=1,NF                                                     GEN01426
ISN 0118             DO 27 I=1,NP3                                                    GEN01428
ISN 0119          27 PREF(J,I)=PREF(J,I)                                              GEN01430
            C    3  3 3   3  3  3  3             SOURCES                              GEN01432
            C           VELOCITY U                                                    GEN01434
ISN 0120         300 DO 307 I=2,NP2                                                   GEN01436
ISN 0121         307 S U(3,I)=PEI*(UM(I+1)-UM(I-1))/RHO(I)/U(I)                       GEN01438
ISN 0122             GO TO (310,312,312), KIN                                         GEN01440
ISN 0123         310 S U(3,2)=(R(1)+.5*(R(2)+R(3)))*YI                                GEN01442
ISN 0124             GO TO 313                                                        GEN01444
ISN 0125         312 S U(3,2)=PEI*UM(3)/RHO(3)/U(3)                                   GEN01446
ISN 0126         313 GO TO (314,315,315),KEX                                          GEN01448
ISN 0127         314 S U (3,NP2)=(R(NP3)+.5*(R(NP1)+R(NP2)))*YE                       GEN01450
ISN 0128             GO TO 316                                                        GEN01452
ISN 0129         315 S U(3,NP2)-PEI*(1.-UM(NP1))/RHO(NP1)/U(NP1)                      GEN01454
ISN 0130         316 CONTINUE                                                         GEN01456
ISN 0131             DO 308 I=2,NP2                                                   GEN01458
ISN 0132         308 US(I)=DPDX(I)*SU(3,I)                                            GEN01460
ISN 0133             IF (NF.EQ.0) RETURN                                              GEN01462
ISN 0135             RETURN                                                           GEN01464
ISN 0136         100 FORMAT(1H ,I8,  1011.5/(9X,1011.5))                              GEN01466
ISN 0137             END                                                              GEN01468
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REQUESTED OPTIONS:

OPTIONS IN EFFECT: NAME(MAIN) NOOPTIMIZE LINECOUNT(57) SIZE(MAX) AUTODBL(NONE)
SOURCE EBCDIC NOLIST NODECK OBJECT NOMAP NOFORMAT NOGOSTMT NOXREF NOALC NOANSF TERM FLA

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ISN 0002          SUBROUTINE STRIDE(ISW)                                          GEN01470
ISN 0003          IMPLICIT REAL*8 (A-H,O-Z)                                       GEN01472
ISN 0004          LOGICAL LADIAB,LEQUIL,LREACT,LDEBUG,LBURN                       GEN01474
ISN 0005          DIMENSION ASUB(20,3)                                            GEN01476
ISN 0006          COMMON                                                          GEN01478
                 1/CCHEM1/CPSUM,FQ,PPLN,RGAS,RGASIN,SMINV,IKINV,ILN,LCONVG,LNRG   GEN01480
                 1/CINDEX/IDCO,IDCO2,IOH2,IOH2O,ION2,IOO2,IHCPS,ILC,ILH,IMAT,ITER, GEN01482
                 2        JJ,N1,N2,N3,NA,NGLOB,NGLOBP,NLM,NQ,NSM                  GEN01484
                 1/CPARAM/ASUB,NI,NE,EMV,ER,HSOEO,NDEBUG,NS,PA,QO,Q1,Q2,Q3,Q4,RHOP, GEN01486
                 2        SM,S1(20),S2(20),IK,LADIAB,LDEBUG,LEQUIL,LREACT         GEN01488
ISN 0007          COMMON/COMA/A(43),AJE(22),AJI(22),B(43),C(43),CSALFA,D(43),DPDX(43GEN01490
                 1),DX,EMU(43),F(22,43),IAX,IEND,IFIN,INDE(22),INDI(22),IOUT,IDUMY, GEN01492
                 2 ISTEP,ITEST,IUTRAP,JS,JSW,JV,JY,KEX,KIN,KRAD,N,ND2,NF,NOVEL,NP1, GEN01494
                 3 NP2,NP3,OM(43),OMD(43),P(43),PEI,PR(22),PREF(22,43),PSIE,PSII,R(4GEN01496
                 43),RHO(43),RME,RMI,RU(43),SD(5,43),TAUE,TAUI,U(43),XD,XU,SU(5,43),GEN01498
                 5 Y(43),YE,YI                                                    GEN01500
ISN 0008          COMMON/COMB/AK,ALMG,ARRCON,EWALL,FR,H,HFU,INERT,MASSTR,NDUMY,   GEN01502
                 1 MODEL,OXOFU,PREEXP,PRESS,UBAR,UFAC                             GEN01504
              C/-------- SUBROUTINE FOR PROGRAM GENMIX 4A                         GEN01506
              C/ THIS SUBROUTINE PERFORMS THE SAME OPERATIONS AS THE ONE IN GENMIX4A GEN01508
              C  BUT MORE ECONOMICALLY. THE A,B,C ARRAYS ARE ONE-DIMENSIONAL. SOME  GEN01510
              C  OFTEN USED FUNCTIONS OF OM ARE STORED, AND A D ARRAY SAVES        GEN01512
              C  UNNECESSARY ARITHMETIC IN THE TDMA OPERATION.                     GEN01514
              C------------------------------------------------------------------GEN01516
ISN 0009          DIMENSION A2(22),ANP2(22),B2(22),BNP2(22),C2(22),CNP2(22),D2(22), GEN01518
                 1 DNP2(22),AHLPT(43),BOMT3(43),FOIFE(22),FOIFI(22),GE(22),GI(22), GEN01520
                 2 PBOM(43),PGOM(43),THLPT(43),TTPF(22)                          GEN01522
ISN 0010          DIMENSION BOM(43),OMPOM(43),OS(43)                              GEN01524
ISN 0011          DIMENSION ISAVE(43),CF(22,43)                                   GEN01526
ISN 0012          DATA SMALL/1.D-6/,TINY/1.D-20/                                  GEN01528
              C                                                                   GEN01530
ISN 0013          EQUIVALENCE (DPDX(1),OS(1))                                     GEN01532
ISN 0014          EQUIVALENCE (ARRCON,S2FUEL)                                     GEN01534
ISN 0015          GO TO (1000,2000,3000,4000), ISW                                GEN01536
              C                                                                   GEN01538
              C**************************************  S T R I D E 1  ***************GEN01540
ISN 0016     1000 IF(ISTEP) 1003,1003,1100                                        GEN01541
ISN 0017     1003 OMI=.5*OM(3)                                                    GEN01542
ISN 0018          OME=.5*(1.-OM(NP1))                                             GEN01544
ISN 0019          DO 1002 I=2,NP2                                                 GEN01548
ISN 0020          BOM(I)=OM(I+1)-OM(I-1)                                          GEN01550
ISN 0021          BOMT3(I)=3.*BOM(I)                                              GEN01552
ISN 0022          OMPOM(I)=OM(I)+OM(I+1)                                          GEN01554
ISN 0023     1002 OMD(I)=OM(I+1)-OM(I)                                            GEN01556
ISN 0024          OMD(1)=BOM(2)                                                   GEN01558
ISN 0025          BPE=1.                                                          GEN01560
ISN 0026          BPI=1.                                                          GEN01562
ISN 0027          Y(1)=0.                                                         GEN01564
ISN 0028          IF(KRAD.EQ.1) GO TO 1100                                        GEN01566
ISN 0030          DO 1001 I=2,NP3                                                 GEN01568
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ISN 0031      1001 R(1)=1.
ISN 0032           R25=1.
ISN 0033           RN15=1.
ISN 0034           IF(ITEST.NE.0) WRITE(6,9010) (R(I),I=1,NP3),R25,RN15
              C--------------------------- CALCULATION OF RHO*U 'S. ----------------
ISN 0036      1100 DO 1101 I=1,NP3
ISN 0037           IF(RHO(I).GT.0.) GO TO 1101
ISN 0039           WRITE(6,1108) RHO(I),I,RHO(I)
ISN 0040      1108 FORMAT(36H ********** NEGATIVE OR ZERO RHO(I)=,2PD11.3,6H AT I=,
                  1 I5,6X,21HSET TO ABS OF RHO(I)=,D11.3,17H ******** STRIDE1)
ISN 0041           RHO(I)=DABS(RHO(I))
ISN 0042      1101 RU(I)=RHO(I)*U(I)
ISN 0043           RU3=RU(3)
ISN 0044           RUN1=RU(NP1)
ISN 0045           DO 1102 I=2,NP1
ISN 0046      1102 RU(I)=.5*(RU(I)+RU(I+1))
ISN 0047           IF(ITEST.NE.0) WRITE(6,9010) (RU(I),I=1,NP3),RUN1,RU3,PE1
              C--------------------------- CALCULATION OF Y 'S AND R 'S ------------
              C   ------------------------------------------- Y'S FOR PLANE GEOMETRY
ISN 0049           Y1=PE1*UM1/(BP1*RU(2))
ISN 0050           Y(3)=Y1+PE1*UM(3)/(RU(2)+RU3)
ISN 0051           Y(2)=2.*Y1-Y(3)
ISN 0052           DO 1103 I=4,NP1
ISN 0053      1103 Y(I)=Y(I-1)+PE1*UMD(I-1)/RU(I-1)
ISN 0054           YN15=Y(NP1)+PE1*UMD(NP1)/(RU(NP1)+RUN1)
ISN 0055           YE=PE1*UME/(BPE*RU(NP1))
ISN 0056           Y(NP3)=YN15+YE
ISN 0057           Y(NP2)=2.*YN15-Y(NP1)
ISN 0058           IF(KRAD.EQ.0) RETURN
              C   --------------------------------- Y'S AND R'S FOR AXISYMMETRICAL GEOMETRY
ISN 0060           IF(CSALFA.EQ.0.) GO TO 1110
              C   ------------------------------------------- CSALFA NE ZERO
ISN 0062           COSD2=.5*CSALFA
ISN 0063           IF(R(1).NE.0.) GO TO 1105
              C---------------------------------------------- R(1)=0.
ISN 0065           DO 1106 I=2,NP3
ISN 0066           Y(I)=DSQRT(DABS(Y(I)/COSD2))
ISN 0067      1106 R(I)=Y(I)*CSALFA
ISN 0068           Y1=DSQRT(DABS(Y1/COSD2))
ISN 0069           YN15=DSQRT(DABS(YN15/COSD2))
ISN 0070           GO TO 1107
              C   ------------------------------------------- R(1) NE 0.
ISN 0071      1105 R1D2=.5*R(1)
ISN 0072           R1D2SQ=R1D2*R1D2
ISN 0073           DO 1104 I=2,NP3
ISN 0074           Y(I)=Y(I)/(R1D2+DSQRT(DABS(R1D2SQ+COSD2*Y(I))))
ISN 0075      1104 R(I)=R(1)+Y(I)*CSALFA
ISN 0076           Y1=Y1/(R1D2+DSQRT(DABS(R1D2SQ+COSD2*Y1)))
ISN 0077           YN15=YN15/(R1D2+DSQRT(DABS(R1D2SQ+COSD2*YN15)))
ISN 0078      1107 R25=R(1)+Y1*CSALFA
ISN 0079           RN15=R(1)+YN15*CSALFA
ISN 0080           YE=Y(NP3)-YN15
ISN 0081           RETURN
              C   ------------------------------------------- CSALFA EQ ZERO
ISN 0082      1110 DO 1111 I=2,NP3
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ISN 0083          Y(1)=Y(1)/R(1)
ISN 0084     1111 R(1)=R(1)
ISN 0085          YI=YI/R(1)
ISN 0086          YN15=YN15/R(1)
ISN 0087          R25=R(1)
ISN 0088          RN15=R(1)
ISN 0089          YE=Y(NP3)-YN15
ISN 0090          RETURN
                C***************************************   S T R I D E 2   ****************
                C  ---------------------------------   PRELIMINARIES FOR COEFFICIENTS
ISN 0091     2000 PX=PEI/DX
ISN 0092          PD8=.125*PX
ISN 0093          PD4=PD8+PD8
ISN 0094          G=RMI-RME
ISN 0095          ARMI=DABS(RMI)
ISN 0096          ARME=DABS(RME)
ISN 0097          GD4=.25*G
ISN 0098          PG=PX+G
ISN 0099          PGD8=.125*PG
ISN 0100          PGD4=PGD8+PGD8
ISN 0101          RMID2=.5*RMI
ISN 0102          DO 2004 I=2,NP2
ISN 0103          PBUM(I)=PX+BUM(I)
ISN 0104     2004 PGUM(I)=PGD4+UMU(I)
ISN 0105          P4UMP=PD4*BUM(2)
                C  ----------------------------------------   GRID POINT 2
                C----------------------------------------   TAUI, BPI, TI
ISN 0106          IF(KIN.NE.1) GO TO 2001
ISN 0108          CALL WF(0,1,BPI,TI,TAUI)
ISN 0109          GO TO 2002
ISN 0110     2001 TI=0.
ISN 0111          IF(KRAD.EQ.0) BPI=.33333+.66667*RU(1)/RU(2)
ISN 0113          IF(KRAD.EQ.1) BPI=(R(1)*(5.*RU(1)+RU(2))+3.*R25*
                 1                     (RU(1)+RU(2)))/6./(R(1)+R25)/RU(2)
                C  ---------------------   BOUNDARY COEFFICIENTS FOR VELOCITY
ISN 0115     2002 HLP=RMID2-GD4*UMPUM(2)
ISN 0116          AHLP=DABS(HLP)
ISN 0117          THLP=HLP+HLP
ISN 0118          THLPT(2)=THLP
ISN 0119          TP=EM U(2)
ISN 0120          TTP=TP+AHLP+DABS(TP-AHLP)
ISN 0121          A(2)=TTP-THLP-TI-PGUM(2)
ISN 0122          B(2)=2.*TI+RMI+ARMI
ISN 0123          C(2)=P4UMP*(3.*U(2)+U(3))-US(2)
ISN 0124          D(2)=A(2)+B(2)+PBUM(2)
                C  ---------------------------------   BOUNDARY COEFFICIENTS FOR F'S
ISN 0125          IF (NF.EQ.0) GO TO 2304
ISN 0127          DO 2300 J=1,NF
ISN 0128          TPF2=TP/PREF(J,2)
ISN 0129          TTPF(J)=TPF2+AHLP+DABS(TPF2-AHLP)
ISN 0130          IF(KIN.NE.1) GO TO 2301
ISN 0132          CALL WF(J,1,FDIFI(J),TIF,GI(J))
ISN 0133          IF(INDI(J).EQ.2) GO TO 2303
ISN 0135          AJI(J)=GI(J)*(F(J,1)-.5*(F(J,2)+F(J,3))-FDIFI(J))
ISN 0136          GO TO 2302
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ISN 0137     2301 TIF=0.                                                        GEN01790
ISN 0138          FDIFI(J)=0.                                                   GEN01792
ISN 0139     2302 A2(J)=TPF(J)-THLP-TIF-PGUM(2)                                 GEN01794
ISN 0140          B2(J)=2.+TIF+RM1+ARM1                                         GEN01796
ISN 0141          D2(J)=A2(J)+B2(J)+PBUM(2)                                     GEN01798
ISN 0142          T=-TIF*FDIFI(J)                                               GEN01800
ISN 0143          GO TO 2305                                                    GEN01802
ISN 0144     2303 A2(J)=TPF(J)-THLP-PGUM(2)                                     GEN01804
ISN 0145          B2(J)=0.                                                      GEN01806
ISN 0146          D2(J)=A2(J)+PBUM(2)                                           GEN01856
ISN 0147          T=RM1*F(J,1)+AJ1(J)*R(1)                                      GEN01808
ISN 0148     2305 TT=3.*F(J,2)+F(J,3)                                           GEN01810
ISN 0149     2300 C2(J)=P4UMF*TT+2.*T                                           GEN01812
             C ---------------------------------------- GRID POINT NP2         GEN01814
             C---------------------------------------- TAUE, BPE, TNP3         GEN01816
ISN 0150     2304 IF(KEX.NE.1) GO TO 2005                                       GEN01818
ISN 0152          CALL WF(0,NP3,BPE,TNP3,TAUE)                                  GEN01820
ISN 0153          GO TO 2310                                                    GEN01822
ISN 0154     2005 TNP3=0.                                                       GEN01824
ISN 0155          IF(KRAD.EQ.0) BPE=.33333+.66667*RU(NP3)/RU(NP1)               GEN01826
ISN 0157          IF(KRAD.EQ.1) BPE=(R(NP3)*(5.*RU(NP3)+RU(NP1))+3.*RN15*       GEN01828
                1              (RU(NP3)+RU(NP1)))/6./(R(NP3)+ RN15)/RU(NP1)     GEN01830
             C ---------------------- BOUNDARY COEFFICIENTS FOR VELOCITY        GEN01832
ISN 0159     2310 HLM=RM1U2-GU4*GMPUM(NP1)                                      GEN01834
ISN 0160          AHLM=DABS(HLM)                                                GEN01836
ISN 0161          THLM=HLM+HLM                                                  GEN01840
ISN 0162          TM=EM U(NP1)                                                  GEN01842
ISN 0163          TTM=TM+AHLM+DABS(TM-AHLM)                                     GEN01844
ISN 0164          P4UMM=PU4*BUM(NP2)                                            GEN01846
ISN 0165          A(NP2)=2.+TNP3-RME+ARME                                       GEN01848
ISN 0166          B(NP2)=TTM+THLM-TNP3-PGUM(NP1)                                GEN01850
ISN 0167          C(NP2)=P4UMM*(3.*U(NP2)+U(NP1))-US(NP2)                       GEN01851
ISN 0168          D(NP2)=A(NP2)+B(NP2)+PBUM(NP2)                                GEN01852
             C ---------------------- BOUNDARY COEFFICIENTS FOR F'S             GEN01853
ISN 0169          DO 2320 J=1,NF                                                GEN01858
ISN 0170          TMF=TM/PREF(J,NP1)                                            GEN01860
ISN 0171          TTMF=TMF+AHLM+DABS(TMF-AHLM)                                  GEN01862
ISN 0172          IF(KEX.NE.1) GO TO 2311                                       GEN01864
ISN 0174          CALL WF(J,NP3,FDIFE(J),TNP3F,GE(J))                           GEN01866
ISN 0175          IF(INDE(J).EQ.2) GO TO 2313                                   GEN01868
ISN 0177          AJE(J)=GE(J)*(.5*(F(J,NP2)+F(J,NP1))+FDIFE(J)-F(J,NP3))       GEN01870
ISN 0178          GO TO 2312                                                    GEN01872
ISN 0179     2311 TNP3F=0.                                                      GEN01874
ISN 0180          FDIFE(J)=0.                                                   GEN01876
ISN 0181     2312 ANP2(J)=2.+TNP3F-RME+ARME                                     GEN01878
ISN 0182          BNP2(J)=TTMF+THLM-TNP3F-PGUM(NP1)                             GEN01880
ISN 0183          DNP2(J)=ANP2(J)+BNP2(J)+PBUM(NP2)                             GEN01882
ISN 0184          T=-TNP3F*FDIFE(J)                                             GEN01884
ISN 0185          GO TO 2315                                                    GEN01886
ISN 0186     2313 ANP2(J)=0.                                                    GEN01888
ISN 0187          BNP2(J)=TTMF+THLM-PGUM(NP1)                                   GEN01890
ISN 0188          DNP2(J)=BNP2(J)+PBUM(NP2)                                     GEN01892
ISN 0189          T=-RME*F(J,NP3)-AJE(J)*R(NP3)                                 GEN01894
ISN 0190     2315 TT=3.*F(J,NP2)+F(J,NP1)                                       GEN01896
ISN 0191     2320 CNP2(J)=P4UMM*TT+2.*T                                         GEN01898
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ISN 0192          RETURN                                                    GEN01900
          C***************************************** S T R I D E 3 ****************GEN01902
ISN 0193     3000 DO 3005 I=3,NP1                                           GEN01904
ISN 0194          THLM=THLP                                                 GEN01906
ISN 0195          HLP=RHIDZ-GD4*UMPUM(I)                                    GEN01908
ISN 0196          THLP=HLP+HLP                                              GEN01910
ISN 0197          THLPT(I)=THLP                                             GEN01912
ISN 0198          AHLP=DABS(HLP)                                            GEN01914
ISN 0199          AHLPT(I)=AHLP                                             GEN01916
ISN 0200          TTM=TTP                                                   GEN01918
ISN 0201          TP=EM U(I)                                                GEN01920
ISN 0202          TTP=TP+AHLP+DABS(TP-AHLP)                                 GEN01922
ISN 0203          A(I)=TTP-THLP-PGUM(I)                                     GEN01924
ISN 0204          B(I)=TTM+THLM-PGUM(I-1)                                   GEN01926
ISN 0205          C(I)=PE4*(EUMT3(I)*U(I)+OMD(I)*U(I+1)+OMD(I-1)*U(I-1))-US(I) GEN01928
ISN 0206          D(I)=A(I)+B(I)+PBUM(I)                                    GEN01930
ISN 0207     3005 CONTINUE                                                  GEN01932
ISN 0208          GO TO (3021,3020), NUVEL                                  GEN01934
ISN 0209     3020 IF(ITEST) 3900,3905,3900                                  GEN01936
ISN 0210     3900 WRITE(6,3901) (A(I),I=2,NP2)                              GEN01938
ISN 0211          WRITE(6,3902) (B(I),I=2,NP2)                              GEN01940
ISN 0212          WRITE(6,3903) (C(I),I=2,NP2)                              GEN01942
ISN 0213          WRITE(6,3904) (D(I),I=2,NP2)                              GEN01944
ISN 0214     3901 FORMAT(7H  A(I) ,1P11D11.3/(7X,11D11.3))                  GEN01946
ISN 0215     3902 FORMAT(7H  B(I) ,1P11D11.3/(7X,11D11.3))                  GEN01948
ISN 0216     3903 FORMAT(7H  C(I) ,1P11D11.3/(7X,11D11.3))                  GEN01950
ISN 0217     3904 FORMAT(7H  D(I) ,1P11D11.3/(7X,11D11.3))                  GEN01952
ISN 0218     3905 CONTINUE                                                  GEN01954
          C------------------------                  ------------------------GEN01956
ISN 0219          IF(KIN.EQ.2.AND.RU(1).NE.0.) U(1)=U(1)-DPDX(1)*DX/RU(1)   GEN01958
ISN 0221          IF(KEX.EQ.2.AND.RU(NP3).NE.0.) U(NP3)=U(NP3)-DPDX(NP3)*DX/RU(NP3) GEN01960
          C------------------------ SOLVE FOR DOWNSTREAM U 'S ---------------GEN01962
ISN 0223          B(2)=(B(2)*U(1)+C(2))/D(2)                                GEN01964
ISN 0224          A(2)=A(2)/D(2)                                            GEN01966
ISN 0225          DO 3048 I=3,NP2                                           GEN01968
ISN 0226          T=D(I)-B(I)*A(I-1)                                        GEN01970
ISN 0227          A(I)=A(I)/T                                               GEN01972
ISN 0228     3048 B(I)=(B(I)*B(I-1)+C(I))/T                                 GEN01974
ISN 0229          DO 3050 IDASH=2,NP2                                       GEN01976
ISN 0230          I=N+4-IDASH                                               GEN01978
ISN 0231          U(I)=A(I)*U(I+1)+B(I)                                     GEN01980
          C      ------------------------------------- TEST FOR NEGATIVE U'S  GEN01982
          C/IUTRAP=0,NO ACTION/ .GT.0,SET TO 1.D-30/ .GT.1,IFIN=-1/ .GT.2,ITEST=1/GEN01984
ISN 0232          IF(IUTRAP.EQ.0.OR.I.EQ.2.OR.I.EQ.NP2) GO TO 3050          GEN01986
ISN 0234          IF(U(I)) 3046,3046,3050                                   GEN01988
ISN 0235     3046 J=ISTEP+1                                                 GEN01990
ISN 0236          WRITE(6,3047) U(I),I,J                                    GEN01992
ISN 0237     3047 FORMAT(25H ********** U (LE ZERO) =,2PD10.3,6H AT I=,I3,  GEN01994
                 1 6H, ISTEP=,I6,34H, SET U TO 1.D-30 ******** STRIDE3)     GEN01996
ISN 0238          U(I)=1.D-30                                               GEN01998
ISN 0239          IFIN=-IUTRAP/2                                            GEN02000
ISN 0240          ITEST=IUTRAP/3                                            GEN02002
ISN 0241     3050 CONTINUE                                                  GEN02004
          C      ----------------------------------------------------       GEN02006
ISN 0242          IF(KIN.EQ.3) U(1)=.5*(U(2)+U(3))                          GEN02008
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ISN 0244          IF(KEX.EQ.3)U(NP3)=.5*(U(NP1)+U(NP2))                        GEN02010
ISN 0246     3021 IF(ITEST) 3011,3013,3011                                     GEN02012
ISN 0247     3011 WRITE(6,3012) (U(I),I=1,NP3)                                 GEN02014
ISN 0248     3012 FORMAT(3H U ,6X,1P11D11.3/(9X,11D11.3))                      GEN02016
            C     -----------------------------------------                    GEN02018
ISN 0249     3013 IF (NF) 3000,3000,3014                                       GEN02020
ISN 0250     3014 CONTINUE                                                     GEN02022
ISN 0251          DO 324 J=1,NF                                                GEN02024
            C----------------------------   SOLVE FOR DOWNSTREAM F 'S  ------------GEN02026
ISN 0252          D(2)=D2(J)                                                   GEN02028
ISN 0253          A(2)=A2(J)/D(2)                                              GEN02030
ISN 0254          B(2)=B2(J)/D(2)                                              GEN02032
ISN 0255          CF(J,2)=C2(J)/D(2)                                           GEN02034
ISN 0256          D(NP2)=DNP2(J)                                               GEN02036
ISN 0257          A(NP2)=ANP2(J)/D(NP2)                                        GEN02038
ISN 0258          B(NP2)=BNP2(J)/D(NP2)                                        GEN02040
ISN 0259          CF(J,NP2)=CNP2(J)/D(NP2)                                     GEN02042
ISN 0260          DO 3002 I=3,NP1                                              GEN02044
ISN 0261          TIMF=TIPF(J)                                                 GEN02046
ISN 0262          TPF=2M U(I)/PRLF(J,I)                                        GEN02048
ISN 0263          TIPF(J)=TPF+AHLPI(I)+DABS(TPF-AHLPI(I))                      GEN02050
ISN 0264          A(I)=TIPF(J)-THLPI(I)-PGUM(I)                                GEN02052
ISN 0265          B(I)=TIMF+THLPI(I-1)-PGUM(I-1)                               GEN02054
ISN 0266          C(I)=PG4+(BUM13(I)*F(J,I)+UMD(I)*F(J,I+1)+UMD(I-1)*F(J,I-1)) GEN02056
ISN 0267          D(I)=A(I)+B(I)+PBUM(I)                                       GEN02058
ISN 0268          A(I)=A(I)/D(I)                                               GEN02060
ISN 0269          B(I)=B(I)/D(I)                                               GEN02062
ISN 0270          CF(J,I)=C(I)/D(I)                                            GEN02064
ISN 0271     3002 CONTINUE                                                     GEN02066
ISN 0272          IF(ITEST) 3906,3907,3906                                     GEN02068
ISN 0273     3906 WRITE(6,3901) (A(I),I=2,NP2)                                 GEN02070
ISN 0274          WRITE(6,3902) (B(I),I=2,NP2)                                 GEN02072
ISN 0275          WRITE (6,3903) (CF(J,I),I=2,NP2)                             GEN02074
ISN 0276          WRITE(6,3904) (D(I),I=2,NP2)                                 GEN02076
ISN 0277     3907 CONTINUE                                                     GEN02078
ISN 0278      324 CONTINUE                                                     GEN02080
            C     -----------------------------------------                    GEN02082
ISN 0279          ICT=0                                                        GEN02084
ISN 0280          DO 61 I=2,NP2                                                GEN02086
ISN 0281          TSAVE(I)=F(NT,I)                                             GEN02088
ISN 0282       61 CONTINUE                                                     GEN02090
            C      ITERATIVE LOOP FOR CREK                                     GEN02092
ISN 0283       62 CONTINUE                                                     GEN02094
ISN 0284          DO 300 I=2,NP2                                               GEN02096
ISN 0285          EMV=D(I)/S D(3,I)                                            GEN02098
ISN 0286          DO 305 J=1,NS                                                GEN02100
ISN 0287          TTM=A(I)*F(J,I+1)+B(I)*F(J,I-1)+CF(J,I)                      GEN02102
ISN 0288          IF (TTM.LT.TINY) TTM=TINY                                    GEN02104
ISN 0290          S1(J)=TTM                                                    GEN02106
ISN 0291          S2(J)=F(J,I)                                                 GEN02108
            C    INSURE HOT ESTIMATE BY S2(K).GT.SMALL  (SEE DATA STATEMENT)   GEN02110
ISN 0292          IF (S2(J).LT.1.D-10) S2(J)=SMALL                             GEN02112
ISN 0294      305 CONTINUE                                                     GEN02114
            C   PREVENT FUEL CONCENTRATION FROM EXCEEDING INLET VALUE          GEN02116
            C   IDCO USED TO IDENTIFY CH4 THE FUEL                             GEN02118
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          C  ARRCON USED TO SAVE INLET STREAM FUEL MOLE NUMBER                GEN02120
ISN 0295        IF (S1(IDCO).GT.S2FUEL) S1(IDCO)=S2FUEL                        GEN02122
ISN 0297        HSUBO=A(I)*F(NF,I+1)+B(I)*F(NF,I-1)+CF(NF,I)                   GEN02124
ISN 0298        TK=F(NT,I)                                                     GEN02126
          C     ESTABLISH CONTACT INDEXES FOR FORWARD AND REVERSE REACTION, IF DESIGEN02128
          C     CALL XIX2                                                      GEN02130
ISN 0299        IF (TK.LT.560.) LREACT=.FALSE.                                 GEN02132
ISN 0301        CALL CREK                                                      GEN02134
ISN 0302        IF (LBURN) LREACT=.TRUE.                                       GEN02136
ISN 0304        DO 306 J=1,NS                                                  GEN02138
ISN 0305        F(J,I)=S2(J)                                                   GEN02140
ISN 0306    306 CONTINUE                                                       GEN02142
ISN 0307        F(NF,I)=HSUBO                                                  GEN02144
ISN 0308        F(NT,I)=TK                                                     GEN02146
ISN 0309        F(NE,I)=EK                                                     GEN02148
ISN 0310        RHO(I)=RHOF                                                    GEN02150
ISN 0311    300 CONTINUE                                                       GEN02152
          C  TEST FOR CONVERGENCE OF THERMOCHEMICAL FIELD                      GEN02154
ISN 0312        IQUIT=0                                                        GEN02156
ISN 0313        DO 114 I=2,NP2                                                 GEN02158
ISN 0314        TEST =DABS(TSAVE(I)-F(NT,I))                                   GEN02160
ISN 0315        IF (TEST.GT.1.) IQUIT=1                                        GEN02162
ISN 0317        TSAVE(I)=F(NT,I)                                               GEN02164
ISN 0318    114 CONTINUE                                                       GEN02166
ISN 0319        IF (IQUIT.EQ.0) GO TO 115                                      GEN02168
ISN 0321        ICI=ICI+1                                                      GEN02170
ISN 0322        IF (ICI.LE.20) GO TO 62                                        GEN02172
ISN 0324        WRITE (6,915) ISTEP,(F(NT,K),K=1,NP3)                          GEN02174
ISN 0325    915 FORMAT (1H0,20X,55H NO CONVERGENCE OF THERMOCHEMICAL FIELD...TEMPSGEN02176
               1ARE    /1X,I5,1P12D10.2/6X,1P12D10.2)                          GEN02178
ISN 0326    115 CONTINUE                                                       GEN02180
          C--------------------------- ADJUST F(J,1) AND F(J,NP3) -------------GEN02182
ISN 0327        DO 3321 J=1,NE                                                 GEN02184
ISN 0328        GO TO (3210,3220,3230),KIN                                     GEN02186
ISN 0329   3210 IF(INDI(J).EQ.2) F(J,1)=FOIFI(J)+.5*(F(J,2)+F(J,3))+AJI(J)/GI(J)  GEN02188
ISN 0331        GO TO 3220                                                     GEN02190
ISN 0332   3230 F(J,1)=.5*(F(J,2)+F(J,3))                                      GEN02192
ISN 0333   3220 GO TO (3310,3320,3330),KEX                                     GEN02194
ISN 0334   3310 IF(INDE(J).EQ.2) F(J,NP3)=FOIFE(J)+.5*(F(J,NP2)+               GEN02196
               1                         F(J,NP1))-AJE(J)/GE(J)                GEN02198
ISN 0336        GO TO 3320                                                     GEN02200
ISN 0337   3330 F(J,NP3)=.5*(F(J,NP1)+F(J,NP2))                                GEN02202
ISN 0338   3320 IF(ITEST) 3322,3321,3322                                       GEN02204
ISN 0339   3322 WRITE(6,3323) J,(F(J,I),I=1,NP3)                               GEN02206
ISN 0340   3323 FORMAT(6H F, J=,I3,1P11D11.3/(9X,11D11.3))                      GEN02208
ISN 0341   3321 CONTINUE                                                       GEN02210
          C     ----------------------------------------------------           GEN02212
ISN 0342   3060 XU=XD                                                          GEN02214
ISN 0343        PSII=PSII-RMI*DX                                               GEN02216
ISN 0344        PSIE=PSIE-RME*DX                                               GEN02218
ISN 0345        PEI=PSIE-PSII                                                  GEN02220
ISN 0346        ISTEP=ISTEP+1                                                  GEN02222
ISN 0347        RETURN                                                         GEN02224
          C*******************************  S T R I D E 4  ********************GEN02226
ISN 0348   4000 CONTINUE                                                       GEN02228
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   ISN 0349             ND2=N/2                                                  GEN02230
   ISN 0350             NP1=N+1                                                  GEN02232
   ISN 0351             NP2=N+2                                                  GEN02234
   ISN 0352             NP3=N+3                                                  GEN02236
   ISN 0353             OM(1)=0.                                                 GEN02238
   ISN 0354             OM(NP3)=1.                                               GEN02240
   ISN 0355             ISTEP=0                                                  GEN02242
   ISN 0356             IEND=10000                                               GEN02244
   ISN 0357             IAX=10000                                                GEN02246
   ISN 0358             IOUT=10000                                               GEN02248
   ISN 0359             XO=1.D-30                                                GEN02250
   ISN 0360             DX=1.D-30                                                GEN02252
   ISN 0361             IFIN=0                                                   GEN02254
   ISN 0362             KIN=1                                                    GEN02256
   ISN 0363             KEX=1                                                    GEN02258
   ISN 0364             LBURN=.TRUE.                                             GEN02260
   ISN 0365             IF (.NOT.LREACT) LBURN=.FALSE.                           GEN02262
   ISN 0367             RETURN                                                   GEN02264
   ISN 0368        9010 FORMAT(1H ,1P11D11.3)                                    GEN02266
   ISN 0369             END                                                      GEN02268

*OPTIONS IN EFFECT*NAME(MAIN) NOOPTIMIZE LINECOUNT(57) SIZE(MAX) AUTODBL(NONE)

*OPTIONS IN EFFECT*SOURCE EBCDIC NOLIST NODECK OBJECT NOMAP NOFORMAT NOGOSTMT NOXREF NOALC NOANSF TERM FLA

*STATISTICS*     SOURCE STATEMENTS =      366, PROGRAM SIZE =     26408, SUBPROGRAM NAME =STRIDE

*STATISTICS*  NO  DIAGNOSTICS GENERATED

****** END OF COMPILATION ******                                 292K BYTES OF CORE NOT USED
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REQUESTED OPTIONS:

OPTIONS IN EFFECT: NAME(MAIN) NOOPTIMIZE LINECOUNT(57) SIZE(MAX) AUTODBL(NONE)
SOURCE EBCDIC NOLIST NODECK OBJECT NOMAP NOFORMAT NOGOSTMT NOXREF NOALC NOANSF TERM FLA

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ISN 0002          SUBROUTINE WF(J,I1,OUT1,OUT2,OUT3)                                GENO2270
ISN 0003          IMPLICIT REAL*8 (A-H,O-Z)                                         GENO2272
ISN 0004          DIMENSION ASUB(20,3)                                              GENO2274
ISN 0005          COMMON/COMA/A(43),AJE(22),AJI(22),B(43),C(43),CSALFA,D(43),DPDX(43GENO2276
                 1),DX,EMU(43),F(22,43),IAX,IEND,IFIN,INDE(22),INDI(22),IOUT,IDUMY, GENO2278
                 2 ISTEP,ITEST,IUTRAP,JS,JSW,JV,JY,KEX,KIN,KRAD,N,ND2,NF,NOVEL,NP1, GENO2280
                 3 NP2,NP3,OM(43),OMD(43),P(43),PEI,PR(22),PREF(22,43),PSIE,PSII,R(4GENO2282
                 43),RHO(43),RME,RMI,RU(43),SD(5,43),TAUE,TAUI,U(43),XD,XU,SU(5,43),GENO2284
                 5 Y(43),YE,YI                                                      GENO2286
ISN 0006          COMMON/COME  /AK,ALMG,ARRCON,EWALL,FR,H,HFO,INERT,MASSTR,NDUMY,   GENO2288
                 1 MODEL,OADFO,PREEXP,PRESS,UBAR,UFAC                               GENO2290
            C                                                                       GENO2292
            C     EFFECTS OF PRESSURE GRADIENT AND MASS TRANSFER ARE INCLUDED       GENO2294
            C     EFFECTS OF RADIUS VARIATION ARE NEGLECTED                         GENO2296
            C     FOR VELOCITY,      OUT1=BP,     OUT2=T,   OUT3=TAU                GENO2298
            C     FOR F*S,           OUT1=FIOIF, OUT2=T,   OUT3=G                   GENO2300
            C                                                                       GENO2302
ISN 0007          DATA SHALF/.04/, BPLAST/.9/                                       GENO2304
ISN 0008          INI=I/I1                                                          GENO2306
ISN 0009          I2=I1-1+2*INI                                                     GENO2308
ISN 0010          I3=I1-2+4*INI                                                     GENO2310
ISN 0011          I25=I3-INI                                                        GENO2312
ISN 0012          IF(J) 100,100,200                                                 GENO2314
            C ------------------------------------------------ VELOCITY             GENO2316
ISN 0013      100 UREF=.5*(U(I2)+U(I3))                                             GENO2318
ISN 0014          RHOREF=.5*RHO(I1)+.25*(RHO(I2)+RHO(I3))                           GENO2320
ISN 0015          RUREF=RHOREF*UREF                                                 GENO2322
ISN 0016          RREF=.5*(R(I2)+R(I3))                                             GENO2324
ISN 0017          VREF=EMU(I1)                                                      GENO2326
ISN 0018          YREF=YI+(YE-YI)*OM(I1)                                            GENO2328
ISN 0019          RE=UREF*RHOREF*YREF/VREF                                          GENO2330
ISN 0020          RRUREF=RREF*RUREF                                                 GENO2332
ISN 0021          AM=(RMI-(RME+RMI)*OM(I1))/RRUREF                                  GENO2334
ISN 0022          EF=YREF*DPDX(I1)/RUREF/UREF                                       GENO2336
ISN 0023          IF(MODEL.EQ.1) GO TO 110                                          GENO2338
ISN 0025          IF(RE.LT.132.25) GO TO 110                                        GENO2340
            C------------------------------------------------EXTENDED LOG LAW      GENO2342
ISN 0027          ER=RE*EWALL                                                       GENO2344
ISN 0028          NIT=0                                                             GENO2346
ISN 0029      101 SHALF1=SHALF                                                      GENO2348
ISN 0030          S=SHALF**2                                                        GENO2350
ISN 0031          SLOC=S+AM+EF                                                      GENO2352
ISN 0032          IF(SLOC.GT.0.) GO TO 104                                          GENO2354
ISN 0034          SLOC=1.D-30                                                       GENO2356
ISN 0035          SHALF=DSQRT(DABS(AM+EF))                                          GENO2358
ISN 0036      104 BEE=DSQRT(SLOC)/AK                                                GENO2360
ISN 0037          ARG=ER*(SHALF+(AM/(1.+BEE)+.5*EF)/SHALF)                          GENO2362
ISN 0038          IF(ARG.GT.11.5*EWALL) GO TO 106                                   GENO2364
ISN 0040          GO TO 110                                                         GENO2366
ISN 0041      106 SHALF=AK/DLOG(ARG)                                                GENO2368
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ISN 0042          IF(DABS(SHALF-SHALF1).LT..0001.OR.NIT.GT.10) GO TO 102     GEN02370
ISN 0044          NIT=NIT+1                                                  GEN02372
ISN 0045          GO TO 101                                                  GEN02374
ISN 0046      102 S=SHALF**2                                                 GEN02376
ISN 0047          SAV=.5*(SHALF**2+SLOC)                                     GEN02378
ISN 0048          OUT1=1./(1.+BEE)                                           GEN02380
ISN 0049          EM U(125)=.25*RHOREF*RREF*DABS(U(13)-U(12))*(AK/OUT1)**2   GEN02382
ISN 0050          GO TO 103                                                  GEN02384
        C ---------------------------------------------- LAMINAR FLOW        GEN02386
ISN 0051      110 AMRE=AM*RE                                                 GEN02388
ISN 0052          FRE=FF*RE                                                  GEN02390
ISN 0053          IF(DABS(AMRE).LT..01) GO TO 111                            GEN02392
ISN 0055          AMRE=DMAX1(-6.D1,DMIN1(6.D1,AMRE))                         GEN02394
ISN 0056          EXPMRE=DEXP(AMRE)                                          GEN02396
ISN 0057          STORE=EXPMRE-1.-AMRE                                       GEN02398
ISN 0058          AMRESQ=AMRE*AMRE                                           GEN02400
ISN 0059          SRE=AMRE*(1.-STORE*FRE/AMRESQ)/(EXPMRE-1.)                 GEN02402
ISN 0060          OUT1=SRE*STORE/AMRESQ+FRE*(STORE-.5*AMRESQ)/(AMRESQ*AMRE)  GEN02404
ISN 0061          GO TO 112                                                  GEN02406
ISN 0062      111 SRE=(2.-FRE*(1.+AMRE/3.))/(2.+AMRE)                        GEN02408
ISN 0063          OUT1=SRE*(.5+AMRE/6.)+FRE*(.16667+AMRE/24.)                GEN02410
ISN 0064      112 IF(SRE.GT.1.D-30) GO TO 113                                GEN02412
ISN 0066          SRE=1.D-30                                                 GEN02414
ISN 0067          OUT1=.33333                                                GEN02416
ISN 0068      113 S=SRE/RE                                                   GEN02418
ISN 0069          EM U(125)=VREF*RREF/DABS(Y(13)-Y(12))                      GEN02420
ISN 0070      103 OUT2=S*RRUREF                                              GEN02422
ISN 0071          OUT3=OUT2*UREF/R(I1)                                       GEN02424
        C         ---------- UNDER-RELAX OUT1.                               GEN02426
ISN 0072          OUT1=.1*OUT1+.9*BPLAST                                     GEN02428
ISN 0073          BPLAST=OUT1                                                GEN02430
ISN 0074          RETURN                                                     GEN02432
        C----------------- STAGNATION ENTHALPY, FUEL, OX-FU/OXDFU            GEN02434
ISN 0075      200 IF(RE.LT.132.25) GO TO 210                                 GEN02436
ISN 0077          IF(MODEL.EQ.1) GO TO 210                                   GEN02438
ISN 0079          PRRAT=PR(J)/PREF(J,125)                                    GEN02440
ISN 0080          PJAY=9.*(PRRAT-1.)/PRRAT**.25                              GEN02442
ISN 0081          S=SAV/PREF(J,125)/(1.+DMAX1(-9.9999D-1,PJAY*DSQRT(DABS(SAV)))) GEN02444
ISN 0082          OUT1=0.                                                    GEN02446
ISN 0083          IF(J.EQ.1) OUT1=(H-1.)*.5*UREF**2                          GEN02448
ISN 0085          OUT2=S*RRUREF                                              GEN02450
ISN 0086          OUT3=OUT2/R(I1)                                            GEN02452
ISN 0087          RETURN                                                     GEN02454
ISN 0088      210 IF(DABS(AMRE).LT..01) GO TO 211                            GEN02456
ISN 0090          S=AM/(DEXP(PR(J)*AMRE)-1.)                                 GEN02458
ISN 0091          GO TO 212                                                  GEN02460
ISN 0092      211 S=1./PR(J)/RE/(1.+.5*PR(J)*AMRE)                           GEN02462
ISN 0093      212 OUT1=0.                                                    GEN02464
ISN 0094          IF(J.EQ.1) OUT1=(PR(J)-1.)*.5*UREF**2                      GEN02466
ISN 0096          OUT2=S*RRUREF                                              GEN02468
ISN 0097          OUT3=OUT2/R(I1)                                            GEN02470
ISN 0098          RETURN                                                     GEN02472
ISN 0099          END                                                        GEN02474
*OPTIONS IN EFFECT*NAME(MAIN) NOOPTIMIZE LINECOUNT(57) SIZE(MAX) AUTODBL(NONE)
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REQUESTED OPTIONS:

OPTIONS IN EFFECT: NAME(MAIN) NOOPTIMIZE LINECOUNT(57) SIZE(MAX) AUTODBL(NONE)
SOURCE EBCDIC NOLIST NODECK OBJECT NOMAP NOFORMAT NOGOSTMT NOXREF NOALC NOANSF TERM FLAG

```
ISN 0002            SUBROUTINE CREK                                                 GEN02476
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)                                       GEN02478
              C                                                                     GEN02480
ISN 0004            DIMENSION ASUB(20,3)                                            GEN02482
ISN 0005            LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LNRG,LREACT                 GEN02484
              C                                                                     GEN02486
ISN 0006            COMMON                                                          GEN02488
                   1/CCHEM1/CPSUM,FQ,PPLN,RGAS,RGASIN,SMINV,TKINV,ILN,LCONVG,LNRG   GEN02490
                   1/CEQUIL/ALT(7,20),ATOM(3,7),BO(7),PI(7)                         GEN02492
                   1/CINDEX/ICO,ICO2,IDH2,IDH2O,IDN2,IDO2,IHCPS,ILC,ILH,IMAT,ITER,  GEN02494
                   2    JJ,N1,N2,N3,NA,NGLCB,NGLCBP,NLM,NQ,NSM                      GEN02496
                   1/CPARAM/ASUB,NT,NE,EMV,ER,HSUBO,NDEBUG,NS,PA,Q0,Q1,Q2,Q3,Q4,RHOP, GEN02498
                   2          SM,S1(20),S2(20),TK,LADIAB,LDEBUG,LEQUIL,LREACT       GEN02500
                   1/CSPEC2/HO(20),SO(20),SMW(20),SSAVE(20),Z(7,2,20)               GEN02502
              C                                                                     GEN02504
              C*************************************************************************GEN02506
              C  THIS SUBROUTINE IS THE MAIN EQUILIBRIUM AND KINETIC SOLUTION ROUTINE.GEN02508
              C  THE CALLING PROGRAM MUST SUPPLY ALL THE VARIABLES EXCEPT RHOP AND SM GEN02510
              C  THROUGH THE LABELLED COMMON BLOCK CPARAM IN SI UNITS.  BOTH EQUIL    GEN02512
              C  SOLUTIONS (LEQUIL=T) -- BY MINIMIZATION OF THE GIBBS FUNCTION --     GEN02514
              C  AND KINETIC (LEQUIL=F) SOLUTIONS ARE CALCULATED BY A NEWTON-RAPHSON  GEN02516
              C  TECHNIQUE.  CREK ALSO CONTROLS THE LOGIC FOR PROBLEM CELLS.          GEN02518
              C  REFERENCE  CREK    (WASHINGTON STATE UNIVERSITY)  MARCH 1976         GEN02520
              C*************************************************************************GEN02522
              C                                                                     GEN02524
ISN 0007            DATA FACTOR/5.0/,SMALL/1.0D-6/                                  GEN02526
              C                                                                     GEN02528
              C                                                                     GEN02530
              C     ***NORMAL SOLUTION***                                           GEN02532
              C                                                                     GEN02534
              C     DETERMINE EQUIVALENCE RATIO AND IF OUTSIDE INTERVAL (0.1,10) ASSUME GEN02536
              C     NO REACTION AND RETURN ADIABATIC NON-REACTED MIXTURE PROPERTIES:  GEN02538
              C     SAVE GIVEN ESTIMATES OR PROGRAM GENERATED ESTIMATES IF TK IS SMALL GEN02540
              C     IF SOLUTION IS SUCCESSFUL, RETURN TO CALLING ROUTINE: OTHERWISE,  GEN02542
              C     ENTER PROBLEM CELL LOGIC BELOW                                  GEN02544
              C                                                                     GEN02546
ISN 0008            Q0=0.                                                           GEN02548
ISN 0009            Q1=6.360D-30                                                    GEN02550
ISN 0010            Q2=-1.190D0                                                     GEN02552
ISN 0011            Q3=2.510-1                                                      GEN02554
ISN 0012            Q4=2.510-1                                                      GEN02556
ISN 0013            CALL ERATIO                                                     GEN02558
ISN 0014            IF (.NOT.LDEBUG) GO TO 30                                       GEN02560
ISN 0016            WRITE(6,10) LREACT,LEQUIL,LADIAB,EMV,ER,HSUBO,Q0,Q1,Q2,Q3,Q4,PA,TKGEN02562
ISN 0017         10 FORMAT(1X,5L3,1P10D12.3)                                        GEN02564
ISN 0018            IF (NDEBUG.EQ.1) GO TO 30                                       GEN02566
ISN 0020            WRITE(6,20) (S1(I),I=1,NS)                                      GEN02568
ISN 0021            WRITE(6,20) (S2(I),I=1,NS)                                      GEN02570
ISN 0022         20 FORMAT((1X,1P10D12.3))                                          GEN02572
ISN 0023         30 IF (.NOT.LREACT) GO TO 400                                      GEN02574
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 ISN 0025        IF (ER.LT.0.1.OR.ER.GT.10.0) GO TO 400                          GEN02576
 ISN 0027        EMVSAV=EMV                                                      GEN02578
           C     11.52609 IS E-LOG OF STD PATM=101325.0 N/M**2                   GEN02580
 ISN 0028        PPLN=DLOG(PA)-11.52609                                          GEN02582
 ISN 0029        TSAVE=TK                                                        GEN02584
 ISN 0030        DO 40 I=1,NS                                                    GEN02586
 ISN 0031     40 SSAVE(I)=SZ(I)                                                  GEN02588
 ISN 0032        IF (TK.LT.SMALL) GO TO 100                                      GEN02590
           C                                                                     GEN02592
 ISN 0034        CALL SPECE                                                      GEN02594
           C                                                                     GEN02596
 ISN 0035        IF (LCONVG) GO TO 900                                           GEN02598
           C                                                                     GEN02600
           C                                                                     GEN02602
           C    ***PROBLEM CELL***                                               GEN02604
           C                                                                     GEN02606
           C    SOLUTION LOGIC IS DIFFERENT FOR FOUR TYPES OF PROBLEMS AS FOLLOWS:  GEN02608
           C       MODE 1 ... LEQUIL = T, LADIAB = T                             GEN02610
           C       MODE 2 ... LEQUIL = T, LADIAB = F                             GEN02612
           C       MODE 3 ... LEQUIL = F, LADIAB = T                             GEN02614
           C       MODE 4 ... LEQUIL = F, LADIAB = F                             GEN02616
           C                                                                     GEN02618
           C    ALWAYS TRY KT=0.0 (LNKG=F) AFTER SOLUTION FAILURE WHEN LEQUIL=F.  GEN02620
           C    LOGIC TO FIND SOLUTION IS CONTROLLED IN CHAPTERS 1 AND 2 BELOW    GEN02622
           C    WHERE IN EACH SECTION, NEW ESTIMATES ARE DETERMINED EITHER BY     GEN02624
           C    SAVED GIVEN ONES, NEW ASSIGNED ONES, OR SOLUTION FUUND NOT AT     GEN02626
           C    REQUIRED CONDITIONS.  THE VARIABLES NEXTOK AND NEXTNG ARE ASSIGNED GEN02628
           C    THE STATEMENT NUMBERS OF WHERE TO GO IF THE SOLUTION ATTEMPT IS   GEN02630
           C    SUCCESSFUL OR NOT, RESPECTIVELY.                                  GEN02632
           C                                                                     GEN02634
 ISN 0037        ASSIGN 900 TO NEXTOK                                            GEN02636
 ISN 0038        ASSIGN 100 TO NEXTNG                                            GEN02638
 ISN 0039        GO TO 520                                                       GEN02640
           C                                                                     GEN02642
           C* * * * * * * * * * * * * * * * * * * * * * CHAPTER 1 * * * * * * *GEN02644
           C* * * * * * * * * * * * * * * * * * * * * * CHAPTER 1 * * * * * * *GEN02646
           C                                                                     GEN02648
           C    ***EQUILIBRIUM***                                                GEN02650
           C    THIS CHAPTER MAKES EQUILIBRIUM ESTIMATES AND INITIATES STRATEGY FOR  GEN02652
           C    CASES IN WHICH CONVERGENCE WAS NOT ACHIEVED ON FIRST CALL TO SPECE   GEN02654
           C                                                                     GEN02656
 ISN 0040    100 MODE=4                                                          GEN02658
 ISN 0041        IF (LEQUIL) MODE=MODE-2                                         GEN02660
 ISN 0043        IF (LADIAB) MODE=MODE-1                                         GEN02662
 ISN 0045        LEQUIL=.TRUE.                                                   GEN02664
 ISN 0046        LADIAB=.TRUE.                                                   GEN02666
 ISN 0047        IF (MODE.LT.3.OR.TK.LT.SMALL) GO TO 130                         GEN02668
           C                                                                     GEN02670
           C-----FIRST USE GIVEN ESTIMATES FOR EQUIL SOLN IN MODE 3 AND 4 PROBLEMS GEN02672
           C                                                                     GEN02674
 ISN 0049        TK=TSAVE                                                        GEN02676
 ISN 0050        DO 120 I=1,NS                                                   GEN02678
 ISN 0051    120 SZ(I)=SSAVE(I)                                                  GEN02680
 ISN 0052        ASSIGN 200 TO NEXTOK                                            GEN02682
 ISN 0053        ASSIGN 150 TO NEXTNG                                            GEN02684
```

```
ISN 0054          GO TO 500
            C
            C
            C-----COMPLETE COMBUSTION ESTIMATE
            C
            C-----IF NO CARBON IN FUEL, SKIP TO GARBAGE ESTIMATES.
ISN 0055      130 IF (ILC.EQ.0) GO TO 170
ISN 0057          X=0.0
ISN 0058          Y=0.0
ISN 0059          DO 132 I=1,NS
ISN 0060          S2(I)=SMALL
ISN 0061          X=X+AL(ILC,I)*S1(I)
ISN 0062          Y=Y+AL(ILH,I)*S1(I)
ISN 0063      132 CONTINUE
ISN 0064          S2(IDN2)=S1(IDN2)
            C
ISN 0065          ER1=(4.0*X+Y)/(2.0*X+Y)
ISN 0066          ER2=2.0+Y/(2.0*X)
ISN 0067          IF (ER.LE.1.0) GO TO 133
ISN 0069          IF (ER.LT.ER1) GO TO 134
ISN 0071          IF (ER.LT.ER2) GO TO 135
            C-----ER.GT.ER2 ---- ALL C AND H IN CO, H2 AND UNBURNED CXHY
ISN 0073          S2(IDCO)=2.0*(X+Y/4.0)
ISN 0074          S2(IDH2)=Y*(1.0+Y/(4.0*X))
            C-----MOLE NUMBER FOR CXHY SHOULD BE (ER-2*(1+Y/(4*X)))
ISN 0075          GO TO 136
            C-----FUEL-LEAN COMBUSTION ---- ONLY CO2 AND H2O FORMED
ISN 0076      133 S2(IDCO2)=X*ER
ISN 0077          S2(IDO2)=(1.-ER)*(X+Y/4.)
ISN 0078          S2(IDH2O)=Y*ER/2.
ISN 0079          GO TO 136
            C-----SLIGHTLY FUEL-RICH ---- CO,CO2, AND H2O PRESENT
ISN 0080      134 S2(IDCO)=2.*(X+Y/4.)*(ER-1.)
ISN 0081          S2(IDCO2)=Y*(1.-ER)/2.+X*(2.-ER)
ISN 0082          S2(IDH2O)=Y*ER/2.
ISN 0083          GO TO 136
            C-----FUEL-RICH ---- CO,H2, AND H2O PRESENT
ISN 0084      135 S2(IDCO)=ER*X
ISN 0085          S2(IDH2)=Y*(ER-1.0)/2.0+X*(ER-2.0)
ISN 0086          S2(IDH2O)=Y/2.+X*(2.-ER)
            C
ISN 0087      136 SM=0.0
ISN 0088          DO 137 I=1,NS
ISN 0089      137 SM=SM+S2(I)
ISN 0090          TK=1500.0
ISN 0091          TKINV=6.6666660D-4
ISN 0092          IHCPS=1
ISN 0093          XLG=TK
ISN 0094          DO 139 K=1,10
ISN 0095          CALL HCPS
ISN 0096          HSUM=0.0
ISN 0097          DO 138 I=1,NS
ISN 0098      138 HSUM=HSUM+HO(I)*S2(I)
ISN 0099          TK=TK+(1.0+(HSUBO+RGASIN*TKINV-HSUM)/CPSUM)
ISN 0100          TKINV=1.0/TK
```

```
ISN 0101            XHI=DABS(TK-XLO)                                                GEN02796
ISN 0102            XLO=TK                                                          GEN02798
ISN 0103            IF (XHI.LT.1.0) GO TO 141                                       GEN02800
ISN 0105        139 CONTINUE                                                        GEN02802
ISN 0106            WRITE(6,140) K,XHI                                              GEN02804
ISN 0107        140 FORMAT(1H0,10X,42HMIXTURE TEMPERATURE FAILED TO CONVERGE IN ,  GEN02806
                   1I2,11H ITERATIONS,5X,17HTEMP DIFFERENCE =,2PD12.3/)             GEN02808
ISN 0108        141 CONTINUE                                                        GEN02810
              C                                                                     GEN02812
ISN 0109            IF (LDEBUG) WRITE(6,142) (S2(K),K=1,NS),SM,TK                   GEN02814
ISN 0111        142 FORMAT(/5X,28HCOMPLETE COMBUSTION ESTIMATE/1P11D10.2/1P11D10.2/) GEN02816
ISN 0112            IF (MODE.EQ.1) ASSIGN 900 TO NEXTOK                             GEN02818
ISN 0114            IF (MODE.EQ.2) ASSIGN 300 TO NEXTOK                             GEN02820
ISN 0116            IF (MODE.GE.3) ASSIGN 200 TO NEXTOK                             GEN02822
ISN 0118            ASSIGN 170 TO NEXTNG                                            GEN02824
ISN 0119            GO TO 500                                                       GEN02826
              C                                                                     GEN02828
              C                                                                     GEN02830
              C-----GARBAGE ESTIMATES  (GORDON AND MCBRIDE)                         GEN02832
              C                                                                     GEN02834
ISN 0120        170 TK=3800.0                                                       GEN02836
ISN 0121            SM=0.1/DFLOAT(NS)                                               GEN02838
ISN 0122            DO 171 I=1,NS                                                   GEN02840
ISN 0123        171 S2(I)=SM                                                        GEN02842
ISN 0124            SM=0.1                                                          GEN02844
ISN 0125            IF (MODE.EQ.1) ASSIGN 900 TO NEXTOK                             GEN02846
ISN 0127            IF (MODE.EQ.2) ASSIGN 300 TO NEXTOK                             GEN02848
ISN 0129            IF (MODE.GE.3) ASSIGN 200 TO NEXTOK                             GEN02850
ISN 0131            ASSIGN 600 TO NEXTNG                                            GEN02852
ISN 0132            GO TO 500                                                       GEN02854
              C                                                                     GEN02856
              C**  **  **  **  **  **  **  **  **  **  **  **  CHAPTER 2  **  **  ** GEN02858
              C**  **  **  **  **  **  **  **  **  **  **  **  CHAPTER 2  **  **  ** GEN02860
              C                                                                     GEN02862
              C   ***KINETIC***                                                     GEN02864
              C   SECTION FOR KINETIC SOLUTION FROM ADIABATIC EQUILIBRIUM ESTIMATES GEN02866
              C   (MODE 3 AND 4 ONLY)                                               GEN02868
              C                                                                     GEN02870
              C-----NEAR-EQUILIBRIUM SOLUTION  (KINETIC WITH EMV=1.0D-3 KG/CU M-SEC) GEN02872
              C                                                                     GEN02874
ISN 0133        200 LEQUIL=.FALSE.                                                  GEN02876
ISN 0134            IX=0                                                            GEN02878
ISN 0135            EMV=1.D0
ISN 0136            XLO=EMV                                                         GEN02882
              C-----INCREASE MINOR SPECIES FROM EQUILIBRIUM ESTIMATES               GEN02884
ISN 0137            DO 201 I=1,NS                                                   GEN02886
ISN 0138            IF (S2(I).LT.SMALL) S2(I)=SMALL                                 GEN02888
ISN 0140        201 CONTINUE                                                        GEN02890
ISN 0141            ASSIGN 250 TO NEXTOK                                            GEN02892
ISN 0142            ASSIGN 210 TO NEXTNG                                            GEN02894
ISN 0143            GO TO 500                                                       GEN02896
              C                                                                     GEN02898
              C                                                                     GEN02900
              C-----FAILURE ON NEAR-EQUIL WITH EMV=XLO, DECREASE EMV BY AN ORDER OF GEN02902
              C-----MAGNITUDE AND ATTEMPT AGAIN, ITERATING THIS WAY UP TO 12 TIMES  GEN02904
```

```
                 C
ISN 0144            210 EMV=EMV*0.1
ISN 0145                XLO=EMV
ISN 0146                IX=IX+1
ISN 0147                IF (IX.EQ.12) GO TO 610
ISN 0149                TK=TSAVE
ISN 0150                DO 211 I=1,NS
ISN 0151            211 S2(I)=SSAVE(I)
ISN 0152                ASSIGN 230 TO NEXTOK
ISN 0153                ASSIGN 210 TO NEXTNG
ISN 0154                GO TO 500
                 C
                 C
                 C-----HAVE NEAR-EQUIL SOLUTION, SO FIRST TRY DIRECTLY TO OBTAIN
                 C-----REQUIRED SOLUTION AT GIVEN EMV
                 C-----HAVE NEAR-EQUIL SOLUTION, SO FIRST TRY DIRECTLY TO OBTAIN
                 C-----REQUIRED SOLUTION AT GIVEN EMV
                 C
ISN 0155            230 EMV=EMVSAV
ISN 0156                IF (MODE.EQ.3) ASSIGN 900 TO NEXTOK
ISN 0158                IF (MODE.EQ.4) ASSIGN 300 TO NEXTOK
ISN 0160                ASSIGN 250 TO NEXTNG
ISN 0161                GO TO 500
                 C
                 C   ***UPPER BRANCH MARCHING***
                 C      HAVE A KINETIC SOLUTION BUT AT EMV .LT. EMVSAV.  START AT
                 C      KNOWN SOLUTION AND INCREASE EMV BY FACTOR TO MOVE TOWARDS
                 C      A SOLN THERE, IF SUCCESSFUL, REPEAT UNTIL EMVSAV IS REACHED; IF
                 C      NOT SUCCESSFUL START HALF INTERVAL SEARCHING DESCRIBED BELOW
                 C
ISN 0162            250 EMV=EMV*1.01
ISN 0163                IF (EMV.GT.EMVSAV) EMV=EMVSAV
ISN 0165                XHI=EMV
ISN 0166                IX=0
ISN 0167                TK=TSAVE
ISN 0168                DO 251 I=1,NS
ISN 0169            251 S2(I)=SSAVE(I)
ISN 0170                ASSIGN 250 TO NEXTOK
ISN 0171                IF (EMV.GE.EMVSAV.AND.MODE.EQ.3) ASSIGN 900 TO NEXTOK
ISN 0173                IF (EMV.GE.EMVSAV.AND.MODE.EQ.4) ASSIGN 300 TO NEXTOK
ISN 0175                ASSIGN 270 TO NEXTNG
ISN 0176                GO TO 500
                 C
                 C   ***HALF-INTERVAL SEARCHING***
                 C   HAVE SOLUTION AT XLO BUT NOT AT XHI, HENCE START INTERVAL
                 C   SEARCHING BY SETTING EMV TO THE LOGARITHMIC AVERAGE;
                 C   IF ITERATING MORE THAN TEN TIMES, TERMINATE.
                 C
ISN 0177            270 IX=IX+1
ISN 0178                TK=TSAVE
ISN 0179                DO 271 I=1,NS
ISN 0180            271 S2(I)=SSAVE(I)
ISN 0181                IF (IX.GT.10) GO TO 620
ISN 0183                EMV=DSQRT(XLO*XHI)
ISN 0184                XHI=EMV
```

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ISN 0185            ASSIGN 250 TO NEXTOK                                            GEN03016
ISN 0186            ASSIGN 270 TO NEXTNG                                            GEN03018
ISN 0187            GO TO 500                                                       GEN03020
              C                                                                     GEN03022
              C***   ***   ***   ***   ***   ***   ***   ***   CHAPTER 3   ***   ***  GEN03024
              C***   ***   ***   ***   ***   ***   ***   ***   CHAPTER 3   ***   ***  GEN03026
              C                                                                     GEN03028
              C   ***NON-ADIABATIC***                                               GEN03030
              C   SECTION FOR NON-ADIABATIC SOLUTIONS FROM ADIABATIC ESTIMATES      GEN03032
              C   (MODE 2 AND 4 ONLY)                                               GEN03034
              C   TRY DIRECTLY TO OBTAIN NON-ADIABATIC SOLUTION; IF NOT SUCCESSFUL, GEN03036
              C   START HALF-INTERVAL SCALING FROM THE ADIABATIC SOLUTION BY        GEN03038
              C   DEFINING A SCALING FACTOR FQ (0.0-1.0) TO MULTIPLY THE NON-ADIABATIC GEN03040
              C   TERM (Q) IN THE ENERGY EQUATION IN SPECE.                         GEN03042
              C                                                                     GEN03044
ISN 0188        300 LADIAB=.FALSE.                                                  GEN03046
ISN 0189            XLO=0.0                                                         GEN03048
ISN 0190            XHI=1.0                                                         GEN03050
ISN 0191            FQ=1.0                                                          GEN03052
ISN 0192            IX=0                                                            GEN03054
ISN 0193        310 ASSIGN 320 TO NEXTOK                                            GEN03056
ISN 0194            ASSIGN 330 TO NEXTNG                                            GEN03058
ISN 0195            GO TO 500                                                       GEN03060
              C                                                                     GEN03062
ISN 0196        320 IF (FQ.EQ.1.0) GO TO 900                                        GEN03064
ISN 0198            XLO=FQ                                                          GEN03066
ISN 0199            FQ=1.0                                                          GEN03068
ISN 0200            XHI=1.0                                                         GEN03070
ISN 0201            IX=0                                                            GEN03072
ISN 0202            GO TO 310                                                       GEN03074
              C                                                                     GEN03076
ISN 0203        330 IX=IX+1                                                         GEN03078
ISN 0204            IF (IX.GT.10) GO TO 340                                         GEN03080
ISN 0206            TK=TSAVE                                                        GEN03082
ISN 0207            DO 331 I=1,NS                                                   GEN03084
ISN 0208        331 S2(I)=SSAVE(I)                                                  GEN03086
ISN 0209            FQ=0.5*(XLO+XHI)                                                GEN03088
ISN 0210            XHI=FQ                                                          GEN03090
ISN 0211            GO TO 310                                                       GEN03092
              C                                                                     GEN03094
ISN 0212        340 CONTINUE                                                        GEN03096
ISN 0213            FQ=1.                                                           GEN03098
ISN 0214            GO TO 630                                                       GEN03100
              C                                                                     GEN03102
              C****   ****   ****   ****   ****   ****   CHAPTER 4   ****   ***GEN03104
              C****   ****   ****   ****   ****   ****   CHAPTER 4   ****   ***GEN03106
              C                                                                     GEN03108
              C   ***FAILURE EXITS***                                               GEN03110
              C   FAILED EQUIL OR KINETIC SOLN OR EQUIV RATIO OUTSIDE (0.1,10)      GEN03112
              C   RETURN ADIABATIC, NON-REACTED MIXTURE PROPERTIES                  GEN03114
              C                                                                     GEN03116
ISN 0215        400 SM=0.0                                                          GEN03118
ISN 0216            DO 401 I=1,NS                                                   GEN03120
ISN 0217            S2(I)=S1(I)                                                     GEN03122
ISN 0218            SM=SM+S2(I)                                                     GEN03124
```

```
ISN 0219        401 CONTINUE
ISN 0220            TK=1000.0
ISN 0221            XLO=TK
ISN 0222            IHCPS=1
ISN 0223            TKINV=1.0D-3
ISN 0224            DO 403 I=1,10
ISN 0225            CALL HCPS
ISN 0226            HSUM=0.0
ISN 0227            DO 402 K=1,NS
ISN 0228            HSUM=HSUM+HO(K)*S2(K)
ISN 0229        402 CONTINUE
ISN 0230            TK=TK*(1.0+(HSUBO*RGASIN*TKINV-HSUM)/CPSUM)
ISN 0231            TKINV=1.0/TK
ISN 0232            XHI=DABS(TK-XLO)
ISN 0233            XLO=TK
ISN 0234            IF (XHI.LT.1.0) GO TO 404
ISN 0236        403 CONTINUE
ISN 0237            WRITE(6,140) I,XHI
ISN 0238        404 CONTINUE
ISN 0239            RHOP=PA/(RGAS*TK*SM)
ISN 0240            GO TO 500
                C
                C*****     *****     *****     *****     *****   CHAPTER 5   *****
                C*****     *****     *****     *****     *****   CHAPTER 5   *****
                C
                C  ***PROBLEM CELL CALL TO SPECE***
                C  TAKE THE ESTIMATES GENERATED IN CHAPTERS 1,2 AND ATTEMPT A SOLUTION
                C  WITH FULL EQUATIONS. IF SUCCESSFUL, UPDATE THE SAVE ANSWERES WITH THE
                C  SOLUTION AND RETURN TO STATEMENT NUMBER NEXTOK.  IF NOT, THE ACTION
                C  DEPENDS ON WHETHER AN EQUILBM OR KINETIC SOLN IS SOUGHT. FAILED
                C  EQUIL SOLN, RETURN TO STATEMENT NUMBER NEXING, WHILE FAILURE IN A
                C  KINETIC SOLN WILL BE FOLLOWED BY AN ATTEMPT WITH LNRG=F ----> KT=0.0
                C  AND SAME ESTIMATES.  SETTING KT=0.0 IMPLIES THAT A CHANGE IN TEMP
                C  FIELD HAS NO EFFECT ON SPECIES DISTRIBUTION FOR THAT PARTICULAR
                C  ITERATION, BUT DOES ALLOW THE SPECIES CHANGES TO INFLUENCE THE TEMP
                C  CHANGE ----> PARTIAL DECOUPLING OF THE ENERGY EQUATION.  IF SUCCESSFUL
                C  WITH LNRG=F, REPEAT WITH LNRG=T (FULL EQUATIONS)! IF STILL NO GOOD,
                C  RETURN TO STATEMENT NUMBER NEXING.
                C
ISN 0241        500 CALL SPECE
ISN 0242            IF (LCONVG) GO TO 540
                C   SOLUTION FAILED TRY KT=0.0
ISN 0244            IF (LNRG) GO TO 520
ISN 0246            LNRG=.TRUE.
ISN 0247        510 GO TO NEXING, (100,130,170,210,250,270,330,600)
ISN 0248        520 IF (LEQUIL) GO TO 510
ISN 0250        530 LNRG=.FALSE.
ISN 0251            GO TO 500
                C   HAVE SOLN BUT WITHOUT KT TERMS, SEND THIS
                C   SOLN AS ESTIMATES WITH KT CALCULATION
ISN 0252        540 IF (LNRG) GO TO 550
ISN 0254            LNRG=.TRUE.
ISN 0255            GO TO 500
                C
                C-----SOLUTION IS SUCCESSFUL, UPDATE SAVE ANSWERS AND CONTINUE.
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                 C                                                                           GEN03236
ISN 0256           550 TSAVE=TK                                                              GEN03238
ISN 0257               DO 560 I=1,NS                                                         GEN03240
ISN 0258           560 SSAVE(I)=S2(I)                                                        GEN03242
                 C                                                                           GEN03244
ISN 0259               GO TO NEXTCK, (200,230,250,300,320,900)                               GEN03246
                 C                                                                           GEN03248
                 C******      ******      ******      ******      CHAPTER 6      ******      GEN03250
                 C******      ******      ******      ******      CHAPTER 6      ******      GEN03252
                 C                                                                           GEN03254
                 C   ***ERROR MESSAGES***                                                    GEN03256
                 C                                                                           GEN03258
ISN 0260           600 WRITE(6,601)                                                          GEN03260
ISN 0261           601 FORMAT(1H0,10X,3(4H****),30H FAILURE TO FIND EQUIL SOLN....,          GEN03262
                      A24HAVG INLET PROPS RETURNED/)                                         GEN03264
ISN 0262               GO TO 650                                                             GEN03266
ISN 0263           610 WRITE(6,611)                                                          GEN03268
ISN 0264           611 FORMAT(1H0,10X,3(4H****),35H FAILURE TO FIND NEAR-EQUIL SOLN....,     GEN03270
                      A24HAVG INLET PROPS RETURNED/)                                         GEN03272
ISN 0265               GO TO 650                                                             GEN03274
ISN 0266           620 WRITE(6,621)                                                          GEN03276
ISN 0267           621 FORMAT(1H0,10X,3(4H****),37H FAILURE TO OBTAIN KINETIC SOLN AFTER,GEN03278
                      A46H TEN INTERVAL HALVING...AVG INLET PROPS RETURNED/)                 GEN03280
ISN 0268               GO TO 650                                                             GEN03282
ISN 0269           630 WRITE(6,631)                                                          GEN03284
ISN 0270           631 FORMAT(1H0,10X,3(4H****),29H NON-ADIABATIC SOLN FAILED....,           GEN03286
                      A19HADIAB SOLN RETURNED/)                                              GEN03288
ISN 0271               GO TO 670                                                             GEN03290
                 C                                                                           GEN03292
                 C-----RESTORE FAILED PROBLEM MODE PRIOR TO RETURN                           GEN03294
                 C                                                                           GEN03296
ISN 0272           650 IF (MODE.EQ.2) LADIAB=.FALSE.                                         GEN03298
ISN 0274               IF (MODE.EQ.3) LEQUIL=.FALSE.                                         GEN03300
ISN 0276               IF (MODE.EQ.4) LADIAB=.FALSE.                                         GEN03302
ISN 0278               GO TO 400                                                             GEN03304
                 C                                                                           GEN03306
                 C-----FAILED NON-ADIABATIC SOLUTION...RETURN ADIABATIC                      GEN03308
                 C-----EQUIL OR KINETIC SOLUTION                                             GEN03310
                 C                                                                           GEN03312
ISN 0279           670 TK=TSAVE                                                              GEN03314
ISN 0280               SM=0.0                                                                GEN03316
ISN 0281               DO 671 I=1,NS                                                         GEN03318
ISN 0282               S2(I)=SSAVE(I)                                                        GEN03320
ISN 0283           671 SM=SM+S2(I)                                                           GEN03322
                 C                                                                           GEN03324
ISN 0284           900 RHOP=PA/(RGAS*TK*SM)                                                  GEN03326
ISN 0285               RETURN                                                                GEN03328
ISN 0286               END                                                                   GEN03330
```

```
NUMBER    LEVEL                                FORTRAN H EXTENDED ERROR MESSAGES

IFE307I    4(W)        NAME FACTOR        THE DATA STATEMENT CONTAINS A VARIABLE THAT IS NOT REFERENCED.

*OPTIONS IN EFFECT*NAME(MAIN) NOOPTIMIZE LINECOUNT(57) SIZE(MAX) AUTODBL(NONE)
```

REQUESTED OPTIONS:

OPTIONS IN EFFECT: NAME(MAIN) NOOPTIMIZE LINECOUNT(57) SIZE(MAX) AUTODBL(NONE)
SOURCE EBCDIC NOLIST NODECK OBJECT NOMAP NOFORMAT NOGOSTMT NOXREF NOALC NOANSF TERM FLAG

```
ISN 0002          SUBROUTINE CPERO
ISN 0003          IMPLICIT REAL*8 (A-H,O-Z)
            C
ISN 0004          LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LMOLES,LNRG,LREACT,LSI
ISN 0005          DIMENSION ASUB(20,3)
ISN 0006          DIMENSION ATOM(7),DATA(12),AT(4)
ISN 0007          DIMENSION B(4)
            C
ISN 0008          COMMON
                 1/CCHEMI/CPSUM,FQ,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LCONVG,LNRG
                 1/CEQUIL/A(7,20),ATOM(3,7),BO(7),PI(7)
                 1/CINDEX/IDCO,IDCO2,IDH2,IDH2O,IDN2,IDO2,IHCPS,ILC,ILM,IMAT,ITER,
                 2        JJ,NI,NE,NS,NA,NGLOB,NGLOBP,NLM,NO,NSM
                 1/CMATRI/HSUM,X(22),Y(22)
                 1/CPARAM/ACOB,NT,NE,EMV,ER,HSUBO,NDEBUG,NS,PA,QO,Q1,Q2,Q3,Q4,RHOP,
                 2        SM,S1(20),S2(20),TK,LADIAB,LDEBUG,LEQUIL,LREACT
                 1/CREACT/BX(36),BX2(36),ID(4,36),MOOR(36),TACT(36),TACT2(36),
                 2        TEN(36),TEN2(36),X1(36),X2(36)
ISN 0009          COMMON  /CSPECE/
                 1        HO(20),SO(20),SMW(20),SSAVE(20),Z(7,2,20)
ISN 0010          DATA ACO/4HCO   /,ACO2/4HCO2 /,AH2/4HH2   /,AH2O/4HH2O /,
                 1 AMCH/4HMECH/,AN2/4HN2   /,AO2/4HO2   /,BLANK/4H    /,ELEM/4HELEM/,
                 2 GLOB/4HGLOB/,REAL/4HREAC/,REVE/4HREVE/,THER/4HTHER/,THIRD/4HM   /
                 3 ,COS/4HCOS /,COMM/4HCOMM/,GAZ/1HG/,MOL/1HM/,BLNK/2H  /,
                 4 CARB/2HC /,HYDR/2HH /
ISN 0011          DATA NSTRM /0/,TENLN/2.3026/,XMAX/.001/,XMIN/.0003/
            C
            C*************************************************************************
            C  THIS SUBROUTINE IS THE INITIALIZING ROUTINE.  THE FIRST CALL READS
            C  (1) ELEMENT DATA DECK, (2) THERMO DATA DECK, AND (3) MECHANISM DATA
            C  DECK.  EACH SUBSEQUENT CALL READS ONE REACTANTS DATA DECK...NO LIMIT
            C  ON NUMBER OF CALLS...ONE FOR EACH DIFFERENT REACTANT STREAM
            C  PRESSURE AND TEMPERATURE OF EACH REACTANT STREAM MUST BE SUPPLIED BY
            C  CALLING PROGRAM IN PA AND TK, RESPECTIVELY
            C  ON RETURN, CALLING PROGRAM MUST STORE MOLE NUMBERS S2(I), PRESSURE,
            C  TEMPERATURE, ENTHALPY AND DENSITY AT APPROPRIATE INLET GRID NODE
ISN 0012       10 READ (5,20) (DATA(I),I=1,12)
ISN 0013       20 FORMAT (12A4)
ISN 0014          WRITE (6,30) (DATA(I),I=1,12)
ISN 0015       30 FORMAT (1H0,5X,12A4)
ISN 0016          IF (DATA(1).EQ.BLANK) GO TO 10
ISN 0018          IF (DATA(1).EQ.ELEM) GO TO 100
ISN 0020          IF (DATA(1).EQ.THER)GO TO 200
ISN 0022          IF (DATA(1).EQ.AMCH) GO TO 300
ISN 0024          IF (DATA(1).EQ.REAC) GO TO 400
ISN 0026          GO TO 10
            C
            C
            C
            C     ***ELEMENTS***
```

```
                C  READ ELEMENT DATA FROM CARDS
                C  ATOM(1,K)=SYMBOL,  ATOM(2,K)=ATOMIC WT   ATOM(3,K)=VALENCE
ISN 0027          100 RGAS=831.4
ISN 0028              RGASIN=1./RGAS
ISN 0029              IDCO=0
ISN 0030              IDCO2=0
ISN 0031              IDH2=0
ISN 0032              IDH2O=0
ISN 0033              IDN2=0
ISN 0034              IDO2=0
ISN 0035              ILC=0
ISN 0036              ILH=0
ISN 0037              LADIAB=.TRUE.
ISN 0038              LDEBUG=.TRUE.
ISN 0039              LDEBUG=.FALSE.
ISN 0040              NLEBUG=5
ISN 0041              LEQUIL=.TRUE.
ISN 0042              LREACT=.TRUE.
ISN 0043              LST=.TRUE.
ISN 0044              LARG=.TRUE.
ISN 0045              FW=1.
ISN 0046              NLM=1
ISN 0047          110 READ (5,120) ATOM(NLM),(ATOM(K,NLM),K=2,3)
ISN 0048          120 FORMAT(A2,7X,2F10.0)
ISN 0049              IF (ATOM(NLM)  .EQ.BLANK) GO TO 140
ISN 0051              WRITE(6,130) ATOM(NLM),(ATOM(K,NLM),K=2,3)
ISN 0052          130 FORMAT(1X,A2,5X,2F15.6/)
ISN 0053              IF (ATOM(NLM)  .EQ.CARB) ILC=NLM
ISN 0055              IF (ATOM(NLM)  .EQ.HYDR) ILH=NLM
ISN 0057              NLM=NLM+1
ISN 0058              GO TO 110
                C
ISN 0059          140 CONTINUE
ISN 0060              NLM=NLM-1
ISN 0061              N1=NLM+1
ISN 0062              N2=NLM+2
ISN 0063              N3=NLM+3
ISN 0064              GO TO 10
                C
                C**  **  **  **  **  **  **  **  **  **  **  **  CHAPTER 2  **  **  **
                C**  **  **  **  **  **  **  **  **  **  **  **  CHAPTER 2  **  **  **
                C
                C   ***THERMO***
                C   READ THERMODYNAMIC DATA CARDS
                C
ISN 0065          200 NS=1
ISN 0066          201 READ(5,210) (DATA(I),I=1,3),DT1,DT2,(AT(J),B(J),J=1,4),PHAZ,
                     1T1,T2,NCO
ISN 0067          210 FORMAT(3A4,6X,2A3,4(A2,F3.0),A1,2F10.3,I15)
ISN 0068              IF (DATA(1).EQ.BLANK) GO TO 200
ISN 0070              WRITE(6,211)(DATA(I),I=1,3),DT1,DT2,(AT(J),B(J),J=1,4),PHAZ,
                     1 T1,T2,NCO
ISN 0071          211 FORMAT(10X,3A4,6X,2A3,2X,4(A2,2X,F3.0),2X,A1,2X,2F10.3,I15)
ISN 0072              IF (PHAZ.NE.GAZ) WRITE(6,212) (DATA(I),I=1,3),PHAZ
ISN 0074          212 FORMAT(1H0,10X,26HWARNING...DATA FOR SPECIES,2X,3A4,3X,
```

```
                A1,HNO) GAS BO',2X,A1//)                                        GEN03542
            C-----READ Z WITH FIRST AND SECOND SUBSCRIPTS REVERSED              GEN03544
ISN 0075        READ(5,213) (Z(J,1,NS),J=1,5),NCD                               GEN03546
ISN 0076    213 FORMAT(5D15.8,I5)                                               GEN03548
ISN 0077        WRITE(6,214) (Z(J,1,NS),J=1,5),NCD                              GEN03550
ISN 0078    214 FORMAT(10X,5D15.8,I5)                                           GEN03552
ISN 0079        READ(5,213) (Z(J,1,NS),J=6,7),(Z(K,2,NS),K=1,3),NCD             GEN03554
ISN 0080        WRITE(6,214) (Z(J,1,NS),J=6,7),(Z(K,2,NS),K=1,3),NCD            GEN03556
ISN 0081        READ(5,215) (Z(J,2,NS),J=4,7),NCD                               GEN03558
ISN 0082    215 FORMAT(4D15.8,I20)                                              GEN03560
ISN 0083        WRITE(6,216) (Z(J,2,NS),J=4,7),NCD                              GEN03562
ISN 0084    216 FORMAT(10X,4D15.8,I20/)                                         GEN03564
            C-----ESTABLISH ATOM STOICHIOMETRY...AL(L,N) = (KG-ATOMS ELEMENT L  GEN03566
            C-----PER KG-MOLECULE OF SPECIES N)                                 GEN03568
            C                                                                   GEN03570
ISN 0085        DO 220 L=1,NLM                                                  GEN03572
ISN 0086    220 AL(L,NS)=0.0                                                    GEN03574
            C                                                                   GEN03576
ISN 0087        SUM=0.0                                                         GEN03578
ISN 0088        DO 240 K=1,4                                                    GEN03580
ISN 0089        IF (B(K).EQ.0.0) GO TO 240                                      GEN03582
ISN 0091        DO 230 L=1,NLM                                                  GEN03584
ISN 0092        IF (ATOM(1,L).NE.AT(K)) GO TO 230                               GEN03586
ISN 0094        AL(L,NS)=AL(L,NS)+B(K)                                          GEN03588
            C                                                                   GEN03590
            C-----ESTABLISH MOLECULAR WEIGHT OF SPECIES                         GEN03592
            C                                                                   GEN03594
ISN 0095        SUM=SUM+ATOM(2,L)*B(K)                                          GEN03596
ISN 0096    230 CONTINUE                                                        GEN03598
ISN 0097    240 CONTINUE                                                        GEN03600
ISN 0098        SMW(NS)=SUM                                                     GEN03602
ISN 0099        S2(NS)=1.0D-6                                                   GEN03604
            C                                                                   GEN03606
            C-----STORE HOLLERITH NAME OF SPECIES                               GEN03608
            C                                                                   GEN03610
ISN 0100        DO 250 I=1,3                                                    GEN03612
ISN 0101    250 ASUB(NS,I)=DATA(I)                                              GEN03614
            C                                                                   GEN03616
            C-----STORE INDEX NUMBER OF SPECIES                                 GEN03618
            C                                                                   GEN03620
ISN 0102        IF (ASUB(NS,1).EQ.ACO)  ICO=NS                                  GEN03622
ISN 0104        IF (ASUB(NS,1).EQ.ACO2) ICO2=NS                                 GEN03624
ISN 0106        IF (ASUB(NS,1).EQ.AH2)  IH2=NS                                  GEN03626
ISN 0108        IF (ASUB(NS,1).EQ.AH2O) IH2O=NS                                 GEN03628
ISN 0110        IF (ASUB(NS,1).EQ.AN2)  IN2=NS                                  GEN03630
ISN 0112        IF (ASUB(NS,1).EQ.AO2)  IO2=NS                                  GEN03632
            C                                                                   GEN03634
ISN 0114        NS=NS+1                                                         GEN03636
ISN 0115        GO TO 201                                                       GEN03638
            C                                                                   GEN03640
ISN 0116    260 NS=NS-1                                                         GEN03642
ISN 0117        NSM=NS+1                                                        GEN03644
ISN 0118        NQ=NS+2                                                         GEN03646
ISN 0119        NA=NS+3                                                         GEN03648
ISN 0120        GO TO 10                                                        GEN03650
```

```
            C
            C***   ***   ***   ***   ***   ***   ***   ***   CHAPTER 3   ***   ***
            C***   ***   ***   ***   ***   ***   ***   ***   CHAPTER 3   ***   ***
            C
            C   ***MECHANISM***
            C   READ MECHANISM/RATE DATA CARDS
            C   THE VARIABLE DT1 (COLUMNS 73/76) IS USED AS A FLAG:
            C   CGS  ----- CGS UNITS, RATE CONSTANTS IN GM-MOLES, CM, SEC
            C             AND EAC IN (KCAL/GM-MOLE)
            C   COMM ----- COMMENT CARD, FIRST 48 CHARACTERS PRINTED OUT
            C   REVE ----- REVERSE RATE DATA, IN SAME UNITS AS FORWARD DATA
            C   GLOB ----- GLOBAL RATE EXPRESSION DATA IN SI UNITS
            C   OTHERWISE THE SI UNITS (KG-MOLES, M, SEC) ARE ASSUMED
            C   DT1 AND DT2 (COL 73/80) CAN HAVE ANYTHING (COMMENTS) IF ABOVE FOUR
            C   WORDS ARE NOT REQUIRED
            C   TACT IS ACTIVATION TEMPERATURE, = EACT/GASCON, DEG K
            C
ISN 0121      300 JJ=1
ISN 0122          NGLOB=0
            C
ISN 0123      310 READ(5,311) (DATA(I),I=1,12),BX(JJ),TEN(JJ),TACT(JJ),DT1,DT2
ISN 0124      311 FORMAT(12A4,3F8.3,2A4)
ISN 0125          IF (DATA(1).EQ.BLANK.AND.DT1.NE.COMM) GO TO 356
            C-----CHECK FOR COMMENT CARD
ISN 0127          IF (DT1.NE.COMM) GO TO 313
ISN 0129          WRITE(6,312) (DATA(I),I=1,12)
ISN 0130      312 FORMAT(1H0,5X,3H***,12A4,3H***)
ISN 0131          GO TO 310
            C-----CHECK FOR REVERSE RATE DATA...ORDER OF CARDS MUST BE CORRECT
            C-----UNITS OF REVERSE DATA ASSUMED SAME AS FORWARD DATA
ISN 0132      313 IF (DT1.NE.REVE) GO TO 315
ISN 0134          J=JJ-1
ISN 0135          BX2(J)=BX(JJ)
ISN 0136          TEN2(J)=TEN(JJ)
ISN 0137          TACT2(J)=TACT(JJ)
ISN 0138          WRITE(6,314) BX2(J),TEN2(J),TACT2(J),DT1,DT2
ISN 0139      314 FORMAT(14X,17HREVERSE RATE DATA,28X,3F15.3,2A4)
            C-----CONVERT BX2 FOR INTERNAL CALCULATIONS
ISN 0140          BX2(J)=BX2(J)*TENLN
ISN 0141          IF (LSI) GO TO 310
ISN 0143          BX2(J)=BX2(J)-TENLN*3.0
ISN 0144          TACT2(J)=TACT2(J)*1000.0/1.987
ISN 0145          IF (MODR(J).EQ.2) BX2(J)=BX2(J)-TENLN*3.0
ISN 0147          GO TO 310
            C-----CHECK FOR UNITS
ISN 0148      315 LSI=.TRUE.
ISN 0149          IF (DT1.EQ.CGS) LSI=.FALSE.
            C
ISN 0151          WRITE(6,316) JJ,(DATA(I),I=1,12),BX(JJ),TEN(JJ),TACT(JJ),DT1,DT2
ISN 0152      316 FORMAT(1H0,5X,I5,4H.    ,12A4,3F15.3,5X,2A4)
ISN 0153          IF (.NOT. LSI) TACT(JJ)=TACT(JJ)*1000./1.987
ISN 0155          IF (DT1.EQ.GLOB) NGLOB=NGLOB+1
            C-----CONVERT BX FOR INTERNAL CALCULATIONS
ISN 0157          BX(JJ)=BX(JJ)*TENLN
            C
```

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              C-----ID(I,J) IS THE INDEX NUMBER OF THE I-TH DISTINCT SPECIES IN      GEN03762
              C-----REACTION J ... I=1,4 AS NO DISTINCT THIRD BODIES ARE CONSIDERED  GEN03764
              C                                                                      GEN03766
ISN 0158            DO 320 I=1,4                                                     GEN03768
ISN 0159        320 ID(I,JJ)=0                                                       GEN03770
              C                                                                      GEN03772
ISN 0160            ND=1                                                             GEN03774
ISN 0161            DO 325 N=1,6                                                     GEN03776
ISN 0162            K=N*2-1                                                          GEN03778
ISN 0163            IF (DATA(K).EQ.BLANK) GO TO 325                                  GEN03780
ISN 0165            IF (DATA(K).NE.THIRD) GO TO 321                                  GEN03782
ISN 0167            DATA(K)=BLANK                                                    GEN03784
ISN 0168            GO TO 325                                                        GEN03786
ISN 0169        321 CONTINUE                                                         GEN03788
ISN 0170            DO 322 I=1,NS                                                    GEN03790
ISN 0171            IF (DATA(K).NE.ASUB(I,1)) GO TO 322                              GEN03792
ISN 0173            IF (DATA(K+1).NE.ASUB(I,2)) GO TO 322                            GEN03794
ISN 0175            I1=I                                                             GEN03796
ISN 0176            GO TO 323                                                        GEN03798
ISN 0177        322 CONTINUE                                                         GEN03800
ISN 0178        323 IF (K.GT.5) GO TO 324                                            GEN03802
ISN 0180            ID(ND,JJ)=I1                                                     GEN03804
ISN 0181            ND=ND+1                                                          GEN03806
ISN 0182            GO TO 325                                                        GEN03808
ISN 0183        324 IF (ND.EQ.2) ND=3                                                GEN03810
ISN 0185            ID(ND,JJ)=I1                                                     GEN03812
ISN 0186            ND=ND+1                                                          GEN03814
ISN 0187        325 CONTINUE                                                         GEN03816
              C                                                                      GEN03818
              C                                                                      GEN03820
              C-----STORE THE TYPE OF REACTION...THREE TYPES                         GEN03822
              C     MODR 1 ... A + B ----> C + D                                     GEN03824
              C     MODR 2 ... AB + M ----> A + B + M                                GEN03826
              C     MODR 3 ... A + B + M ----> AB + M                                GEN03828
              C                                                                      GEN03830
ISN 0188            MODR(JJ)=1                                                       GEN03832
ISN 0189            IF (ID(2,JJ).EQ.0) MODR(JJ)=2                                    GEN03834
ISN 0191            IF (ID(4,JJ).EQ.0) MODR(JJ)=3                                    GEN03836
              C                                                                      GEN03838
              C                                                                      GEN03840
              C     THE FOLLOWING SECTION, UP TO STATEMENT 355 INCLUSIVE, MAY BE     GEN03842
              C     ELIMINATED IF REVERSE (AS WELL AS FORWARD) RATE DATA IS SUPPLIED GEN03844
              C     FOR ** ALL ** REACTIONS.                                         GEN03846
              C                                                                      GEN03848
              C     CALCULATES REVERSE RATE CONSTANTS FROM EQUILIBRIUM CONSTANTS     GEN03850
              C     AND FORWARD RATE CONSTANTS FOR FIFTEEN POINTS                    GEN03852
              C     OVER THE TEMPERATURE RANGE 1000 TO 3000 DEG K                    GEN03854
ISN 0193            BA2(JJ)=0.                                                       GEN03856
ISN 0194            TEN2(JJ)=0.                                                      GEN03858
ISN 0195            FACT2(JJ)=0.                                                     GEN03860
ISN 0196            IF (DT1.EQ.GLOB) GO TO 355                                       GEN03862
ISN 0198            DX=(XMAX-XMIN)/14.0                                              GEN03864
ISN 0199            SUMX=0.0                                                         GEN03866
ISN 0200            SUMY=0.0                                                         GEN03868
ISN 0201            INCPS=2                                                          GEN03870
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```
ISN 0202          DO 351 N=1,15                                                    GEN03872
ISN 0203          X(N)=XMIN+DX*DFLOAT(N-1)                                         GEN03874
ISN 0204          SUMX=SUMX+X(N)                                                   GEN03876
ISN 0205          TKINV=X(N)                                                       GEN03878
ISN 0206          TK=1.0/TKINV                                                     GEN03880
ISN 0207          TLN=DLOG(TK)                                                     GEN03882
ISN 0208          CALL HCPS                                                        GEN03884
ISN 0209          SUMI=0.0                                                         GEN03886
ISN 0210          DO 350 ND=1,4                                                    GEN03888
ISN 0211          K=ID(ND,JJ)                                                      GEN03890
ISN 0212          IF (K.EQ.0) GO TO 350                                            GEN03892
ISN 0214          GF=H0(K)-S0(K)                                                   GEN03894
ISN 0215          IF (ND.LT.3) SUMI=SUMI+GF                                        GEN03896
ISN 0217          IF (ND.GE.3) SUMI=SUMI-GF                                        GEN03898
ISN 0219      350 CONTINUE                                                         GEN03900
ISN 0220          TMI=0.0                                                          GEN03902
ISN 0221          IF (ID(2,JJ).EQ.0) TMI=TLN-2.50034                               GEN03904
ISN 0223          IF (ID(4,JJ).EQ.0) TMI=2.50034-TLN                               GEN03906
ISN 0225          Y(N)=TMI-SUMI+TEN(JJ)*TLN-TACT(JJ)*TKINV+BX(JJ)                  GEN03908
ISN 0226          SUMY=SUMY+Y(N)                                                   GEN03910
ISN 0227      351 CONTINUE                                                         GEN03912
ISN 0228          XBAR=SUMX/15.0                                                   GEN03914
ISN 0229          YBAR=SUMY/15.0                                                   GEN03916
ISN 0230          SUMX=0.0                                                         GEN03918
ISN 0231          SUMI=0.0                                                         GEN03920
ISN 0232          SUMY=0.0                                                         GEN03922
ISN 0233          DO 352 N=1,15                                                    GEN03924
ISN 0234          SUMX=SUMX+Y(N)*(X(N)-XBAR)                                       GEN03926
ISN 0235          SUMI=SUMI+(X(N)-XBAR)**2                                         GEN03928
ISN 0236          SUMY=SUMY+(Y(N)-YBAR)**2                                         GEN03930
ISN 0237      352 CONTINUE                                                         GEN03932
ISN 0238          TEN2(JJ)=0.0                                                     GEN03934
ISN 0239          TACT2(JJ)=-SUMX/SUMI                                             GEN03936
ISN 0240          BX2(JJ)=(YBAR+TACT2(JJ)*XBAR)/TENLN                              GEN03938
ISN 0241          SUMX=0.0                                                         GEN03940
ISN 0242          DO 353 N=1,15                                                    GEN03942
ISN 0243          SUMX=SUMX+(Y(N)+TACT2(JJ)*X(N)-TENLN*BX2(JJ))**2                 GEN03944
ISN 0244      353 CONTINUE                                                         GEN03946
ISN 0245          SUMY=DSQRT(1.0-SUMX/SUMY)                                        GEN03948
ISN 0246          SUMX=DSQRT(SUMX/14.0)                                            GEN03950
ISN 0247          DTHCC  =TACT2(JJ)                                                GEN03952
ISN 0248          IF (.NOT.LSI) DTHCC  =TACT2(JJ)*1.987*.001                       GEN03954
ISN 0250          WRITE (6,354) BX2(JJ),TEN2(JJ),DTHCC  ,SUMX,SUMY                 GEN03956
ISN 0251      354 FORMAT (6X,57H CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEFGEN03958
                 1 =    ,3F15.3,4X,2P2D10.3)                                       GEN03960
            C-----CONVERT BX2 FOR INTERNAL CALCULATIONS                            GEN03962
ISN 0252          BX2(JJ)=BX2(JJ)*TENLN                                            GEN03964
            C                                                                      GEN03966
ISN 0253      355 JJ=JJ+1                                                          GEN03968
            C-----CONVERT ALL RATE DATA TO SI UNITS                                GEN03970
ISN 0254          IF (LSI) GO TO 310                                               GEN03972
ISN 0256          J=JJ-1                                                           GEN03974
ISN 0257          BX(J)=BX(J)-TENLN*3.0                                            GEN03976
ISN 0258          BX2(J)=BX2(J)-TENLN*3.0                                          GEN03978
ISN 0259          IF (MODR(J).EQ.2) BX2(J)=BX2(J)-TENLN*3.0                        GEN03980
```

```
ISN 0261          IF (MODR(J).EQ.3) BX(J)=BX(J)-TENLN*3.0
ISN 0263          GO TO 310
            C
ISN 0264      356 JJ=JJ-1
ISN 0265          NGLDBP=NGLDB+1
            C
            C-----PRINT OUT ARRAY OF STOICHIOMETRIC COEFFICIENTS
            C
ISN 0266          DO 372 J=1,JJ
ISN 0267          DO 370 N=1,6
ISN 0268          K=N*2-1
ISN 0269          L=N
ISN 0270          IF (N.GT.3) L=N-1
ISN 0272          DATA(K)=BLANK
ISN 0273          DATA(K+1)=BLANK
ISN 0274          IF (N.EQ.3) GO TO 370
ISN 0276          IF (N.EQ.6) GO TO 370
ISN 0278          IF (ID(L,J).EQ.0) GO TO 370
ISN 0280          IDLJ=ID(L,J)
ISN 0281          DATA(K)=ASUB(IDLJ,1)
ISN 0282          KPLUS1=K+1
ISN 0283          DATA(KPLUS1)=ASUB(IDLJ,2)
ISN 0284      370 CONTINUE
ISN 0285          IF (ID(2,J).EQ.0) DATA(5)=THIRD
ISN 0287          IF (ID(4,J).EQ.0) DATA(5)=THIRD
ISN 0289          DATA(11)=DATA(5)
ISN 0290          WRITE(6,371) J,(DATA(K),K=1,12)
ISN 0291      371 FORMAT(5X,I5,1H.,5X,6A4,4H---,6X,6A4/)
ISN 0292      372 CONTINUE
            C
            C-----PRINT OUT ALL RATE DATA IN SI UNITS
            C
ISN 0293          WRITE(6,380)
ISN 0294      380 FORMAT(//1H0,40X,29HKINETIC RATE DATA IN SI UNITS/
                 A1H0,6X,1HJ,6X,4HMODR,12X,2HID,19X,2HBX,10X,3HTEN,9X,4HTACT,
                 B13X,3HBX2,9X,4HTEN2,9X,5HTACT2/)
ISN 0295          DO 382 J=1,JJ
ISN 0296          TM1=BX(J)/TENLN
ISN 0297          TM2=BX2(J)/TENLN
ISN 0298          WRITE(6,381) J,MODR(J),(ID(I,J),I=1,4),TM1,TEN(J),TACT(J),
                 1TM2,TEN2(J),TACT2(J)
ISN 0299      382 CONTINUE
ISN 0300      381 FORMAT((5X,I2,1H.,I8,3X,4I5,2(3X,3F13.3)))
            C
            C-----SET CONTACT INDEXES TO UNITY
ISN 0301          DO 390 J=1,JJ
ISN 0302          X1(J)=1.0
ISN 0303          X2(J)=1.0
ISN 0304      390 CONTINUE
            C
ISN 0305          RETURN
            C
            C****     ****     ****     ****     ****     ****     CHAPTER 4     ****     ***
            C****     ****     ****     ****     ****     ****     CHAPTER 4     ****     ***
            C
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              C   ***REACTANTS***
              C   READ REACTANTS DATA CARDS FOR EACH INLET STREAM
              C
ISN 0306        400 NSTRM=NSTRM+1
ISN 0307            LMOLES=.FALSE.
              C-----SCRUB SPECIES MOLE NUMBER ARRAY
ISN 0308            DO 405 I=1,NS
ISN 0309        405 S2(I)=0.0
ISN 0310            SUM1=0.0
              C
ISN 0311        410 READ(5,411) (AT(I),B(I),I=1,4),(DATA(I),I=1,2),PECWT,MOLE,PHAZ
ISN 0312        411 FORMAT(4(A2,F7.5),2A4,1X,F7.5,A1,9X,A1)
ISN 0313            IF (AT(1).EQ.BLNK) GO TO 450
ISN 0315            WRITE(6,412) (AT(I),B(I),I=1,4),(DATA(I),I=1,2),PECWT,MOLE,
                   1PHAZ,NSTRM
ISN 0316        412 FORMAT(1X,4(2X,A2,F9.5),2X,2A4,2X,F9.5,2X,A1,2X,A1,2X,I5)
ISN 0317            IF (MOLE.EQ.MOL) LMOLES=.TRUE.
              C
              C-----ESTABLISH MOLE NUMBERS (KG-MOL I/KGM MIXTURE) IN INLET STREAM
              C
ISN 0319            TRINV=1.0/TR
ISN 0320            DO 430 I=1,NS
              C-----SCREEN FOR SPECIES NAME
ISN 0321            IF (DATA(1).NE.ASUB(I,1)) GO TO 430
ISN 0323            IF (DATA(2).NE.ASUB(I,2)) GO TO 430
ISN 0325            DO 420 L=1,NLM
              C-----SCREEN FOR ATOMIC COMPOSITION
ISN 0326            DO 420 K=1,4
ISN 0327            IF (ATOM(L)   .NE.AT(K)) GO TO 420
ISN 0329            IF (AL(L,I).NE.B(K)) GO TO 430
ISN 0331        420 CONTINUE
              C-----IF PECWT IS RELATIVE MASS, CONVERT TO RELATIVE MOLE NUMBERS
ISN 0332            AMOLE=PECWT/SMW(I)
ISN 0333            IF (LMOLES) AMOLE=PECWT
ISN 0335            S2(I)=S2(I)+AMOLE
ISN 0336            SUM1=SUM1+AMOLE*SMW(I)
ISN 0337            GO TO 410
ISN 0338        430 CONTINUE
              C
ISN 0339            WRITE(6,440)
ISN 0340        440 FORMAT(1H0,10X,45H REACTANT ABOVE NOT FOUND IN THERMO LIBRARY  /)
ISN 0341            GO TO 410
              C
ISN 0342        450 CONTINUE
              C
              C-----ESTABLISH MIXTURE ENTHALPY
              C
ISN 0343            IHCPS=1
ISN 0344            CALL HCPS
              C
ISN 0345            WRITE(6,460) NSTRM
ISN 0346        460 FORMAT(1H0,19H*** REACTANT STREAM,I3,4H ***/
                   A1H0,5X,1HI,4X,7HSPECIES,14X,16HMOLECULAR WEIGHT,5X,
                   B12HMOLE NUMBERS,8X,14HMASS FRACTIONS/32X,17H(KGMOLE I)/(KG I),
                   C4X,17H(KGMOLE I)/(KG X),5X,13H(KG I)/(KG X)/)
```

```
ISN 0347          HSUM=0.0                                                 GEN04202
ISN 0348          SM=0.0                                                   GEN04204
ISN 0349          DO 480 I=1,NS                                            GEN04206
ISN 0350          S2(I)=S2(I)/SUM1                                         GEN04208
            C-----S2(I) IN MOLE NUMBERS, KG-MOLES I/KG MIXTURE             GEN04210
ISN 0351          HSUM=HSUM+H0(I)*S2(I)                                    GEN04212
ISN 0352          SM=SM+S2(I)                                              GEN04214
ISN 0353          DTHLD=S2(I)*SMW(I)                                       GEN04216
ISN 0354          WRITE(6,470) I,(ASUB(I,J),J=1,3),SMW(I),S2(I),DTHLD      GEN04218
ISN 0355      470 FORMAT(5X,I2,1H.,4X,3A4,2P3D20.3)                        GEN04220
ISN 0356      480 CONTINUE                                                 GEN04222
            C-----HSUB0 IN JOULES/KG REACTANT MIXTURE                      GEN04224
ISN 0357          HSUB0=HSUM*RGAS*TK                                       GEN04226
            C-----RHOP IS MASS DENSITY, KG/CU M                            GEN04228
ISN 0358          RHOP=PA/(RGAS*TK*SM)                                     GEN04230
            C                                                              GEN04232
ISN 0359          SMINV=1.0/SM                                             GEN04234
ISN 0360          WRITE(6,490) TK,HSUB0,PA,RHOP,SMINV                      GEN04236
ISN 0361      490 FORMAT(1H0//12X,13HTEMPERATURE =,2PD12.3,3X,5HDEG K/     GEN04238
                 A12X,10HENTHALPY =,3X,2PD12.3,3X,9HJOULES/KG/             GEN04240
                 B12X,10HPRESSURE =,3X,2PD12.3,3X,6HN/M**2/                GEN04242
                 C12X,9HDENSITY =,4X,2PD12.3,3X,7HKG/M**3/                 GEN04244
                 D12X,13HMEAN MOL WT =,2PD12.3,3X,9HKG/KGMOLE//)           GEN04246
            C                                                              GEN04248
            C-----ON RETURN, CALLING PROGRAM MUST STORE MOLE NUMBERS S2(I),  GEN04250
            C-----PRESSURE, TEMPERATURE, ENTHALPY AND DENSITY AT APPROPRIATE INLET GEN04252
            C-----INLET GRID NODE                                          GEN04254
            C                                                              GEN04256
ISN 0362          RETURN                                                   GEN04258
ISN 0363          END                                                      GEN04260
```

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*OPTIONS IN EFFECT*NAME(MAIN) NOOPTIMIZE LINECOUNT(57) SIZE(MAX) AUTODBL(NONE)

*OPTIONS IN EFFECT*SOURCE EBCDIC NOLIST NODECK OBJECT NOMAP NOFORMAT NOGOSTMT NOXREF NOALC NOANSF TERM FLA

*STATISTICS*     SOURCE STATEMENTS =     362, PROGRAM SIZE =     10620, SUBPROGRAM NAME = CREKO

*STATISTICS*  NO  DIAGNOSTICS GENERATED

****** END OF COMPILATION ******                              308K BYTES OF CORE NOT USED
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REQUESTED OPTIONS:

OPTIONS IN EFFECT: NAME(MAIN) NOOPTIMIZE LINECOUNT(57) SIZE(MAX) AUTODBL(NONE)
SOURCE EBCDIC NOLIST NODECK OBJECT NOMAP NOFORMAT NOGOSTMT NOXREF NOALC NOANSF TERM FLA

```
ISN 0002          SUBROUTINE SPECE
ISN 0003          IMPLICIT REAL*8 (A-H,O-Z)
            C
ISN 0004          DIMENSION ASUB(20,3)
ISN 0005          LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LNRG,LREACT
            C
ISN 0006          COMMON
                 1/CCHEM1/CPSUM,FQ,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LCONVG,LNRG
                 1/CEQUIL/AL(7,20),ATOM(3,7),BO(7),PI(7)
                 1/CINDEX/IDCO,IDCO2,IDH2,IDH2O,IDN2,IDO2,IHCPS,ILC,ILH,IMAT,ITER,
                 2         JJ,N1,N2,N3,NA,NGLOB,NGLOBP,NLM,NQ,NSM
                 1/CMATRX/HSUM,X(22),Y(22)
                 1/CPARAM/ASUB,NT,NE,EMV,EK,HSUBO,NDEBUG,NS,PA,Q0,Q1,Q2,Q3,Q4,RHOP,
                 2         SM,S1(20),S2(20),TK,LADIAB,LDEBUG,LEQUIL,LREACT
                 1/CSPECE/HO(20),SO(20),SMW(20),SSAVE(20),Z(7,2,20)
            C
            C*********************************************************************
            C     THIS SUBROUTINE CALLS CALC TO COMPUTE THE CORRECTIONS TO THE
            C     CHEMICAL SPECIES AND TEMP AND DETERMINES THE UNDERRELAXATION
            C     PARAMETER PRIOR TO THE APPLICATION OF THESE CORRECTIONS TO THE
            C     ESTIMATES FOR BOTH EQUILIBRIUM AND KINETIC STATIONARY STATES
            C     FOR EACH ITERATION.  SPECE ALSO CONTROLS THE CONVERGENCE TESTS
            C     REFERENCE CREK     (WASHINGTON STATE UNIVERSITY)   MARCH 1976
            C*********************************************************************
            C
ISN 0007          DATA ITMAX/70/,TINY/1.0D-20/,TNY/-46.0517/
            C
ISN 0008          LCONVG=.FALSE.
ISN 0009          SM=0.0
ISN 0010          DO 20 I=1,NS
ISN 0011          IF (S2(I).GT.TINY) GO TO 10
ISN 0013          S2(I)=TINY
ISN 0014          Y(I)=TNY
ISN 0015          GO TO 20
ISN 0016       10 SM=SM+S2(I)
ISN 0017          Y(I)=DLOG(S2(I))
ISN 0018       20 CONTINUE
ISN 0019          TKINV=1.0/TK
ISN 0020          TLN=DLOG(TK)
ISN 0021          Y(NSM)=DLOG(SM)
ISN 0022          SMINV=1.0/SM
ISN 0023          Y(NQ)=TLN
            C
            C* * * * * * * * * * * * * * * * * * * * * * * CHAPTER 1 * * * * * * *
            C* * * * * * * * * * * * * * * * * * * * * * * CHAPTER 1 * * * * * * *
            C
            C  ***SOLVE FOR CORRECTIONS***
            C  INITIATE THE ITER LOOP AND CALL CALC TO SET UP AND CALCULATE THE
            C  CORRECTIONS FOR EITHER EQUILIBRIUM OR KINETIC SOLUTION
            C
```

```
ISN 0024          ETA=1.0                                                                        GEN04362
ISN 0025          ETAO=ETA                                                                       GEN04364
ISN 0026          NDEC=0                                                                         GEN04366
ISN 0027          NRLX=0                                                                         GEN04368
ISN 0028          DO 550 ITER=1,ITMAX                                                            GEN04370
            C                                                                                    GEN04372
ISN 0029          CALL CALC                                                                      GEN04374
            C                                                                                    GEN04376
ISN 0030          IF (IMAT.EQ.NQ) GO TO 300                                                      GEN04378
            C                                                                                    GEN04380
            C                                                                                    GEN04382
            C**  **   **   **   **   **   **   **   **   **   **   **   CHAPTER 2   **   **   **   GEN04384
            C**  **   **   **   **   **   **   **   **   **   **   **   CHAPTER 2   **   **   **   GEN04386
            C                                                                                    GEN04388
            C  ***CONSTRUCT CORRECTIONS FOR EQUILIBRIUM SPECIES***                               GEN04390
            C  CHECK FOR SINGULAR MATRIX (LCONVG SET TO TRUE AT END OF CALC)                     GEN04392
ISN 0032          IF (.NOT.LCONVG) GO TO 200                                                     GEN04394
ISN 0034          LCONVG=.FALSE.                                                                 GEN04396
ISN 0035          RETURN                                                                         GEN04398
            C                                                                                    GEN04400
ISN 0036      200 DO 210 L=1,NLM                                                                 GEN04402
ISN 0037      210 PI(L)=X(L)                                                                     GEN04404
ISN 0038          X(NSM)=X(N1)                                                                   GEN04406
ISN 0039          X(NQ)=X(N2)                                                                    GEN04408
ISN 0040          DO 230 I=1,NS                                                                  GEN04410
ISN 0041          X(I)=HO(I)*X(NQ)-(HO(I)-SO(I)+Y(I)+PPLN-Y(NSM))+X(NSM)                         GEN04412
ISN 0042          DO 220 L=1,NLM                                                                 GEN04414
ISN 0043          X(I)=X(I)+AL(L,I)*PI(L)                                                        GEN04416
ISN 0044      220 CONTINUE                                                                       GEN04418
ISN 0045      230 CONTINUE                                                                       GEN04420
            C                                                                                    GEN04422
            C***   ***   ***   ***   ***   ***   ***   ***   CHAPTER 3   ***   ***               GEN04424
            C***   ***   ***   ***   ***   ***   ***   ***   CHAPTER 3   ***   ***               GEN04426
            C                                                                                    GEN04428
            C  ***CALCULATE UNDERRELAXATION PARAMETER ETA***                                     GEN04430
            C  UNDERRELAXATION TESTS ARE DIFFERENT FOR MAJOR AND MINOR SPECIES WITH              GEN04432
            C  ETA = MIN(ETA1,ETA2,1)  WHERE                                                     GEN04434
            C  MAJOR SPECIES ---- S2(I)/SM > 1.0D-6                                              GEN04436
            C  MINOR SPECIES ---- S2(I)/SM   1.0D-6                                              GEN04438
            C  AND ONLY POSITIVE CORRECTION CHANGES FOR MOLE NUMBERS ARE MONITORED               GEN04440
            C  ETA1 = MAJOR SPECIES CONTROL                                                      GEN04442
            C  ETA2 = MINOR SPECIES CONTROL                                                      GEN04444
            C                                                                                    GEN04446
ISN 0046      300 ETAO=ETA                                                                       GEN04448
ISN 0047          ETA=1.0                                                                        GEN04450
ISN 0048          ETA1=1.0                                                                       GEN04452
ISN 0049          SUM=DABS(X(NSM))                                                               GEN04454
ISN 0050          TM1=DABS(X(NQ))                                                                GEN04456
ISN 0051          IF (TM1.GT.SUM) SUM=TM1                                                        GEN04458
ISN 0053          DO 320 I=1,NS                                                                  GEN04460
ISN 0054          IF (X(I).LE.0.0) GO TO 320                                                     GEN04462
ISN 0056          IF (S2(I)*SMINV.LE.1.0D-6) GO TO 310                                           GEN04464
            C-----MAJOR SPECIES                                                                  GEN04466
ISN 0058          IF (X(I).GT.SUM) SUM=X(I)                                                      GEN04468
ISN 0060          GO TO 320                                                                      GEN04470
```

```
              C-----MINOR SPECIES
ISN 0061        310 TST1=DABS((Y(NSM)-Y(I)-9.2103404)/(X(I)-X(NSM)))
ISN 0062            IF (TST1.LT.ETA1) ETA1=TST1
ISN 0064        320 CONTINUE
ISN 0065            IF (SUM.GT.2.0) ETA=2.0/SUM
ISN 0067            IF (ETA1.LT.ETA) ETA=ETA1
              C
              C   ***CONVERGENCE MONITORING***
              C   AFTER TEN SUCCESSIVE UNDERRELAXED ITERATIONS, IN WHICH ETA DOES NOT
              C   INCREASE BY TWICE OR MORE, OR AFTER SIX ITERATIONS IN WHICH ETA
              C   DECREASES, DIVERGENCE IS ASSUMED AND THE SOLUTION TERMINATED
              C
              C   LNRG=.TRUE. ----> FULL EQUATIONS
ISN 0069            IF (ETA.EQ.1.0) NRLX=-1
ISN 0071            IF ((ETA/ETAO).GE.2.0) NRLX=-1
ISN 0073            NRLX=NRLX+1
ISN 0074            IF (NRLX.GT.10) GO TO 900
ISN 0076            IF (ETA.LT.ETAO) NDEC=NDEC+1
ISN 0078            IF (.NOT.LNRG) NDEC=1
ISN 0080            IF (NDEC.GT.6) GO TO 900
              C
              C****     ****     ****     ****     ****     ****     CHAPTER 4     ****     ***
              C****     ****     ****     ****     ****     ****     CHAPTER 4     ****     ***
              C
              C   APPLY CORRECTIONS TO ESTIMATES
              C
              C
ISN 0082            DO 420 I=1,NS
ISN 0083            Y(I)=Y(I)+ETA*X(I)
ISN 0084            IF (Y(I).LT.TNY) GO TO 410
ISN 0086            S2(I)=DEXP(Y(I))
ISN 0087            GO TO 420
              C
ISN 0088        410 Y(I)=TNY
ISN 0089            S2(I)=TINY
              C-----INSURE CONVERGENCE TEST PASSED WHENEVER Y(I)=TNY
ISN 0090            X(I)=0.0
ISN 0091        420 CONTINUE
ISN 0092            Y(NSM)=Y(NSM)+ETA*X(NSM)
ISN 0093            SM=DEXP(Y(NSM))
ISN 0094            SMINV=1.0/SM
ISN 0095            Y(NQ)=Y(NQ)+ETA*X(NQ)
ISN 0096            TLN=Y(NQ)
ISN 0097            TK=DEXP(TLN)
ISN 0098            TKINV=1.0/TK
              C
ISN 0099            IF (.NOT.LDEBUG) GO TO 500
ISN 0101            IF (NDEBUG.GE.3) WRITE(6,430) ITER,ETA,LREACT,LEQUIL,LADIAB,
                   1                              LNRG,HSUBO,SM,EMV,TK
ISN 0103            IF (NDEBUG.GE.4) WRITE(6,440) (I,ASUB(1,I),S1(I),S2(I),Y(I),
                   1                              X(I),H0(I),S0(I),I=1,NS)
ISN 0105        430 FORMAT(2X,I3,2PD12.3,4L8,2P4D12.3)
ISN 0106        440 FORMAT(20X,7HSPECIES,4X,5HS1(I),7X,5HS2(I),7X,4HY(I),8X,
                   A4HX(I),8X,5HH0(I),7X,5HS0(I)/(16X,I2,3X,A4,2X,2P6D12.3))
              C
```

```
                C*****      *****      *****      *****      *****   CHAPTER 5    *****
                C*****      *****      *****      *****      *****   CHAPTER 5    *****
                C
                C   CONVERGENCE CHECK...ALL MOLE NUMBER CORRECTIONS MUST BE .LT. 1.0 PCT
                C
  ISN 0107        500 IF (ETA.LT.1.0) GO TO 550
  ISN 0109            DO 510 I=1,NS
  ISN 0110            IF (DABS(X(I)).GT.0.10) GO TO 550
  ISN 0112        510 CONTINUE
  ISN 0113            LCONVG=.TRUE.
  ISN 0114            HSUBO=HSUM*RGAS*TK
  ISN 0115            RETURN
                C
  ISN 0116        550 CONTINUE
                C
                C
  ISN 0117            RETURN
                C
                C******     ******     ******     ******      CHAPTER 6    ******
                C******     ******     ******     ******      CHAPTER 6    ******
                C
  ISN 0118            ENTRY ERATIO
                C
                C   CALCULATES FUEL/AIR EQUIV RATIO, GIVEN MOLE NUMBERS IN SI ARRAY,
                C   USING POSITIVE AND NEGATIVE OXIDATION STATES (VALENCES)
                C
  ISN 0119            VP=0.0
  ISN 0120            VM=0.0
  ISN 0121            DO 610 I=1,NS
  ISN 0122            IF (SI(I).LE.TINY) GO TO 610
  ISN 0124            DO 600 L=1,NLM
  ISN 0125            IF (AL(L,I).EQ.0.) GO TO 600
  ISN 0127            IF (ATOM(3,L).GT.0.0) VP=VP+AL(L,I)*ATOM(3,L)*SI(I)
  ISN 0129            IF (ATOM(3,L).LT.0.0) VM=VM+AL(L,I)*ATOM(3,L)*SI(I)
  ISN 0131        600 CONTINUE
  ISN 0132        610 CONTINUE
                C
  ISN 0133            VM=-VM
  ISN 0134            IF (VM.LT.TINY) GO TO 620
  ISN 0136            IF (VP.LT.TINY) GO TO 630
  ISN 0138            ER=VP/VM
  ISN 0139            RETURN
                C
  ISN 0140        620 ER=1000000.0
  ISN 0141            RETURN
                C
  ISN 0142        630 ER=0.0
                C
  ISN 0143        900 RETURN
  ISN 0144            END
```

*OPTIONS IN EFFECT*NAME(MAIN) NOOPTIMIZE LINECOUNT(57) SIZE(MAX) AUTODBL(NONE)

*OPTIONS IN EFFECT*SOURCE EBCDIC NOLIST NODECK OBJECT NOMAP NOFORMAT NOGOSTMT NOXREF NOALC NOANSF TERM FL

STATISTICS SOURCE STATEMENTS = 143, PROGRAM SIZE = 4020, SUBPROGRAM NAME = SPECE

REQUESTED OPTIONS:

OPTIONS IN EFFECT: NAME(MAIN) NOOPTIMIZE LINECOUNT(57) SIZE(MAX) AUTODBL(NONE)
SOURCE EBCDIC NOLIST NODECK OBJECT NOMAP NOFORMAT NOGOSTMT NOXREF NOALC NOANSF TERM FL

```
ISN 0002            SUBROUTINE CALC
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
              C
ISN 0004            LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LREACT,LNRG
ISN 0005            DIMENSION ASUB(20,3)
              C
              C     THE FOLLOWING DOUBLE PRECISION REQUIRED ONLY FOR IBM MACHINES
              C     DOUBLE PRECISION A,DIMI
              C
ISN 0006            COMMON
                   1/CCHEM1/EPSUM,FO,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LCONVG,LNRG
                   1/CEQUIL/AL(7,20),ATOM(3,7),EO(7),PI(7)
                   1/CINDEX/IOCO,IOCO2,IOH2,IOH2O,ION2,IOO2,IHCPS,ILC,ILH,IMAT,ITER,
                   2     JJ,N1,N2,N3,NA,NGLOB,NGLOBP,NLM,NQ,NZM
                   1/CMATRI/HSUM,X(22),Y(22)
                   1/CPARAM/FSUB,NT,NE,EMV,ER,HSUBO,NDEBUG,NS,PA,QC,Q1,Q2,Q3,Q4,RHOP,
                   2         SM,S1(20),S2(20),TK,LADIAB,LDEBUG,LEQUIL,LREACT
                   1/CREACT/BX(30),BX2(30),ID(4,30),MODR(30),TACT(30),TACT2(30),
                   2         TEN(30),TEN2(30),X1(30),X2(30)
ISN 0007            COMMON  /CSPECE/
                   1        HO(20),SO(20),SMW(20),SSAVE(20),Z(7,2,20)
              C
              C*************************************************************************
              C  THIS SUBROUTINE CONSTRUCTS THE NEWTON-RAPHSON DERIVATIVE MATRIX FOR
              C  BOTH KINETIC AND EQUILIBRIUM SOLUTIONS AND SOLVES IT BY PIVOTAL
              C  GAUSSIAN REDUCTION.  WHENEVER TEMP IS LESS THAN 1500K, THE REVERSE
              C  RATE IS CALCULATED FROM THE FORWARD RATE AND EQUILIBRIUM CONSTANT.
              C  PROVISION IS MADE FOR GLOBAL REACTIONS
              C  REFERENCE  CREK    (WASHINGTON STATE UNIVERSITY)  MARCH 1976
              C*************************************************************************
              C
ISN 0008            DIMENSION A(22,23)
              C
ISN 0009            DATA BIG/46.051/
              C
ISN 0010            DO 10 I=1,NQ
ISN 0011            DO 10 K=1,NA
ISN 0012         10 A(I,K)=0.0
              C
ISN 0013            IHCPS=1
ISN 0014            IF (LEQUIL) IHCPS=2
ISN 0016            IF (TK.LT.1500.0) IHCPS=2
ISN 0018            CALL HCPS
ISN 0019            HIN=HSUBO*RGASIN*TKINV
ISN 0020            Q=0.
ISN 0021            QCRV=0.
ISN 0022            IF (LADIAB) GO TO 20
              C-----Q AND QCRV ARE NON-DIMENSIONAL
ISN 0024            TM1=FO/(EMV*RGAS)
ISN 0025            Q=(((Q4*TK+Q3)*TK+Q2)*TK+Q1+Q0*TKINV)*TM1
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ISN 0026          QDRV=(((4.*Q4*TK+3.*Q3)*TK+2.*Q2)*TK+Q1)*TM1                    GEN04782
ISN 0027       20 CONTINUE                                                        GEN04784
              C                                                                   GEN04786
ISN 0028          IF (LEQUIL) GO TO 300                                           GEN04788
              C                                                                   GEN04790
ISN 0030          RHSM=PA*RGASIN*TKINV                                            GEN04792
ISN 0031          RHOP=RHSM*SMINV                                                 GEN04794
ISN 0032          RHSQ=RHOP**2                                                    GEN04796
              C                                                                   GEN04798
              C* * * * * * * * * * * * * * * * * * * * * * * CHAPTER 1 * * * * * * *GEN04800
              C* * * * * * * * * * * * * * * * * * * * * * * CHAPTER 1 * * * * * * *GEN04802
              C                                                                   GEN04804
              C    ***GLOBAL REACTION***                                          GEN04806
              C    GLOBAL RATE EQUATIONS FOR HYDROCARBON PYROLYSIS...             GEN04808
              C    GLOBAL RATE EXPRESSION DUE TO EDELMAN OF GASL                  GEN04810
              C       CXHY + (X/2) O2 -----> X CO + (Y/2) H2                      GEN04812
              C                                                                   GEN04814
ISN 0033          IF (NGLOB.EQ.0) GO TO 110                                       GEN04816
ISN 0035          IF (TK.LT.500.) GO TO 110                                       GEN04818
ISN 0037          DO 100 J=1,NGLOB                                                GEN04820
ISN 0038          I=ID(1,J)                                                       GEN04822
ISN 0039          K=IDO2                                                          GEN04824
ISN 0040          M=IDCO                                                          GEN04826
ISN 0041          N=IDH2                                                          GEN04828
ISN 0042          XC=AL(ILC,I)                                                    GEN04830
ISN 0043          YH=AL(ILH,I)                                                    GEN04832
ISN 0044          TK1=TACT(J)*TKINV                                               GEN04834
ISN 0045          TM2=TK1-BX(J)+(0.815*PPLN)                                      GEN04836
ISN 0046          IF (DABS(TM2).GT.BIG) GO TO 100                                 GEN04838
ISN 0048          R1=DEXP(-TM2)                                                   GEN04840
              C                                                                   GEN04842
              C-----PROVISION FOR CONTACT INDEX                                   GEN04844
ISN 0049          R1=X1(J)*R1                                                     GEN04846
ISN 0050          R1=(0.0009*TK-0.5)*R1*(RHOP*S2(K))*DSQRT(RHOP*S2(I))            GEN04848
ISN 0051          TM1=R1*0.5                                                      GEN04850
ISN 0052          A(I,I)=A(I,I)+TM1                                               GEN04852
ISN 0053          A(I,K)=A(I,K)+R1                                                GEN04854
ISN 0054          A(K,I)=A(K,I)+R1*XC*0.25                                        GEN04856
ISN 0055          A(K,K)=A(K,K)+TM1*XC                                            GEN04858
ISN 0056          A(M,I)=A(M,I)-TM1*XC                                            GEN04860
ISN 0057          A(M,K)=A(M,K)-R1*XC                                             GEN04862
ISN 0058          A(N,I)=A(N,I)-R1*YH*0.25                                        GEN04864
ISN 0059          A(N,K)=A(N,K)-TM1*YH                                            GEN04866
              C-----A(ANY,M)=A(ANY,N)=0 BECAUSE NO REVERSE REACTION ASSUMED       GEN04868
ISN 0060          RN=R1*1.5                                                       GEN04870
ISN 0061          A(I,NSM)=A(I,NSM)-RN                                            GEN04872
ISN 0062          A(K,NSM)=A(K,NSM)-RN*XC*0.5                                     GEN04874
ISN 0063          A(M,NSM)=A(M,NSM)+RN*XC                                         GEN04876
ISN 0064          A(N,NSM)=A(N,NSM)+RN*YH*0.5                                     GEN04878
ISN 0065          A(I,NA)=A(I,NA)-R1                                              GEN04880
ISN 0066          A(K,NA)=A(K,NA)-R1*XC*0.5                                       GEN04882
ISN 0067          A(M,NA)=A(M,NA)+R1*XC                                           GEN04884
ISN 0068          A(N,NA)=A(N,NA)+R1*YH*0.5                                       GEN04886
ISN 0069          IF (.NOT.ENRG) GO TO 100                                        GEN04888
ISN 0071          R1=R1*(TK1+1.0/(1.0-555.5*TKINV)-1.5)                           GEN04890
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ISN 0072           A(I,NQ)=A(I,NQ)+RT                                              GEN04892
ISN 0073           A(K,NQ)=A(K,NQ)+RT*XC*0.5                                       GEN04894
ISN 0074           A(M,NQ)=A(M,NQ)-RT*XC                                           GEN04896
ISN 0075           A(N,NQ)=A(N,NQ)-RT*YH*0.5                                       GEN04898
ISN 0076       100 CONTINUE                                                        GEN04900
ISN 0077       110 CONTINUE                                                        GEN04902
             C                                                                     GEN04904
ISN 0078           DO 270 J=NGLOBP,JJ                                              GEN04906
             C                                                                     GEN04908
             C**  **  **  **  **  **  **  **  **  **  **  **  CHAPTER 2  **  **  ** GEN04910
             C**  **  **  **  **  **  **  **  **  **  **  **  CHAPTER 2  **  **  ** GEN04912
             C                                                                     GEN04914
             C                                                                     GEN04916
             C  ***REACTION RATES***                                               GEN04918
             C  CALCULATE FORWARD AND REVERSE RATES R1 AND R2                      GEN04920
             C  THREE TYPES OF REACTIONS                                           GEN04922
             C                                                                     GEN04924
             C     MODE 1 ... A + B ---> C + D                                     GEN04926
             C     MODE 2 ... AB + M ---> A + B + M                                GEN04928
             C     MODE 3 ... A + B + M ---> AB + M                                GEN04930
             C                                                                     GEN04932
ISN 0079           I=ID(1,J)                                                       GEN04934
ISN 0080           K=ID(2,J)                                                       GEN04936
ISN 0081           M=ID(3,J)                                                       GEN04938
ISN 0082           N=ID(4,J)                                                       GEN04940
ISN 0083           MODE=MODR(J)                                                    GEN04942
             C                                                                     GEN04944
ISN 0084           R1=0.0                                                          GEN04946
ISN 0085           R2=0.0                                                          GEN04948
ISN 0086           TM1=0.0                                                         GEN04950
ISN 0087           TM2=0.0                                                         GEN04952
ISN 0088           RN=0.0                                                          GEN04954
ISN 0089           RT=0.0                                                          GEN04956
             C                                                                     GEN04958
ISN 0090           TK1=TACT(J)*TKINV                                               GEN04960
ISN 0091           TM2=TK1-BX(J)                                                   GEN04962
ISN 0092           IF (TEN(J).NE.0.) TM2=TM2-TEN(J)*TLN                            GEN04964
ISN 0094           IF (DABS(TM2).GT.BIG) GO TO 205                                 GEN04966
ISN 0096           R1=DEXP(-TM2)                                                   GEN04968
             C-----PROVISION FOR CONTACT INDEX                                     GEN04970
ISN 0097           R1=R1*X1(J)                                                     GEN04972
ISN 0098           IF (MODE-2) 200,201,202                                         GEN04974
ISN 0099       200 R1=R1*S2(I)*RHSQ*S2(K)                                          GEN04976
ISN 0100           RN=R1*2.0                                                       GEN04978
ISN 0101           IF (LNRG)  RT=R1*(TEN(J)+TK1-2.0)                               GEN04980
ISN 0103           GO TO 205                                                       GEN04982
             C                                                                     GEN04984
ISN 0104       201 R1=R1*RHSM*RHOP*S2(I)                                           GEN04986
ISN 0105           RN=R1                                                           GEN04988
ISN 0106           IF (LNRG) RT=R1*(TEN(J)+TK1-2.0)                                GEN04990
ISN 0108           GO TO 205                                                       GEN04992
             C                                                                     GEN04994
ISN 0109       202 R1=R1*RHSM*S2(I)*RHSQ*S2(K)                                     GEN04996
ISN 0110           RN=R1*2.0                                                       GEN04998
ISN 0111           IF (LNRG) RT=R1*(TEN(J)+TK1-3.0)                                GEN05000
```

```
                C
ISN 0113          205 TM1=R1
                C
                C
                C-----CALCULATE REVERSE RATE CONST FROM FWD RATE CONST AND EQUIL CONST
                C-----WHENEVER TEMP IS LESS THAN 1500 K
                C
ISN 0114              IF (TK.GT.1500.0) GO TO 220
                C
ISN 0116              HH=H0(I)-H0(M)
ISN 0117              SS=S0(I)-S0(M)
ISN 0118              IF (MODE-2) 210,211,212
                C
ISN 0119          210 HH=HH+H0(K)-H0(N)
ISN 0120              SS=SS+S0(K)-S0(N)
ISN 0121              BXX=BX(J)+SS
ISN 0122              TK2=TK1+HH
ISN 0123              TN2=TEN(J)
ISN 0124              GO TO 230
                C
ISN 0125          211 HH=HH-H0(N)
ISN 0126              SS=SS-S0(N)
                C     -2.500304 IS E-LOG OF GAS CONST 0.08206 M**3-ATM/KGMOL-DEG K.
ISN 0127              BXX=BX(J)+SS-2.500304
ISN 0128              TK2=TK1+HH
ISN 0129              TN2=TEN(J)+1.0
ISN 0130              GO TO 230
                C
ISN 0131          212 HH=HH+H0(K)
ISN 0132              SS=SS+S0(K)
ISN 0133              BXX=BX(J)+SS+2.500304
ISN 0134              TK2=TK1+HH
ISN 0135              TN2=TEN(J)-1.0
ISN 0136              GO TO 230
                C
ISN 0137          220 BXX=BX2(J)
ISN 0138              TK2=TAC2(J)*TKINV
ISN 0139              TN2=TEN2(J)
                C
ISN 0140          230 TM2=TK2-BXX
ISN 0141              IF (TN2.NE.0.) TM2=TM2-TN2*TLN
ISN 0143              IF (DABS(TM2).GT.BIG) GO TO 250
ISN 0145              R2=DEXP(-TM2)
                C-----MULTIPLY HOMOGENEOUS RATE CONSTANT BY CONTACT INDEX
ISN 0146              R2=R2*X2(J)
                C
ISN 0147              IF (MODE-2) 240,241,242
                C
ISN 0148          240 R2=R2*S2(M)*RHSQ*S2(N)
ISN 0149              RN=RN-R2*2.0
ISN 0150              IF (LNRG) RT=RT-R2*(TN2+TK2-2.0)
ISN 0152              GO TO 250
                C
ISN 0153          241 R2=R2*RHSM*S2(M)*RHSQ*S2(N)
ISN 0154              RN=RN-R2*2.0
```

```
ISN 0155           IF (LNRG) RT=RT-R2*(TN2+TK2-3.0)                               GEN05112
ISN 0157           GO TO 250                                                      GEN05114
             C                                                                    GEN05116
ISN 0158       242 R2=R2*RHSM*RHOP*S2(M)                                          GEN05118
ISN 0159           RN=RN-R2                                                       GEN05120
ISN 0160           IF (LNRG) RT=RT-R2*(TN2+TK2-2.0)                               GEN05122
             C                                                                    GEN05124
ISN 0162       250 TM1=TM1-R2                                                     GEN05126
             C                                                                    GEN05128
             C                                                                    GEN05130
             C    ***KINETIC***                                                   GEN05132
             C    DERIVATIVE AND FUNCTION MATRIX FOR KINETIC SOLUTION             GEN05134
             C                                                                    GEN05136
ISN 0163           A(I,I)=A(I,I)+R1                                               GEN05138
ISN 0164           A(M,I)=A(M,I)-R1                                               GEN05140
ISN 0165           A(I,M)=A(I,M)-R2                                               GEN05142
ISN 0166           A(M,M)=A(M,M)+R2                                               GEN05144
ISN 0167           A(I,NSM)=A(I,NSM)-RN                                           GEN05146
ISN 0168           A(M,NSM)=A(M,NSM)+RN                                           GEN05148
ISN 0169           A(I,NQ)=A(I,NQ)+RT                                             GEN05150
ISN 0170           A(M,NQ)=A(M,NQ)-RT                                             GEN05152
ISN 0171           A(I,NA)=A(I,NA)-TM1                                            GEN05154
ISN 0172           A(M,NA)=A(M,NA)+TM1                                            GEN05156
ISN 0173           IF (MODE.EQ.3) GO TO 260                                       GEN05158
             C                                                                    GEN05160
ISN 0175           A(N,I)=A(N,I)-R1                                               GEN05162
ISN 0176           A(N,M)=A(N,M)+R2                                               GEN05164
ISN 0177           A(I,N)=A(I,N)-R2                                               GEN05166
ISN 0178           A(M,N)=A(M,N)+R2                                               GEN05168
ISN 0179           A(N,N)=A(N,N)+R2                                               GEN05170
ISN 0180           A(N,NSM)=A(N,NSM)+RN                                           GEN05172
ISN 0181           A(N,NQ)=A(N,NQ) - RT                                           GEN05174
ISN 0182           A(N,NA)=A(N,NA)+TM1                                            GEN05176
ISN 0183           IF (MODE.EQ.2) GO TO 270                                       GEN05178
             C                                                                    GEN05180
ISN 0185       260 CONTINUE                                                       GEN05182
ISN 0186           A(K,I)=A(K,I)+R1                                               GEN05184
ISN 0187           A(I,K)=A(I,K)+R1                                               GEN05186
ISN 0188           A(K,K)=A(K,K)+R1                                               GEN05188
ISN 0189           A(M,K)=A(M,K)-R1                                               GEN05190
ISN 0190           A(K,M)=A(K,M)-R2                                               GEN05192
ISN 0191           A(K,NSM)=A(K,NSM)-RN                                           GEN05194
ISN 0192           A(K,NQ)=A(K,NQ)+RT                                             GEN05196
ISN 0193           A(K,NA)=A(K,NA)-TM1                                            GEN05198
ISN 0194           IF (MODE.EQ.3) GO TO 270                                       GEN05200
             C                                                                    GEN05202
ISN 0196           A(N,K)=A(N,K)-R1                                               GEN05204
ISN 0197           A(K,N)=A(K,N)-R2                                               GEN05206
             C                                                                    GEN05208
ISN 0198       270 CONTINUE                                                       GEN05210
             C                                                                    GEN05212
ISN 0199           HSUM=0.0                                                       GEN05214
ISN 0200           DO 280 I=1,NS                                                  GEN05216
ISN 0201           S2I=S2(I)                                                      GEN05218
ISN 0202           A(I,I)=A(I,I)+EMV*S2I                                          GEN05220
```

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ISN 0203          A(I,NA)=A(I,NA)+EMV*(S1(I)-S21)
ISN 0204          A(NSM,I)=S21
ISN 0205          A(NSM,NA)=A(NSM,NA)-S21
ISN 0206          A(NQ,I)=H0(I)*S21
ISN 0207          HSUM=HSUM+A(NQ,I)
ISN 0208      280 CONTINUE
            C
ISN 0209          A(NSM,NSM)=-SM
            C-----A(NSM,NQ) AND A(NQ,NSM) ARE EQUAL TO ZERO.
ISN 0210          A(NSM,NA)=A(NSM,NA)+SM
ISN 0211          A(NQ,NQ)=CPSUM+QDRV
ISN 0212          A(NQ,NA)=HIN-Q-HSUM
            C
ISN 0213          IMAT=NQ
ISN 0214          GO TO 400
            C
            C***   ***   ***   ***   ***   ***   ***   ***   CHAPTER 3   ***   ***
            C***   ***   ***   ***   ***   ***   ***   ***   CHAPTER 3   ***   ***
            C
            C   ***EQUILIBRIUM***
            C   DERIVATIVE AND FUNCTION MATRIX FOR EQUILIBRIUM SOLUTION
            C
ISN 0215      300 DO 310 L=1,NEM
ISN 0216      310 B0(L)=0.0
            C
ISN 0217          HSUM=0.0
ISN 0218          SUM=0.0
ISN 0219          DO 340 I=1,NS
ISN 0220          SUM=SUM+S2(I)
ISN 0221          TM1=H0(I)*S2(I)
ISN 0222          HSUM=HSUM+TM1
ISN 0223          TM2=(H0(I)-S0(I)+Y(I)-Y(NSM)+PPLN)*S2(I)
ISN 0224          A(N1,N3)=A(N1,N3)+TM2
ISN 0225          A(N2,N2)=A(N2,N2)+H0(I)*TM1
ISN 0226          A(N2,N3)=A(N2,N3)+H0(I)*TM2
            C
ISN 0227          DO 330 L=1,NEM
ISN 0228          IF (AL(L,I).EQ.0.0) GO TO 330
ISN 0230          TM3=AL(L,I)*S2(I)
            C-----CROSS-DERIVATIVES OF ELEMENT EQUATIONS, D F(L)/D PI(K)
ISN 0231          DO 320 K=L,NEM
ISN 0232          IF (AL(K,I).EQ.0.0) GO TO 320
ISN 0234          A(L,K)=A(L,K)+AL(K,I)*TM3
ISN 0235      320 CONTINUE
            C-----DERIVATIVES OF L-ELEMENT EQN W.R.T. LN SM AND LN T
ISN 0236          A(L,N1)=A(L,N1)+TM3
ISN 0237          A(L,N2)=A(L,N2)+AL(L,I)*TM1
            C-----NEGATIVE OF L-ELEMENT EQN, F(L)
ISN 0238          A(L,N3)=A(L,N3)+AL(L,I)*TM2
ISN 0239          B0(L)=B0(L)+AL(L,I)*S1(I)
ISN 0240      330 CONTINUE
ISN 0241      340 CONTINUE
            C
ISN 0242          A(N1,N1)=SUM-SM
ISN 0243          A(N1,N3)=A(N1,N3)-(SUM-SM)
```

```
ISN 0244          A(N1,N2)=HSUM
ISN 0245          A(N2,N2)=A(N2,N2)+CPSUM+QDRV
ISN 0246          A(N2,N3)=A(N2,N3)+HIN-HSUM-Q
            C
            C-----NEGATIVE OF L-ELEMENT EQNS, F(L)
ISN 0247          DO 350 L=1,NEM
ISN 0248          A(L,N3)=A(L,N3)+BO(L)-A(L,N1)
ISN 0249      350 CONTINUE
            C
            C-----STORE SYMMETRIC ELEMENTS OF MATRIX
            C
ISN 0250          DO 360 I=1,N2
ISN 0251          DO 360 J=1,N2
ISN 0252          A(J,I)=A(I,J)
ISN 0253      360 CONTINUE
            C
            C-----INTERCHANGE SM-EQN WITH ELEMENT ROW L WITH LARGEST A(L,N1) TO
            C-----AVOID POTENTIAL ZERO IN DIAGONAL ELEMENT A(N1,N1)
            C
ISN 0254          TM1=0.0
ISN 0255          DO 370 L=1,NEM
ISN 0256          IF (A(L,N1).LT.TM1) GO TO 370
ISN 0258          TM1=A(L,N1)
ISN 0259          LL=L
ISN 0260      370 CONTINUE
            C
ISN 0261          DO 380 J=1,N3
ISN 0262          TM1=A(N1,J)
ISN 0263          A(N1,J)=A(LL,J)
ISN 0264          A(LL,J)=TM1
ISN 0265      380 CONTINUE
ISN 0266          IMAT=N2
            C
            C****     ****     ****     ****     ****     ****     CHAPTER 4     ****     ***
            C****     ****     ****     ****     ****     ****     CHAPTER 4     ****     ***
            C
            C   ***MATRIX SOLUTION***
            C   SOLVE FOR CORRECTIONS BY STANDARD PIVOTAL GAUSSIAN ELIMINATION
            C
ISN 0267      400 KMAT=IMAT+1
            C-----OPTIONAL OUTPUT OF INTERMEDIATE VALUES FOR DEBUGGING
ISN 0268          IF (.NOT.LDEBUG) GO TO 410
ISN 0270          IF (NDEBUG.LT.5) GO TO 410
ISN 0272          WRITE(6,401)
ISN 0273      401 FORMAT(1H0,10X,36HELEMENTS A(I,K) OF CORRECTION MATRIX/)
ISN 0274          DO 403 K=1,IMAT
ISN 0275          WRITE(6,402) (A(K,I),I=1,KMAT)
ISN 0276      402 FORMAT(1X,1P16D8.0)
ISN 0277      403 CONTINUE
ISN 0278      410 CONTINUE
ISN 0279          DO 450 NN=1,IMAT
ISN 0280          IF (A(NN,NN).EQ.0.0) GO TO 500
            C-----CHANGE 1.0D0 TO 1.0 FOR NON-IBM MACHINES NOT REQUIRING DOUBLE PRE
ISN 0282          DTM1=1./A(NN,NN)
ISN 0283          K=NN+1
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ISN 0284          DO 420 J=K,KMAT                                              GEN05442
ISN 0285          A(NN,J)=A(NN,J)*DIMI                                         GEN05444
ISN 0286      420 CONTINUE                                                     GEN05446
ISN 0287          IF (K.EQ.KMAT) GO TO 450                                     GEN05448
ISN 0289          DO 440 I=K,IMAT                                              GEN05450
ISN 0290          IF (A(I,NN).EQ.0.0) GO TO 440                                GEN05452
ISN 0292          DO 430 J=K,KMAT                                              GEN05454
ISN 0293          A(I,J)=A(I,J)-A(I,NN)*A(NN,J)                                GEN05456
ISN 0294      430 CONTINUE                                                     GEN05458
ISN 0295      440 CONTINUE                                                     GEN05460
ISN 0296      450 CONTINUE                                                     GEN05462
            C                                                                  GEN05464
            C-----BACK SOLVE FOR CORRECTION VECTOR                             GEN05466
            C                                                                  GEN05468
ISN 0297          K=IMAT                                                       GEN05470
ISN 0298      460 J=K+1                                                        GEN05472
ISN 0299          DSUM=0.                                                      GEN05474
ISN 0300          X(K)=0.0                                                     GEN05476
ISN 0301          IF (IMAT.LT.J) GO TO 480                                     GEN05478
ISN 0303          DO 470 I=J,IMAT                                              GEN05480
ISN 0304          DSUM=DSUM+A(K,I)*X(I)                                        GEN05482
ISN 0305      470 CONTINUE                                                     GEN05484
ISN 0306      480 CONTINUE                                                     GEN05486
ISN 0307          X(K)=A(K,KMAT)-DSUM                                          GEN05488
ISN 0308          K=K-1                                                        GEN05490
ISN 0309          IF (K.NE.0) GO TO 460                                        GEN05492
            C                                                                  GEN05494
ISN 0311          RETURN                                                       GEN05496
            C                                                                  GEN05498
            C*****     *****     *****     *****     *****   CHAPTER 5   *****  *GEN05500
            C*****     *****     *****     *****     *****   CHAPTER 5   *****  *GEN05502
            C                                                                  GEN05504
            C   ***SINGULAR MATRIX***                                          GEN05506
            C                                                                  GEN05508
ISN 0312      500 WRITE(6,501)                                                 GEN05510
ISN 0313      501 FORMAT(1H0,10X,3(4H****),16HSINGULAR MATRIX/)                GEN05512
            C-----SET LCONVG=.TRUE. TO NOTIFY SPECE OF SINGULAR MATRIX         GEN05514
ISN 0314          LCONVG=.TRUE.                                                GEN05516
ISN 0315          RETURN                                                       GEN05518
ISN 0316          END                                                          GEN05520
*OPTIONS IN EFFECT*NAME(MAIN) NOOPTIMIZE LINECOUNT(57) SIZE(MAX) AUTODBL(NONE)
*OPTIONS IN EFFECT*SOURCE EBCDIC NOLIST NODECK OBJECT NOMAP NOFORMAT NOGOSTMT NOXREF NOALC NOANSF TERM FLA
*STATISTICS*     SOURCE STATEMENTS =      315, PROGRAM SIZE =     15604, SUBPROGRAM NAME =  CALC
*STATISTICS*  NO  DIAGNOSTICS GENERATED
****** END OF COMPILATION ******                                   316K BYTES OF CORE NOT USED
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ORIGINAL PAGE IS
OF POOR QUALITY

REQUESTED OPTIONS:

OPTIONS IN EFFECT: NAME(MAIN) NOOPTIMIZE LINECOUNT(57) SIZE(MAX) AUTODBL(NONE)
SOURCE EBCDIC NOLIST NODECK OBJECT NOMAP NOFORMAT NOGOSTMT NOXREF NOALC NOANSF TERM FL

```
ISN 0002          SUBROUTINE HCPS
ISN 0003          IMPLICIT REAL*8 (A-H,O-Z)
            C
ISN 0004          DIMENSION ASUB(20,3)
ISN 0005          LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LNRG,LREACT
            C
ISN 0006          COMMON
                 1/CCHEM1/CPSUM,FQ,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LCONVG,LNRG
                 1/CINDEX/ICO,ICO2,IH2,IH2O,IN2,IO2,IHCPS,ILC,ILH,IMAT,ITER,
                 2        JJ,N1,N2,N3,NA,NGLOB,NGLOBP,NLM,NQ,NSM
                 1/CPARAM/ASUB,NT,NE,EMV,ER,HSUBO,NDEBUG,NS,PA,Q0,Q1,Q2,Q3,Q4,RHOP,
                 2        SM,S1(20),S2(20),TK,LADIAB,LDEBUG,LEQUIL,LREACT
                 1/CSPECE/HO(20),SO(20),SMW(20),SSAVE(20),Z(280)
            C
            C*********************************************************************
            C   THIS SUBROUTINE CALCULATES THE NON-DIMENSIONAL, 1-ATM VALUES OF
            C   ENTHALPY, SPECIFIC HEAT, AND ENTROPY FOR A GIVEN VALUE OF TEMPERATURE
            C   (DEG K)  THE Z ARRAY IS REFERENCED AS HAVING ONLY ONE SUBSCRIPT
            C   TO SAVE INTERNAL SUBSCRIPT CALCULATIONS.
            C   Z(IC,IT,IS) ----> Z(IC+7*(IT-1)+7*2*(IS-1)) FOR Z(7,2,20)
            C   WHERE IC=1,7. COEF FOR TEMP RANGE IT=1 OR 2. FOR SPECIES IS=1,NS.
            C   NOTE THAT THE FIRST 2 SUBSCRIPTS ARE REVERSED FROM THE
            C   GORDON AND MCBRIDE PRACTICE
            C   REFERENCE  GORDON AND MCBRIDE  (NASA SP-273, 1971)
            C*********************************************************************
            C
ISN 0007          DATA ICIT/14/
            C
ISN 0008          IT=0
ISN 0009          IF (TK.LT.1000.0) IT=7
            C
ISN 0011          TKSQ=TK**2
ISN 0012          TKCU=TKSQ*TK
ISN 0013          TK4=TKCU*TK
ISN 0014          CPSUM=0.0
ISN 0015          IF (IHCPS.NE.1) GO TO 20
            C
            C-----IHCPS=1 ----> JUST CPSUM AND HO(I) REQUIRED
            C
ISN 0017          DO 10 I=1,NS
ISN 0018          K=IT+ICIT*(I-1)
ISN 0019          CP1=Z(K+1)
ISN 0020          CP2=TK*Z(K+2)
ISN 0021          CP3=TKSQ*Z(K+3)
ISN 0022          CP4=TKCU*Z(K+4)
ISN 0023          CP5=TK4*Z(K+5)
ISN 0024          CPSUM=CPSUM+(CP1+CP2+CP3+CP4+CP5)*S2(I)
ISN 0025          HO(I)=0.2*CP5+0.25*CP4+0.33333333*CP3+0.5*CP2+CP1+TKINV*Z(K+6)
ISN 0026       10 CONTINUE
ISN 0027          RETURN
```

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                    C                                                                      GEN05622
                    C-----IHCPS=2 ---> CPSUM, HO(I) AND SO(I) REQUIRED                     GEN05624
                    C                                                                      GEN05626
   ISN 0028            20 CONTINUE                                                         GEN05628
   ISN 0029               DO 30 I=1,NS                                                     GEN05630
   ISN 0030               K=IT+IC(I)*(I-1)                                                 GEN05632
   ISN 0031               CP1=Z(K+1)                                                       GEN05634
   ISN 0032               CP2=TK*Z(K+2)                                                    GEN05636
   ISN 0033               CP3=TKSQ*Z(K+3)                                                  GEN05638
   ISN 0034               CP4=TKCU*Z(K+4)                                                  GEN05640
   ISN 0035               CP5=TK4*Z(K+5)                                                   GEN05642
   ISN 0036               CPSUM=CPSUM+(CP1+CP2+CP3+CP4+CP5)*S2(I)                          GEN05644
   ISN 0037               HO(I)=0.2*CP5+0.25*CP4+0.3333333*CP3+0.5*CP2+CP1+TKINV*Z(K+6)    GEN05646
   ISN 0038               SO(I)=0.25*CP5+0.3333333*CP4+0.5*CP3+CP2+TLN*CP1+Z(K+7)          GEN05648
   ISN 0039            30 CONTINUE                                                         GEN05650
   ISN 0040               RETURN                                                           GEN05652
   ISN 0041               END                                                              GEN05654
```

*OPTIONS IN EFFECT*NAME(MAIN) NOOPTIMIZE LINECOUNT(57) SIZE(MAX) AUTODBL(NONE)

*OPTIONS IN EFFECT*SOURCE EBCDIC NOLIST NODECK OBJECT NOMAP NOFORMAT NOGOSTMT NOXREF NOALC NOANSF TERM FL

STATISTICS   SOURCE STATEMENTS =   40, PROGRAM SIZE =   1300, SUBPROGRAM NAME = HCPS

STATISTICS NO DIAGNOSTICS GENERATED

****** END OF COMPILATION ******   372K BYTES OF CORE NOT USED

```
ELEMENTS
C         12.011150        4.000000
H          1.007970        1.000000
O         15.999400       -2.000000
N         14.006700        0.0

THERMO FOR CH4/AIR COMBUSTION
CH2                     J 6/69  C     1.H     2.0     0.0     0.  G     300.000  5000.000     1
 0.25649263D+01 0.45499925D-02-0.16974415D-05 0.29273414D-09-0.19116560D-13    2
 0.45355512D+05 0.57255698D+01 0.27277046D+01 0.33512361D-02 0.11455341D-05    3
-0.25591076D-08 0.12457256D-11 0.45304444D+05 0.52009628D+01                   4

CH3                     J 6/69  C     1.H     3.0     0.0     0.  G     300.000  5000.000     1
 0.28400327D+01 0.60869086D-02-0.21740338D-05 0.36042576D-09-0.22725300D-13    2
 0.16449813D+05 0.55056751D+01 0.34066350D+01 0.38313845D-02 0.10111220D-05    3
-0.18659236D-08 0.66803182D-12 0.16313104D+05 0.24172192D+01                   4

CH4                     J 3/61  C     1.H     4.00    0.00    0.  G     300.000  5000.000     1
 0.15027072D+01 0.10416798D-01-0.39181522D-05 0.67777899D-09-0.44283706D-13    2
-0.99787078D+04 0.10707143D+02 0.38261932D+01-0.39794581D-02 0.24558340D-04    3
-0.22732926D-07 0.69626957D-11-0.10144950D+05 0.86690075D+00                   4

HCO                     J12/70  H     1.C     1.0     1.0     0.  G     300.000  5000.000     1
 0.34738348D+01 0.34370227D-02-0.13632664D-05 0.24928645D-09-0.17044331D-13    2
 0.39594005D+04 0.60453340D+01 0.36840192D+01-0.82974448D-03 0.77900809D-05    3
-0.70616962D-08 0.19971730D-11 0.40563860D+04 0.48354133D+01                   4

CH2O                    J 3/61  C     1.H     2.0     1.0     0.  G     300.000  5000.000     1
 0.28364249D+01 0.68605298D-02-0.26882647D-05 0.47971258D-09-0.32118406D-13    2
-0.15236031D+05 0.78531169D+01 0.37963783D+01-0.25701785D-02 0.18548815D-04    3
-0.17869177D-07 0.55504451D-11-0.15088947D+05 0.47548163D+01                   4

CO                      J 9/65  C     1.O     1.00    0.00    0.  G     300.000  5000.000     1
 0.29840696D+01 0.14891390D-02-0.57899684D-06 0.10364577D-09-0.69353550D-14    2
-0.14245228D+05 0.63479156D+01 0.37100928D+01-0.16190964D-02 0.36923594D-05    3
-0.20319674D-08 0.23953344D-12-0.14356310D+05 0.29555351D+01                   4

CO2                     J 9/65  C     1.O     2.00    0.00    0.  G     300.000  5000.000     1
 0.44608041D+01 0.30981719D-02-0.12392571D-05 0.22741325D-09-0.15525954D-13    2
-0.48961442D+05-0.98635982D+00 0.24007797D+01 0.87350957D-02-0.66070878D-05    3
 0.20021861D-08 0.63274039D-15-0.48377527D+05 0.96951457D+01                   4

H                       J 9/65  H     1.00    0.00    0.00    0.  G     300.000  5000.000     1
 0.25000000D+01 0.0            0.0            0.0            0.0               2
 0.25471627D+05-0.46011763D+00 0.25000000D+01 0.0            0.0               3
 0.0            0.0            0.25471627D+05-0.46011762D+00                   4

H2                      J 3/61  H     2.0     0.0     0.0     0.  G     300.000  5000.000     1
 0.31001901D+01 0.51119464D-03 0.52644210D-07-0.34909973D-10 0.36945345D-14    2
-0.87738042D+03-0.19629421D+01 0.30574451D+01 0.26765200D-02-0.58099162D-05    3
 0.55210391D-08-0.18122739D-11-0.98890474D+03-0.22997056D+01                   4

H2O                     J 3/61  H     2.0     1.00    0.00    0.  G     300.000  5000.000     1
 0.27167633D+01 0.29451374D-02-0.80224374D-06 0.10226682D-09-0.48472145D-14    2
-0.29905826D+05 0.66305671D+01 0.40701275D+01-0.11084499D-02 0.41521180D-05    3
-0.29637404D-08 0.80702103D-12-0.30279722D+05-0.32270046D+00                   4
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HO2              J 3/64  H    1.0    2.00   0.00   0.   G     300.000  5000.000      1
 0.37866280D+01 0.27665404D-02-0.16168708D-05 0.17183946D-09-0.11021852D-13    2
 0.11868500D+04 0.48147611D+01 0.35094850D+01 0.11499670D-02 0.58784259D-05    3
-0.77955190D-08 0.29607885D-11 0.13803331D+04 0.68276325D+01                   4

N                J 3/61  N    1.00   0.00   0.00   0.   G     300.000  5000.000      1
 0.24502682D+01 0.10661458D-03-0.74653373D-07 0.18796524D-10-0.10259839D-14    2
 0.56116640D+05 0.44487581D+01 0.25030714D+01-0.21800181D-04 0.54205287D-07    3
-0.56475602D-10 0.20999044D-13 0.56098904D+05 0.41675764D+01                   4

NO               J 6/63  N    1.0    1.00   0.00   0.   G     300.000  5000.000      1
 0.31890000D+01 0.13382280D-02-0.52899318D-06 0.95919332D-10-0.64847932D-14    2
 0.98283290D+04 0.67458120D+01 0.40459521D+01-0.34181783D-02 0.79819190D-05    3
-0.61139316D-08 0.15919076D-11 0.97453934D+04 0.29974988D+01                   4

NO2              J 9/64  N    1.0    2.00   0.00   0.   G     300.000  5000.000      1
 0.46240771D+01 0.25260332D-02-0.10609498D-05 0.19879239D-09-0.13799384D-13    2
 0.22899900D+04 0.13324136D+01 0.34589236D+01 0.20647064D-02 0.66866067D-05    3
-0.95556725D-08 0.36195588D-11 0.28152265D+04 0.83116983D+01                   4

N2               J 9/65  N    2.0    0.0    0.0    0.   G     300.000  5000.000      1
 0.28963194D+01 0.15154866D-02-0.57235277D-06 0.99807393D-10-0.65223555D-14    2
-0.90586184D+03 0.61615148D+01 0.36748261D+01-0.12081500D-02 0.23240102D-05    3
-0.63217559D-09-0.22577553D-12-0.10611588D+04 0.23580424D+01                   4

N2O              J12/64  N    2.0    1.00   0.00   0.   G     300.000  5000.000      1
 0.47306679D+01 0.28258461D-02-0.11558115D-05 0.21260383D-09-0.14504667D-13    2
 0.81617052D+04-0.17151745D+01 0.26189196D+01 0.86439610D-02-0.68110624D-05    3
 0.22275077D-08-0.[illegible]D-13 0.87590123D+04 0.92260952D+01                   4

O                J 6/62  O    1.00   0.00   0.00   0.   G     300.000  5000.000      1
 0.25420596D+01-0.27550619D-04-0.31028033D-08 0.45510674D-11-0.43680515D-15    2
 0.29230803D+05 0.49203080D+01 0.29464287D+01-0.16381665D-02 0.24210316D-05    3
-0.16028432D-08 0.38906964D-12 0.29147644D+05 0.29639949D+01                   4

OH               J12/70  O    1.H    1.0    0.0    0.   G     300.000  5000.000      1
 0.29131230D+01 0.95418248D-03-0.19084325D-06 0.12730795D-10 0.24803941D-15    2
 0.39647060D+04 0.54288735D+01 0.38365518D+01-0.10702014D-02 0.94849757D-06    3
 0.20845575D-09-0.23384265D-12 0.36715867D+04 0.49805456D+00                   4

O2               J 9/65  O    2.0    0.0    0.0    0.   G     300.000  5000.000      1
 0.36219535D+01 0.73618264D-03-0.19652228D-06 0.36201558D-10-0.28945627D-14    2
-0.12019825D+04 0.36150960D+01 0.36255985D+01-0.18782184D-02 0.70554544D-05    3
-0.67635137D-08 0.21555993D-11-0.10475226D+04 0.43052778D+01                   4
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MECHANISM - CY WALSMANS ULTRASYSTEM CH4/AIR

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   1.   HCO              M          CO        H        M        17.398     -1.500      8460.000   WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =            9.091      0.0      -1195.308   56.035D-0398.293D-02

   2.   HCO     H                   CO        H2                 7.477      1.000         0.0     WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =           11.982      0.0      47022.495   99.890D-0399.995D-02

   3.   CH2O    O                   HCO       OH                 8.301      1.000      2215.000
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =           16.541      0.0      10298.286   10.935D-0299.881D-02

   4.   HCO     OH                  CO        H2O                7.477      1.000         0.0     WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =           12.615      0.0      54014.418   80.200D-0399.996D-02

   5.   HCO     O                   CO        OH                 [illegible]  1.000   [illegible]  WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =           [illegible]  0.0    [illegible]  [illegible]

   6.   CH3     O                   CH2O      H                  [illegible]  0.500   [illegible]  WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =           [illegible]  0.0      25693.751   [illegible]

   7.   CH4     O                   CH3       OH                 7.000      1.000      4028.000   WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =            8.918      0.0       4466.562   16.965D-0299.406D-02
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   8.   CH4      H                      CH3      H2                                   7.700         1.000         5635.000      WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                 9.975         0.0           6546.927      11.2270-0299.7070-02

   9.   CH4      OH                     CH3      H2O                                 10.477         0.0           2516.000      WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                 9.704         0.0           9964.560      31.0970-0399.9950-02

  10.   HCO      O2                     CO       HO2                                  9.903         0.0              0.0        WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                10.259         0.0          10286.826      16.6850-0399.9990-02

  11.   CO       OH                     CO2      H                                    6.602         0.500            0.0        WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                10.473         0.0          11918.292      40.3360-0299.9650-02

  12.   CO2               M             CO       O        M                          12.000         0.0          56353.000      WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                 6.719         0.0         -12217.960      81.7600-0399.9550-02

  13.   H        OH                     H2       O                                    6.903         1.000         3525.000      WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                10.942         0.0           6255.656      62.4990-0399.8960-02

  14.   H2O               M             OH       H        M                          12.477         0.0          52870.000      WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                 8.250         0.0          -7256.561      22.9960-0399.9950-02

  15.   H        HO2                    OH       OH                                  11.398         0.0            957.000
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                10.410         0.0          20915.565      42.2570-0399.9960-02

  16.   OH       H2                     H        H2O                                 10.390         0.0           2618.000      WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                11.032         0.0          10279.922      15.7460-0399.9960-02

  17.   H        O        M             OH                M                           9.903         0.0              0.0        WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                13.153         0.0          51481.213      67.9350-0412.0000-01

  18.   OH       O                      H        O2                                  10.398         0.0              0.0        WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                11.495         0.0           8066.454      24.5100-0399.9970-02

  19.   H        O2       M             HO2               M                           9.176         0.0            503.500      WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                12.317         0.0          23959.693      22.8000-0399.9990-02

  20.   OH       OH                     H2O      O                                    9.778         0.0            503.500      WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                10.769         0.0           9148.788      17.1660-0399.9960-02

  21.   OH       N                      H        NO                                   8.778         0.500         4028.000      WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                11.048         0.0          29029.744      14.6540-0310.0000-01

  22.   H        N2O                    OH       N2                                  10.903         0.0           7553.000      WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                 9.609         0.0          40513.129      77.3670-0399.9960-02

  23.   N        NO                     N2       O                                   10.176         0.0              0.0        WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                10.831         0.0          37862.229      53.5260-0412.0000-01

  24.   N        O2                     NO       O                                    6.778         1.000         3172.000      WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                 9.791         0.0          20935.934      66.6220-0399.9690-02

  25.   N2O      O                      NO       NO                                  11.000         0.0          15000.000      WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                 9.480         0.0          34270.998      55.4300-0399.9970-02

  26.   N2O               M             N2       O        M                          11.000         0.0          25170.000      ALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                 6.456         0.0           6654.916      8[illegible].3140-0399.6410-02

  27.   HCO      CH3                    CH2      CH2O                                 8.176         0.700         2014.000      ALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                11.776         0.0          -6657.[illegible]06    65.0570-0499.9960-02

  28.   HCO      CH4                    CH2O     CH3                                  8.903         0.600         4532.000      WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                10.792         0.0         -20598.551      36.0050-0399.6940-02

  29.   CH3      H                      CH2      H2                                   8.301         0.700         1151.000      WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                10.010         0.0            -41.067      59.1060-0312.5500-02

  30.   CH3      OH                     CH2      H2O                                  7.778         0.700         1067.000      WALD
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                                10.426         0.0           1950.516      46.1120-0399.5120-02
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   31.   CH2      O2                     CH2O     O                                 6.699        0.500       3525.000     ALO
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                              10.982        0.0        34709.372    22.2570-0310.0000-01

   32.   CH3      O2                     CH2O     OH                               10.477        0.0        15106.000
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                              10.499        0.0        42055.652    64.6110-0410.0000-01

   33.   CH4               M             CH3      H        M                       14.301        0.0        44310.000     HALO
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                               9.257        0.0        -6319.941    54.2460-0399.9500-02

   34.   CH3      HO2                    CH4      O2                                8.000        0.500       3021.000     HALO
CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF =                              11.714        0.0        53073.393    48.0950-0410.0000-02
    1.    HCO              M      ---->     CO       H        M
    2.    HCO     H               ---->     CO       H2
    3.    CH2O    O               ---->     HCO      OH
    4.    HCO     OH              ---->     CO       H2O
    5.    HCO     O               ---->     CO       OH
    6.    CH3     O               ---->     CH2O     H
    7.    CH4     O               ---->     CH3      OH
    8.    CH4     H               ---->     CH3      H2
    9.    CH4     OH              ---->     CH3      H2O
   10.    HCO     O2              ---->     CO       HO2
   11.    CO      OH              ---->     CO2      H
   12.    CO2              M      ---->     CO       O        M
   13.    H       OH              ---->     H2       O
   14.    H2O              M      ---->     OH       H        M
   15.    H       HO2             ---->     OH       OH
   16.    OH      H2              ---->     H        H2O
   17.    H       O        M      ---->     OH                M
   18.    OH      O               ---->     H        O2
   19.    H       O2       M      ---->     HO2               M
   20.    OH      OH              ---->     H2O      O
   21.    OH      N               ---->     H        NO
   22.    H       N2O             ---->     OH       N2
   23.    N       NO              ---->     N2       O
   24.    N       O2              ---->     NO       O
   25.    N2O     O               ---->     NO       NO
   26.    N2O              M      ---->     N2       O        M
   27.    HCO     CH3             ---->     CH4      CO
```

ORIGINAL PAGE IS
OF POOR QUALITY

I	SPECIES	MOLECULAR WEIGHT	MOLE NUMBERS	MASS FRACTIONS
7.	CO2	44.010D+00	0.0	0.0
8.	H	10.080D-01	0.0	0.0
9.	H2	20.159D-01	0.0	0.0
10.	H2O	18.015D+00	0.0	0.0
11.	HO2	33.007D+00	0.0	0.0
12.	N	14.007D+00	0.0	0.0
13.	NO	30.006D+00	0.0	0.0
14.	NO2	46.005D+00	0.0	0.0
15.	N2	28.013D+00	0.0	0.0
16.	N2O	44.013D+00	0.0	0.0
17.	O	15.999D+00	0.0	0.0
18.	OH	17.007D+00	0.0	0.0
19.	O2	31.999D+00	0.0	0.0

```
TEMPERATURE =    10.000D+02    DEG K
ENTHALPY =      -22.871D+05    JOULES/KG
PRESSURE =       10.000D+04    N/M**2
DENSITY =        19.295D-02    KG/M**3
MEAN MOL WT =    16.043D+00    KG/KGMOLE
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REACTANTS-2 *AIR*
O   2.00000   0.0   0.0   0.0   O2   1.00000 M G   2
N   2.00000   0.0   0.0   0.0   N2   3.76000 M G   2
```

*** REACTANT STREAM 2 ***

I	SPECIES	MOLECULAR WEIGHT (KGMOLE I)/(KG I)	MOLE NUMBERS (KGMOLE I)/(KG X)	MASS FRACTIONS (KG I)/(KG X)
1.	CH2	14.027D+00	0.0	0.0
2.	CH3	15.035D+00	0.0	0.0
3.	CH4	16.043D+00	0.0	0.0
4.	HCO	29.019D+00	0.0	0.0
5.	CH2O	30.026D+00	0.0	0.0
6.	CO	28.011D+00	0.0	0.0
7.	CO2	44.010D+00	0.0	0.0
8.	H	10.080D-01	0.0	0.0
9.	H2	20.159D-01	0.0	0.0
10.	H2O	18.015D+00	0.0	0.0
11.	HO2	33.007D+00	0.0	0.0
12.	N	14.007D+00	0.0	0.0
13.	NO	30.006D+00	0.0	0.0
14.	NO2	46.005D+00	0.0	0.0
15.	N2	28.013D+00	27.379D-03	76.699D-02
16.	N2O	44.013D+00	0.0	0.0
17.	O	15.999D+00	0.0	0.0
18.	OH	17.007D+00	0.0	0.0
19.	O2	31.999D+00	72.818D-04	23.301D-02

```
TEMPERATURE =    10.000D+02    DEG K
ENTHALPY =       75.291D+04    JOULES/KG
PRESSURE =       10.000D+04    N/M**2
DENSITY =        34.700D-02    KG/M**3
MEAN MOL WT =    28.851D+00    KG/KGMOLE
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KARE  N

KASE=  1 LESSON=  0 MODEL=  1 MASSTR=  1 INERT=  2
 UA          UB          UC          UD          TA          TB          TC          TD          RA          RB          FL          KL
0.347D+00 0.347D+00 0.463D+00 0.463D+00 0.160D+04 0.100D+04 0.100D+04 0.100D+04 0.0         0.0         0.353D-02 0.150D-02
 XEND        XOUT        XCLAST      TAN         PRESS       PREEXP      KEY         EQRAT       AMACH
 0.0         0.0         0.200D+01   0.0         0.160D+06   0.0         0.640D+02   0.100D+07
       7  0.0          0.0         0.526D-01   0.105D+05   0.158D+00   0.211D+00   0.263D+00   0.316D+00   0.368D+00   0.421D+00   0.474D+00
          0.526D+00    0.579D+00   0.632D+00   0.684D+00   0.737D+00   0.789D+00   0.842D+00   0.895D+00   0.947D+00   0.100D+01   0.100D+01

ISTEP=     0 IAX=     0 IEND=     0 IOUT=     0 KIN= 3 KEX= 2 DX=  0.335D-06 PSII=  0.0        PSIE=  0.784D-07
RMI=  0.0        RME= -0.234D-02 PEI=  0.784D-07
XU=  0.100D-29 UFLUX= -0.915D-08 PRESS=  0.0          AEXP=  0.0          FLUX(J)=
 -0.269D-42  -0.269D-42   0.466D-06  -0.269D-42  -0.269D-42  -0.269D-42  -0.269D-42  -0.269D-42  -0.269D-42  -0.269D-42
 -0.269D-42  -0.269D-42  -0.269D-42  -0.269D-42  -0.215D-08  -0.269D-42  -0.265D-42  -0.269D-42  -0.571D-09  -0.256D+00

       9  0.0          0.514D-01   0.251D-03   0.496D-03   0.608D-03   0.702D-03   0.785D-03   0.860D-03   0.929D-03   0.995D-03   0.103D-02
          0.111D-02    0.116D-02   0.122D-02   0.127D-02   0.131D-02   0.136D-02   0.140D-02   0.145D-02   0.149D-02   0.153D-02   0.155D-02
      10  0.347D+00    0.347D+00   0.347D+00   0.347D+00   0.347D+00   0.347D+00   0.347D+00   0.347D+00   0.347D+00   0.347D+00   0.347D+00
          0.347D+00    0.347D+00   0.347D+00   0.347D+00   0.347D+00   0.347D+00   0.347D+00   0.347D+00   0.347D+00   0.347D+00   0.463D+00
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MASS FRACTIONS,ENTHALPY,TEMP,F/A EQUIV RATIO,CELL LEADING EDGE (KG/M 3-S), CELL RES TIME

STA.	CH2 / NB	CH3 / NO2	CH4 / N2	HCO / N2O	CH2O / O	CO / OH	CO2 / O2	H / H (J/KG)	H2 / T (K)	H2O / EQ RATIO	HO2 / KG/M3-S	RES (S)
1	0.0 0.0	0.0 0.0	1.000D+00 0.0	0.0 0.0	0.0 0.0	0.0 0.0	0.0 0.0	0.0 -2.290D+06	0.0 1.000D+03	0.0 1.000D+06	0.0 0.0	0.0 0.0
2	0.0 0.0	0.0 0.0	1.000D+00 0.0	0.0 0.0	0.0 0.0	0.0 0.0	0.0 0.0	0.0 -2.290D+06	0.0 1.000D+03	0.0 1.000D+06	0.0 0.0	0.0 0.0
3	0.0 0.0	0.0 0.0	1.000D+00 0.0	0.0 0.0	0.0 0.0	0.0 0.0	0.0 0.0	0.0 -2.290D+06	0.0 1.000D+03	0.0 1.000D+06	0.0 0.0	0.0 0.0
4	0.0 0.0	0.0 0.0	1.000D+00 0.0	0.0 0.0	0.0 0.0	0.0 0.0	0.0 0.0	0.0 -2.290D+06	0.0 1.000D+03	0.0 1.000D+06	0.0 0.0	0.0 0.0
5	0.0 0.0	0.0 0.0	1.000D+00 0.0	0.0 0.0	0.0 0.0	0.0 0.0	0.0 0.0	0.0 -2.290D+06	0.0 1.000D+03	0.0 1.000D+06	0.0 0.0	0.0 0.0
6	0.0 0.0	0.0 0.0	1.000D+00 0.0	0.0 0.0	0.0 0.0	0.0 0.0	0.0 0.0	0.0 -2.290D+06	0.0 1.000D+03	0.0 1.000D+06	0.0 0.0	0.0 0.0
7	0.0 0.0	0.0 0.0	1.000D+00 0.0	0.0 0.0	0.0 0.0	0.0 0.0	0.0 0.0	0.0 -2.290D+06	0.0 1.000D+03	0.0 1.000D+06	0.0 0.0	0.0 0.0
8	0.0 0.0	0.0 0.0	1.000D+00 0.0	0.0 0.0	0.0 0.0	0.0 0.0	0.0 0.0	0.0 -2.290D+06	0.0 1.000D+03	0.0 1.000D+06	0.0 0.0	0.0 0.0
9	0.0 0.0	0.0 0.0	1.000D+00 0.0	0.0 0.0	0.0 0.0	0.0 0.0	0.0 0.0	0.0 -2.290D+06	0.0 1.000D+03	0.0 1.000D+06	0.0 0.0	[illegible] [illegible]
10	0.0 0.0	0.0 0.0	1.000D+00 0.0	0.0 0.0	0.0 0.0	0.0 0.0	0.0 0.0	0.0 -2.290D+06	0.0 1.000D+03	0.0 1.000D+06	0.0 0.0	[illegible] [illegible]
11	0.0 0.0	[illegible]	1.000D+00 [illegible]	[illegible]	0.0 [illegible]	[illegible]	0.0 [illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
12	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

13	0.0	0.0	1.000D+00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-2.290D+06	1.000D+03	1.000D+06	0.0	0.0
14	0.0	0.0	1.000D+00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-2.290D+06	1.000D+03	1.000D+06	0.0	0.0
15	0.0	0.0	1.000D+00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-2.290D+06	1.000D+03	1.000D+06	0.0	0.0
16	0.0	0.0	1.000D+00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-2.290D+06	1.000D+03	1.000D+06	0.0	0.0
17	0.0	0.0	1.000D+00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-2.290D+06	1.000D+03	1.000D+06	0.0	0.0
18	0.0	0.0	1.000D+00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-2.290D+06	1.000D+03	1.000D+06	0.0	0.0
19	0.0	0.0	1.000D+00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-2.290D+06	1.000D+03	1.000D+06	0.0	0.0
20	0.0	0.0	1.000D+00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-2.290D+06	1.000D+03	1.000D+06	0.0	0.0
21	0.0	0.0	1.000D+00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-2.290D+06	1.000D+03	1.000D+06	0.0	0.0
22	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	7.670D-01	0.0	0.0	0.0	2.330D-01	7.530D+05	1.000D+03	0.0	0.0	0.0

```
ISTEP=     1 IAX=     0 IEND=     6 IOUT=     0 KIN= 3 KEX= 2 UX=  0.315D-06 PSII=  0.0        PSIE=  0.792D-07
RMI=  0.0        RME= -0.252D-02 PEI=  0.792D-07
XU=  0.355D-06 UFLUX= -0.913D-08 PRESSD=  0.0        AEXD=  0.0        FLUX(J)=
 -0.269D-42  -0.269D-42   0.489D-08  -0.269D-42  -0.269D-42  -0.269D-42  -0.269D-42  -0.269D-42  -0.269D-42  -0.269D-42
 -0.269D-42  -0.269D-42  -0.269D-42  -0.269D-42  -0.215D-08  -0.269D-42  -0.269D-42  -0.269D-42  -0.572D-09  -0.239D+00

      9  0.0         0.514D-11  0.353D-03  0.499D-03  0.611D-03  0.706D-03  0.789D-03  0.864D-03  0.933D-03  0.998D-03  [illegible]
         0.112D-02   0.117D-02  0.122D-02  0.127D-02  0.132D-02  0.137D-02  0.141D-02  0.145D-02  0.150D-02  0.153D-02  0.153D-0[illegible]
     10  0.347D+00   0.347D+00  0.347D+00  0.347D+00  0.347D+00  0.347D+00  0.347D+00  0.347D+00  0.347D+00  0.347D+00  [illegible]
         0.347D+00   0.347D+00  0.347D+00  0.347D+00  0.347D+00  0.347D+00  0.347D+00  0.347D+00  0.350D+00  0.366D+00  [illegible]
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MASS FRACTIONS,ENTHALPY,TEMP,F/A EQUIV RATIO,CELL LOADING EMV (KG/M 3-S), CELL RES TIME

STA.	CH2 NO	CH3 NO2	CH4 N2	HCO N2O	CH2O O	CO OH	CO2 O2	H H (J/KG)	H2 T (K)	H2O EQ RATIO	HO2 KG/M3-S	M RES (S)
1	0.0	0.0	1.000D+00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-2.290D+06	1.000D+03	1.000D+06	0.0	0.0
2	0.0	0.0	1.000D+00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-2.290D+06	1.000D+03	1.000D+06	0.0	1.000D+06
3	0.0	0.0	1.000D+00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-2.290D+06	1.000D+03	1.000D+06	0.0	1.000D+06
4	0.0	0.0	1.000D+00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-2.290D+06	1.000D+03	1.000D+06	0.0	1.000D+06
5	0.0	0.0	1.000D+00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-2.290D+06	1.000D+03	1.000D+06	0.0	1.000D+06
6	0.0	0.0	1.000D+00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-2.290D+06	1.000D+03	1.000D+06	0.0	1.000D+06
7	0.0	0.0	1.000D+00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-2.290D+06	1.000D+03	1.000D+06	0.0	1.000D+06
8	0.0	0.0	1.000D+00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-2.290D+06	1.000D+03	1.000D+06	0.0	1.000D+06

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  9  0.0        0.0        1.000D+00  0.0        0.0        0.0        0.0         0.0        0.0        0.0        0.0        0.0
     0.0        0.0        0.0        0.0        0.0        0.0        0.0        -2.229D+06  1.000D+03  1.000D+06  0.0        1.000D+06
 10  0.0        0.0        1.000D+00  0.0        0.0        0.0        0.0         0.0        0.0        0.0        0.0        0.0
     0.0        0.0        0.0        0.0        0.0        0.0        0.0        -2.229D+06  1.000D+03  1.000D+06  0.0        1.000D+06
 11  0.0        0.0        1.000D+00  0.0        0.0        0.0        0.0         0.0        0.0        0.0        0.0        0.0
     0.0        0.0        0.0        0.0        0.0        0.0        0.0        -2.229D+06  1.000D+03  1.000D+06  0.0        1.000D+06
 12  0.0        0.0        1.000D+00  0.0        0.0        0.0        0.0         0.0        0.0        0.0        0.0        0.0
     0.0        0.0        0.0        0.0        0.0        0.0        0.0        -2.229D+06  1.000D+03  1.000D+06  0.0        1.000D+06
 13  0.0        0.0        1.000D+00  0.0        0.0        0.0        0.0         0.0        0.0        0.0        0.0        0.0
     0.0        0.0        0.0        0.0        0.0        0.0        0.0        -2.229D+06  1.000D+03  1.000D+06  0.0        1.000D+06
 14  0.0        0.0        1.000D+00  0.0        0.0        0.0        0.0         0.0        0.0        0.0        0.0        0.0
     0.0        0.0        0.0        0.0        0.0        0.0        0.0        -2.229D+06  1.000D+03  1.000D+06  0.0        1.000D+06
 15  0.0        0.0        1.000D+00  0.0        0.0        0.0        0.0         0.0        0.0        0.0        0.0        0.0
     0.0        0.0        0.0        0.0        0.0        0.0        0.0        -2.229D+06  1.000D+03  1.000D+06  0.0        1.000D+06
 16  0.0        0.0        1.000D+00  0.0        0.0        0.0        0.0         0.0        0.0        0.0        0.0        0.0
     0.0        0.0        0.0        0.0        0.0        0.0        0.0        -2.229D+06  1.000D+03  1.000D+06  0.0        1.000D+06
 17  0.0        0.0        1.000D+00  0.0        0.0        0.0        0.0         0.0        0.0        0.0        0.0        0.0
     0.0        0.0        0.0        0.0        0.0        0.0        0.0        -2.229D+06  1.000D+03  1.000D+06  0.0        1.000D+06
 18  0.0        0.0        1.000D+00  0.0        0.0        0.0        0.0         0.0        0.0        0.0        0.0        0.0
     0.0        0.0        0.0        0.0        0.0        0.0        0.0        -2.229D+06  1.000D+03  1.000D+06  0.0        1.000D+06
 19  0.0        0.0        1.000D+00  0.0        0.0        0.0        0.0         0.0        0.0        0.0        0.0        0.0
     0.0        0.0        0.0        0.0        0.0        0.0        0.0        -2.229D+06  1.000D+03  1.000D+06  0.0        1.000D+06
 20  0.0        0.0        1.000D+00  0.0        0.0        0.0        0.0         0.0        0.0        0.0        0.0        0.0
     0.0        0.0        0.0        0.0        0.0        0.0        0.0        -2.229D+06  1.000D+03  1.000D+06  0.0        1.000D+06
 21  0.0        0.0        6.870D-01  0.0        0.0        0.0        0.0         0.0        0.0        0.0        0.0        0.0
     0.0        0.0        2.460D-01  0.0        0.0        0.0        7.290D-02  -1.340D+06  1.000D+03  3.760D+01  0.0        1.000D+06
 22  0.0        0.0        0.0        0.0        0.0        0.0        0.0         0.0        0.0        0.0        0.0        0.0
     0.0        0.0        7.670D-01  0.0        0.0        0.0        2.330D-01   7.530D+05  1.000D+03  0.0        0.0        0.0

ISTEP=    2 IAX=    0 IEND=    0 IOUT=    0 KIN= 3 KEX= 2 DX=  0.292D-06 PSII=  0.0        PSIE=  0.799D-07
RMI=  0.0        RME= -0.274D-02 PEI=  0.799D-07
XU=  0.649D-06 UFLUX= -0.913D-08 PRESSU=  0.0           AEAU=  0.0        FLUX(J)=
 -0.269D-42  -0.269D-42   0.496D-08  -0.269D-42  -0.269D-42  -0.269D-42  -0.269D-42  -0.269D-42  -0.269D-42  -0.269D-42
 -0.269D-42  -0.269D-42  -0.269D-42  -0.269D-42  -0.215D-08  -0.269D-42  -0.269D-42  -0.269D-42  -0.572D-09  -0.235D+00

      9  0.0        0.160D-09  0.355D-03  0.501D-03  0.614D-03  0.709D-03  0.793D-03  0.868D-03  0.938D-03  0.100D-02  0.106D-02
         0.112D-02  0.118D-02  0.125D-02  0.128D-02  0.133D-02  0.137D-02  0.142D-02  0.146D-02  0.150D-02  0.154D-02  0.155D-02
     10  0.347D+00  0.347D+00  0.347D+00  0.347D+00  0.347D+00  0.347D+00  0.347D+00  0.347D+00  0.347D+00  0.347D+00  0.347D+00
         0.347D+00  0.347D+00  0.347D+00  0.347D+00  0.347D+00  0.347D+00  0.347D+00  0.348D+00  0.358D+00  0.410D+00  0.465D+00

   MASS FRACTIONS,ENTHALPY,TEMP,F/A EQUIV RATIOCELL LOADING EMV (KG/M 3-S), CELL RES TIME

 STA. CH2        CH3        CH4        HCO        CH2O       CO         CO2         H          H2         H2O        HO2        W
      NO         NO2        N2         N2O        O          OH         O2          H (J/KG)   T (K)      EQ RATIO   KG/M3-S    RES T (S)

  1  0.0        0.0        1.000D+00  0.0        0.0        0.0        0.0         0.0        0.0        0.0        0.0        0.0
     0.0        0.0        0.0        0.0        0.0        0.0        0.0        -2.229D+06  1.000D+03  1.000D+06  0.0        0.0
  2  0.0        0.0        1.000D+00  0.0        0.0        0.0        0.0         0.0        0.0        0.0        0.0        0.0
     0.0        0.0        0.0        0.0        0.0        0.0        0.0        -2.229D+06  1.000D+03  1.000D+06  0.0        [illegible]
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C-2