A HYBRID COMPUTER PROGRAM FOR RAPIDLY SOLVING FLOWING OR STATIC CHEMICAL KINETIC PROBLEMS INVOLVING MANY CHEMICAL SPECIES

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A hybrid chemical kinetic computer program has been assembled which provides a rapid solution to problems involving flowing or static, chemically reacting, gas mixtures. The computer program uses subroutines from the program of NASA TN D-6586 for problem setup, initialization, and preliminary calculations and incorporates the stiff ordinary differential equation solution technique of C. W. Gear.

A number of the check cases presented in NASA TN D-6586 were recomputed with the hybrid program and the results were almost identical to the results published in NASA TN D-6586. The computational time saving is demonstrated with a propane-oxygen-argon shock tube combustion problem involving 31 chemical species and 64 reactions. This case yielded comparable results and a computational time almost an order of magnitude lower than that for the program of NASA TN D-6586. Information is presented in the appendixes to enable potential users to prepare an input data deck for the calculation of a problem.

Chemical kinetics
Shock waves
Combustion
Gas phase reactions

Subject Category 25

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A HYBRID COMPUTER PROGRAM FOR RAPIDLY SOLVING FLOWING OR STATIC CHEMICAL KINETIC PROBLEMS INVOLVING MANY CHEMICAL SPECIES

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SUMMARY

A hybrid chemical kinetic computer program has been assembled which provides a rapid solution to problems involving flowing or static, chemically reacting, gas mixtures. The computer program makes use of subroutines from the program of NASA TN D-6586 for problem setup, initialization, and preliminary calculations. However, the method of solution of the resulting ordinary differential equations is that presented by C. W. Gear. The Gear numerical solution technique uses a highly efficient strategy in altering step size and order in combination with an extensive history array to achieve a stable, rapid solution to a problem involving a number of stiff simultaneous differential equations. Therefore, the chief advantage of using the hybrid program of this paper instead of the program of NASA TN D-6586 is realized when the reacting system contains more than 15 different chemical species, although the use of the program for a smaller number of reacting species does not penalize the user with respect to computational time.

A number of the check cases presented in NASA TN D-6586 were recomputed with the hybrid program and the results were almost identical to the results published in NASA TN D-6586. The saving in computational time is demonstrated with a propane-oxygen-argon shock tube combustion problem which involves 31 chemical species and 64 reactions. This case yielded comparable results between the hybrid program and the program of NASA TN D-6586; however, the computational time for the program of this paper was almost an order of magnitude lower than that for the program of NASA TN D-6586.

INTRODUCTION

Recent interest in problems associated with energy conservation and pollution abatement has led to increased use of computer codes to study kinetically controlled chemical reactions in the combustion processes of static and flowing hydrocarbon fuel. In energy-associated research, if a set of realistic kinetic steps is given, simulation of combustion

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processes could be studied by a variation of input parameters to find the conditions that would provide optimum extraction of energy from a fuel. In pollution research, the conditions where pollutant levels would be reduced could be studied with some insurance that the predicted changes would actually result. Sets of kinetic steps, or reaction mechanisms, which adequately describe the chemical processes appear to grow longer as the fuels increase in molecular weight. At present, only the reaction mechanism for the oxidation of the smallest hydrocarbon, methane, is understood sufficiently to allow a reliable prediction of product distribution during combustion. A recently published reaction mechanism for methane (ref. 1) contains over 20 reactions and approximately 15 species. Higher molecular weight hydrocarbons, such as propane and eventually heptanes, octanes, and other constituents of present fuels, will require many more species and reactions to describe their combustion behavior. Each additional species adds to the computational difficulties associated with solving the differential equations in the mathematical model of the reacting system.

The differential equations become "stiff" because so many of their terms change very rapidly at the same time other terms are hardly changing at all. This stiffness is a local situation and may occur in some regions of the independent variable but not in other regions. The stiffness causes many finite-difference solution procedures to fail unless the increment of the independent variable is reduced significantly in size. The reduced step size, although needed only in certain regions of the independent variable, increases the computational time for a solution over the entire range of the independent variable. Therefore, most computer programs using finite-difference techniques automatically vary increment size in regions where the equations become stiff. The chemical kinetic computer program of reference 2 uses such a strategy for varying increment size to achieve a more efficient use of computer time. However, as the number of equations increase, the strategy and numerical technique used by the program of reference 2 become less efficient and the computational time increases dramatically. For these reasons, a solution technique which was derived specifically for stiff systems of equations was sought.

A hybrid chemical kinetic computer program has been assembled which provides a rapid solution to problems associated with flowing or static, chemically reacting, gas mixtures. The program is designated as hybrid because it combines the desirable portions of two existing and well-documented computer programs. The program uses subroutines from the computer program of reference 2 for problem setup, initialization, and preliminary calculations with the solution technique presented in references 3 and 4. The listing of the resulting computer program is presented in this report. Several of the check cases presented in reference 2 have been computed with the program of this report and the computed results and computational times are compared. To illustrate the savings in computational time for a calculation involving a large number of chemical species, the computed results for the stoichiometric combustion of a propane, oxygen, and argon
mixture in a shock tube obtained by using the hybrid program and the program of reference 2 are compared. Information is presented to enable possible users to calculate a specific problem.

SYMBOLS

A  area, m²

species production function described in equation (5), sec⁻¹

enthalpy production function described in equation (6), sec⁻¹

specific heat at constant pressure

\[ f_i = \frac{dy_i}{dt} \]

enthalpy of species \( i \)

Mach number, \( \sqrt{\frac{V^2 M_w}{\gamma RT}} \)

molecular weight

pressure of gas mixture, atm

universal gas constant

temperature, K

time

initial time

velocity

net species production rate, moles/vol·sec

general dependent variable

initial value of dependent variable
\[ \gamma \quad \text{specific heat ratio,} \quad \frac{C_p}{C_p - \frac{R}{M_w}} \]

\[ \rho \quad \text{density} \]

\[ \sigma_i \quad \text{concentration, moles of species } i \text{ per unit mass of mixture} \]

**DIFFERENTIAL EQUATIONS FOR CHEMICALLY REACTING, FLOWING OR STATIC SYSTEM**

The computer program of this paper, as indicated, is a hybrid combination of two existing and well-documented computer programs. This hybrid program uses the subroutines of reference 2 for setting up the system of differential equations for a specific flowing or static, chemically reacting problem. The system of differential equations is then solved by using subroutines from reference 3 based on the methods developed in reference 4.

The system of equations may be derived with respect to either time or distance and may have either assigned area or pressure profiles. For example, the differential equations which must be solved with respect to time for a one-dimensional steady-state flow through an arbitrary assigned area profile would be

\[ \frac{d\sigma_i}{dt} = \frac{w_i}{\rho} \quad (i = 1, 2, \ldots, N) \quad (1) \]

\[ \frac{dV}{dt} = \frac{V}{M^2 - 1} \left( \frac{1}{A} \frac{dA}{dt} - \mathcal{A} \right) \quad (2) \]

\[ \frac{dp}{dt} = -p \left[ \frac{M^2}{M^2 - 1} \left( \frac{1}{A} \frac{dA}{dt} - \mathcal{A} \right) + \mathcal{A} \right] \quad (3) \]

\[ \frac{dT}{dt} = -T \left[ \frac{(\gamma - 1)M^2}{M^2 - 1} \left( \frac{1}{A} \frac{dA}{dt} - \mathcal{A} \right) + \mathcal{B} \right] \quad (4) \]

where

\[ \mathcal{A} = \frac{RT}{p} \sum_{i=1}^{N} w_i - \mathcal{B} \quad (5) \]

and

\[ \mathcal{B} = \frac{1}{p} \frac{\gamma - 1}{\gamma} \sum_{i=1}^{N} h_i w_i \quad (6) \]
This relationship represents a system of \( N + 3 \) equations with \( N + 3 \) unknowns (where \( N \) is the number of species in the system). Problems with distance as the independent variable would yield a similar system of \( N + 3 \) equations. If the assigned variable were pressure, \( N + 3 \) equations with respect to time or distance would also be possible. Reference 2 offers a complete derivation of the different systems of equations.

**SOLUTION OF DIFFERENTIAL EQUATIONS**

The system of equations derived for the particular problem described in the previous section forms a nonlinear, coupled set of differential equations which can be represented in the following form:*\n
\[
\frac{dy_i}{dt} = f_i\left(t, y_1, \ldots, y_N\right) \quad (i = 1, 2, \ldots, N)
\] (7)

The equations in this form can be solved by using a numerical solution technique. The subroutine package from reference 3 provides the user with two basically different methods for the solution of such a system of equations. The two basic methods are (1) the Adams implicit methods and (2) the stiffly stable, linear multistep methods of Gear. If the system of equations is not considered to be excessively stiff, the Adams methods may be used to solve the problem efficiently. However, if the problem is judged to be stiff (a condition which may be aggravated by considering a large number of additional equations inherent with the consideration of additional chemical species), the Gear methods should be used. With these methods, the incremental step size is restricted to small values, because of accuracy requirements, only where the solution is active. In this region accuracy is achieved by varying both step size and order of the method of solution. The step sizes in regions of stiffness are unrestricted because of small time constants until the terms become active again. This condition requires that the method be implicit and a system of generally nonlinear equations be solved at each step. For a detailed discussion of the mathematical derivation of this solution technique, reference 4 should be obtained. Reference 3 provides additional information about the method of Gear and is linked directly to the developed subroutine package.

Since the subroutines presented in reference 3 are user-oriented, a reiteration of the mathematical development is not believed to be justified. If equations (1) to (4) are given in the general form of equation (7) with an initial value of the vector \( y(t_0) = y_0 \) and

*\( \text{(Here } i \text{ refers to a particular dependent variable } y, \text{ and } N \text{ is the total number of equations in which the variable } y \text{ changes with the independent variable } t. \text{ Specifically, } y_1, y_2, \text{ and } y_3 \text{ are } V, \rho, \text{ and } T, \text{ respectively, and } y_4 \text{ to } y_N \text{ are the total number of chemical species.)} \)
a subroutine for the calculation of $f_k$ values, the subroutine package of reference 3 computes a numerical solution at values of the independent variable $t$ in intervals desired by the user.

Although the package of subroutines of reference 3 was obtained primarily for the stiffly stable methods of Gear, both the Adams methods and the Gear methods are functional in this program. Comparative calculations which will be performed later in this paper utilize the method of Gear with the internal approximation of the Jacobian by finite differences. The user accessibility to all the methods available with this program is presented in appendix A.

PROGRAM DESCRIPTION

The computer program described in reference 2 has been altered to allow the solution of the differential equations by the methods described in reference 4. The program organization is still very similar to that presented in reference 2. Table I lists the subroutines of the program of reference 2 and describes the type of changes, if any, which were affected.

An overall schematic diagram of the computer program is shown in figure 1 with the Gear package of reference 3 enclosed by the dashed line. The direction of the arrows indicates calls from one routine to another with normal returns from the called routine after completion of its task. The three subroutines numbered (1) GPAK, (2) KINP, and (3) DRIVES indicate the general order followed during the solution of any of the problems which the program can handle. The program starts in subroutine GPAK and calls KINP for reading the input data (reactions, inert species, third body reactants, and namelists), storing thermodynamic data, initializing variables, and performing initial calculations. The equilibrium property calculations are also obtained in the subroutine. This can be seen by observing the subroutines at the left of figure 1. The return to GPAK is followed by printout of preliminary data. Subroutine DRIVES (ref. 3) is then called and control is maintained by DRIVES until the desired interval of the independent variable is achieved.

The flow diagrams for the main program GPAK and the control subroutine DRIVES are presented in figures 2 and 3, respectively. The flow diagram for subroutine STIFF is shown in figure 4 as it appeared in reference 3 to allow the reader to follow its logic. Subroutine DRIVES calls subroutine STIFF to obtain a solution for the system of differential equations for each increment of the independent variable. After each successful step, DRIVES regains control and calls for output of the calculated data. If printout is desired at specific locations of the independent variable, subroutine YOUT is called for calculation of the dependent variables at the print location through interpolation of the history array.
<table>
<thead>
<tr>
<th>Subroutines from program of reference (2)</th>
<th>Alteration performed</th>
</tr>
</thead>
<tbody>
<tr>
<td>GCKP</td>
<td>1. All monitoring of integration removed.</td>
</tr>
<tr>
<td>KINP</td>
<td>2. Calls for output removed.</td>
</tr>
<tr>
<td>CIMAGE</td>
<td>3. Problem control yielded to subroutine DRIVES of reference 3 for looping and error treatment coding.</td>
</tr>
<tr>
<td>NAMBLK</td>
<td>4. Subroutine renamed GPAK.</td>
</tr>
<tr>
<td>BLCK</td>
<td>Minor modifications as to variable initialization and printout scheme setup. In OUTP printing format changed to conserve paper.</td>
</tr>
<tr>
<td>INIT</td>
<td>No changes made.</td>
</tr>
<tr>
<td>OUTF</td>
<td>Combined and renamed DIFFUN. Internal changes made for updating dependent variables at print location without altering array values for continuation of problem after printing.</td>
</tr>
<tr>
<td>COMB</td>
<td>Renamed PEDERV.</td>
</tr>
<tr>
<td>SHOK</td>
<td>No changes made.</td>
</tr>
<tr>
<td>SHOCKS</td>
<td>These subroutines completely removed and replaced with subroutines of reference 3. The subroutines used are YOUT, COSET, YOUTD, DECOMP, DRIVES, SOLVE, STIFF.</td>
</tr>
</tbody>
</table>
The flow diagram for subroutine YOUT is shown in figure 5. Flow diagrams of subroutines DIFFUN (which is a combination of routine PRED and DERV) and PEDERV (which is basically subroutine PARD) can be seen in reference 2.

The resulting modified program is presented in appendix B. Obvious changes in the computer program made to facilitate its use with the Control Data Corporation 6000 Series computers are not enumerated specifically.

The details of program input and error messages are shown in appendix A. The format is the same as that described in reference 2 and its related bulletin.

RESULTS OF CALCULATIONS

Several of the check cases presented in reference 2 were calculated by using the modified program of this paper. For ease of comparison, the results of these calculations for check cases 1, 5, 6, and 8 of reference 2 are shown in appendix C alongside results obtained from the program of reference 2. The comparison for check case 1, which is bromine decomposition in a shock tube, is shown first in appendix C. The input card image and the first page of computer output are shown for the modified program alone to show the similarity with output information shown in appendix E of reference 2. The remaining printout for check case 1 enables the reader to see the closeness of the computed results for species concentrations, temperatures, velocities, densities, etc. The one parameter which shows a difference worth mentioning is the dependent variable (time) for this particular case. An explanation as to the reason for this difference is presented to prevent concern by the reader.

The difference is caused by the fact that the selected step sizes are not the same for both programs. This difference is more easily understood by considering the equation by which the dependent variable is calculated by either program.

Time as dependent variable: For time as a dependent variable,

\[ \text{DVAR} = \text{DVAR} + \frac{2(\text{present step size})}{V_1 + V_2} \]

It is apparent that increments of larger or smaller step size influence the summed DVAR since the average velocity computed is different. Both the program of reference 2 and this program based on different strategies increase the step size automatically. Achieving identical results in DVAR between the two programs is therefore practically impossible.
Distance as dependent variable: For distance as a dependent variable,

\[ \text{DVAR} = \text{DVAR} + \frac{V_1 + V_2}{2} \times \text{(Present step size)} \]

Present step size in time units

Similarly, a different average velocity would have an effect in this dependent variable.

For this one reaction system involving three chemical species, the time for computation is presented at the end of the case in appendix C. The comparison for this case is very close.

Check cases 5 and 6 from reference 2 were run together to test the repeat option. The comparison of the output information is shown in appendix C. As can be seen, the computed times, distances, areas, flow, and chemical properties were very close to the computed quantities obtained by using the program of reference 2. The computational time using the program of this report was roughly one half the time for the program of reference 2. This is presented at the end of both cases in appendix C.

Check case 8 from reference 2 was also computed with both programs and the results are also compared in appendix C. The results were again comparable. The computational time was reduced slightly by using the program of this paper.

The results of the comparisons obtained by computing check cases 1, 5, 6, and 8 of reference 2 by the program of this paper and the program of reference 2 indicate that even for as few as eight species, computational time was reduced. The memory required for the program of this paper was 71100b as compared with 66700b for the program of reference 2. The memory for the program of this report can be reduced somewhat if subroutine PEDERV is made a dummy routine. However, if partial derivatives are to be calculated in PEDERV (an option used if the second digit of MF equals 1), care must be taken to restore the subroutine's computational ability.

As was shown, the program of this report reduced the usage of computer time for systems with few reacting species. Significantly larger savings in computer time can be expected for kinetic problems involving a very large number of chemical species. This is illustrated by the case shown in appendix D. This case involves the shock tube combustion of propane. The mechanism illustrated in appendix D contains 31 different chemical species in 64 reactions. The bulk of this reaction mechanism is from reference 5 by Chinitz and Baurer. The steps for methane combustion were taken from reference 1 and substituted for the appropriate steps in reference 5. This was done primarily because of the correlation of this methane mechanism with experimental shock tube results.

Reaction number 2 in the list of reactions was input to cause some rapid changes in the species concentrations, since it was found that the basic reaction mechanism from reference 5 caused the combustion of propane to proceed very slowly. The thermochemical
The reaction mechanism presented for the combustion of propane was used merely to illustrate the savings in time for a reaction system involving a large number of chemical species. The need for such an extensive list of chemical species and reactions to describe the combustion of a hydrocarbon similar to those in fuels presently used is evident. The trends established in the studies of methane, ethane, ethylene, and acetylene indicate that extensive reaction mechanisms with numerous chemical species will have to be considered.

CONCLUDING REMARKS

A hybrid computer program for solving flowing or static chemical kinetic problems has been assembled from subroutines of NASA TN D-6586 and the subroutine package of the Lawrence Livermore Laboratory Computer document UCID-30001 based on the solution methods presented by C. W. Gear. The resulting computer program has been used to calculate check cases presented in NASA TN D-6586. Comparisons of the check-case results obtained by using the computer program of this paper with those calculated by the program of NASA TN D-6586 have shown a reduction in computer time for equivalent results. For a calculation involving 31 chemical species and 64 reactions, the computer time for using the program of this report was almost an order of magnitude less.

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Hampton, Va. 23665
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APPENDIX A

DETAILS OF PROGRAM INPUT AND ERROR MESSAGES

Input

The first card of an input data deck instructs the computer to read a thermodynamic data file. The word, CARDS or TAPE, indicates where the thermodynamic data are located. The thermodynamic data are read from the input location (cards or tape) and stored on tape unit for subsequent use by the computer program. The first record of the thermodynamic data set specifies the temperature range limits. The rest of the thermodynamic data is composed of four card sets for each chemical species. The first card contains the species name, the names of its chemical elements, their stoichiometric coefficients, and reference information. The remaining three cards contain the curve-fitted polynomial coefficients for the upper and lower temperature ranges. The upper temperature range runs from 1000 K to 5000 K and the lower range runs from 300 K to 1000 K.

The data cards in the order that they appear in the data deck are described in the following sections.

(1) Title – The first card contains a description of the type case to be run. All 80 locations on one card may be used. The title data are read with an alphanumeric format and appear on the first page of output.

(2) Reactions – Chemical reactions are listed one per card. Each card describes the reaction of the type

\[ aA + bB \rightarrow dD + eE \]

where the lower case letters, \( a, b, d, \) and \( e \) are stoichiometric coefficients between 1 and 9 and the capital letters, \( A, B, D, \) and \( E, \) refer to chemical species. To the right of each card, the rate constant parameters are presented. Species \( A \) or \( E \) may be omitted to specify reactions of the types:

(a) Unimolecular decomposition to one or two products

(b) Third-body influenced reactions (where one or two reactants form one or two products with the aid of a third body)

(c) Two reactants forming one product.

The photochemical irreversible decomposition as described in the bulletin of reference 2 can also be used. It is of the form

\[ h\nu + bB \rightarrow dD + eE \]
APPENDIX A

The format for the reaction cards as reprinted from the bulletin of reference 2 is:

<table>
<thead>
<tr>
<th>Card column</th>
<th>FORTRAN format</th>
<th>Content</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>I1</td>
<td>Stoichiometric coefficient of first reactant — default is one</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td>Blank (not read)</td>
</tr>
<tr>
<td>3 to 10</td>
<td>A8</td>
<td>(a) Name of first reactant (left justified) (b) M for third body collision (c) HNU for photochemical reaction</td>
</tr>
<tr>
<td>11</td>
<td></td>
<td>Not read</td>
</tr>
<tr>
<td>12</td>
<td>I1</td>
<td>Stoichiometric coefficient of second reactant (left justified) or first reactant for decomposition</td>
</tr>
<tr>
<td>13</td>
<td></td>
<td>Not read</td>
</tr>
<tr>
<td>14 to 21</td>
<td>A8</td>
<td>Name of second reactant (left justified) — first reactant for decomposition</td>
</tr>
<tr>
<td>22 to 24</td>
<td></td>
<td>Not read</td>
</tr>
<tr>
<td>25</td>
<td>I1</td>
<td>Stoichiometric coefficient for first product</td>
</tr>
<tr>
<td>26</td>
<td></td>
<td>Not read</td>
</tr>
<tr>
<td>27 to 34</td>
<td>A8</td>
<td>Name of first product (left justified)</td>
</tr>
<tr>
<td>35</td>
<td></td>
<td>Not read</td>
</tr>
<tr>
<td>36</td>
<td>I1</td>
<td>Stoichiometric coefficient of second product</td>
</tr>
<tr>
<td>37</td>
<td></td>
<td>Not read</td>
</tr>
<tr>
<td>38 to 45</td>
<td>A8</td>
<td>(a) Name of second product (left justified) (b) M if thick body recombination</td>
</tr>
</tbody>
</table>
APPENDIX A

<table>
<thead>
<tr>
<th>Card column</th>
<th>FORTRAN format</th>
<th>Content</th>
</tr>
</thead>
<tbody>
<tr>
<td>46 to 49</td>
<td></td>
<td>Not read</td>
</tr>
<tr>
<td>50 to 60</td>
<td>E11.4</td>
<td>A factor of rate equation $K = AT^{N-E/RT}$</td>
</tr>
<tr>
<td>61 to 62</td>
<td></td>
<td>Not read</td>
</tr>
<tr>
<td>63 to 70</td>
<td>F8.4</td>
<td>N factor of rate equation</td>
</tr>
<tr>
<td>71 to 72</td>
<td></td>
<td>Not read</td>
</tr>
<tr>
<td>73 to 80</td>
<td>F8.4</td>
<td>$E$, activation energy, cal/mole</td>
</tr>
</tbody>
</table>

The end of the reaction list is signaled by a blank card. The program listed in appendix B is limited to 50 reactions. The dimensions of the program at Langley can be altered quickly, however, by the use of one card with the Control Data UPDATE program management system.

(3) Inert species — A species may be declared inert by placing the species name or names in column 1, 17, 33, or 49 on the next card. A blank card indicates no inert species desired and a blank field after a species name indicates the end of the inert species list.

(4) Version and units — One card specifies the independent variable (time or distance) and the assigned variable (area or pressure). The input and output units may also be specified on this card.

The card punch locations are as follows (from ref. 2):

<table>
<thead>
<tr>
<th>Columns</th>
<th>Contents</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 to 8</td>
<td>Time</td>
<td>Time fundamental variable</td>
</tr>
<tr>
<td></td>
<td>Distance</td>
<td>Distance fundamental variable</td>
</tr>
<tr>
<td>11 to 18</td>
<td>Pressure</td>
<td>Pressure is assigned variable</td>
</tr>
<tr>
<td></td>
<td>Area</td>
<td>Area is assigned variable</td>
</tr>
<tr>
<td></td>
<td>(Blank)</td>
<td>Velocity zero (static case)</td>
</tr>
<tr>
<td>21 to 23</td>
<td>cgs</td>
<td>Input in internal cgs units</td>
</tr>
</tbody>
</table>
### APPENDIX A

<table>
<thead>
<tr>
<th>Columns</th>
<th>Contents</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Blank)</td>
<td>Input in internal units cgs</td>
<td></td>
</tr>
<tr>
<td>fps</td>
<td>Input in fps units</td>
<td></td>
</tr>
<tr>
<td>SI</td>
<td>Input in SI units</td>
<td></td>
</tr>
<tr>
<td>31 to 33</td>
<td>cgs</td>
<td>Output in cgs units</td>
</tr>
<tr>
<td>(Blank)</td>
<td>Output in cgs units</td>
<td></td>
</tr>
<tr>
<td>fps</td>
<td>Output in fps units</td>
<td></td>
</tr>
<tr>
<td>SI</td>
<td>Output in SI units</td>
<td></td>
</tr>
</tbody>
</table>

(5) Controls – The controlling variables are input in NAMELIST PROB and are listed below. Default options are underlined. Most of the variables are the same as listed in reference 2. The variable names followed by (√) will be found only in the program of this paper. The variables deleted from the program are shown as deleted.

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>HMIN</td>
<td>0.0001</td>
<td>Minimum step size in cm or sec</td>
</tr>
<tr>
<td></td>
<td>5.0 \times 10^{-8}</td>
<td>cm (if DISTANCE on version card)</td>
</tr>
<tr>
<td>HMAX</td>
<td>0.1000</td>
<td>Maximum step size</td>
</tr>
<tr>
<td></td>
<td>5.0 \times 10^{-5}</td>
<td>cm (if DISTANCE version)</td>
</tr>
<tr>
<td>HINT</td>
<td>. . . .</td>
<td>No longer input (assumes value of HMIN initially)</td>
</tr>
<tr>
<td>EMAX</td>
<td>0.0001</td>
<td>Maximum error acceptable (becomes EPS in Gear package)</td>
</tr>
</tbody>
</table>
### APPENDIX A

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALLM1</td>
<td>TRUE</td>
<td>Third body efficiencies equal to 1. None input</td>
</tr>
<tr>
<td></td>
<td>FALSE</td>
<td>Third body efficiencies to be input. Those not input remain equal to one</td>
</tr>
<tr>
<td>ELIM</td>
<td>.      . . .</td>
<td>Deleted</td>
</tr>
<tr>
<td>CONC</td>
<td>TRUE</td>
<td>Concentration output as molar concentrations if SI or fps output designated</td>
</tr>
<tr>
<td></td>
<td>FALSE</td>
<td>Mass fractions output if SI or fps output designated</td>
</tr>
<tr>
<td>ITPSZ</td>
<td>1</td>
<td>An area or pressure table input</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>Area or pressure specified by polynomial equation</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>LSUBM and ETA will be input for area equation</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>D, VISC, BETA, and ETA will be input for area equation</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>Zero velocity, no assigned pressure</td>
</tr>
<tr>
<td>IPRCOD</td>
<td>1</td>
<td>Distance against area profile given</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>Distance against pressure profile given</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>Time against area profile given</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>Time against pressure profile given</td>
</tr>
<tr>
<td>XTB</td>
<td>. . . .</td>
<td>Array for time or distance portion of profile, must be in correct user units</td>
</tr>
<tr>
<td>ATB</td>
<td>. . . .</td>
<td>Array for area or pressure profile, must be in user units</td>
</tr>
<tr>
<td>Name</td>
<td>Value</td>
<td>Explanation</td>
</tr>
<tr>
<td>--------</td>
<td>-------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td>NTB</td>
<td></td>
<td>Total entries in area or pressure table, must be less than or equal to 40</td>
</tr>
<tr>
<td>CX3</td>
<td></td>
<td>Coefficient of cubed component of pressure/area polynomial equation</td>
</tr>
<tr>
<td>CX2</td>
<td></td>
<td>Coefficient of squared component of pressure/area polynomial equation</td>
</tr>
<tr>
<td>CX1</td>
<td></td>
<td>Coefficient of pressure/area to the first power in polynomial equation</td>
</tr>
<tr>
<td>CX0</td>
<td></td>
<td>Constant term in pressure/area polynomial equation</td>
</tr>
<tr>
<td>LSUBM</td>
<td></td>
<td>Characteristic shock tube reaction length for special area equation (see ref. 2)</td>
</tr>
<tr>
<td>ETA</td>
<td></td>
<td>Dimensionless exponent in special area equation for boundary layer (see ref. 2)</td>
</tr>
<tr>
<td>D</td>
<td></td>
<td>Hydraulic diameter of shock tube</td>
</tr>
<tr>
<td>VISC</td>
<td></td>
<td>Viscosity coefficient</td>
</tr>
<tr>
<td>BETA</td>
<td></td>
<td>Dimensionless boundary-layer parameter used to calculate LSUBM</td>
</tr>
<tr>
<td>END</td>
<td></td>
<td>Changed from reference 2, must always be input</td>
</tr>
<tr>
<td>DELP</td>
<td></td>
<td>Deleted (from ref. 2)</td>
</tr>
<tr>
<td>PRINT</td>
<td></td>
<td>Deleted (from ref. 2)</td>
</tr>
<tr>
<td>APRINT</td>
<td></td>
<td>Deleted (from ref. 2)</td>
</tr>
<tr>
<td>NPRNTS</td>
<td></td>
<td>Deleted (from ref. 2)</td>
</tr>
</tbody>
</table>
# APPENDIX A

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>EVSTEP</td>
<td>. . . .</td>
<td>Deleted (from ref. 2)</td>
</tr>
<tr>
<td>DEBUG0</td>
<td>FALSE</td>
<td>Changed, prints output parameters in more concise format</td>
</tr>
<tr>
<td></td>
<td>TRUE</td>
<td>Prints format same as reference 2 with exception of derivatives, increment, and relative error information</td>
</tr>
<tr>
<td>PAPS(✓)</td>
<td>FALSE</td>
<td>Program prints at every (5) iterations or number specified by IPRINT</td>
</tr>
<tr>
<td></td>
<td>TRUE</td>
<td>Prints at specific stations specified by END and IDEL or a TPRINT table</td>
</tr>
<tr>
<td>IDEL(✓)</td>
<td>. . . .</td>
<td>Number of increments derived (50 maximum)</td>
</tr>
<tr>
<td>IPRINT(✓)</td>
<td>5</td>
<td>Number specifying integration steps between printing</td>
</tr>
<tr>
<td>TPRINT(✓)</td>
<td>. . . .</td>
<td>Table of 50 values for specifying printing location (filled automatically by specifying IDEL)</td>
</tr>
<tr>
<td>NPRINT(✓)</td>
<td>. . . .</td>
<td>Number of values in TPRINT table</td>
</tr>
</tbody>
</table>
| MF(✓) | 22 | Positive integer specifying method to be used in solving the problem. Composed of two digits  
1st digit – 1 Adams Methods  
2 Gear Methods  
2nd digit – 0 functional iteration  
1 chord method where Jacobian supplied by subroutine PEDERV  
2 chord method where Jacobian approximated internally by finite differences  
3 chord method where Jacobian replaced by diagonal matrix |
APPENDIX A

(See ref. 3 for extensive explanation of mathematics involved in different methods.)

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>COMBUS</td>
<td>TRUE</td>
<td>Perform equilibrium combustion calculation</td>
</tr>
<tr>
<td></td>
<td>FALSE</td>
<td>Do not perform equilibrium combustion calculation</td>
</tr>
<tr>
<td>SHOCK</td>
<td>TRUE</td>
<td>Perform frozen and equilibrium shock calculations</td>
</tr>
<tr>
<td></td>
<td>FALSE</td>
<td>Do not perform shock calculation</td>
</tr>
<tr>
<td>TCON</td>
<td>TRUE</td>
<td>Hold temperature constant</td>
</tr>
<tr>
<td></td>
<td>FALSE</td>
<td>Do not hold temperature constant</td>
</tr>
<tr>
<td>RHOCON</td>
<td>TRUE</td>
<td>Hold volume (density) constant</td>
</tr>
<tr>
<td></td>
<td>FALSE</td>
<td>Do not hold volume (density) constant</td>
</tr>
</tbody>
</table>

(6) Third-body efficiencies – To input third-body efficiencies ALLM1 in NAMELIST PROB must be set to FALSE; otherwise, all efficiencies are equal to one and no cards are needed in this section. The third-body efficiency card format is as follows (from bulletin of ref. 2):

<table>
<thead>
<tr>
<th>Card column</th>
<th>FORTRAN format</th>
<th>Content</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 to 45</td>
<td></td>
<td>Reaction as written in section (2) of this appendix for inputting reactions</td>
</tr>
<tr>
<td>46 to 48</td>
<td></td>
<td>Not read</td>
</tr>
<tr>
<td>49 to 56</td>
<td>A8</td>
<td>Name of species to be assigned third body ratio other than unity</td>
</tr>
<tr>
<td>57</td>
<td></td>
<td>Not read</td>
</tr>
<tr>
<td>58 to 63</td>
<td>F6.3</td>
<td>Efficiency ratio for species in columns 49 to 56</td>
</tr>
<tr>
<td>64 to 65</td>
<td></td>
<td>Not read</td>
</tr>
</tbody>
</table>
APPENDIX A

<table>
<thead>
<tr>
<th>Card column</th>
<th>FORTRAN format</th>
<th>Content</th>
</tr>
</thead>
<tbody>
<tr>
<td>66 to 73</td>
<td>A8</td>
<td>Name of species to be assigned third body ratio other than unity</td>
</tr>
<tr>
<td>74</td>
<td></td>
<td>Not read</td>
</tr>
<tr>
<td>75 to 80</td>
<td>F6.3</td>
<td>Efficiency ratio for species in columns 66 to 73</td>
</tr>
</tbody>
</table>

The end of the list of third-body efficiencies is signaled by a blank card following the last efficiency card.

(7) Initial conditions – The initial conditions for a problem are input through NAMELIST START. The parameters are as follows:

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time</td>
<td></td>
<td>Time in seconds</td>
</tr>
<tr>
<td></td>
<td>0.</td>
<td>For default</td>
</tr>
<tr>
<td>X</td>
<td></td>
<td>Distance</td>
</tr>
<tr>
<td></td>
<td>0.</td>
<td>For default</td>
</tr>
<tr>
<td>MACH</td>
<td></td>
<td>Mach number</td>
</tr>
<tr>
<td></td>
<td>0.</td>
<td>For default</td>
</tr>
<tr>
<td>U</td>
<td></td>
<td>Velocity</td>
</tr>
<tr>
<td>RHO</td>
<td></td>
<td>Density</td>
</tr>
<tr>
<td>T</td>
<td></td>
<td>Temperature</td>
</tr>
<tr>
<td>Area</td>
<td></td>
<td>Area for a flow calculation</td>
</tr>
<tr>
<td>MDOT</td>
<td></td>
<td>Mass flow rate for a flow calculation</td>
</tr>
<tr>
<td>MM Hg</td>
<td>TRUE</td>
<td>Pressure input in mm of mercury</td>
</tr>
<tr>
<td></td>
<td>FALSE</td>
<td>Pressure input in user's choice of input units</td>
</tr>
</tbody>
</table>
APPENDIX A

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOLEF</td>
<td>TRUE</td>
<td>Mole fractions input</td>
</tr>
<tr>
<td></td>
<td>FALSE</td>
<td>Mass fractions input</td>
</tr>
</tbody>
</table>

The starting mixture is input as mole fraction or mass fraction of the individual component species. The sum of the individual species mass fractions or mole fraction must be one.

(8) Permanently neglected species – The program of this paper does not neglect species from error consideration, and no cards from this section are necessary.

(9) Final card – The word FINIS in columns 1 to 5 designates that the input data list for a particular case is complete.

As can be seen there are very few new input variables and the input data deck structure is very near that described in reference 2. Multiple cases can be run as described in reference 2.

Error Messages

The error messages built into the program are listed in the following section; their meanings are indicated.

The subroutine where the error was printed is also indicated. There are 16 remaining from the original program of reference 2 and 6 from the Gear package of reference 3. They are as follows:

Main Program GPAK:

(1) End of this case – read data for next case.
Normal end of case reached.

(2) A fatal error has occurred – case terminated.
Indicates that an unrecoverable error has occurred during the call to subroutine KINP and the logical variable NEXT has been set true. This message will be preceded by message from subroutine KINP and the subroutines KINP calls.

Subroutine KINP:

(3) The input reaction list does not contain the reaction (- + - = - + -).
Indicates error made in specifying third-body ratio information or during multiple case execution.

(4) The master species list does not contain the species . . . .
Indicates that the printed species is not in the master species list, ALSP in BLOCK DATA.
APPENDIX A

(5) The input species list does not contain the species . . . .
    Indicates an error in entering third-body efficiencies.

(6) Invalid input composition  Sum = x.xxxx.
    Indicates input composition does not sum to one.

Subroutine SHOCKS:

(7) Equilibrium shock calculation failed.
    Indicates iteration of equilibrium shock equations failed to converge.

(8) Frozen shock calculation failed.
    Indicates iteration of frozen shock equations failed to converge.

Subroutine EQLBRM:

(9) Derivative matrix singular.
    Indicates a singular derivative matrix encountered during an equilibrium calculation.

(10) Singular matrix.
    Indicates a singular matrix encountered in an equilibrium calculation.

(11) XX iterations did not satisfy convergence requirements.
    Indicates iteration of equilibrium equations failed to converge.

(12) Restart.
    Indicates equilibrium calculation restarted.

Subroutine OUTP:

(13) Invalid composition.
    Indicates that mass fractions do not sum to one.

Subroutine DIFFUN:

(14) Warning Mach number – x.xxx is approaching 1.0.
    Indicates that for assigned area calculations numerical problems could be encountered if the Mach number is between 0.9 and 1.1.

Subroutine THRHM:

(15) Error  T = xxxx.xx  is out of range.
    Indicates a temperature above the range of the thermodynamic data has been submitted to THRHM for calculation of properties.

(16) Warning  T = xxxx.xx  is out of range extrapolated values returned.
    Indicates a temperature below the range of the thermodynamic data has been submitted to THRHM for calculation of properties.
A number of error messages may be printed if an error condition is encountered in subroutine STIFF. These messages are output as follows from Hollerith format contained in DRIVES.

(17) KFLAG = -1 from STIFF at T = xxxx.xx
    Error test failed with ABS (H) = HMIN
    H has been reduced to 0.xxxx and STEP will be retried.
    This message is encountered often at the start of a problem if HMIN (which
is the initial step size) is too large. After 10 reductions of 10 orders of
magnitude in step size, and the error condition still exists, the next message
is printed.

PROBLEM APPEARS UNSOLVABLE WITH GIVEN INPUT
    At this point, the user may elect to retry the problem with a much smaller
HMIN.

(18) KFLAG = -2 from STIFF at T = xxxx.xx H = 0.xxxx
    The requested error is smaller than can be handled.

    At this point, subroutine YOUTD is called and intermediate printout can be used to enable
    the user to decide on his next course of action — perhaps relax the relative error require-
ments. Subroutine YOUTD may be changed by the user to provide the variables he wishes
    to view.

(19) KFLAG = -3 from STIFF at T = xxxx.xx
    Corrector convergence could not be achieved.

    This error message will be followed by the messages in section 1 and ultimately the
user may be required to alter the program internally if a solution with the present input
is desired.

(20) Illegal Input EPS LE 0
    Indicates the maximum error is zero or negative.

(21) Illegal Input N LE 0
    Indicates the number of equations to be solved is zero or negative.

(22) Illegal Input (TO - TLAST) * HO GE 0.
    Indicates that initial time or distance is greater or equal to final time or
distance
    or
    initial step to be taken in a negative direction
    or
    the final time is negative.

Error messages (20), (21), and (22) are the results of faulty input and may be
corrected easily by retyping the pertinent variable value on the input cards.
APPENDIX B

HYBRID PROGRAM LISTING

The entire hybrid program listing is contained herein.

PROGRAM GPKIINPUT, OUTPUT, TAPE5=INPUT, TAPE6=OUTPUT, TAPE4, TAPE7
C***********************************************************************
C**** THIS PROGRAM HAS BITTKERS INPUT AND OUTPUT WITH THE GEAR
C**** PACKAGE USED FOR INTEGRATION.
C***********************************************************************
LOGICAL NEXT
LOGICAL KTCON
LOGICAL KUP
DIMENSION Y(28,13), YDOT(56)
COMMON/GJUNK/TLAST
COMMON/CONO/OUM1(51,XI28), DUM2(2), NEXT
COMMON/STCOM1/N, T, H, HMIN, HMAX, EPS, MF, KFLAG, JSTART
COMMON/KTCON
COMMON/UPOT/KUP
C READ AND CONVERT INPUT, PERFORM PRE-KINETIC CALCULATIONS
CALL KINP
1 IF (NEXT) GO TO 1000
C PRINT REACTIONS, ASSIGNED VARIABLE PROFILE, INTEGRATION CONTROLS
CALL OUT1
C COMPUTE (NON-INPUT) INITIAL CONDITIONS
DO 17 I=1,56
   YDOT(I) = 0.
17 CONTINUE
METH = MF/10
DO 19 I=1,28
   DO 15 J=1,13
      Y(I,J) = 0.
15 CONTINUE
DO 20 I=1,N
   Y(I,1) = X(I)
20 CONTINUE
IFN = 0
NPEOV = 0
K2 = 0
IF (METH .EQ. 1) GO TO 23
K2=6
23 CONTINUE
KTCON = .FALSE.
CALL DIFFUN(N, T, Y, YDOT, IFN, NPEOV, K2)
KTCON = .FALSE.
C PRINT ALL INITIAL CONDITIONS
CALL OUT2
IF INEXT GO TO 1000
CALL DRIVES(N, T, TLAST, V, HMIN, EPS, MF, KFLAG, K2)
IF (KFLAG .EQ. -4) NEXT = .TRUE.
IF (NEXT) GO TO 1000
100 WRITE (6,101)
101 FORMAT (7HAPPENDIX B, 5X, END OF THIS CASE — READ DATA FOR NEXT CASE
   *SE;
   GU TO 13
1000 WRITE (6,1001)
1001 FORMAT (7HAPPENDIX B, 5X, FATAL ERROR HAS OCCURRED — CASE TERMINATED
   *ATED)
13 CONTINUE
CALL RINP
GO TO 1
END
SUBROUTINE KINP

C INPUT CAN BE ACCEPTED IN (1) INTERNAL (CGS) UNITS, (2) FPS UNITS,
C (3) SI UNITS

C THE FOLLOWING UNITS ARE USED INTERNALLY
C * DISTANCE CM
C * AREA CM²
C * MASS FLOW RATE GM/SEC
C * PRESSURE ATM
C * TIME SEC
C * VELOCITY CM/SEC
C * DENSITY GM/CC
C * TEMPERATURE DEG K
C * CONCENTRATION MOLE(I)/MASS

C INTERNAL CORRESPONDENCE
C * DVAR - DEPENDENT VARIABLE
C * IVAR - INDEPENDENT VARIABLE
C * AVAR - ASSIGNED VARIABLE

C THE FOLLOWING LOGICAL TAPE UNITS ARE REQUIRED
C * LTHM (4) - FOR THERMODYNAMIC DATA
C * DAT (5) - FOR TEMPORARY STORAGE OF DATA CARDS
C LOGICAL TAPE UNIT ASSIGNMENTS ARE SPECIFIED IN *NAM8LK*

C THE STOICHIOMETRIC COEFFICIENT OF A
C REACTANT (LEFT HAND SIDE) IS NEGATIVE
C PRODUCT (RIGHT HAND SIDE) IS POSITIVE

LOGICAL ALLM1, CONC, DBUGO, EXCHR, MELEF, MMHG, NEXT
LOGICAL COMBUS, RHCON, SHOCK, TCON
LOGICAL PAPS

INTEGER STOIC

REAL MDIT, IVAR, M, N, NSUBM, MIXMH, M2, NEW

DIMENSION ISTOICI(4)
DIMENSION ISSI(25), TBR(3), TMC(7, 2)
DIMENSION SP(4), DP(4), SPP(2, DSPP(2), SMNM(28), DSNM(28)
DIMENSION LK(4), SUBS(4), GL(25, 4), CN(4, 25), C(25), CX(4)
DIMENSION CJA(2), FJA(2), SUA(2), CUI(1, 2), CUP2(2), SUP1(12), SUP2(12)
DIMENSION LMT(4), SUBS(14), C(25), CX(4)
DIMENSION CJA(2), FJA(2), SUA(2), CUI(1, 2), CUP2(2), SUP1(12), SUP2(12)
COMMON/TUS/LTHM,DAT,NBLANK,NPHOTO
COMMON/DPST/VERS1, T1MEV, VERSA, AREAV, TCON, RHCON, IPACOD
COMMON/COND/VAR, AREA, MDIT, P, IVAR, Y, M, T, SIGMA(25), LSP3, NEXT
COMMON/KRAT1(50), YS(50), EAVT(50), EAVT(50), EAVT(50), ALLM1
COMMON/MVNS(14), TPS1, LSUBM, ETA, V, VISC, BETA
COMMON/SPC, SNAM(31), M(25), SW(25), I(25), STOIC(25)
COMMON/SCON, TPR, HMIN, HMAX, ENA, MF, FFLAG, JSTART
COMMON/FCOFCT(17, 25), FLOW, TMO, TTH
COMMON/XTS(25), TOS(25), TOS(25), TOS(25)
COMMON/SNMM/DLS(75), ALM(75)

COMMON/GR1T/TOT, UNITG, CONG, EXCHR, DELM(50), FPS, SIN, OBUGO
COMMON/GHS/CRT(25), HRT(25), SRT(25), CPR(25), CPRP(25)
COMMON/HECC, REAC, M, M2, GAMMA, TGPA
COMMON/MS/GT, TT, PP, PRO, HRO, ENS, SUN, ESH(25), LGMT(15), BD(15)
COMMON/IN/TP, HP, NLM, NS(1), CONV, KRAT, IMAT
COMMON/SCFS/MSCFCS(4), EQUL1(50), EQUL2(50)
COMMON/SNOB/CXT(40), CXTB(40), NSOB(40)
COMMON/GJUNK/TLAST
COMMON/SECON/IAP1, PAPS
COMMON/PAIN/TPRINT(50), NPRINT, NCON

EQUIVALENCE (1, SIGMA), (SPNM, DSNNM), (SP, DSPP), (SP, DSPP), (SP, SP)
EQUIVALENCE (SP, SUNAM), (TEFF, SPM(26)), (BLANK, SPM(27)),
EQUIVALENCE (MMU, SPM(28)),
EQUIVALENCE (CXX, SPM(29))

DATA CU, F, SU, TZN, 2HFT, 2HM / DATA CUA, HCM**, 1H2, FUA, 4HFT**, 1H2, SUA, 4HMM**, 1H2 / DATA CUP, 1HMM**, 1F, L/CUP, 2HATM, 1H, F/LHBF, 2HAT, 1H2, SU, L/HMM**

DATA NEW, CHANGE, REPEAT, 3HNEW, 4HCHANG, 4HREP,
DATA TAPEND, CARDS, 3HNEW, 4HCRF
EQUIVALENCE (3HNEW, 4HCHANG, 4HREP,
* IPACOD, TP, SG, T, AB, NTB, CXX, CXTB, CXT, JSUBM, ETA, V, VISC, BETA
* CURUSM, SHOCK, TCON, RHCON, NF
* IPRIT
* TPRINT, NPRINT, PAPS, IDEL

C THERMODYNAMIC DATA WILL BE INPUT FROM #UNIT# REWDYN LTHM
READ (9, 99) UNIT
99 FORMAT (30) IF UNIT = NE CARDS GO TO 3
C REWDYN LTHM
READ (9, 98) LTHM, TMO, TTH
98 FORMAT (3P10.3) WRITE (LTHM, 99) TMO, TTH, T
1 READS (9, 97) SPT, LMT(1), SUBS(1), I = 1, 4
97 FORMAT (A, 10K4, 1, A, 4) #END# CARD SIGNALS END OF THERMODYNAMIC DATA IFIPST, EQ. TAPEND GO TO 2

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APPENDIX B

WRITE(LTHM,97) SP,T((LM1(I),SUBS(I),I=1,4))
READ (5,96) ((LTHM(I),I=1,17),I=1,2)
96 FORMAT (2(13,5X,F8.3))
WRITE (LTHM,96) ((LTHM(I),I=1,17),I=1,2)
GO TO 1
2 WRITE(LTHM,97) SP
REWIND LTHM
3 CALL CIMAGE

C READ OUTPUT TITLE
READ (LDA9.99) NAME
ACTION = NEW
GO TO 4

4 ENTRY RINP
NCQ = 0
IDEL = 1
PAPS=.FALSE.
NEXT = .FALSE.
PRINT LTHM
3 CALL CIMAGE

C READ NEW OUTPUT TITLE
READ (LDA9.99) NAME
ACTION = CHANGE
READ SWITCH
READ (LDA9.99) TITLE
READ ACTION
READ (LDA9.99) TITLE
ACTION = CHANGE
READ (LDA9.99) TITLE
ACTION = NEW
GO TO 4

5 NL1=1,25
DO 1=1,25
1 CONTINUE

C INITIALIZE
NEXT = .FALSE.
NL1 = 0
NL2 = 0
LB = 0
L = 0
L = 0
DO 6 = 1,50
6 CONTINUE
NL1 = 0

C SET STANDARD OPTIONS
4 CONC = .TRUE.
EXCHR = .FALSE.
COMBUS = .FALSE.
SHOCK = .FALSE.
TCON = .FALSE.
KCON = .FALSE.
DBUGO = .FALSE.
MF=22
NCQ = 0
IDEL = 1
PAPS = .FALSE.
IPRIT = 5
EMAX = 0.0001
ITPSZ = 5
ALLMI = .TRUE.
DO 5 = 1,25
DO 5 = 1,25
5 M,L,I,J) = 1.

C ADJUST STOICHIOMETRIC COEFFICIENTS
DO 801 1=1,25
801 USTOIC(I,J) = 0
DO 802 1=1,50
802 STQIC(I,J) = 0
CONTINUE

9 IF (ACTION .NE. CHANGE) GO TO 13
C READ REACTION AND (CHANGED) REACTION RATE
10 READ(LOAI.99) LISTOIC(I),SP(I),1=1,41,TA,IN.TEA
95 FORMAT(2(11,1X,A2),(1X,2(11,1X,A2),(11,1X,F8.4))
C BLANK CARD SIGNALS END OF CHANGE REACTION LIST
IF(ISP(I)) .EQ. BLANK) GO TO 12
C ADJUST STOICHIOMETRIC COEFFICIENTS
DO 510 = 1,25
510 CONIINUE
ISTOIC(I) = -ISTOIC(I)
ISTOIC(I) = -ISTOIC(I)
C SEARCH INPUT REACTION LIST
DO 11 J=1,LA
11 CONTINUE

9 IF (ACTION .NE. CHANGE) GO TO 13
APPENDIX B

A(I,J) = TA
N(I,J) = TN
EACT(I,J) = TEA
GO TO 10

11 CONTINUE
C ERROR MESSAGE - NO MATCH FOUND
ISTOCIC(1) = -ISTOCIC(1)
ISTOCIC(2) = -ISTOCIC(2)
WRITE(6,101) (ISTOCIC(I),S,1=1,4)
101 FORMAT ((TH0(KINP)),5X,S55THE INPUT REACTION LIST DOES NOT CONTAIN T
*HE REACTION ,U,1H*.A8,3H = ,U,1H*.A8,3H = ,U,1H*.A8,3H + ,
* U,1H*.A8
NEXT = .TRUE.
GO TO 10

12 READ (LDAT,99) ACTION
13 IF (ACTION .EQ. REPEAT) GO TO 33
14 LSULD = LS
LSELD = LS
C READ (NEW OR ADDED) REACTION AND REACTION RATE
15 READ (LOAD,95) (ISTOCIC(I),S,1=1,4),TA,TEA
C BLANK CARD SIGNALS END OF NEW OR ADDED REACTION LIST
IF (SPI(2) .EQ. BLANK) GO TO 21
C ADJUST STOICHIOMETRIC COEFFICIENTS
DO 515 (=1,4)
IF (ISTOCIC(I) .NE. 0) GO TO 515
IF (SPI(I) .EQ. EFFM) GO TO 19
IF (SPI(2) .EQ. BLANK) GO TO 219
IF (SPI(I) .EQ. HMU) GO TO 319
515 CONTINUE
ISTOCIC(1) = 1
ISTOCIC(2) = -ISTOCIC(2)
LX = LX + 1
ALX(I) = TA
N(LX) = TN
EACT(LX) = TEA
GO TO 20

515 CONTINUE
C MATCH INPUT SPECIES AGAINST INPUT SPECIES LIST
DO 16 I=1,LS
IF (ISP(II) .EQ. 2 .OR. I .EQ. 3) GO TO 215
IF (SPI(I) .EQ. EFFM) GO TO 19
IF (SPI(2) .EQ. BLANK) GO TO 219
IF (SPI(I) .EQ. HMU) GO TO 319
215 IF (LS .EQ. 0) GO TO 17
C MATCH INPUT SPECIES AGAINST MASTER SPECIES LIST
DO 18 I=1,75
IF (DALSP(II) .NE. DSP(I)) GO TO 18
LSRI(I,LR) = II
ISTOCIC(I,LR) = ISTOCIC(I,LR) + ISTOCIC(I)
GO TO 20
16 CONTINUE

C Match INPUT SPECIES AGAINST MASTER SPECIES LIST
17 DO 18 I=1,75
IF (DALSP(II) .EQ. DSP(I)) GO TO 18
LS = LS + 1
LSDRI(U) = LS
ISTOCIC(LS,LR) = ISTOCIC(I)
SPNM(LS) = SPI(I)
MW(LS) = ALMW(II)
ISS(LS) = II
GO TO 20
18 CONTINUE
C ERROR MESSAGE - NO MATCH FOUND
WRITE(6,102) SPI(I)
102 FORMAT ((TH0(KINP)),5X,S55THE MASTER SPECIES LIST DOES NOT CONTAIN T
*HE SPECIES tASI
C ** RUN TERMINATED - ERROR IN INPUT REACTION LIST
STOP

19 LSRI(I,LR) = NTHRD
GO TO 20
219 LSRI(I,LR) = NBLANK
GO TO 20

319 IF (I .EQ. 2) GO TO 320
ISTOCIC(I) = -ISTOCIC(I)
ISTOCIC(2) = -ISTOCIC(2)
WRITE(6,106) (ISTOCIC(I),S1=1,4)
106 FORMAT (*(TH0(KINP)),5X,S55THE INPUT REACTION LIST DOES NOT CONTAIN T
*HE SPECIES tASI
STOP

320 LSRI(I,LR) = NPHOTO
20 CONTINUE
GO TO 15

21 IF (ACTION .EQ. NEW) GO TO 25
C READ INERT SPECIES (1 PER CARD)
22 READ (LOAD,94) SPI(I),S1=1,4
94 FORMAT (4(A8,8X))
DO 29 I=1,4
C BLANK FIELD SIGNALS END OF INERT SPECIES LIST
IF (SPI(I) .EQ. BLANK) GO TO 25
C SEARCH MASTER SPECIES LIST
DO 23 I=1,75
IF (DALSP(II) .EQ. DSP(I)) GO TO 23
LS = LS + 1
SPNM(LS) = SPI(I)
MW(LS) = ALMW(II)
23 CONTINUE
GO TO 15

29 CONTINUE
GO TO 25
APPENDIX B

155(LS) = 11
GO TO 24

23 CONTINUE

C ERROU MESSAGE - NO MATCH FOUND
WRITE(6,102) SPII
NEXT = .TRUE.
LS = LS + 1
ML(LS) = 1.
24 CONTINUE
go to 22

25 IF (LS .EQ. LSOLD) GO TO 30
C GET THERMODYNAMIC COEFFICIENTS FROM TAPE
LSP = LSOLD + 1
II = LSOLD
READ (LTHM,98) TLOW,TMID,THI
26 READ(LTHM,97) SPII
IF(SPII .EQ. TAPEND) GO TO 29
READ (LTHM,96) (THMC(I,K),K=1,7,I=1,2)
DO 28 I=LSP,LSP+L5
IF (DSPNM(I) .NE. OSP(I)) GO TO 28
DO 27 K=1,2
DO 27 K=1,7
27 TCI(K,KK) = THMC(I,KK)
II = II + 1
IF (II .LT. LS) GO TO 26
GO TO 230

29 CONTINUE
GO TO 26
C ERROR MESSAGE - END OF THERMO TAPE REACHED
WRITE 16,103
103 FORMAT (7HOUINPI. 5X.42HEND OF THERMO TAPE - NOT ALL SPECIES FOUND
NEXT = .TRUE.
230 REWIND LTHM

30 LRPI = LSOLD + 1
C GET SPECIES ENTHALPY AT REFERENCE T
TREF = 298.15
CALL THRM (TREF.O.I
TRAL " TREF>1.98716
C COMPUTE HEAT OF REACTION
DO 32 J=1,LR
DELH(J) = 0.
80 READ (LDAT,PROB) M = MMIN
IF (.NOT. PAPS) GO TO 1001
IF (IDEL .EQ. 1) GO TO 1001
PRINT * END/1DEL
DO 1000 I=1,1DEL
PRINT(I) = PRINT(I) + 1
1000 CONTINUE
1001 CONTINUE
PRINT * IDEL
IF (.NOT. ALLM) GO TO 36
DO 77 J=1,25
DO 77 J=1,25
77 M(J,J) = 1 -
GO TO 40
C READ THERM BODIY RATIOS
36 READ(LMAT,91) (ISTOIC(I),SPI(I),I=1,4), (SPP(I),TBRI(I),I=1,2)
91 FORMAT(2I11,1X,8A8,1X,2F9.3,2X,1I8,2X,1F6.3)
C BLANK CARD SIGNALS END OF THIRD BODY RATIO LIST
37 IF (SPI2 .EQ. BLANK) GO TO 40
C ADJUST STOICHIOMETRIC COEFFICIENTS
DO 532 I=1,4
IF (ISTOIC(I) .NE. 0) GO TO 532
IF (ISTOIC(I) .NE. OSP(I)) GO TO 532
IF (SPP(I) .EQ. BLANK) ID = 532
532 CONTINUE
C SEARCH INPUT REACTION LIST
DO 39 J=1,LR
DO 39 J=1,LR
39 M(J,J) = 1 -
GO TO 39
C SEARCH INPUT SPECIES LIST
DO 37 J=1,LR
DO 37 J=1,LR
37 M(J,J) = 1 -
GO TO 37
C RESET STANDARD OPTIONS
LSP = LS + 3
C
APPENDIX B

33 MOLEF = .TRUE.
    MMHG = .FALSE.
C INITIALIZE
END = 0.
NTB = 0
AREA = 0.
MDOT = 0.
P = 0.
V = 0.
RHO = 0.
T = 0.
C READ NAME OF INDEPENDENT VARIABLE, NAME OF ASSIGNED VARIABLE,
C INPUT UNITS, OUTPUT UNITS
READ (LOAF,92) VERSA,UNITV,UNITO
92 FORMAT (4X,4,4X)
    IF (VERSA .EQ. BLANK) VERSA = AREA
C INITIALIZE STEP SIZE LIMITS
    IF (VERSI .EQ. TIMEV) GO TO 70
    HMIN = 0.0001
    HMAX = 0.1000
    IPRCOD = 2
    GO TO 79
70 HMIN = 0.500E-07
    HMAX = 0.500E-04
    IPRCOD = 4
79 IF (VERSA .EQ. AREAV) IPRCOD = IPRCOD + 1
C READ INTEGRATION CONTROLS, PROFILE OPTIONS,
C PRINT OPTIONS, SPECIALTY SWITCHES
37 CONTINUE
C ERROR MESSAGE - NO MATCH FOUND
WRITE(6,104) SPPL(1)
104 FORMAT (7HOUINPI,5X,33HTHE INPUT SPECIES LIST DOES NOT CONTAIN THE
     # SPECIES A,B)
NEXT = .TRUE.
38 CONTINUE
GO TO 36
39 CONTINUE
C SET INITIAL STEP SIZE
48 IF (ITPSZ .GT. 2) GO TO 53
    IF (ITPSZ .EQ. 1 .AND. NIB .EQ. 0) GO TO 53
    IF INTB .NE. 0) NT » NTB
    NZ = NTB
    CONV = 1.
    CON2 = 1.
    IF (VERSA .NE. AREAV) GO TO 203
    XU = CUS
    AUEI1 = CUA(I)
    AUE2 = CUA(2)
C CONVERT AREA PROFILE TO INTERNAL UNITS
    IF (UNITI .NE. FPSI) GO TO 201
    IF (UNIT .EQ. 2) GO TO 202
    IF (UNIT .EQ. 0) NT = NTB
    NZ = NTB
    CONV = 1.
    CONV = 1.
    IF (VERSA .NE. AREAV) GO TO 203
    XU = CUS
    AUEI1 = CUA(I)
    AUE2 = CUA(2)
C CONVERT PRESSURE PROFILE TO INTERNAL UNITS
    IF (UNITI .NE. FPSI) GO TO 201
    IF (UNIT .EQ. 2) GO TO 202
    IF (UNIT .EQ. 0) NT = NTB
    NZ = NTB
    CONV = 1.
    CONV = 1.
    IF (VERSA .NE. AREAV) GO TO 203
    XU = CUS
    AUEI1 = CUA(I)
    AUE2 = CUA(2)
APPENDIX B

```
AUL(1) = FUP(02)
CONV = 30.48
CON = 1./110.2
GO TO 205
204 IF (UNITI .NE. 51) GO TO 205
XU = SU
AUL(1) = SUP(1)
AUL(2) = SUP(2)
CONV = 100.
CON = 1./1.01325E+05
205 IF (.NOT. MMHGI) GO TO 206
AUL(1) = CUP(01)
AUL(2) = CUP(02)
CON = 1./100.2
206 IF (VERSI .EQ. TIMEVI) CONV = 1.
IF (LIPSZ .EQ. 21) GO TO 208
GO 207 = 1.4
LX(01) = LX(01)*CONV
207 CATB(01) = CATB(01)*CON
GO TO 53
208 DO 209 = 1.4
209 CN(01) = CN(01)*CON
CONTINUE
53 CONTINUE
59 IF (LIPSZ .EQ. 11) CALL CUBS (CTXB, CTXB, NT)
   IF (UNITI .NE. FPS) GO TO 63
   CONVERT FROM FPS UNITS TO INTERNAL (CGS) UNITS
   IF (VERSI .NE. TIMEVI) GO TO 60
   DVAR = DVAR*30.48
   GO TO 61
60 IVAR = IVAR*30.48
61 IF (MMHGI) P = P*2.7845
   P = P/110.2
   AREA = AREA*929.0304
   MDDT = MDDT*5.59237
   V = V*30.48
   RHO = RHO/62.43
   T = T/760.
   IF (VERSI .EQ. TIMEVI) GO TO 68
   CEND = UNCEND*30.48
   GO TO 68
63 IF (UNITI .NE. SI) GO TO 67
   CONVERT FROM SI UNITS TO INTERNAL (CGS) UNITS
   IF (VERSI .NE. TIMEVI) GO TO 64
   DVAR = DVAR*100.
   GO TO 65
64 IVAR = IVAR*100.
65 IF (MMHGI) P = P*133.3224
   P = P/1.01325E+05
   AREA = AREA*10000.
   MDDT = MDDT*1000.
   V = V*100.
   RHO = RHO/100.
   T = T/760.
   IF (VERSI .EQ. TIMEVI) GO TO 68
   CEND = UNCEND*100.
   GO TO 68
67 CEND = UNCEND
IF (.NOT. MMHGI) P = P/760.
68 MIXMN = 0.
   IF (.NOT. MLEF) GO TO 71
   MOLE FRACTION TO MOLES(I)/MASS(MIXTURE)
   DO 69 = 1, LS
   MIXMN = MIXMN + C(II)*MM(II)
   GO TO 71
69 SIGMA(II) = C(II)/MIXMN
   GO TO 73
70 SIGMA(II) = C(II)/MIXMN
   GO TO 73
71 DO 72 = 1, LS
   SIGMA(II) = C(II)/MIXMN
   MIXMN = 1/MIXMN
   GO TO 73
C mass fraction to moles(I)/mass(mixture)
72 DO 72 = 1, LS
   SIGMA(II) = C(II)/MIXMN
   MIXMN = 1/MIXMN
   GO TO 73
C universal gas constant in atm-cc/mole-deg K
73 R = 82.056
C universal gas constant in ergs/mole-deg K
74 CPRO = CPRO + CPR(II)*SIGMA(II)
   GAMMA = CPRO/CPR(II) + 1./MIXMN
   IF (V .EQ. 0.1) GO TO 81
   CALL THRM (II, 1.)
   CPRO = 0.
   GO TO 72
   CPRO = CPRO + CPR(II)*SIGMA(II)
   GAMMA = CPRO/CPR(II) + 1./MIXMN
   IF (V .EQ. 0.1) GO TO 81
   CALL THRM (II, 1.)
   CPRO = 0.
61 IF (LIPSZ .EQ. 0.1) GO TO 82
   RHO = RHO/MIXMN
   GO TO 75
82 RHO = RHO/RR*MIXMN
   GO TO 75
```
APPENDIX B

83 IF (IPRCCD .GT. 21) GO TO 84
   X = IVAR
   IF (IVERSI .EQ. TIMEVI) X = DVAR
   CALL CNPI(MATB,CXTB,INT,X,IVAR,DUM1,DUM2)
   GO TO 85
84 TIME = DVAR
   IF (IVERSI .EQ. TIMEVI) TIME = IVAR
   CALL CNPI(MATB,CXTB,INT,TIME,IVAR,DUM1,DUM2)
85 IF (IVERSA .EQ. AREAVI) GO TO 86
   P = DVAR
   GO TO 81
86 AREA = DVAR
   rho = NDOT/CAREA/VI
   GO TO 82
75 IF (MOOT .EQ. 0.) MOOT = rho*AREA/VI
   NO*LSP3
   TLAST>ENO
   IF (.NOT. ICOMBUS .OR. SHOCK!) RETURN
   rho = 0.
   .76 I-LS
   76 rho = rho + HRT(I)*SIGMA(I)
   rho = rho + M2
   2 = V*V/F*MIXM/GAMNA
C EQUILIBRIUM COMBUSTION
   IF (COMBUS) CALL COMB
C EQUILIBRIUM AND FROZEN SHOCK
   IF (SHOCK) CALL SHOCK
   RETURN
END

BLOCK DATA
C ALPHANUMERIC DATA FOR TESTING AND OUTPUT
   COMMON/LTUS/LTHM,LOAT,NTHRD,NBLANK,NPHOTO
   COMMON/OPTS/DUM3,TIME,DUM2,AREA,DUM5
   COMMON/SPEC/SNAM(3),DUM125,FPPS,ST,DUM7
C LOGICAL TAPE UNIT ASSIGNMENTS
   DATA LTHM,LOAT/4,7/
C SPECIES SUBSCRIPTS FOR M,BLANK, AND HNU
   DATA NTHRD,NBLANK,NPHOTO/26,27,28/
C ALPHANUMERIC DATA
   DATA TIME,AREA/4HTIME,4HAREAS
   DATA SNAM,EFFM,BLANK/IHV^HRHO, 1HT,1HM,1H /
   DATA HNU/3HHNU/
   DATA PPS,SI/3HFPS,2HSI/
END

BLOCK DATA
C SPECIES NAMES AND MOLECULAR WEIGHTS
   COMMON/SNAM/ALSP(75),ALMM(75)
   DATA ALSP/
   * BMAR  BMCH4M  BMCH4M11  BMCH4M12  BMCH2MCD  *
   * BMCH2MCD  BMCH2MCD1  BMCH2MCD11  BMCH2MCD12  *
   * BMCH2MCD1  BMCH2MCD11  BMCH2MCD12  BMCH2MCD13  *
   * BMCH2MCD13  BMCH2MCD14  BMCH2MCD15  BMCH2MCD16  *
   * BMCH2MCD16  BMCH2MCD17  BMCH2MCD18  BMCH2MCD19  *
   * BMCH2MCD19  BMCH2MCD20  BMCH2MCD21  BMCH2MCD22  *
   * BMCH2MCD22  BMCH2MCD23  BMCH2MCD24  BMCH2MCD25  *
   * BMCH2MCD25  BMCH2MCD26  BMCH2MCD27  BMCH2MCD28  *
   * BMCH2MCD28  BMCH2MCD29  BMCH2MCD30  BMCH2MCD31  *
   * BMCH2MCD31  BMCH2MCD32  BMCH2MCD33  BMCH2MCD34  *
   * BMCH2MCD34  BMCH2MCD35  BMCH2MCD36  BMCH2MCD37  *
   * BMCH2MCD37  BMCH2MCD38  BMCH2MCD39  BMCH2MCD40  *
   * BMCH2MCD40  BMCH2MCD41  BMCH2MCD42  BMCH2MCD43  *
   * BMCH2MCD43  BMCH2MCD44  BMCH2MCD45  BMCH2MCD46  *
   * BMCH2MCD46  BMCH2MCD47  BMCH2MCD48  BMCH2MCD49  *
   * BMCH2MCD49  BMCH2MCD50  BMCH2MCD51  BMCH2MCD52  *
   * BMCH2MCD52  BMCH2MCD53  BMCH2MCD54  BMCH2MCD55  *
   * BMCH2MCD55  BMCH2MCD56  BMCH2MCD57  BMCH2MCD58  *
   * BMCH2MCD58  BMCH2MCD59  BMCH2MCD60  BMCH2MCD61  *
   * BMCH2MCD61  BMCH2MCD62  BMCH2MCD63  BMCH2MCD64  *
   * BMCH2MCD64  BMCH2MCD65  BMCH2MCD66  BMCH2MCD67  *
   * BMCH2MCD67  BMCH2MCD68  BMCH2MCD69  BMCH2MCD70  *
   * BMCH2MCD70  BMCH2MCD71  BMCH2MCD72  BMCH2MCD73  *
   * BMCH2MCD73  BMCH2MCD74  BMCH2MCD75  BMCH2MCD76  *
   * BMCH2MCD76  BMCH2MCD77  BMCH2MCD78  BMCH2MCD79  *
   *)
   DATA ALMM/
   * 39.948, 78.114, 83.154, 86.162, 58.081,
   * 73.105, 46.070, 44.036, 42.065, 40.086,
   * 45.042, 31.015, 63.013, 79.009, 159.820,
   * 12.011, 85.170, 86.170, 13.019, 14.021,
   * 15.035, 16.043, 26.011, 26.011, 44.010,
   * 43.096, 25.030, 26.038, 28.054, 38.029,
   * 112.212, 113.224, 43.089, 42.081, 40.065,
   * 29.062, 1.00797, 27.026, 36.461, 20.066,
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33.005, 2.019, 18.014, 34.014, 4.0026,
* 14.007, 11.423, 98.139, 99.139, 16.293,
* 17.031, 30.006, 46.006, 23.013, 32.045,
* 127.001, 92.004, 109.209, 15.999, 10.009,
* 31.997, 31.014, 24.022, 131.300, 15.015,
* 29.0186, 30.026, 126.263, 37.063, 64.097,
* 127.251, 128.259, 30.070, 47.988, 62.0049

END

SUBROUTINE THRM (T,holm)
C THIS ROUTINE CALCULATES (DIMENSIONLESS) THERMODYNAMIC PROPERTIES
C FROM POLYNOMIAL CURVE FITS
LOGICAL NEXT
COMMON/CONO/DUMI, LS, LSP, NEXT
COMMON/GMGC/GRT, MF(25), SR(25), CPR(25), DCPR(25)
COMMON/TCOF/CI(7,25), TLOW, TMID, THI
FIT = A1*10(A2*10(A3*10(A4*10(A5)))
IF (T.EQ. 298.15) TPREV = 0.
IF (T .EQ. TPREV) RETURN
IF (0.35*TLOW .LE. T .AND. T .LE. THI) GO TO 3
IF (T .LE. 1.20*TMID) GO TO 2
WRITE (6,100) T
100 FORMAT (6,I10) T
NEXT = .TRUE.
RETURN
2 WRITE (6,101) T
101 FORMAT (6,I10) T
101 FORMAT (6,I10) T
NEXT = .FALSE.
RETURN
C LOCATE PROPER TEMPERATURE RANGE
3 K = 2
IF (T .GT. TMID) K = 1
DO 4 I = 1, 25
4 COMPUTE H/(R*T)
A1 = C(I,6,1)*C(I,6,1)/T
A2 = C(I,2,6,1)/2.
A3 = C(I,3,6,1)/6.
A4 = C(I,4,6,1)/4.
A5 = C(I,5,6,1)/5.
HRT(I) = FIT
IF (HOML .LT. 0.0) RETURN
TPREV = T
DO 5 I = 1, 25
5 COMPUTE G/(R*T)
A1 = C(I,6,1)*C(I,6,1)*C(I,7,1) - C(I,7,1)
A2 = -C(I,3,6,1)/2.
A3 = C(I,3,6,1)/6.
A4 = C(I,4,6,1)/12.
A5 = C(I,5,6,1)/20.
GRT(I) = FIT
C COMPUTE S/R
A1 = C(I,6,1)*C(I,7,1) + C(I,6,1)/T - C(I,7,1)
A2 = C(I,2,6,1)/2.
A3 = C(I,3,6,1)/6.
A4 = C(I,4,6,1)/12.
A5 = C(I,5,6,1)/20.
SRT(I) = FIT
C COMPUTE CP/R
A1 = C(I,6,1)
A2 = C(I,2,6,1)
A3 = C(I,3,6,1)
A4 = C(I,4,6,1)
A5 = C(I,5,6,1)
CPRI(I) = FIT
C COMPUTE DCP/DF1/R
A1 = C(I,6,1)
A2 = C(I,2,6,1)
A3 = C(I,3,6,1)
A4 = C(I,4,6,1)
A5 = 0.
DCPRI(I) = FIT
RETURN
END
SUBROUTINE CUBS(X,Y,N,X1,Y1,DX,DY)
C THIS ROUTINE IS USED TO CALCULATE VALUES OF THE ASSIGNED VARIABLE
C AND ITS DERIVATIVES

REAL LSUBM
DIMENSION X(N),Y(N)
DIMENSION D,X(U),S(U),V(U)
DIMENSION A3(V),A2(U),A1(U),A0(U)
COMMON/AFUN/C3,C2,C1,C0,ITPSZ,LSUBM,ETA,DIAM,VISC,BETA
EQUIVALENCE IStA31,IT.A2It(U,AlI) , 1V,AO)

C COMPUTE CUBIC SPLINE COEFFICIENTS FROM INPUT TABLE
C THIS ROUTINE WILL ACCEPT END CONDITIONS OF THE FORM
C F**(X(1)I = ALPHA1«F»*(XI2) » BETA1»F»«IX(3) I * GAMMA1
C F**(X(N)I = ALPHAN*F*»(X(N-1II » BETAN*F**(X(N-2I) » GAMMAN
C THE CURRENT END CONDITIONS GIVE A PARABOLIC RUNOUT
C F**(X(1)) = 0
C F**(X(N)) = 0
C F**(X(N-1)) = 0
C COMPUTE CUBIC SPLINE COEFFICIENTS

C CONSTRUCT (TRIAGONAL) COEFFICIENT MATRIX
S=DIAGONAL, T=SUBDIAGONAL, U=SUBDIAGONAL, V=CONSTANTS

C GET Oil) AND DIN) FROM END CONDITIONS

C COMPUTE CUBIC SPLINE COEFFICIENTS

APPENDIX B
APPENDIX B

RETURN

ENTRY CINP
NM=1
GO TO (7,10,11,13,14,15)

C COMPUTE Y, DY/DX, DZY/DX2 FROM CUBIC SPLINE COEFFICIENTS
7 DO B = 1, NM
II = I
IF (XI[I] = XI[I]) GO TO 9
8 CONTINUE
WRITE (6,100) XI[I], Y[I], XI[I-1], XI[I+1]
100 FORMAT (5X,5H IN=,5X,F13.5,17H OUT OF RANGE/5X, 5I, 5X, 5H(I)=,F13.5,5X,5H(I)=,F13.5)
DY = (3*A3[I]*XI[I] + 2*A2[I]*XI[I] + A1[I])
DZY = 6*A3[I]*XI[I] + 2*A2[I])
RETURN

C COMPUTE Y, DY/DX, DZY/DX2 FROM INPUT POLYNOMIAL
10 Y[I] = ((C3*X*I + C2*X*I + C1)*XI + C0)
DY = (3*C3*X*I + 2*C2*X*I + C1)
DZY = C3*X*I + 2*C2
RETURN

C COMPUTE Y, DY/DX, DZY/DX2 FROM INPUT SPECIAL FUNCTION
C EXCEPTIONAL CASE AT X=0
11 IF (X[I] .LE. 0.0) GO TO 12
TERM = X[I]/LSUBM
Y[I] = G(TERM)
DY = DGY[I]
DZY = D2GY[I]Y[I]
RETURN
12 Y[I] = 1.
C FIT A CUBIC THROUGH THE POINTS I0 = Y[I], I0.05 = Y[I+1], I0.05 = Y[I+2], AND I0.10 = Y[I+3]
IN ORDER TO FIND Y[I] AND Y[I+2]
TERM = .05/LSUBM
Y2 = G(TERM)
Y2P = DGY2
Y2PP = D2GY2
TERM = .10/LSUBM
Y3 = G(TERM)
Y3P = DGY3
Y3PP = D2GY3
DY = (.05*Y3PP - Y2PP)/(.10 - .05) - Y2P
DZY = Y2PP - .05*Y3PP - Y2P/(.10 - .05)
RETURN

C Y=0 CASE - ASSIGNED AREA IS NOT REQUIRED
13 Y[I] = 1.
DY = 0.
DZY = 0.
RETURN

END

SUBROUTINE INIT (ISS, NMHGS, MLEFS)

C READ INITIAL CONDITIONS
LOGICAL NMHG, MLEF, NMHGS, MLEFS
REAL IVAR, MDOT, M2, MACH
REAL N, NF, NF2, NF3, NH2, NH3, NO, N2, N2H4, N2O, N2O4, NE, KR, NH, NOP, NO3
DIMENSION ISS(25), TINP(25)

COMMON/LUS/LTHM, DAT, NTHRO, NLANK, NPNAME
COMMON/OPTS/VERS, TIME, DUM(5)
COMMON/CIND/IVAR, AREA, MDOT, P, IVAR, V, RHO, f, CONC(25), LS, DUM2(2)
COMMON/NECC/DUM3(2), M2, DUM4(3)
COMMON/FRAKE/

C C6H12 C6H11 C6H10 C6H9 C6H8 C6H7 C6H6 C6H5 C6H4 C6H3 C6H2 C6H1 C6
C C6H13 C6H12 C6H11 C6H10 C6H9 C6H8 C6H7 C6H6 C6H5 C6H4 C6H3 C6H2 C6H1 C6
C C6H13 C6H12 C6H11 C6H10 C6H9 C6H8 C6H7 C6H6 C6H5 C6H4 C6H3 C6H2 C6H1 C6
C C6H13 C6H12 C6H11 C6H10 C6H9 C6H8 C6H7 C6H6 C6H5 C6H4 C6H3 C6H2 C6H1 C6
C C6H13 C6H12 C6H11 C6H10 C6H9 C6H8 C6H7 C6H6 C6H5 C6H4 C6H3 C6H2 C6H1 C6
C C6H13 C6H12 C6H11 C6H10 C6H9 C6H8 C6H7 C6H6 C6H5 C6H4 C6H3 C6H2 C6H1 C6

APPENDIX B

EQUIVALENCE (ITINP(I), AR)

NAMELIST/START/X,A,EA,NOOT,P,TIME,V,RHO,T, MACH, MMHG,MOLEF,
  AR, BR, C2H5CO, C2H40H, C, CH3, C6H6, C6H13, C2H30, C8H16, C2H5,
  C8H18, C2H5, H02, N, NH3, N20, O2, H2O, C9H19, C6H6, C2H50H, CH20H,
  C6H13, CH*, C2H, C8H17, H, H2, C8H18, NO, N20*, HNO, C9H20, C6H11,
  C6H12, CH30H, BR, CH, CO, C2H4, C3H6, HCL, H202, C7H15, N2, 0,
  XE, C2H3, 03

X = 0.
TIME = 0.
MACH = 0.
DO 1 I=1,75
1 TINPI(I) = 0.
MMHG = MMHG
MOLEF = MOLEF
READ (LOAT,START)

MMHG = MMHG
MOLEF = MOLEF
IF (VERSI .EQ. TIMEV) GO TO 2
IVAR = X
OVAR = TIME
GO TO 3
2 IVAR = TIME
OVAR = X
3 M2 = MACH*MACH
DO 4 I=1,15
JJ = I$X(I)
4 CONCII(I) = TINPI(I)
RETURN
END

SUBROUTINE CIMAGE
C THIS ROUTINE HEADS EACH DATA CARD, PRINTS A CARD IMAGE, AND STORES
C THE IMAGE FOR LATER FORMATTED INPUT
DIMENSION CARD(20)
COMMON/LTUS/LTHM,LDAT,NTHRD,NBLANK,NPHOTO
EQUIVALENCE (MORD,CARO)
DATA FINIS,-,BLANK/*HFINI.IH /
READ (5,101) CARD
101 FORMAT (20A)
998 STOP
999 CONTINUE
REWIND LDAT
WRITE (6,102) CARD
102 FORMAT (28X,20A4)
IF (MORD .EQ. FINIS) GO TO 6
WRITE (LOAT,101) CARD
GO TO 1
6 REMIND LDAT
RETURN
END
APPENDIX B

SUBROUTINE OUTP
C OUTPUT CAN BE GIVEN IN (1) INTERNAL (CGS) UNITS, (2) FPS UNITS
C (3) SI UNITS

LOGICAL ALLM, CONC, OBUGO, EXCHR, NEXT, RHOCON, TCON
REAL MDDT, IVAR, N, M, M2, MIXMM, MACH, LSUBM
DIMENSION SPNM(28), PRC(25), PRX(50), XXH(50)
COMMON/OEV/TOEV
COMMON/LUS/LTM, LDT, NTRO, NBLANK, NMPYTO
COMMON/LFVS/TVS, TVERS, TVAR, TND, THRO, NBLANK, NMPYTO
COMMON/LCON/CONV, AREA, MQ, CON, NVAR, V, RHOT, SIGMA, MPYTO, NEX
COMMON/XMC/OMX, NHY, MAX, FM, RFLG, ESTART
COMMON/NEC/PR, MIXMM, N2, GAMMA, TCPM, R
COMMON/KDIF/TITLE(1),UNIT, UNITI, CONC, EXCHR, DEL(HI50), FPS, SI, OBUGO
COMMON/EAC/ELR, I(50), X(50), RATE(50), LKEG(50), DLKEQ(50), HM, LM
COMMON/RAT(A(50), (50), EAC(50), B(50), M(25), S0, ALLM)
COMMON/AU/AVC(30), ICTH, SUBM, ETA, D, VISC, BETA, L
COMMON/ELS/EXP(125), (50), MM(25), M(50), SIGMA(50, LS, LSP3, NEXT
COMMON/REAC/LSRI4, 50), XX(50), LK89(50), DLKE0(50), M(50), LR
COMMON/SP/SPNM(31), N(25), -1(25), STOIC(25, 50), DMEGA(25, 50)
COMMON/XVS/XTV(100), ADB(100), NT, XA, AU(12), CK(4)
COMMON/GHC/GRT(25), HRT(25), SR(25), CPR(25), DCRP(25)
COMMON/STC/STOIC(4, 50), EQUI(50)
EQUIVALENCE (SPNM, SNAM(4))
EQUIVALENCE (PRX(11), XH(11))
ENTRY OUTP

C ** TITLE PAGE
 IF (VERSI .EQ. TIMEVI) GO TO 98
 I = 2
 GO TO 99
98 I = 4
99 IF (VERSA .EQ. AREAV) I = 1 - 1
 GO TO (I00, 200, 300, 400),
100 WRITE (6, 101)
101 FORMAT (1H9, 14X, 21"DISTANCE-AREA VERSION!
 GO TO 3
200 WRITE (6, 201)
201 FORMAT (1H9, 12X, 25"DISTANCE-PRESSURE VERSION)
 GO TO 3
300 WRITE (6, 301)
301 FORMAT (1H9, 16X, 17"TIME-AREA VERSION)
 GO TO 3
400 WRITE (6, 401)
401 FORMAT (1H9, 14X, 21"TIME-PRESSURE VERSION)
3 WRITE (6, 102) (TITLE!!), I = 1, 20
102 FORMAT (1H9, 49X, "GENERAL CHEMICAL KINETICS PROGRAM", 9X, "NASA LANGLE
 RESEARCH CENTER", 39X, "LANGLEY RESEARCH CENTER VERSION OF LEWIS PROGRAM T IP D-658
 26* USING STEFF DDE", 9X, "SOLUTION TECHNIQUE DEVELOPED BY C.U. GEAR
 3 */ 28X, 22X, 1//, 5X, "REACTION", 31X, "REACTION", 42X, "REACTION RATE VA
 3 6X, 4X, F10.2)
4 WRITE (6, 103) J, NSTOIC(2), SPNM(2), N(2), M(2), SIGMA(2)
103 FORMAT (8I2, 12X, 11L4, AB, 2X, 1, H4, 12X, 11L4, A, 25X, E12.5, 5X
 * F10.4, 9X, F10.2)
 IF (INJ .EQ. NBLANKM) GO TO 4
 IF (INJ .LE. LS) GO TO 203
 WRITE (6, 105) SPNM(I)
105 FORMAT (21X, A8, 2X, H4)
 GO TO 4
203 WRITE (6, 106) N(2), M(2), SIGMA(2)
 WRITE (6, 107) N(2), M(2), SIGMA(2)
204 FORMAT (1H9, 14X, 21"TIME-AREA VERSION!
 IF (INJ .EQ. NBLANKM) GO TO 4
 IF (INJ .LE. LS) GO TO 304
 WRITE (6, 108) SPNM(I)
304 FORMAT (1H9, 14X, 21"TIME-PRESSURE VERSION)
 IF (INJ .EQ. NBLANKM) GO TO 4
 IF (INJ .LE. LS) GO TO 304
 WRITE (6, 109) SPNM(I)
305 FORMAT (1H9, 16X, 17"TIME-AREA VERSION)
 CONVERT ACTIVATION ENERGY TO B-FACTOR
 6 B0J = EACT(2J) / 1.987165
 IF (J .NOT. ALLM) GO TO 7
 WRITE (6, 105) SPNM(I)
7 WRITE (6, 106)
106 FORMAT (1H9, 14X, 21"TIME-AREA VERSION!
 IF (INJ .EQ. NBLANKM) GO TO 4
 IF (INJ .LE. LS) GO TO 304
 WRITE (6, 109) SPNM(I)
304 FORMAT (1H9, 14X, 21"TIME-PRESSURE VERSION)
107 FORMAT (1H9, 49X, "ALL THIRD BODY RATIOS ARE 1.0")
 GO TO 13
7 WRITE (6, 107)
107 FORMAT (1H9, 49X, "ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING"
 * NG/1)
 K = 0
 DO 12 I = 1, LS
 DO 12 J = 1, LS
APPENDIX B

IF (M(1,J) .EQ. 1) GO TO 12
K = K + 1
IF (K .EQ. 51) K = 1
GO TO 10
10 WRITE(6,108) SPN(I,J), M(1,J)
108 FORMAT(5X,2HM(,A8.1H,,12.3H) = .F10.5)
GO TO 12
11 WRITE(6,110) SPN(I,J), M(1,J)
110 FORMAT(1H",",A8.1H,,I2.3H) = .F10.5)
GO TO 12
12 CONTINUE

13 IF (VERS .EQ. TIME) GO TO 14
WRITE (6,112) HM_MIN, HM_MAX, HINT, HM_MAX
GO TO 15
14 WRITE (6,113) HM_MIN, HM_MAX, HINT, HM_MAX

C ** SECOND PAGE
15 WRITE (6,114)
114 FORMAT (1H",",50X,31H"ASSIGNED VARIABLE PROFILE "//)
GO TO (16,18,19,19,20), IPRTC

16 GO TO (116,216,316,416), IPRTC
116 WRITE (6,117) XU, AU
117 FORMAT (34X,64HTHE AREA IS CALCULATED BY INTERPOLATION FROM THE FOLLOWING TABLE///36X,7HSTATION,10X,17HAXIAL DISTANCE, A2,1H),10X,17HAREA, (,A4,A1,1H))
GO TO 516
216 WRITE (6,217) XU, AU
217 FORMAT (32X,58HTHE PRESSURE IS CALCULATED BY INTERPOLATION FROM THE FOLLOWING TABLE///36X,7HSTATION,10X,17HAXIAL DISTANCE, A2,1H),15X,11HPRESSURE , (2A4,1H))
GO TO 516
316 WRITE (6,317) AU
317 FORMAT (3*X,68HTHE AREA IS CALCULATED BY INTERPOLATION FROM THE FOLLOWING TABLE///36X,7HSTATION,16X,UTIME, A2,1H), 16X, 7HAREA, (,A4,A1,1H))
GO TO 516
416 WRITE (6,417) AU
417 FORMAT (32X,68HTHE PRESSURE IS CALCULATED FROM THE FOLLOWING POLYNOMIAL///23X,6HAREA, (,A4,A1,5H) = I , 1PE12.5,9H)X*«3 t (,E12.5,9H)X*«2 » (,E12.5,6H)X t (,E12.5,1H))
GO TO 21
516 DO 17 I = 1, NTS
17 WRITE (6,016) I, XDATA, I)
616 FORMAT (38X,14X,1PE12.5,15X,E12.5)
GO TO 21
18 GO TO (218,318,418,518), IPRTC
19 WRITE (6,219) AU, CX
219 FORMAT (40X,52HTHE AREA IS CALCULATED FROM THE FOLLOWING POLYNOMIAL///46X,16HAREA = 1 - (X/,F10.3,4H)»*(,F10. 5, 1H))
IF (ITPSZ .EQ. 4) WRITE (6,018) E, HM_VISC
018 FORMAT (16X,20HHYDRAULIC DIAMETER =,F8.4,3H CM,7X,23HVISCOSITY COEFFICIENT =,E12.4,10H GM/CM-SEC,7X.6HETA =,F7.4)
GO TO 21
C SPECIAL AREA FUNCTION
19 WRITE (6,118) LSMBETA
118 FORMAT (41X,50HTHE AREA IS CALCULATED FROM THE FOLLOWING FUNCTION/ ///48X,14HAREA = - (E/F10.3,4H) = .F10.5,1H))
IF (IPRTC .EQ. 4) WRITE (6,119) E, HM_VISC
119 FORMAT (70X,20HYDRAULIC DIAMETER =,F8.4,3H CM,7X,23HVISCOSITY COE //,IFFICIENT =,E12.4,10H GM/CM-SEC,7X,6MBETA =,F7.4)
GO TO 21
C ZERO VELOCITY - ASSIGNED VARIABLE NOT REQUIRED
20 WRITE (6,119)
119 FORMAT (32X,50HTHIS IS A V= 0 PROBLEM - AN ASSIGNED VARIABLE IS NOT # REQUIRED)
GO TO 21
21 CONTINUE
APPENDIX B

212 IF (RHOCONI WRITE (16,126)
1126 FORMAT (///38,5HTHE VOLUME (DENSITY) WILL BE HELD CONSTANT FOR T
**HIS CASE)
IF (ITCONI WRITE (16,2126)
2126 FORMAT (///40,5HTHE TEMPERATURE WILL BE HELD CONSTANT FOR THIS C
**ASE)
RETURN
ENTRY OUT2

C INITIAL CONDITIONS
WRITE (16,127)
127 FORMAT (I///38X,56HTME VOLUME (DENSITY) WILL BE HELD CONSTANT FOR T
**HIS CASE)
WRITE (16,2127)
2127 FORMAT (///40X, 51HT ME TEMPERATURE WILL BE HELD CONSTANT FOR THIS C
**ASE)
RETURN
ENTRY OUT3

C GENERAL OUTPUT
WRITE (16,128)
128 FORMAT (//)

29 MACH = SQRT(22)
MAX = MAX(1LS,LR)
TENT = 0.
CSUM = 0.
PMLOG = ALOG(P*MIXMM)
C TOTAL ENTRPY AND MASS FRACTION SUM
DO 30 I=1,LS
SIGMA(I) = SIGMA(I)**R(I)
TENT = TENT + SIGMA(I)**R(I)
30 CSUM = CSUM + SIGMA(I)**R(MII)
TENT = TENT*1.987165
TXH = 0.
C ENERGY EXCHANGE RATES
DO 31 J=1,LR
XXHU = XXH(J)*OELH(J)
31 TXXH = TXXH + XXH(J)
IF (IVERST .EQ. TIMEV) GO TO 32
TIME = TIME + DVAR
X = XVAR
GO TO 33
32 TIME = XVAR
X = XVAR
33 IF (UNITU .NE. FPS) GO TO 48
; CONVERT FROM INTERNAL ICGS) UNITS TO FPS UNITS
X = X/30.48
AREAA = AREA/929.0304
DOTM = DOTM/453.59237
PP = PP/2116.2
VV = V/30.48
RHOO = RHO*62.43
IT = IT!B
WRITE (6,129) TIME,AREAA,X,PP, VV, RHOO,
 * T,TDOT,TENT, MACH,GAMMA
129 FORMAT (16X,TIME*,E14.5,* SEC*,16X,*AREA*,E14.5,* SQ FT*,
 14X,MAXAL POSITION*,E14.5,* FT*,/20X,HUM PROPERTIES*,4X,
 2 *INTEGRATION INDICATORS//22X,*PRESSURE*,E22.5,*30X*,
 3 *STEPS FROM LAST PRINT*,I13X,23X,*LB/FT**,21X,*VELOCITY*,
 4 E22.5,*30X,*AVERAGE STEP SIZE**23X,*3FT/SEC**22X,*DENSITY*,
 5 E23.5,*30X,*CONTROLLING VARIABLE**23X,*3LB/FT**3*3FT/SEC**3*
 6 22X,*TEMPERATURE*,E19.5/23X,*DEG R**,22X,*MASS FLOW RATE*,
 7 E10.5/23X,*3LB/SEC**22X,*ENERGY EXCHANGE RATE*,E23.5,30X,*RELATIVE ERROR*/
 8 23X,*BTU/SEC**22X,*MACH NUMBER*,E19.5/22X,*GAMMA*,E25.5)
34 WRITE (6,131)
131 FORMAT (///56,19HCHEMICAL PROPERTIES//)

C PRINT MASS FRACTIONS AND REACTION CONVERSION RATES
WRITE (16,132)
132 FORMAT (16X,FORMA1X,TIME*,E14.5,* SEC*,16X,*AREA*,E14.5,* SQ FT*,
 14X,MAXAL POSITION*,E14.5,* FT*,/20X,HUM PROPERTIES*,4X,
 2 *INTEGRATION INDICATORS//22X,*PRESSURE*,E22.5,*30X*,
 3 *STEPS FROM LAST PRINT*,I13X,23X,*LB/FT**,21X,*VELOCITY*,
 4 E22.5,*30X,*AVERAGE STEP SIZE**23X,*3FT/SEC**22X,*DENSITY*,
 5 E23.5,*30X,*CONTROLLING VARIABLE**23X,*3LB/FT**3*3FT/SEC**3*
 6 22X,*TEMPERATURE*,E19.5/23X,*DEG R**,22X,*MASS FLOW RATE*,
 7 E10.5/23X,*3LB/SEC**22X,*ENERGY EXCHANGE RATE*,E23.5,30X,*RELATIVE ERROR*/
 8 23X,*BTU/SEC**22X,*MACH NUMBER*,E19.5/22X,*GAMMA*,E25.5)
34 WRITE (6,131)
C PRINT MASS FRACTIONS AND ENERGY EXCHANGE RATES
WRITE (6,134)
134 FORMAT (16X,FORMA1X,TIME*,E14.5,* SEC*,16X,*AREA*,E14.5,* SQ FT*,
 14X,MAXAL POSITION*,E14.5,* FT*,/20X,HUM PROPERTIES*,4X,
 2 *INTEGRATION INDICATORS//22X,*PRESSURE*,E22.5,*30X*,
 3 *STEPS FROM LAST PRINT*,I13X,23X,*LB/FT**,21X,*VELOCITY*,
 4 E22.5,*30X,*AVERAGE STEP SIZE**23X,*3FT/SEC**22X,*DENSITY*,
 5 E23.5,*30X,*CONTROLLING VARIABLE**23X,*3LB/FT**3*3FT/SEC**3*
 6 22X,*TEMPERATURE*,E19.5/23X,*DEG R**,22X,*MASS FLOW RATE*,
 7 E10.5/23X,*3LB/SEC**22X,*ENERGY EXCHANGE RATE*,E23.5,30X,*RELATIVE ERROR*/
 8 23X,*BTU/SEC**22X,*MACH NUMBER*,E19.5/22X,*GAMMA*,E25.5)
34 WRITE (6,131)
C PRINT MASS FRACTIONS AND ENERGY EXCHANGE RATES
WRITE (6,134)
APPENDIX B

135 FORMAT (5X,16HMOLE/FT**3/SEC),11X,6HNUMBER,8X,21HBTU-FT**3/LB**
2/SEC,6X,13HTIVE DIR RATE)
C COMPUTE MASS FRACTIONS
37 DO 38 I=1,LS
38 PRXIJI = SIGMA(I)*HOO
GO TO 40
39 IF (.NOT. CONCI .OR. EXCHRI) GO TO 41
C PRINT MOLAR CONCENTRATIONS AND REACTION CONVERSION RATES
WRITE (6,136)
136 FORMAT (1X,7HSPECIES,4X,13HCONCENTRATION,3X,13HMOLE FRACTION,3X,
# 27NET SPECIES PRODUCTION RATE,5X,6HREACTION,3X,28NET REACTION C
ADDITION RATE,4X,14HNET RATE/POSIT)
WRITE (6,137)
137 FORMAT (12X,13HMOLES/FT**3),25X,16HMOLE/FT**3/SEC),11X,6HNUMBER,
# 7X,22HMOLE-FTE**3/LB**2/SEC),6X,13HTIVE DIR RATE)
DO 40 J=1,LR
40 PRX(J) = XX(J)
CONV = 1./62.43
GO TO 42
C PRINT MOLAR CONCENTRATIONS AND ENERGY EXCHANGE RATES
41 WRITE (6,138)
138 FORMAT (1X,7HSPECIES,4X,13HCONCENTRATION,3X,13HMOLE FRACTION,3X,
# 27NET SPECIES PRODUCTION RATE,5X,6HREACTION,5X,24HNET ENERGY EXT
ECHANGE RATE,4X,14HNET RATE/POSIT)
WRITE (6,139)
139 FORMAT (12X,13HMOLES/FT**3),25X,16HMOLE/FT**3/SEC),11X,6HNUMBER,
# 8X,21HBTU-FT**3/LB**2/SEC),6X,13HTIVE DIR RATE)
C COMPUTE MOLAR CONCENTRATIONS
42 DO 43 (I=1,LS
43 PRXI(J) = SIGMA(I)*HOO
44 DO 47 JJ=1,MAX
IF (JJ.GT.LS) GO TO 45
FMOL = SIGMA(JJ)*HOO
MM = M(JJ)/62.43
XXX = PRX(JJ)*CONV
WRITE (6,140) SPNMI(JJ),PRC(JJ),FMOL,MM,XXX,EQUIL(JJ)
45 IF (JJ.GT.LS) GO TO 46
FMQL = SIGMA(JJ)*HOO
MM = M(JJ)/62.43
WRITE (6,141) SPNMI(JJ),PRC(JJ),FMQL,MM
46 XXX = PRX(JJ)*CONV
WRITE (6,142) XXX,EQUIL(JJ)
47 CONTINUE
C XXH = XXH*0.02383
WRITE (6,143) XXH,CSUM
143 FORMAT (49X,21H(BTU-FT**3/LB**2/SEC),6X,13HTIVE DIR RATE)
GO TO 78
48 IF (UNITO .NE. 41) GO TO 63
C CONVERT FROM INTERNAL (CGS) UNITS TO SI UNITS
X = X*0.01
AREA = AREA*0.01
DOTM = DOTM*0.001
PP = PP*1.01325E+05
VV = VV*0.01
RHO = RHO*1000.
TENT = TENT*418.4
WHITE (6,145) TIME,AREA,x,PP, VV, RHO,
* TTI,DOTM,HOO, MACH,GAMMA
145 FORMAT (6X,TIME,15.5,* SEC),14X,AREA,1E4.5,* SQ M*,
1 4X,AXIAL POSITION,1E4.5,* M ///20X,*FLOW PROPERTIES,45X,
2 *INTEGRATION INDICATORS,9//22X,*PRESSURE,1E2.5,30X,
3 *STEPS FROM LAST PRINT,15X,23X,*IN/M=-2 19//22X,*VELOCITY*,
# 22X,*TEMPERATURE,1E19.5/23X,*DEG K/*22X,*MASS FLOW RATE*,
7 1E5.5/23X,*M/SEC/*22X,*TEMPERATURE,1E19.5/23X,*DEG K/*22X,*MASS FLOW RATE*,
8 23X,*M/SEC/*22X,*MACH NUMBER,1E19.5/22X,*GAMMA,1E25.5)
49 WRITE (6,131)
CONV = 4.1840
IF (CONC .OR. EXCHRI) GO TO 51
C PRINT MASS FRACTIONS AND REACTION CONVERSION RATES
WRITE (6,132)
132 FORMAT (6X,16HMOLE/FT**3/SEC),12X,6HNUMBER,7X,21HMOLE-H**2/3/SEC,6X,13HTIVE DIR RATE)
DO 50 J=1,LR
50 PRX(J) = XX(J)
CONV = 0.001
GO TO 52

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APPENDIX B

51 IF (CONC .OR. (.NOT. EXCHR)) GO TO 54
C PRINT MASS FRACTIONS AND ENERGY EXCHANGE RATES
WRITE (6, 134)
WRITE (6, 147)
147 FORMAT (5DX, 15H MOLE/M**3/SEC), 12X, 6H NUMBER, TX, 22H JOULE-M**3/KG**2/SEC, 6X, 13HTIVE DIR RATE)
C COMPUTE MASS FRACTIONS
52 DO 53 I=1,LS
53 PRC(I) = SIGMA(I)**W(I)
GO TO 59
54 IF (.NOT. CONC) .OR. EXCHR) GO TO 56
C PRINT MOLAR CONCENTRATIONS AND REACTION CONVERSION RATES
WRITE (6, 139)
WRITE (6, 149)
149 FORMAT (12X, 12H MOLES/M**3), 26X, 13H MOLE/M**3/SEC), 12X, 6H NUMBER, TX, 22H JOULE-M**3/KG**2/SEC, 6X, 13HTIVE DIR RATE)
DO 55 J=1,LR
55 CONV = 0.001
GO TO 57
C COMPUTE MOLAR CONCENTRATIONS
57 DO 58 J=1,LS
58 PRC(I) = SIGMA(I)**W(I)
59 DO 60 J=1,MAX
60 IF (I .GT. IJ .OR. IJ .GT. LR) GO TO 63
FMOL = SIGMA(IJ)**W(IJ)
M = SIGMA(IJ)**W(IJ)
XXX = PRC(IJ)*CONV
WRITE (6, 140) SIGMA(IJ), PRC(IJ), FMOL, XXX, CONV
61 IF (I .GT. IJ .OR. IJ .GT. LR) GO TO 63
FMOL = SIGMA(IJ)**W(IJ)
M = SIGMA(IJ)**W(IJ)
XXX = PRC(IJ)*CONV
WRITE (6, 142) SIGMA(IJ), PRC(IJ), FMOL, XXX
62 CONTINUE
63 XXX = PRC(IJ)*CONV
GO TO 58
C PRINT MOLAR CONCENTRATIONS AND ENERGY EXCHANGE RATES
WRITE (6, 143)
WRITE (6, 153)
153 FORMAT (12X, 12H MOLES/M**3), 26X, 13H MOLE/M**3/SEC), 12X, 6H NUMBER, TX, 22H JOULE-M**3/KG**2/SEC, 6X, 13HTIVE DIR RATE)
DO 65 J=1,LR
65 CONV = 0.001
GO TO 57
C COMPUTE MOLAR CONCENTRATIONS
67 DO 68 J=1,LS
68 PRC(I) = SIGMA(I)**W(I)
C PRINT MASS FRACTIONS AND REACTION CONVERSION RATES
WRITE (6, 132)
WRITE (6, 142)
142 FORMAT (12X, 12H MOLES/M**3), 26X, 13H MOLE/M**3/SEC), 12X, 6H NUMBER, TX, 22H JOULE-M**3/KG**2/SEC, 6X, 13HTIVE DIR RATE)
DO 69 J=1,LS
69 IF (.NOT. CONC) .OR. (.NOT. EXCHR)) GO TO 66
C PRINT MOLAR CONCENTRATIONS AND ENERGY EXCHANGE RATES
WRITE (6, 133)
WRITE (6, 152)
152 FORMAT (12X, 12H MOLES/M**3), 26X, 13H MOLE/M**3/SEC), 12X, 6H NUMBER, TX, 22H JOULE-M**3/KG**2/SEC, 6X, 13HTIVE DIR RATE)
C COMPUTE MOLAR CONCENTRATIONS
60 DO 61 J=1,LS
61 PRC(I) = SIGMA(I)**W(I)
C PRINT MOLAR CONCENTRATIONS AND REACTION CONVERSION RATES
WRITE (6, 134)
WRITE (6, 153)
153 FORMAT (12X, 12H MOLES/M**3), 26X, 13H MOLE/M**3/SEC), 12X, 6H NUMBER, TX, 22H JOULE-M**3/KG**2/SEC, 6X, 13HTIVE DIR RATE)
C PRINT MOLAR CONCENTRATIONS AND ENERGY EXCHANGE RATES
WRITE (6, 135)
WRITE (6, 154)
154 FORMAT (12X, 12H MOLES/M**3), 26X, 13H MOLE/M**3/SEC), 12X, 6H NUMBER, TX, 22H JOULE-M**3/KG**2/SEC, 6X, 13HTIVE DIR RATE)
APPENDIX B

70 PRINT MOLAR CONCENTRATIONS AND ENERGY EXCHANGE RATES
GO TO 72

C PRINT MOLAR CONCENTRATIONS AND ENERGY EXCHANGE RATES
71 WRITE (6,1381)
WRITE (6,1551)
155 FORMAT (1X,3HUNITS/CM**3),2X,16HMOLE/CM**3/SEC),1X,6HNUMBER,
* 8X,2HICAL-ML/CM**3/SEC),6X,13HTIME DIV DIX RATE)

C COMPUTE MOLAR CONCENTRATIONS
72 DO 73 I=1,LS
73 PRC(I) = SIGMA(I)*RHO
PROD = PRC(1)*PRC(3)

74 DO 77 IJ=1,MAX
IF (IJ.GT.LS.OR.IJ.GT.LR) GO TO 75
FMOL = SIGMA(IJ)*MIX
WRITE(I6,40) SPNM(IJ),PRC(IJ),FMOL,PRC(IJ),EQUI(IJ)
GO TO 77
75 IF (IJ.GT.LS) GO TO 76
FMOL = SIGMA(IJ)*MIX
WRITE(I6,40) SPNM(IJ),PRC(IJ),FMOL,PRC(IJ),EQUI(IJ)
GO TO 77
76 WRITE (6,142) IJ,PRC(IJ),EQUI(IJ)
77 CONTINUE
GO TO 705

700 CONTINUE
WRITE (6,171)
701 FORMAT(1XA8,2X,E12.5,E16.5,7X,E12.5,7X,E12.5)
DO 703 I=1,LS
FMOL = SIGMA(I)*MIX
PRC(I) = SIGMA(I)*RHO
WRITE(I6,704) SPNM(I),PRC(I),FMOL,PRC(I),SIGMA(I),I(1)
703 CONTINUE
PROD = PRC(1)*PRC(3)
OCD = PRC(3)*W(I) + PRC(1)*W(I) = E15.5
705 CONTINUE
WRITE (6,20001) PROD
2000 FORMAT(3X,PRODUCT OF SPECIES 1 AND SPECIES 3 MOLAR CONCENTRATIONS = 1PE12.5)
WRITE (6,1550)
1550 FORMAT(15HICAL-ML/CM**3/SEC)
WRITE (6,20001) PROD
1590 FORMAT(*UTEMP/OIVAR = *,E16.5)
78 CONTINUE
82 IF (ABS(I-LS).LE.0.001) RETURN
WRITE (6,1630)
1630 FORMAT(3X,INVALID COMPUTATIONAL DI\U00000000)UTPUT)
NEXT = .TRUE.
RETURN
END

SUBROUTINE DIFFUNI(TI,T,Y,YDOT,IFN.3PE0VX.32)
C PERFORM ALL NECESSARY PRE-DERIVATIVE CALCULATIONS

LOGICAL ALLN,LTCON,NEXT,RHOCON
LOGICAL LKCON
LOGICAL LKUP

INTEGER STOIC
REAL IVAR,MDQT,LKE3iHM,N,M
DIMENSION YINI,K2),YDOT(56)

COMMON/DERV3/TDERV
COMMON/STCOM8/TPREV,HN1
COMMON/STCOM9/VOLD
COMMON/CONT/KCON
COMMON/UPOT/KUP
COMMON/RHAT/AI,NI,EACTI,50,OMEGA1,50
COMMON/GHSC/3RT,HR1,SH1,CPRI,25,M30)
COMMON/NECC/R,R,MIX**M2,GAMMA
COMMON/STCS/NSTOIC!*50),EQUIL50)
COMMON/SNOB/CAT8I40),CATBCtO),NZ
COMMON/ORN/FI28)

APPENDIX B

40
APPENDIX B

COMMON/SAMY,SP1,SP2,AA,BB,OTERM
EQUIVALENCE (T0,Y,F111)
PRINT(10) = VVYV0Z + DVYV0A
DAGRI(10) = 102/Y - DVYV0A

IUPH = 1
YV(Y1)
YV(Y1)
YV(Y1)
YV(Y1)

200 CONTINUE
IF(ktcon) GO TO 400
VNTY IYK1
IF (ktcon) GO TO 5

400 CONTINUE
WARNING = 0

C THERMODYNAMIC PROPERTIES
CALL THM (T1,T2)
ALGRT = ALOG(THM)
AN A = 1/1,L

C #FACTOR RATE CONSTANT
RATE(J) = 1J1/J(1)EXP(-BIJ/T)

C IN KF0 AND DILN KDE1/DDT
DKETC = 1.
NLEG = 0.
NREL = 0.
ON = 1.4
44 = (LPK1,JI)
IF (jun .GT. 15) GO TO 2
STOC = NTOJ(J1,JI)
NLEG = NLEG + STOC
NREL = NREL + STOC

2 CONTINUE
LTE(J1) = -DELG - DELSTC + ALGRT
LTE(J1) = IDELM - DELSTC/F

4 CONTINUE

C *TEXTURE MOLECULAR WEIGHT
5 NP1 = 0.
ON A = 1.1,15
6 NP1 = DPL + SIGMA(I)
STUP = DPL
MPSUM = 1.1/SSUM

C ******* UPDATE INDEPENDENT AND DEPENDENT VARIABLES
IF (KUP(J1) .GT. 400 GO TO 600
TUP = T1
600 CONTINUE
IF (KUP(J1) .EQ. TIMEV) GO TO 700
Y = YUP
IF (KCONV) TIME = OVAR
IF (KUP(J1) .LT. UP) AND (.NOT. KTCON) TIME + OVAR +2.*K1 = TPREV + VOLD + T1(J1)
IF (KUP(J1) .EQ. OVAR
G77(105
700 CONTINUE
TIME = TUP
IF (KCONV) Y = OVAR
STUP(J1) = OVAR + (.NOT. KTCON) X-OVAR + (11-TPREV)*VOLD + Y(J1)
17=
IF (KUP(J1) .EQ. OVAR
701 CONTINUE

C ASSIGNED VARIABLE
IF (KUP(J1) .LT. 21) GO TO 7
CALL CINP(J1,CA1,CA2,CA3,AVAR,DA,D2A)
70 TN 8
8 CONTINUE
CALL CINP(J1,CA1,CA2,CA3,TIME,AVAR,DA,D2A)

C CALCULATED VARIABLE
B IF (KUP(J1) .EQ. AREA) GO TO 9
P = AVAP
IF (YV .LT. 0.1) AREA = MDDT/IRHet
50 TN 10
9 AREA = AVAP
P = PHMM/TABM

C MASS FLOW RATE
MT + MTHAREAV
10 TN (L1)=L1
41 = (L1,J1)
42 = (L1,J2)
43 = (L1,J3)
44 = (L1,J4)

IF (KN1) .EQ. NPHOTO) GO TO 13

C WHEN PHASE FACTOR
WJ(J1) = 0.
IF (KN1 .LT. NHROI) AND (.NE. 1) NPHOTO GO TO 13
I(J1) = 1100 GO TO 12
41 TN 111+1,15
11 WJ(J1) = WJ(J1) + M1,J1*SIGMA(I)
70 TN 13
APPENDIX B

12 MM(J) = SSUM

13 IF (LREQ(J), GT, 0.0) GO TO 14
EXP3 = EXP(-LREQ(J)/3.0)
EXP1 = RATE(J)*EXP3
GO TO 15

14 EXP1 = EXP(ALOGI(RATE(J)) - LREQ(J))
EXP3 = 1.

C NET REACTION CONVERSION RATE

15 SIGMA1 = 0.
IF (N1 .LE. LS1) SIGMA1 = SIGMA(N1)
SIGMA = 0.
IF (N4 .LE. LS4) SIGMA4 = SIGMA(N4)
NC = -NSTOIC(JM,J) - NSTOIC(4,J)
DI = POWER(4, NPHOTO) GO TO 18
NC = NSTOIC(3,J) + NSTOIC(4,J) - 2
DP2 = EXP3*POWER(RHO, NC) EXP1*POWER(SIGMA1, NSTOIC(JM,J))
* POWER(SIGMA4, NSTOIC(4,J))

16 XX(J) = DPI - DP2
IF (N1 .EQ. NPHOTO) GO TO 20
EQUILIJ = 0.
GO TO 20

17 IF (XX(J).LT. 0.0) GO TO 20
EQUILIJ = XX(J)/DP2
IF (N1 .EQ. NTHRD) EQUILIJ = XX(J)/RHO
EQUILIJ = EQUILIJ/(MM(J)*RHO)
GO TO 20

C TOTAL CP/R

20 CONTINUE
RH02 = RHO*RHO
TCPR = 0.
DO 22 I=1, LS
C NET SPECIES PRODUCTION RATE
TCPR = TCPR + CPRI(J)*SIGMA(I)
DI = 0.
DO 21 J=1, LR
STOC = STOC(J)
OMEGA(J) = RH02*STOC*XX(J)
21 DPI = DPI + OMEGA(J)
WII = DPI
22 CONTINUE

C GAMMA (FROZEN)

GAMMA = TCPR/(TCPR - 1./MM)

C MACH NUMBER SQUARED
M2 = V/RH/PMMA/GAMMA

1 IF (VERSA .NE. TIMEVI) M2 = V/RH/PMMA/GAMMA
* GO TO 23
MACH = SQRT(M2)
WRITE (6, 101) MACH
101 FORMAT (15H MACH =, F8.4, 15H IS APP
* MACH = MACH + 1
IF (MACH .LT. 5) GO TO 23
WRITE (6, 102)
102 FORMAT (6H MACH =, F8.4)
NEXT = .TRUE.
RETURN

23 CONTINUE

C COMPUTE DERIVATIVES WRT THE INDEPENDENT VARIABLE

C

DP51 = 0.
DP52 = 0.
DO 51 I=1, LS
FIIJ = 0.
1 CONTINUE
DENM = RHO
IF (VERSI .NE. TIMEVI) DENM = RHO/V
DO 50 I=1, LS
50 CONTINUE

C SIGMA/DIVAR
I = I + 3
FIIJ = WIJ/DENM

C S1 FOR AA
DP51 = DP51 + FIIJ
C S2 FOR BB
50 DP52 = DP52 + HRT(J)*FIIJ
S1 = MIXWOP51
S2 = MIXWOP52

42
CONTINUE
ON 1 T=T+EXP3
ON 1 K+1 EXP3
3.

IF (T>4) GO TO 5

IF (M=0 AND V<0. AND NOT. ICON I) IRHO = ?
ON 2 J-1 EXP
ON 2 T-1 EXP
2.

PXXSTG(J,J) = 0.

C.

L X Y Z W R

INU(J) WRT RN(J), SIGMA(J)
NO 4 J-1 EXP
4 = LXX(J)
N = LXX(J)
BUY(J) = 0.

IF (INU(J), EQ, AND, (1, T = 0) GO TO 3
EXP = EXP-LEDE(J)/3.
EXP = RATE(J)*EXP3
GO TO 4.
3.

EXP = EXPIAOG(RATE(J)) - LKSG(J)
EXP = 1.

4.

SIGMA(J) = 0.
IF (INU(J), EQ, 4, SIGMA(J) = SIGMA(J)
SIGMA(J) = 0.
IF (N4, EQ, L5, SIGMA(J) = SIGMA(J)
N4 = NSTOIC(1,JJ) + NSTOIC(2,JJ) - 2
C1 = N4
C1 = NSTOIC(J,J) + NSTOIC(1,JJ) + NSTOIC(2,JJ) - 2
C0 = C1

PXXSTG(J,J) = C1*POWER(RHO,NC1-1)*RATE(J)*POWER(SIGMA(J),NSTOIC(1,JJ))

PXXSTG(J,J) = C1*POWER(RHO,NC1-1)*RATE(J)*POWER(SIGMA(J),NSTOIC(1,JJ))

PXXSTG(J,J) = C1*POWER(RHO,NC1-1)*RATE(J)*POWER(SIGMA(J),NSTOIC(1,JJ))

IF (N1, EQ, L5, SIGMA(J) = SIGMA(J)

SIGMA(J) = SIGMA(J)

N1 = NSTOIC(J,JJ) - 2
C1 = NSTOIC(J,JJ) + NSTOIC(1,JJ) + NSTOIC(2,JJ) - 2
C0 = C1

PXXSTG(J,J) = C1*POWER(RHO,NC1-1)*RATE(J)*POWER(SIGMA(J),NSTOIC(1,JJ))

PXXSTG(J,J) = C1*POWER(RHO,NC1-1)*RATE(J)*POWER(SIGMA(J),NSTOIC(1,JJ))

PXXSTG(J,J) = C1*POWER(RHO,NC1-1)*RATE(J)*POWER(SIGMA(J),NSTOIC(1,JJ))

J.

PXXSTG(J,J) = FLOAT(STDIC(1,JJ)*POWER(RHO,NC1-1)*POWER(SIGMA(J),NSTOIC(1,JJ))

PXXSTG(J,J) = FLOAT(STDIC(1,JJ)*POWER(RHO,NC1-1)*POWER(SIGMA(J),NSTOIC(1,JJ))

PXXSTG(J,J) = FLOAT(STDIC(1,JJ)*POWER(RHO,NC1-1)*POWER(SIGMA(J),NSTOIC(1,JJ))

GO TO 7.
7.

C1 = -NSTOIC(1,JJ) - 2
C0 = C1

PXXSTG(J,J) = C1*POWER(RHO,NC1-1)*RATE(J)*POWER(SIGMA(J),NSTOIC(1,JJ))

PXXSTG(J,J) = C1*POWER(RHO,NC1-1)*RATE(J)*POWER(SIGMA(J),NSTOIC(1,JJ))

PXXSTG(J,J) = C1*POWER(RHO,NC1-1)*RATE(J)*POWER(SIGMA(J),NSTOIC(1,JJ))

GO TO 8.

8.

MMRHO = MMJ+MMRHO

PXXSTG(J,J) = MMRHO*(C1,J)*POWER(RHO,NC1-1)*RATE(J)*POWER(SIGMA(J),NSTOIC(1,JJ))

PXXSTG(J,J) = MMRHO*(C1,J)*POWER(RHO,NC1-1)*RATE(J)*POWER(SIGMA(J),NSTOIC(1,JJ))

PXXSTG(J,J) = MMRHO*(C1,J)*POWER(RHO,NC1-1)*RATE(J)*POWER(SIGMA(J),NSTOIC(1,JJ))

GO TO 9.

9.

PXXSTG(J,J) = MMRHO*PXXSIG(J,J)

PXXSTG(J,J) = MMRHO*PXXSIG(J,J)

PXXSTG(J,J) = MMRHO*PXXSIG(J,J)

PXXSTG(J,J) = MMRHO*PXXSIG(J,J)

GJ = 2

GAMMA = GAMMA(Gamma - 1)

GAMMA = GAMMA(Gamma - 1)

GAMMA = GAMMA(Gamma - 1)

C.

GAMMA WRT SIGMA(I) AND MACH NUMBER SQUARED WRT SIGMA(I)
NO 10 T-1 EXP
SIGMA(J) = SIGMA(J) + MMRHO*SIGMA(J)
SIGMA(J) = SIGMA(J) + MMRHO*SIGMA(J)
SIGMA(J) = SIGMA(J) + MMRHO*SIGMA(J)
SIGMA(J) = SIGMA(J) + MMRHO*SIGMA(J)
GAMMA = GAMMA(Gamma - 1)

C.

GAMMA WRT T

GAMMA = -GAMMA(T)*PXXSIG(J,J)

GAMMA = -GAMMA(T)*PXXSIG(J,J)

GAMMA = -GAMMA(T)*PXXSIG(J,J)

GAMMA = -GAMMA(T)*PXXSIG(J,J)

C.

MACH NUMBER SQUARED WRT V

MVM = 2.*M*NV*GAMMA(Gamma - 1)

MVM = 2.*M*NV*GAMMA(Gamma - 1)

MVM = 2.*M*NV*GAMMA(Gamma - 1)

MVM = 2.*M*NV*GAMMA(Gamma - 1)
APPENDIX B

C MACH NUMBER SQUARED WRT T
PM2T = -M2*(1./T + PGAMT/GAMMA)
TERM = RHO
IF (VERSI .LE. TIMEV) GO TO 12
TERM = RHO/V
C DSIGMA/DIVAR WRT V
DO II = 1,LS3
11 BETAI(I,1) = -F(I)/V
C DSIGMA/DIVAR WRT RHO AND DSIGMA/DIVAR WRT T
12 DO II = 1,LS3
   I = II - 3
   DO 13 JJ = 1,LR
   STOC = STOIC(J,J)
   BETAI(I,J) = BETAI(I,J) + STOC*PM2RHO(J)
   DO 13 J = 1,LR
   BETAI(I,J) = F(I)/RHO + TERM*BETAI(I,J)
14 BETAI(I,3) = TERM*BETAI(I,3)
C DSIGMA(I)/DIVAR WRT SIGMA(K)
DO II = 1,LS3
   I = II - 3
   DO 16 KK = 1,LS3
   K = KK - 3
   DO 15 J = 1,LR
   STOC = STOIC(J,J)
   BETAI(K,J) = BETAI(K,J) + STOC*PM2SIG(I)
   DO 15 J = 1,LR
   BETAI(K,J) = F(I)/RHO + TERM*BETAI(K,J)
16 BETAI(K,K) = TERM*BETAI(K,K)
C S1 WRT V,RHO,T,SIGMA(I) AND S2 WRT V,RHO,T,SIGMA(I)
PS1V = 0.
PS1RHO = 0.
PS1T = 0.
PS2V = 0.
PS2RHO = 0.
PS2T = 0.
DO 18 II = 1,LS3
   I = II - 3
   PS1V = PS1V + BETAI(I,1)
   PS1RHO = PS1RHO + BETAI(I,2)
   PS1T = PS1T + BETAI(I,3)
   PS2V = PS2V + TERM*BETAI(I,1)
   PS2RHO = PS2RHO + TERM*BETAI(I,2)
   PS2T = PS2T + TERM*BETAI(I,3)
18 PS1SIG(I) = 0.
PS2SIG(I) = 0.
DO 17 KK = 1,LS3
   K = KK - 3
   PS1SIG(I) = PS1SIG(I) + BETAI(K,I)
   PS2SIG(I) = PS2SIG(I) + BETAI(K,I)
17 PS1SIG(I) = PS1SIG(I) + BETAI(KK,1)
18 PS2SIG(I) = PS2SIG(I) + BETAI(KK,2)
PS1V = PS1V + TERM*PS1V
PS1RHO = PS1RHO + TERM*PS1RHO
PS1T = PS1T + TERM*PS1T
PS2V = PS2V + TERM*PS2V
PS2RHO = PS2RHO + TERM*PS2RHO
PS2T = PS2T + TERM*PS2T
GAMDG = (GAMMA - 1.)/GAMMA
SGDG = 2./GAMMA/GAMMA
C DVB WRT V
PBVV = GAMDG*PS2V
C DVB WRT RHO
PBVRHO = GAMDG*PS2RHO
C DVB WRT T
PBVT = GAMDG*PS2T + S2DG2*PGAMT
C DAA WRT V
PAAV = PS1V - PBVV
C DAA WRT RHO
PAARHO = PS1RHO - PBVRHO
C DAA WRT T
PAAT = PS1T - PBVT
C DBB WRT SIGMA(I) AND DAA WRT SIGMA(I)
DO 19 II = 1,LS3
   PBBSIG(I) = GMDG*PS2SIG(I) + S2DG2*PS2SIG(I)
19 PABSIG(I) = PS1SIG(I) - PBBSIG(I)
IF (VERSI .LE. AREAV) GO TO 24
C ASSIGNED AREA EQUATIONS
T1 = 1./(M2 - 1.)
GAM1 = GAMMA - 1.
C DVO/DIVAR WRT V
   BETAI(1,1) = T1*(TERM - F(I)*PM2V - V*PAAV)
C DVO/DIVAR WRT RHO
   BETAI(1,2) = -V*PAARHO
C DVO/DIVAR WRT T
   BETAI(1,3) = T1*(V*PAAT + F(I)*PM2T)
C DVO/DIVAR WRT SIGMA(I)
   DO 20 II = 1,LS3
      I = II - 3
20 BETAI(I,1) = -T1*(V*PABSIG(I) + F(I)*PM2SIG(I))
IF (RHOCON) GO TO 22
C DRHO/DIVAR WRT V
45
APPENDIX B

FUNCTION POWER (X, N)

POWER = 1.
IF (X NE. 0.) RETURN
POWER = N.
RETURN
2 IF (X NE. 1.) GO TO 3
POWER = X
RETURN
3 POWER = X**N
RETURN
END

FUNCTION COMB

FUNCTION FUEL***RCM

LOGICAL TR, HP
SUBROUTINE SHOK

EQUILIBRIUM AND FROZEN SHOCK CALCULATIONS

LOGICAL TP, HP, EOL

REAL MIXNM

DIMENSION AI2(25), AI3(25)

C EQUILIBRIUM SHOCK

CALL ELEMNT (LS, SPNM, SIGMA)

GAM = GAMMA

ENI = 0.1/FLOAT(AI2)

IF (.FALSE.) . THEN

ENDIF = ENI

EQL = .TRUE.

CALL SHOCKS (EQL)

CALL ESOUT

RETURN

END

SUBROUTINE SHOCKS (EQL)

SHOCK EQUATIONS

LOGICAL EQL, NEXT

REAL MIXNM, M2

DIMENSION AI2(25), AI3(25)

C FROZEN SHOCK

WM = MIXNM

DLVTP = 1.

GAM = GAMMA

DO 3 I = 1, LS

ENI(I) = SIGMA(I)

EQL = .FALSE.

CALL SHOCKS (EQL)

CALL FSOUT

RETURN

END

SUBROUTINE SHOCKS (EQL)

SHOCK EQUATIONS

LOGICAL EQL, NEXT

REAL MIXNM, M2

DIMENSION AI2(25), AI3(25)

C EQUILIBRIUM SHOCK

CALL ELEMNT (LS, SPNM, SIGMA)

GAM = GAMMA

ENI = 0.1/FLOAT(AI2)

ENDIF = ENI

EQL = .TRUE.

CALL SHOCKS (EQL)

CALL ESOUT

RETURN

END
APPENDIX B

C INITIAL ESTIMATE OF PRESSURE AND TEMPERATURE RATIOS
P21 = (2/2.GAMMA - GAMMA + 1.)/(GAMMA + 1.)
T21 = P21/2.1/GAMMA + 1.1(GAMMA + 1.)
IF (EQ .AND. 1.1/P21 .GT. 2000.) T21 = 0.7*T21 + 600./T

C ITERATE ON PRESSURE AND TEMPERATURE RATIOS
C ************ ITERATIONS SET AT 99 ARBITRARILY BY AGM ************
DO 4 K = 1,99
IF (K .GT. 81) GO TO 8795
GO TO 8796

8795 KRITE 16,8797) K
8797 FORMAT(9HO<SHOCKS),5X,36HEQUILIBRIUM SHOCK CALCULATION FAILED)
NEXT = .FALSE.
RETURN
6 WRITE 16,101)
101 FORMAT (9HO<SHOCKS),5X,31HFROZEN SHOCK CALCULATION FAILED)
NEXT = .TRUE.
RETURN
END

SUBROUTINE ELEHNT (LS,DSPEC,SIGMA)
C COLLECT ELEMENT DATA FOR EQUILIBRIUM SHOCK OR COMBUSTION
DIMENSION DSP EC 125),SIGMA(25),LMT(*),SUBS(41
COMMON/LTUS/LTHM,L0AT,NTHRO,NBLANK,NPHOTO
COMMUN/MISC/OUM1(7),LLMTI15),80(15)
COMMON/[NOX/TP,HP,NLM.NS,IQ1,OJM2(3)
EQUIVALENCE (DSP,SI>)
IF (ILS .NE. SS) GO TO 10

C CONSTRUCT LIST OF ELEMENTS PRESENT
READ (LTHM,99) DUMMY
NSP = NS * 1
READ(LTHM,94) SP, I LMT(K),SUBS IK) ,K-1,4) iDUMMl,DUMM2,DUMM3
99 FORMAT(A8,16X,*(A2,F3.0)/A1/A1/A1)
DU 8 I=NSP,LS
IF (DSPEC(I) .NE. DSP) GO TO 8
DO 3 L = 1,5
3 AIL,I) = 0.
IF (NLM .NE. 0) GO TO 4
NLM = 1
4 CONTINUE
5 IF (.NOT. EQL GU TO 6
WRITE (6,100)
100 FORMAT ((HO<SHOCKS),5X,36HEQUILIBRIUM SHOCK CALCULATION FAILED)
NEXT = .FALSE.
RETURN
6 WRITE (6,101)
101 FORMAT ((HO<SHOCKS),5X,31HFROZEN SHOCK CALCULATION FAILED)
NEXT = .TRUE.
RETURN
END

SUBROUTINE ELEHNT (LS,DSPEC,SIGMA)
C COLLECT ELEMENT DATA FOR EQUILIBRIUM SHOCK OR COMBUSTION
DIMENSION DSP EC 125),SIGMA(25),LMT(*),SUBS(41
COMMON/LTUS/LTHM,L0AT,NTHRO,NBLANK,NPHOTO
COMMUN/MISC/OUM1(7),LLMTI15),80(15)
COMMON/[NOX/TP,HP,NLM.NS,IQ1,OJM2(3)
EQUIVALENCE (DSP,SI>)
IF (ILS .NE. 45) GO TO 10

C CONSTRUCT LIST OF ELEMENTS PRESENT
READ (LTHM,99) DUMMY
NSP = NS * 1
2 READ(LTM,44) SP LMTIK),SUBS IK) ,K-1,4) OUM1,DUMM2,DUMM3
99 FORMAT(A8,16X,*(A2,F3.0)/A1/A1/A1)
DU 8 I=NSP,LS
IF (DSPEC(I) .NE. DSP) GO TO 8
DO 3 L = 1,5
3 AIL,I) = 0.
IF (NLM = NE. 0) GO TO 4
NLM = 1

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```fortran
LLMT(NLM) = LMT(1)
DO 4 K=1,4
IF (SUBSIK) .EQ. 0.) GO TO 7
DO 5 L=1,NLM
IF (LLMT(L) .NE. LMT(I)) AU(L) = SUBSIK
GO TO 6
5 CONTINUE
NL = NL + 1
LLMT(NLM) = LMT(K)
AU(NLM) = SUBSIK
6 CONTINUE
7 NS = NS + 1
IF (NS .LT. LS) GO TO 2
GO TO 9
8 CONTINUE
GO TO 2
9 REMIND LTHM
C
C COMPUTE ELEMENT CONCENTRATION IN GM-ATOMS/GM
DO 11 1=1,LS
C(1) = C(1) + LLMT(1)*SIGMA(1)
11 RETURN
END
SUBROUTINE EQLBRM
C CALCULATE EQUILIBRIUM COMPOSITION AND PROPERTIES
LOGICAL CONVG,ISING,LOGV,TP,NEXT
DIMENSION PR3HI18)
COMMON/POINTS/DLVTP,DLVPT,GAMMA,MN
COMMON/SPACES/ENLN(25J),ENLIN(25J),DELN(25J),A(15,25)
COMMON/SC/T,PP,CPRO,MSURD,ENM,SURM,ENML,LMLM(15),BMLM(15)
COMMON/INDO/TP,HP,NLM,NS,IQL,CONVG,KMAT,IMAT
COMMON/GHS/GRT(25),WRT(25),SR(25),CPRI25),DLPR(25)
COMMON/MATX/GI28,29),XI26
COMMON/NEC1/NUM141,CPSUM,DUM2
COMMON/COND/NUM335),NEXT
C INITIALIZE
SMALL = 1.0D-06
SMALL = -13.815511
SIZE = 18.0
SIZEF = 0.
CONVG = .FALSE.
ISING = .FALSE.
LOGV = .FALSE.
ITN = 300
ITNUMB = ITN
SUM = ENN
IAGM = 0
TLN = ALOGTTI
TP = ALOGPP/ENN
ENN = ALOGENN
CALL THERM(TT,1.)
CPSUM = 0.
DO 2 I=1,NS
2 CPSUM = CPSUM + CPRID'ENIII
DO 3 CALL MATRIX
NUMB = ITN-1 ITNUMB = ITN
IAGM = IAGM + 1
IQL = IQL + 1
IF (IQL .LT. CONVG) G3 TO 67
IF (LOGV) GU TO 63
DO 182 L=1,NLM
182 PROWIL) = GIIQ(I.L)
GO TO 72
C LOGV = .TRUE. --- SET UP MATRIX TO SOLVE FOR DLVP
DO 63 IQL=1,182
63 G(IQL,IQL) = ENN
IQL = IQL + 1
DO 777 I=1,12
777 G(I,IQL) = G(I,IQL)
72 IMAT = IMAT + 1
67 ITST = IMAT
CALL GAUSS
IF (ITST .NE. IMAT) GO TO 774
IF (LOGV) GU TO 171
SUM = 0.
DO 175 L=1,NLM
175 SUM = SUM + PROWIL(XILI)
OLVP = 1. + (G(IQL,IQL) SUM/ENN - X(IQL)
CPEP = G(IQL,IQL) - SUM/ENN - X(IQL)
DO 170 L=1,121
170
```

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176 CCPR = CCPR - (GIQ2) *(I) *X(I)
LODV = .TRUE.
GO TO 43

C SINGULAR MATRIX
774 IF (.NOT. CONVG) GO TO 871
WRITE (6,172)
172 FORMAT (9HOIEQLRM),5X,26DERIVATIVE MATRIX SINGULAR
GO TO 871
871 WRITE (6,74)
74 FORMAT (9HOIEQLRM),5X,15SINGULAR MATRIX
IF (ISING) GO TO 873
ISING = .TRUE.
DO 970 I=1,NS
IF (EN(I) .NE. 0.) GO TO 970
EN(I) = SMALL
ENL(I) = SMALL
970 CONTINUE
WRITE (6,775)
775 FORMAT (9HOIEQLRM),5X,THRESTART
GO TO 43

85 ITNUMB = ITNUMB - 1
C OBTAIN CORRECTIONS TO THE ESTIMATES
IF (TP) XIQ2) = 0.
DLNT = XIQ2)
SUM = XIQ2)
DO 101 I=1,NS
DEL(I) = HRT(I),DLNT - HRT(I) * (SK(I) - ENL(I)) - TM) + SUM
DO 99 L=1,NS
99 DEL(I) = DEL(I) + AL(I),KL
101 CONTINUE
AMBD = 1.
AMBD1 = 1.
SUM = ABS(XI02)
IF (ABS(DLNT) .GT. SUM) SUM = ABS(DLNT)
DO 917 I=1,NS
IF (EN(I) .GT. 0.) .AND. DEL(I) .GT. 0. .OR. DEL(I) .LE. 0.) GO TO 917
SUM = (-9.212 - EN(I)) * DEL(I) / (DEL(I) - XIQ2)
SUM = ABS(SUM)
IF (SUM .LT. AMBD1) AMBD1 = SUM
917 CONTINUE
IF (SUM .GT. 1.0E-05) AMBD = 2./SUM
IF (AMBD1 .LT. AMBD) AMBD = AMBD1
C APPLY CORRECTIONS TO ESTIMATES
SUM = 0.
DO 113 I=1,NS
ENL(I) = ENL(I) + AMBD * DEL(I)
EN(I) = 0.
IF (ENL(I) .LE. 0.) GO TO 113
EN(I) = EXP(ENL(I))
SUM = SUM + EN(I)
113 CONTINUE
CPSUM = CPSUM + CI02) * EN(I)
CPSUM = CPSUM * CPRID*ENL(I)
ENL = EXP(ENL(I))
TM = LOG(PP/ENN)
C TEST FOR CONVERGENCE
IF (ITNUMB .EQ. 0) GO TO 13
IF (AMBD1 .LT. 1.) GO TO 43
SUM = ENN - SUM/ENN
SUM = ABS(SUM)
IF (SUM .GT. 0.5E-05) GO TO 43
DO 130 I=1,NS
AA = ABS(DLNT) / SUM
130 CONTINUE
13 CONVG = .TRUE.
IF (ITNUMB .NE. 0) GO TO 160
WRITE (6,973) ITN
973 FORMAT (9HOIEQLRM),4X,13,1*ITERATIONS - NO CONVERGENCE*
GO TO 873
160 IF (.NOT. (TP .AND. CONVG)) GO TO 143
CALL THRM (TT,1.)
CPSUM = 0.
DO 4 IT=1,NS
4 CPSUM = CPSUM + CI02) * EN(I)
143 ITNUMB = ITN
GO TO 43
C CALCULATE EQUILIBRIUM PROPERTIES
1171 OLVP = -1.
OLVP = 1.
CCPR = CPSUM
GO TO 199
171 SUM = 0.
DO 179 L=1,NS
179 SUM = SUM + EN(I)
1171 OLYP = -1.
OLYP = 1.
CCPR = CPSUM
GO TO 199
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179 SUM = SUM + PROD(L1*X1L)
DLVPT = -2. * SUM/ENN + XI(Q1)
199 GAMMA = 1./(DLVPT + DLVTP*DLVTP*ENN/CPRI)
JN = J/ENN
872 ENI1 = EXPENLN(111)
RETURN
873 WRITE(6,900)
900 FORMAT(1H10,E4.0)
NEXT = TRUE.
GO TO 171
END

SUBROUTINE SPOUT

LOGICAL FRZQ
REAL MIXMW,M2,MACH1,MACHF,M21,LSUBM
COMMON/KOin/OUMU21,UNITO,OUM2152,FPS,SI,DBUGO
COMMON/COND/AREA,MACH,F,EJA,MACHF,M21,GAMMA,TCP,R
COMMON/NECC/MR,M2,GAMMA,TCP,R
COMMON/SPC/SRT(25),SR(25),CPF(25),OCPR(25)
COMMON/SPEC/DUM(35),PMH(25),DUM(25),1021
COMMON/AFUN/CX3,CX2,CXI,CXO,IPSZ,LSUBM.ETA,0,VISC,SETA
COMMON/MISC/TF,P,F,CPR,HRO,ENN,DUM(32)
COMMON/POINTS/DLVTI,BLVTI,GAMMAF,WN
ENTRY ECOUT

EOUILIBRIUM COMBUSTION OUTPUT
WRITE(6,101)
101 FORMAT (1H1,50X,30M"* EOUILIBRIUM COMBUSTION *\)
VI = 0.
GO TO 2
ENTRY ESOUT
EOUILIBRIUM SHOCK OUTPUT
WRITE(6,102)
102 FORMAT (1H1,7X,37.-I"* EOUILIBRIUM SHOCK CALCULATION *\)
V = V
2 PI = P
RHO = RHO
T = T
P21 = PF/P1
T21 = TF/T1
RHO21 = P21/T21
P = PF
V = VI/RHO21
RHO = RHO21/RH021
T = T*T1
GAMMAF = TCPF/(TCP - 1./MIXMW)
FRZQ = FALSE.
GO TO 3
ENTRY FSOUT
FROZEN SHOCK OUTPUT
WRITE(6,103)
103 FORMAT (1H1,14X,32."* FROZEN SHOCK CALCULATION *\)
P = P
V = V
RHO = RHO
T = T
P21 = PF/P1
T21 = TF/T1
RHO21 = P21/T21
P = PF
V = VI/RHO21
RHO = RHO1*RH021
T = T*T1
GAMMAF = TCPF/(TCP - 1./MIXMW)
FRZQ = TRUE.
3 CALL THER(TT,1.,1.)
PMDL = ALOG(P/MIXMW)
S = 0.
DO 4 1 = LS
IF (SIGMA(1) .EQ. 0.) GO TO 4
S = S + SIGMA(1)*(SR(1) - ALOG(SIGMA(1)) - PMDL)
4 CONTINUE
S = S*1.987165
MACHI = SQRT(S)
VF = VI/RHO21
RHOF = RHO1*H021
CALL THER(EF,1.,1.)
PMDL = ALOG(P/FW)
SP = S.
DO 5 1 = LS
IF(E(1) .EQ. 0.) GO TO 5
SP = SP + E(1)*(SR(1) - ALOG(E(1)) - PMDL)
5 CONTINUE
SP = SP*1.987165
MACHF = SQRT(V/FVF/TFW/GAMMAF)
521 = SF/S
G21 = GAMMAF/GAMMA1

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IF (SVI .EQ. 0.) GO TO 205
SVF = VI/MACHI
V2I = VF/VI
M2I = MACHF/MACHI
SV2I = SVF/SVI
GO TO 305

205 MACHI = 0.
SVI = 0.
SVF = 0.
V2I = 0.
M2I = 0.
SV2I = 0.

305 IF (N azi NOT .EQ. 0.) IFPSZ .NE. N屁股 GO TO 405
C CALCULATE L(M) FOR KINETIC AREA FUNCTION
PST = 1.
RSVST = (GAMMA/SVI)**(1.0/3252546)*0
LSUM = (1./PST)*(RHO21/(RHO21-1.))*(RSVST/IPST*VISC*MACHI)**(1.0/32)
**ETAI*EPAI***(4.0-ETA)***(1./ETA)

405 WRITE (4,104)
104 FORMAT (4/Ii,L1#INITIAL STATE,17I,H#FINAL STATE,17X,1#INITIAL RATIO//)
C IF UNUSED NE, FPS) GO TO 6
CONVERT FROM INTERNAL (CGS) UNITS TO FPS UNITS
P1 = P1*2116.2
PF = PF*2116.2
VF = VF*30.48
VF = VF*30.48
RHODI = RHODI*62.43
ROHF = ROHF*62.43
T1 = T1*1.8
TF = TF*1.8
SV1 = SV1*30.48
SVF = SVF*30.48
WRITE(6,105) P1,PF,V1,VI,V2I,ROHF,ROHF,RHO21,T1,TF,T2I,S,SV1,SVF,SV2I
105 FORMAT (10X,8H(PRESSURE,F35.5,E29.5,E32.5/I,11X,11H(TEMPERATURE,E32.5,E29.5,E32.5/11X,9H(DENSITY,E36.5,E29.5,E32.5/11X,10H(ITEMP,E32.5,E29.5,E32.5/I1X,11H(VELATURATE,E32.5,E29.5,E32.5/I1X,10H(ENTROPY,E32.5,E29.5,E32.5/I1X,14H(GAMMA,E32.5,E29.5,E32.5/I1X,14H(SONIC VELOCITY,E29.5,E29.5,E32.5/I1X,8H(FT/SEC)))
GO TO 8

6 IF UNUSED NE, SI) GO TO 7
C CONVERT FROM INTERNAL (CGS) UNITS TO SI UNITS
P1 = P1*1.0132546*05
PF = PF*1.0132546*05
VF = VF*0.01
VF = VF*0.01
RHODI = RHODI*1000.
ROHF = ROHF*1000.
S = S*4184.0
SF = SF*4184.0
SV1 = SV1*0.01
SVF = SVF*0.01
WRITE(6,106) P1,PF,V1,VI,V2I,ROHF,ROHF,RHO21,T1,TF,T2I,S,SV1,SVF,SV2I
106 FORMAT (10X,8HPRESSURE,F35.5,E29.5,E32.5/I1X,8H(TEMPERATURE,F32.5,E29.5,E32.5/I1X,RHOCM/E36.5,E29.5,E32.5/I1X,10H(TEMPERATURE,F32.5,E29.5,E32.5/I1X,10H(DENSITY,F32.5,E29.5,E32.5/I1X,11H(VOLUME,E32.5,E29.5,E32.5/I1X,11H(GAMMA,E32.5,E29.5,E32.5/I1X,14H(SONIC VELOCITY,F29.5,E29.5,E32.5/I1X,8H(M/SEC)))
GO TO 8

7 WRITE(6,107) P1,PF,V1,VI,V2I,ROHF,ROHF,RHO21,T1,TF,T2I,S,SV1,SVF,SV2I
107 FORMAT (10X,8HPRESSURE,F35.5,E29.5,E32.5/I1X,8H(TEMPERATURE,F32.5,E29.5,E32.5/I1X,10H(DENSITY,F32.5,E29.5,E32.5/I1X,11H(VOLUME,F32.5,E29.5,E32.5/I1X,11H(GAMMA,E32.5,E29.5,E32.5/I1X,14H(SONIC VELOCITY,F29.5,E29.5,E32.5/I1X,8H(M/SEC)))
GO TO 8

C CONVERSION FROM INTERNAL (CGS) UNITS TO SI UNITS
WRITE(6,108) P1,PF,V1,VI,V2I,ROHF,ROHF,RHO21,T1,TF,T2I,S,SV1,SVF,SV2I
108 FORMAT (10X,8HPRESSURE,F35.5,E29.5,E32.5/I1X,8H(TEMPERATURE,F32.5,E29.5,E32.5/I1X,10H(DENSITY,F32.5,E29.5,E32.5/I1X,11H(VOLUME,F32.5,E29.5,E32.5/I1X,11H(GAMMA,E32.5,E29.5,E32.5/I1X,14H(SONIC VELOCITY,F29.5,E29.5,E32.5/I1X,8H(M/SEC)))
GO TO 8

8 WRITE (6,109)
109 FORMAT (6BX,A8,E15.5)
9 CONTINUE
WRITE(6,110) WSPECIES,5X,13HMOLE FRACTION
WRITE(6,110) SPECIES(ENI),ENII)*WM
110 FORMAT (6X,10H) 8(20X,13HMOLES)#(20X,13HMOLES)
GO TO 6

RETURN
END
APPENDIX B

SUBROUTINE MATRIX

LOGICAL TP, HP, CONVG

COMMON/SPCES/ENI(25), EMLN(25), DELM(25), AI(15,25)
COMMON/NMCS/FT, PP, CP, HSUB, ENN, SUMN, ENNL, LMTN(25), BON15)
COMMON/INDX/TP, HP, L, NS, I101, CONVG, KMAT, IEN
COMMON/GHC/RT(25), HR(25), SR(25), CP(25), DCP(25)
COMMON/MAT/GR28, XX, KLZB)
COMMON/NEC/DUM41, CPSUM, DUM2

I02 = I01 + 1
I03 = I02 + 1
KMAT = I03
IF (IDOT, CONVG, AND, TP) KMAT = I02
(KMAT = KMAT - 1)

C CLEAR MATRIX STORAGES TO ZERO

DO 211 I = 1, KMAT
DO 211 J = 1, KMAT
G(I, J) = 0.
211 CONTINUE

SSS = 0.
HSUM = 0.

C BEGIN SETUP OF ITERATION MATRIX

KK = L
TM = ALOG(PP/ENN)
DO 65 J = 1, NS
H = HRT(J) + ENL(J) + TNI*EN(J)
F = HRT(J) - SR(J) - ENL(J) - TM*EN(J)
SS = H - F
TERM = H
IF (KMAT .EQ. I02) TERM = F
DO 55 I = 1, L
G(I, J) = G(I, J)*TERM
55 CONTINUE

C CALCULATE THE ELEMENTS RIIKI

IF (AI(J) .EQ. O.) GO TO 35
TERM = A(I, J)*EN(J)
DO 15 KM = 1, L
G(I, KM) = G(I, I)*TERM
15 CONTINUE

G(I, I) = G(I, I)*TERM
G(I, I) = G(I, I)*TERM

IF (CONVG, OR, TP) GO TO 55
G(I, I) = G(I, I) + SS
G(I, I) = G(I, I) + SS
G(I, I) = G(I, I) + SS

C REFLECT SYMMETRIC PORTIONS OF THE MATRIX

ISYM = I02
IF (HP, OR, CONVG, ISYM) I02 = I02 + 1
ISYM = ISYM + 1
G(I, J) = G(J, I)
102 CONTINUE

C COMPLETE THE RIGHT HAND SIDE

IF (CONVG) GO TO 175
DO 145 I = 1, L
G(I, KMAT) = G(I, KMAT) + BON(I) - G(I, I01)
G(I, I01) = G(I, I01) + ENV + SUMN
145 CONTINUE

C COMPLETE ENERGY ROW AND TEMPERATURE COLUMN

IF (KMAT .EQ. I02) RETURN
IF (HP) ENERGY = HSUB - RT*HNS
G(I02, I03) = G(I02, I03) + ENERGY
175 G(I02, I03) = G(I02, I03) + CPSUM
RETURN
END
APPENDIX B

SUBROUTINE GAUSS
C SOLVE ANY LINEAR SET OF UP TO 20 EQUATIONS
DIMENSION COEFX(20)
COMMON/MATX/G(28,28),XI28)
COMMON/INDX/TP,H,P.NLM:NS,CONVG,KMAT,IUSE
DATA BIGNO/1.E38/

C BEGIN ELIMINATION OF NNTH VARIABLE
IUSE1=IUSE+1
6 DO 45 NN=1,IUSE
IF (NN-IUSE) 8,83,8
45 CONTINUE
C SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW
8 DO 18 I=NN,IUSE
COEFX(J) = BIGNO
IF (ABS(COEFX(J)) .GT. BIGNO) GO TO 18
COEFX(I) = 0.
10 DO J=NN,IUSE1
SUM = SUM + COEFX(I)*X(J)
IF (J .EQ. NN) GO TO 9
20 CONTINUE
IF (SUM .GT. COEFX(J) * SUM) COEFX(J) = SUM
9 CONTINUE
C INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NNTH
C VARIABLE FROM THE REMAINING EQUATIONS
C INTERCHANGE EQUATIONS I AND NN
28 IF (NN-I) 29,31,29
29 DO 30 J=NN,IUSE1
Z = G(J,NN)
G(J,NN) = G(28,NN)
G(28,J) = Z
30 CONTINUE
C NOW DIVIDE NNTH ROW BY NNTH DIAGONAL ELEMENT AND ELIMINATE THE NNTH
C VARIABLE FROM THE REMAINING EQUATIONS
31 K = NN + 1
33 DO 36 J = K, IUSE1
SM = SUM + COEFX(J)*X(J)
36 CONTINUE
C BACKSOLVE FOR THE VARIABLES
K = IUSE1
47 J = K - 1
X(K) = 0.
SUM = 0.D0
IF (IUSE) 51,48,48
48 DO 50 I = J, IUSE1
SUM = SUM + G(I,J)*X(J)
50 CONTINUE
51 X(K) = G(K,IUSE1) - SUM
K = K - 1
IF (K) 47,151,47
23 IUSE = IUSE - 1
151 RETURN
END

SUBROUTINE YOUT(NO,TLAST,Y,NO42)
C ***** PRINT OUT INFORMATION
C IN NAMELIST PABP THE PRINTING VARIABLES ARE
C 1 PAPS - SET TRUE IF PRINTING AT SPECIFIC STATIONS DESIRED
C 2 TPROMP - A TABLE OF PRINT STATIONS INPUT 50 VALUES AT MOST
C 3 NPRINT - THE NUMBER OF PRINT STATIONS

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APPENDIX B

4 IDEL - INCREMENT FOR AUTOMATIC CALCULATION OF AT MOST 50 PRINT
STATIONS. IDEL NOT INPUT - A TABLE OF IPRINTS MUST BE
INPUT IF PAPS = TRUE
IF PAPS = FALSE IPRIT INPUT WILL CAUSE PRINTING EVERY IPRIT
ITERATIONS
END MUST ALWAYS BE SPECIFIED

***********************************************************************
LOGICAL KUP
LOGICAL TCON
LOGICAL OVUTO
REAL IVAR
DIMENSION YINO,K2I,YPRINT(28)
COMMON/PRINT/PRINT(50),NPRINT,NCO
COMMON/STCORN/NI,H,MMIN,MMAX,NSDI,MPI,KFLAG1,JSTART
COMMON/COND/VAR,AREA,MODT,P,IVAR,Y,AND,J,SIGMA(251),LS,LOP,LOP1
COMMON/UPDT/KUP
COMMON/STCORN/TPREV,HMI
COMMON/STCORN/VOLD
COMMON/OPTS/VERSI,FIMEV,DNUM2(2),TCON,AGCUCON,DUM3
OVUOT = .FALSE.
IF IINCDS .EQ. 13) GO TO 10
INT=1
NCO=1
11 CONTINUE
IT=INT,INT, IPRINT(INT) AND, IPRINT(INT),LE, 1) GO TO 10
IF (OVUOT) GO TO 13
ENTRY YOUT1

1F (IVOSI .LE. 0., FIMEV) GO TO 12
YVAR = IVAR / TPREC/IVOLD + Y(I))
GO TO 16
17 CONTINUE
YVAR = DVAR + IT - FPREV/IVOLD + Y(I),/2.
GO TO 14
13 CONTINUE
IF (IVOSI .LE. 0., FIMEV) GO TO 17
YVAR = DVAR + IT - IVAR/IVOLD + Y(I))
GO TO 16
18 CONTINUE
IF (INT .LT. NCO) GO TO 10

10 CONTINUE
V = YPRINT(INT)
MO = YPRINT(2)
1 = YPRINT(3)
10 FOR I = 1,L3
SIGMA(I) = YPRINT(I)
280 CONTINUE
IF (IVOSI .LE. 0., FIMEV) GO TO 14
VOL3 = TPRINT(INT) - IVAR
YVAR = DVAR + 2.*IVAR/VOL3
GO TO 14
15 CONTINUE
YVAR = DVAR + TPRINT(INT) - TPREV
IF (IVOSI .LE. 0., FIMEV) GO TO 14
VOL3 = TPRINT(INT) - IVAR
YVAR = DVAR + 2.*IVAR/VOL3
GO TO 14
16 CONTINUE
YVAR = DVAR + TPRINT(INT)
KUP = .TRUE.
CALL DIFF
KUP = .FALSE.
GO TO 400
380 CONTINUE
IF (IVOSI .LE. 0., FIMEV) GO TO 390
VOL3 = TPRINT(INT) - TPREV/IVOLD + Y(I11)/2.
GO TO 390
391 YVAR = DVAR + IT - TPREV/IVOLD + Y(I11)/2.
400 CONTINUE
CALL OUT
INT = INT + 1
IF (INT .LE. NPRINT) GO TO 11
RETURN
SUBROUTINE YOUTD (Y,NQ)
DIMENSION Y(28,6)
WRITE(6,7)
7 FORMAT(5X,*KFLAG NOT EQUAL TO 0*)
RETURN
END

SUBROUTINE DRIVESC11,TC,TLAS1,T,HO,EPS,HF,KFLAG,K2)
LOGICAL PAPS
COMMON/ STCOM1/ N, T, H, HMIN, UMAX, EPS1, MF1,KFLAG1, JSTART
COMMON/ STCOM2/YMAX(28)
COMMON/ STCOH3/ERRO*(28)
COMMON/ STCOH5/FSAVE(561
COMMON/ STCOM<>/IPRIT
PAPS
DIMENSION YINO(K2),YOOT(56),INIS4(812)
9999 CONTINUE
LOUT=H
IF (EPS.LE.0.1) GO TO 400
IF (NO.LE.O) GO TO 410
IF((TO-TLASTI)*HO.GE.O) GO TO 420
N = NO
T = TO
H = HO
HMIN = ABS(HO)
HMIN = AMIN1HMIN,.1*HMAX)
EPS1 = EPS
MF1 = MF
JSTART = 0
KFLAG = 0
C
NCOUNT=0
NIS4 = NO*(NO+1)
10 CONTINUE
HNI = H
TPREV = T
CALL STIFFd.NO,TNI S4.NI S4 , K2)
NU = JSTART
C
KGO = 1 - KFLAG1
GO TO 1200,300,KGU
C KFLAG1 = Of 'I i -it -3
C
20 CONTINUE
IF(PAPS) GO TO 9998
CALL YOUT1
NCOUNT = NCOUNT + I
IF(INCOUNT .NE. IPRINT) GO TO 888
CALL QUT3
NCOUNT = 0
888 CONTINUE
GO TO 9997
9998 CONTINUE
CALL YOUTD(NO,TLAST,Y,NQ,K2)
9997 CONTINUE
IF(T-TLAST*.H.LT.O) GO TO 10
C THE PROBLEM IS FINISHED. HERE CALL YOUT AND/OR OTHER ROUTINES
C TO OBTAIN DESIRED FINAL RESULTS.
CALL QUT3
GO TO 500
C
100 WRITE (LOUT,105) T
105 FORMAT(/30H KFLAG = -1 FROM STIFF AT T = ,616.8/, 1 36H ERROR TEST FAILED WITH ABS(H) = HMIN/,)
110 IF((KFLAG,.EQ.10)) GO TO 150
KFLAG = KFLAG + 1
HMIN = HMIN*1.0
H = HMIN
WRITE (LOUT,115) H
115 FORMAT(24H M HAS BEEN REDUCED TO ,E16.8, 1 20H AND STEP WILL BE RETRIED/)
JSTART = -1
GO TO 10
C
150 WRITE (LOUT,155)
155 FORMAT(/44H PROBLEM APPEARS UNSOLVABLE WITH GIVEN INPUT/,)
C
C MMIN HAS BEEN CUT BY 1O ORDERS OF MAGNITUDE WITH NO SUCCESS.
C THIS POINT, OUTPUT INFORMATION NEEDED FOR DEBUGGING.
C
C CALL YOUTDIY(NQ)
GO TO 500
C
200 WRITE (LOUT,205) T,H
205 FORMAT(/30H KFLAG = -2 FROM STIFF AT T = ,E16.8,5H H =,E16.8/, 1 52H THE REQUESTED ERROR IS SMALLER THAN CAN BE HANDLED/,)
C AT THIS POINT, OUTPUT INFORMATION NEEDED FOR DEBUGGING.
CALL YOUTDIY(NQ)
GO TO 500
C
56
APPENDIX B

300 WRITE (LOUT,305) T
305 FORMAT(/30H KFLAG * -3 FROM STIFF AT T = .616.8/)
GO TO 110

C
400 WRITE (LOUT,405)
405 FORMAT(/2I>H ILLEGAL INPUT.. EPS.LE.O.//)
KFLAG = -4
RETURN

C
410 WRITE (LOUT,4151
415 FORMAT(/23H ILLEGAL INPUT.. N.LE.O//I
KFLAG = -4
RETURN

C
420 WRITE (LOUT,425)
425 FORMAT(/3BH ILLEGAL INPUT.. (TO-TLAST)«HO .SE. 0.//J
KFLAG = -4
RETURN

C
500 KFLAG = KFLAG1
TO = T
HO = M
RETURN

END
SUBROUTINE STIFF(Y,N,P,W,N1S4,K2)
DIMENSION PMINIS4iYINOiK2I.ELI13).TQI41
COMMON/STCON1/N.T.H.HMIN.HNAX.EPS.MF,KFLAG,JSTART
COMMON/STCOM9/VOLD
COMMON/STCOM2/YHAXI28)
COMMON/STCOM3/ERRORI28I
COMMON/STCOM5/FSAVE(56)
DATA (ANOISE = 1.E-14I
VOLD ' VII)
NPEDV • NO
KFLAG - 0
TOLO - T
IF (JSTART.GT.0) GO TO 200
IF (JSTART.NE.O) GO TO 120

C* ON THE FIRST CALL, THE ORDER IS SET TO 1 AND THE INITIAL
C* DERIVATIVES ARE CALCULATED. YMAX IS INITIALIZED USING THE INITIAL
C* Y AND YDOT. IF BOTH ARE INITIALLY ZERO IN ANY COMPONENT, THE DEFAULT
C* VALUE IS 1. RMAX IS THE MAXIMUM RATIO BY WHICH H CAN BE INCREASED
C* IN A SINGLE STEP. IT IS INITIALLY 1.44 TO COMPENSATE FOR THE SMALL
C* INITIAL H, BUT THEN IS NORMALLY EQUAL TO 10. IF A FAILURE
C* OCCURS (IN CORRECTOR CONVERGENCE OR ERROR TEST), RMAX IS SET AT 2
C* FOR THE NEXT INCREASE. EPSJ IS USED AS THE RELATIVE INCREMENT
C* TO Y WHEN GETTING PARTIALS BY FINITE DIFFERENCING.

NS4 = NO*NO
NSQ1 = NS4 + 1
NO = NO + 1
CALL DIFFUN(N,T,Y,FSAVE,0,NPEOV,K2)
DO 110 1 = 1,N
Y(I,2) = FSAVE(I)*H
AYI = ABS(YI2)
IF (AYI.E(l.O.I AYI = ABSYI2)
110 YMAXI = AYI
NO = 1
T = 2
RMAX = 1.44
EPSJ = SQRTIANOISEI
METH = 0
METH = 0
MTER = 0
MTER = 0
VOLD = H

C* IF THE CALLER HAS CHANGED METH, OR IF JSTART = 0, COSET IS CALLED
C* TO SET THE COEFFICIENTS OF THE METHOD. IF THE CALLER HAS CHANGED
C* EPS OR METH, THE CONSTANTS E, EDN, EUP, AND BND MUST BE RESET.
C* E IS A COMPARISON FOR ERRORS OF THE CURRENT ORDER NO. EUP IS
C* TO TEST FOR INCREASING THE ORDER, EDN FOR DECREASING THE ORDER.
C* BND IS USED TO TEST FOR CONVERGENCE OF THE CORRECTOR ITERATES.
C* IF THE CALLER HAS CHANGED H, Y MUST BE RESCALED.
C* IF R OR METH HAS BEEN CHANGED, IDOUB IS RESET TO L = 1 TO PREVENT
C* FURTHER CHANGES IN H FOR THAT MANY STEPS. ALSO, RC IS RESET.
C* RC IS THE RATIO OF NEW TO OLD VALUES OF THE COEFFICIENT L(I040M.
C* WHEN RC DIFFERS FROM 1 BY MORE THAN 30 PERCENT, OR THE CALLER HAS
C* CHANGED MTER, I HEVAL IS SET TO MTER TO FORCE THE PARTIALS TO BE
C* UPDATED, IF PARTIALS ARE USED.

120 IF (MFEQ,MFEQ) GO TO 130
MEO = MEH
MIO = MTER
METH = MFLO
MTER = RF - 10*METH
MFEQ = RF

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APPENDIX B

IF (MTER .NE. MIO) IWEVAL = MTER
IF (METH .EQ. MEOI) GO TO 150
I = 1
IRET = 1
CALL COSET(METH,NO,EL,TQ,MAXDER)
RC = RC * EL / W
ELDO = EL
140 E0Y = (TQI) * EPS)**2
E = (TQ2) * EPS)**2
EPS = (TQ3) * EPS)**2
BND = (TQ4) * EPS)**2
GO TO 160, 170, 200, J, IREF
150 IF (EPS .EQ. EPSOLD) GO TO 160
IRET = 1
GO TO 140
160 LMAX = MAXDER + 1
EPSOLD = EPS
IF (H .EQ. HOLD) GO TO 200
DO 180 J = 1, N
R1 = R1 * H
DO 180 1 = 1, N
180 Y(I,J) = Y(I,J) * R1
RC = RC * H
BND = BND + 1
IF (T .LE. TOLD) GO TO 690
C THIS SECTION COMPUTES THE PREDICTED VALUES BY EFFECTIVELY
C MULTIPLYING THE Y ARRAY BY THE PASCAL TRIANGLE MATRIX.
200 IF (ABS(RC - 1.) .GT. 0.3) IHEVAL = MITER
T = T * H
DO 210 J1 = 1, NO
DO 210 I = 1, N
210 Y(I, J1) = Y(I, J1) * Y(1, J1)
C UP TO 3 CORRECTOR ITERATIONS ARE TAKEN. CONVERGENCE IS TESTED
C BY REQUIRING CHANGES TO BE LESS THAN BND, WHICH IS DEPENDENT ON
C EPS, IN EUCLIDEAN NORM. THE SUM OF THE CORRECTIONS IS ACCUMULATED
C IN THE VECTOR ERRORS(I). IT IS APPROXIMATELY EQUAL TO THE L-TH
C DERIVATIVE OF Y MULTIPLIED BY H**L / FACTORIAL(L - 1) * EL(L1), AND IS
C OTHERWISE PROPORTIONAL TO THE ACTUAL ERRORS TO THE LOWEST POWER OF
C H PRESENT (H**L).
C THE Y ARRAY IS NOT ALTERED IN THE CORRECTION LOOP. THE UPDATED
C VECTOR IS STORED TEMPORARILY IN FSAVE. THE NORM OF THE
C ITERATE DIFFERENCE IS STORED IN D.
220 DO 230 J = 1, N
230 FSAVE = D*0.
IF (IWEVAL .LE. 0) GO TO 340
C IF NECESSARY, THE PARTIALS ARE REEVALUATED PRIOR TO STARTING THE
C CORRECTOR ITERATION. IWEVAL IS THEN SET TO 0 AS AN INDICATOR
C THAT THIS HAS BEEN DONE.
C IF MTER = 1 OR 2, THE MATRIX P = I - L(0) * JACOBIAN IS STORED
C IN PW AND SUBJECTED TO LU DECOMPOSITION, WITH THE RESULTS ALSO
C STORED IN PW. IF MTER = 3, THE MATRIX USED IS P = I - L(0) * D,
C WHERE D IS A DIAGONAL MATRIX.
C GO TO 1240, 1260, 310, J, MTER
240 CALL PEDERV(N,T,Y,FSAVE,0,NPEOV,K2I)
R = -ELI
DO 250 I = 1, NSQ
250 PW(I) = PHI(I)*R
GO TO 300
260 D = 0.
DO 270 I = 1, N
270 D = D + FSAVE(T,NO)**2
RD = ABS(R)**2*H**2*EPS**2*ANOISE
J1 = NO
DO 290 J = 1, N
J1 = J1 + NO
YJ = Y(J1)
R = EPS**2*MAX(R)
R = AMAX1(R, RD)
YJ = YJ + R
D = -EL(I)*H/R
CALL DIFFUN(N,T,FSAVE,0, NPEOV,K2I)
DO 280 J = 1, N
280 PW(J) = FSAVE(J) - FSAVE(J)*NO
290 YJ = YJ
300 DO 305 I = 1, N
305 PW(I)*NO = PW(I)*NO + 1.
IWEVAL = 0
RC = 1.
CALL DECOMP(NO,N,PW(NSQ),FSAVE,IER)
IF (IER .NE. 1) GO TO 420
GO TO 360
APPENDIX B

310 R = EL111.*1
DO 320 I = 1,N
320 PM(I) = Y(I) + P*FSAVE(I)*NO - Y(I,2)
CALL DIFFUN(T,P,PM,FSAVE,N,PMDFV,K2)
DO 330 I = 1,N
EQ = PM(I) - Y(I)
 CALL DIFFUN(N,T,FSAVE,0,NPENV,K2)
GO TO 340

410 IF (M,NE,0) CRATE = MAX((1.,CRATE)/DI)
IF (M,EQ.3) GO TO 420
CALL DIFFUN(T,FSAVE,FSAVE,N,NPENV,K2)
GO TO 330

420 IF (MITER,NE.0) GO TO I 360, 360 , 400 I, NITER
C THE CORRECTOR HAS CONVERGED. IHEVAL IS SET TO -1 IF PARTIAL
C ERRORS WERE USED TO SIGNAL THAT THEY WERE NOT UPDATED ON
C SUBSEQUENT STEPS. THE ERROR TEST IS MADE AND CONTROL PASSES TO
C STATEMENT 500 IF IT FAILS.
C
450 DO = 0.
DO 460 J = 1,N
460 D = D + ERROR(I)/YMAX(I)**2
IF (M,NE,0) IHEVAL = -1
IF (D,GT.1) GO TO 500
C THE CASE OF THE CH3RO METHOD, COMPUTE THE CORRECTOR ERROR,
C SUB(M), AND SOLVE THE LINEAR SYSTEM WITH THAT AS RIGHT-HAND
C SIDE AND P AS COEFFICIENT MATRIX, USING THE LU DECOMPOSITION
C IF MITER = 1 OR 2.
360 DO 370 I = 1,N
370 FSAVE(I)*NO - FSAVE(I)*NO - Y(I,2) - ERROR(I)
CALL SOLVE(NO,P,FSAVE,FSAVE,PMDFV)
380 DO 400 I = 1,N
400 ERROR(I) = ERROR(I) + FSAVE(I,1)**2
GO TO 410
C TEST FOR CONVERGENCE. IF M,GT.0, AN ESTIMATE OF THE CONVERGENCE
C RATE CONSTANT IS STORED IN CRATE, AND THIS IS USED IN THE TEST.
C USE IN A POSSIBLE ORDER INCREASE ON THE NEXT STEP.
C IF A CHANGE IN H IS CONSIDERED, AN INCREASE OR DECREASE IN ORDER
C BY ONE IS MADE ONLY IF IT IS BY A
C FACTOR OF AT LEAST 1.1. IF NOT, IDUB IS SET TO 10 TO PREVENT
C TESTING FOR THAT MANY STEPS.
APPENDIX B

C******************************************************************************
KFLAG = 0
DO 470 J = 1,L
DO 470 I = 1,N
470 Y(I,J) = Y(I,J) + ELIJ*ERROR(I)
DO 480 I = 1,N
480 YMAXI = AMAX1(Y(I),ABS(Y(I)))
IF (DOUB.EQ.1) GO TO 520
DOUB = DOUB - 1
IF (DOUB.OF.1) GO TO 700
IF (NO.EQ.MAXDER) GO TO 700
DO 490 I = 1,N
490 Y(I,LMAX) = ERROR(I)
GO TO 700
C******************************************************************************
C* THE ERROR TEST FAILED. KFLAG KEEPS TRACK OF MULTIPLE FAILURES.
C* IF 3 OR MORE FAILURES HAVE OCCURRED, THE CODE TAKES A CHANGE OF ORDER.
C* IT IS ASSUMED THAT THE DERIVATIVES THAT HAVE ACCUMULATED IN THE
C* Y ARRAY HAVE ERRORS OF THE WRONG ORDER. HENCE THE FIRST
C* DERIVATIVE IS RECOMPUTED, AND THE ORDER IS SET TO 1. THEN
C* H IS REDUCED BY A FACTOR OF 10, AND THE STEP IS RETRIED.
C* AFTER A TOTAL OF 7 FAILURES, AN EXIT IS TAKEN WITH KFLAG = -2.
C******************************************************************************
500 KFLAG = KFLAG - 1
T = TOLD
DO 510 J = 1,NQ
510 YII.JI = Y(I,J) - VI I,JH(I)
RNAX = 2.
IF (ABS(HI.LE.HMIN)I GO TO 660
IF (KFLAG.LE.-31 GO TO 640
PR3 = 1.E+20
GO TO 540
520 PR3 = 1.E+20
IF (NQ.EQ.MAXOER) GO TO 540
D = 0.
DO 530 I = 1,N
530 D = D + ((ERROR(I) - Y(I,LMAX))/YMAX(I))**2
ENQ3 = 0.5/FLOAT(I)
PR3 = (DI/EI)**ENQ3*1.4 + 1.4E-6
540 ENQ2 = 0.5/FLOAT(I)
PR2 = (DI/EI)**ENQ2*1.2 + 1.2E-6
PR1 = 1.E+20
IF (NO.EQ.1) GO TO 560
D = 0.
DO 550 I = 1,N
550 D = D + ((ERROR(I) - Y(I,LMAX))/YMAX(I))**2
ENQ1 = 0.5/FLOAT(I)
PR1 = (DI/EI)**ENQ1*1.3 + 1.3E-6
560 IF (PR2.LE.PR3) GO TO 570
IF (PR3.LT.PR1) GO TO 590
570 IF (PR2.LT.PR1) GO TO 580
NEWQ = NQ
RH = 1./PR2
GO TO 620
580 NEWQ = NQ - 1
RH = 1./PR1
GO TO 620
590 NEWQ = L + 1
RH = 1./PR3
IF (RM.LT.1.1) GO TO 610
DO 600 I = 1,N
600 YII.NEWQ) = ERROR(I)*ELIJ/FLOAT(L)
GO TO 630
610 DOUB = 10
GO TO 700
620 IF ((KFLAG.EQ.0),AND.(RM.LT.1.1)) GO TO 610
C******************************************************************************
C* IF THERE IS A CHANGE OF ORDER, RESET NO., L, AND THE COEFFICIENTS.
C* IN ANY CASE H IS RESET ACCORDING TO RH AND THE Y ARRAY IS RESCALED.
C* THEN H IS REDUCED BY A FACTOR OF 10, AND THE STEP IS RETRIED.
C* AFTER A TOTAL OF 7 FAILURES, AN EXIT IS TAKEN WITH KFLAG = -2.
C******************************************************************************
630 NO = NEWQ
L = NO + 1
IRET = 2
GO TO 130
C******************************************************************************
C* CONTROL REACHES THIS SECTION IF 3 OR MORE FAILURES HAVE OCCURRED.
C* IT IS ASSUMED THAT THE DERIVATIVES THAT HAVE ACCUMULATED IN THE
C* Y ARRAY HAVE ERRORS OF THE WRONG ORDER. HENCE THE FIRST
C* DERIVATIVE IS RECOMPUTED, AND THE ORDER IS SET TO 1. THEN
C* H IS REDUCED BY A FACTOR OF 10, AND THE STEP IS RETRIED.
C* AFTER A TOTAL OF 7 FAILURES, AN EXIT IS TAKEN WITH KFLAG = -2.
C******************************************************************************
640 IF (KFLAG.EQ.-7) GO TO 670
RH = .1
RM = AMAX1(HMIN/ABS(H),RH)
H = HMIN
CALL DDIFFUN(T,Y,FSAVE,D,NPDEV,K2)
APPENDIX B

SUBROUTINE CDSETETH, NQ, EL, TO, MAXDER

C* COSET IS CALLED BY STIFF AND SETS COEFFICIENTS FOR USE THERE.
C* THE VECTOR EL, OF LENGTH NQ + 1, DETERMINES THE BASIC METHOD.
C* THE VECTOR TO, OF LENGTH 3, IS INVOLVED IN ADJUSTING THE STEP SIZE
C* IN RELATION TO TRUNCATION ERROR. ITS VALUES ARE GIVEN BY THE
C* PERST ARRAY.
C* THE VECTORS EL AND TO DEPEND ON METH AND NO.
C* COSET ALSO SETS MAXDER, THE MAXIMUM ORDER OF THE METHOD AVAILABLE.
C* CURRENTLY IT IS 12 FOR THE ADAMS METHODS AND 5 FOR THE GEAR METHODS.
C* LMAX DER = MAXDER + 1 IS THE NUMBER OF COLUMNS IN THE Y ARRAY.
C* THE MAXIMUM ORDER USED MAY BE REDUCED SIMPLY BY CHANGING THE
C* THE NUMBERS IN STATEMENTS 1 AND 2 BELOW.
C*
C* THE COEFFICIENTS IN PERST NEED BE GIVEN TO ONLY ABOUT
C* ONE PERCENT ACCURACY. THE ORDER IN WHICH THE GROUPS APPEAR BELOW
C* IS.... COEFFICIENTS FOR ORDER NO - 1, COEFFICIENTS FOR ORDER NO,
C* COEFFICIENTS FOR ORDER NO + 1. WITHIN EACH GROUP ARE THE
C* GEAR METHODS.
C* THE FOLLOWING COEFFICIENTS SHOULD BE DEFINED TO
C* MACHINE ACCURACY. FOR EACH ORDER NO, THEY CAN BE CALCULATED
C* FROM THE GENERATING POLYNOMIAL,
### APPENDIX B

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**GO TO 900**

C* 900 GO 910 K=1,1

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APPENDIX B

910 TQ(K) = PERTSTIQ(METH,K)
TQ(K) = .5*QI2(I)/FLOAT(N+2)
RETURN

C********************************************************** END OF CODE **********************************************************
END

SUBROUTINE OECOMPMDIM, N, LU, IPS, SCALES, IER
C
C LINEAR SYSTEMS SUBROUTINE
C
C DECOMPOSE THE N X N MATRIX A INTO TRIANGULAR L AND U SO THAT
C L * U = P * A FOR SOME PERMUTATION MATRIX P.
C
C NDIM THE NUMBER OF ROWS IN THE DIMENSION STATEMENT FOR THE
C MATRIX A IN THE CALLING PROGRAM.
C N THE NUMBER OF ROWS OR COLUMNS IN THE MATRIX
C LU ON INPUT, THE MATRIX A TO BE DECOMPOSED.
C IPS ON OUTPUT, THE ARRAY WHERE L AND U ARE STORED.
C IER THE ERROR RETURN FLAG. IT IS 1 FOR ALL ZERO ELEMENTS
C IN A ROW, 2 FOR A ZERO PIVOT, AND 0 FOR NO ERROR.
C
REAL LU(NDIM,N)
DIMENSION IPS(N), SCALES(N)
INTEGER PIVR3M

C INITIALIZE IER, IPS, LU, SCALES
C
IE=0
DO 5 I = 1, N
IPS(I) = 1
MOWNRM = .0
DO 2 J = 1, N
MOWNRM = AMAX1(MOWNRM, ABS(IPS(I), J))
2 CONTINUE

C TEST FOR MATRIX WITH ZERO ROW.
C
IF (MOWNRM .EQ. 0.0) GO TO 95
SCALES(I) = 1.0 / MOWNRM
9 CONTINUE

C GAUSSIAN ELIMINATION WITH PARTIAL PIVOTING
C
NM1 = N - 1
DO 11 I = 1, NM1
BIG = .0
10 KP = IPS(I)
SIZE = ABS(IPS(KP, I)) * SCALES(KP)
IF (SIZE .LE. BIG) GO TO 11
BIG = SIZE
11 CONTINUE

C TEST FOR ZERO PIVOT
C
IF (BIG .EQ. 0.0) GO TO 96

C INTERCHANGE ROW IF NECESSARY
C
IF (EPSIROW .EQ. 0.0) GO TO 15
J = IPS(KP)
IPS(KP) = IPS(EPSIROW)
IPS(EPSIROW) = J
15 CONTINUE

C TEST FOR LAST PIVOT
C
IF (IPS(KP) .EQ. 0.0) GO TO 96
LU(KP, K) = PIVOT
KP = 1 + 1
DO 16 I = KP, N
EM = LU(IP, K)
LU(IP, K) = EM
LU(IP, K) = EM
16 CONTINUE

C END OF CODE.
SUBROUTINE SOLVEINOIM, N, LU, B, X, IPS)
C
C LINEAR SYSTEM PACKAGE
C
C SOLVE A X = B USING L U FROM SUBROUTINE DECOMP.
C
C SEE DECOMP FOR DESCRIPTION OF PARAMETERS
C
DIMENSION BINI, XINI, IPS(N)
REAL LUNITDIM, Nl
NP1 = N * 1

C FORWARD SUBSTITUTION - SOLVE L * Z = B
C
IP = IPS(1)
X(1) = B(IP)
DO 2 I = 2, N
   IP = IPS(I)
   IM1 = I - 1
   SUM = 0.0
   DO 1 J = 1, IM1
      1 SUM = SUM + LUIIP, J) * X(J)
   2 X(I) = B(IP) - SUM

C BACKWARD SUBSTITUTION - SOLVE U * X = Z, WHERE L * Z = B.
C
DO 4 IBACK = 2, N
   IP = IPS(N)
   X(N) = X(N) * LU(IP, N)
   DO 3 J = IBACK, N - 1
      3 SUM = SUM + LU(IP, J) * X(J)
   4 X(I) = X(I) - SUM * LU(IP, I)

RETURN
END
APPENDIX C

CHECK CASE OUTPUT COMPARISONS

Check case output comparisons are made in this appendix. The output from the program of this paper is always on the left-hand side of the page and the output from the program of NASA TN D-6586 is always on the right-hand side of the page.

Card Input Images

** DATA CARDS **

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BROMINE DISSOCIATION IN A SHOCK TUBE

CASE 1

** DATA CARDS **

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METHANE - AIR COMBUSTION (ASSIGNED AREA - TIME INTEGRATION)

CASE 6

TIME AREA

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<th>TIME</th>
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<td>710</td>
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APPENDIX C

** DATA CARDS **

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METHANE-AIR COMBUSTION AT CONSTANT P: ONE UNIMOLECULAR REACTION CASE 5

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H2-O2 LOW TEMPERATURE REACTION AT CONSTANT VOLUME (ADJUSTED KATES) C-8

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Check Case 1

**APPENDIX C**

**Distance-Area Version**

**General Chemical Kinetics Program**

**NASA Langley Research Center**

**Langley Version of Lewis Program (TN U-05**

**Solution Technique Developed by C. W. Deal**

**Bromine Dissociation in a Shock Tube**

**Case 1**

<table>
<thead>
<tr>
<th>Reaction Number</th>
<th>Reaction</th>
<th>Reaction Rate Variable</th>
<th>Activation Energy</th>
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<tbody>
<tr>
<td>1</td>
<td>H + 1<em>BR2 = 1</em>BR + 1*BR</td>
<td>A</td>
<td>6.99000E+11</td>
</tr>
<tr>
<td></td>
<td></td>
<td>N</td>
<td>5.000</td>
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<tr>
<td></td>
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<td>35500.00</td>
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</table>

All third body ratios are 1.0 except the following.

\[ \text{NIBR2} = 1.0 \times 3.80000 \]

**Integration Controls**

- Minimum Step Size: 1.00000E-04 CM
- Maximum Step Size: 1.00000E-01 CM
- Initial Step Size: 1.00000E-04 CM
- Maximum Relative Error: 0.0010

**Assigned Variable Profile**

The area is calculated from the following function.

\[ \frac{1}{\text{AREA}} = 1 - (x/32200.00) \times (0.5000) \]

**Equilibrium Shock Calculation**

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<tr>
<th>Initial State</th>
<th>Final State</th>
<th>Final/Initial Ratio</th>
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</thead>
<tbody>
<tr>
<td>Pressure (atm)</td>
<td>0.1227</td>
<td>1.6130</td>
</tr>
<tr>
<td>Velocity (cm/sec)</td>
<td>57875.78</td>
<td>18108.11</td>
</tr>
<tr>
<td>Density (g/cm³)</td>
<td>65.60921E-05</td>
<td>20.94992E-04</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>299.40</td>
<td>1231.22</td>
</tr>
<tr>
<td>Entropy (cal/g/deg K)</td>
<td>2.3421</td>
<td>3.576</td>
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<td>Mach Number</td>
<td>3.2646</td>
<td>5.171</td>
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<tr>
<td>Gamma</td>
<td>1.6586</td>
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<tr>
<td>Sonic Velocity (cm/sec)</td>
<td>17728.29</td>
<td>59015.45</td>
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**Species Mole Fraction**

- BR2: 8.12239E-03
- BR: 3.11805E-03
- XE: 9.808160E-01

**Mixture Molecular Weight**

131.3405d
** FROZEN SHOCK CALCULATION **

| PRESSURE [ATM] | 1.0141E+00 |
| VELOCITY [CM/SEC] | 57875.78 |
| DENSITY [GM/CM**3] | 65.60921E-05 |
| TEMPERATURE [DEG K] | 299.90 |
| ENTROPY | .3421 |
| (CAL/GM/DEG K) | 3.2846 |
| MACH NUMBER | 1.0586 |
| GAMMA | .9994 |
| SONIC VELOCITY [CM/SEC] | 17720.29 |

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<th>SPECIES</th>
<th>MOLE FRACTION</th>
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<td>BR2</td>
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<tr>
<td>BR</td>
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<tr>
<td>XE</td>
<td>9.90000E+01</td>
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</tbody>
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MIXTURE MOLECULAR WEIGHT 131.58520

| TIME | 0.0 |
| AXIAL POSITION | 0.0 |
| AREA | 1.00000E+00 |

| PRESSURE [ATM] | 1.6017 |
| VELOCITY [CM/SEC] | 218410.72 |
| TEMPERATURE [K] | 1245.3146 |
| DENSITY [GM/CC] | 2.04950E-03 |
| FLOW RATE [GM/SEC] | 3.0791E+01 |
| ENTROPY [CAL/GM-K] | .35751 |
| MACH NUMBER | .50977 |
| GAMMA | 1.65767 |

<table>
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MIXTURE MOLECULAR WEIGHT 131.58520
## APPENDIX C

### TOTAL ENERGY EXCHANGE RATE
(\( \text{CAL/CM}^3/\text{GM2/SEC} \))

<table>
<thead>
<tr>
<th>Species</th>
<th>Mole Fraction</th>
<th>Net Species Production Rate (MOLES/GC-SEC)</th>
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<tbody>
<tr>
<td>MR2</td>
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<td>-3.6831E-05</td>
</tr>
<tr>
<td>BR</td>
<td>1.2804E-04</td>
<td>7.3663E-05</td>
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<tr>
<td>XE</td>
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**MIXTURE MOLECULAR WEIGHT**: 131.5767

**TOTAL ENERGY EXCHANGE RATE**: 3.9733E+05

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<th>Net Species Production Rate (MOLES/GC-SEC)</th>
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**MIXTURE MOLECULAR WEIGHT**: 131.5767

**TOTAL ENERGY EXCHANGE RATE**: 3.9682E+05

### FLOW PROPERTIES

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<th>Time</th>
<th>2.72635E-05 SEC</th>
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<tr>
<td>Axial Position</td>
<td>5.00000E-01 CM</td>
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<tr>
<td>Area</td>
<td>1.00396E+00 SQ CM</td>
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</tbody>
</table>

**PRESSURE**: 1.6058 ATM
**VELOCITY**: 18314.41 CM/SEC
**TEMPERATURE**: 1245.8185 K
**DENSITY**: 2.04652E-03 GM/CC
**FLOW RATE**: 3.79007E+01 GM/SEC
**ENTROPY**: 35752 CAL/GM-K
**MACH NUMBER**: 50698
**GAMMA**: 1.65772

### CHEMICAL PROPERTIES

**SPECIES**
- **MR2**: 9.9354E-03
- **BR**: 1.2804E-04
- **XE**: 9.8999E-01

**MIXTURE MOLECULAR WEIGHT**: 131.4906

**TOTAL ENERGY EXCHANGE RATE**: 3.9733E+05

**PRESSURE**: 1.6058 ATM
**VELOCITY**: 18314.41 CM/SEC
**TEMPERATURE**: 1245.8185 K
**DENSITY**: 2.04652E-03 GM/CC
**FLOW RATE**: 3.79007E+01 GM/SEC
**ENTROPY**: 35752 CAL/GM-K
**MACH NUMBER**: 50698
**GAMMA**: 1.65772
### APPENDIX C

**TOTAL ENERGY EXCHANGE RATE**

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<th>Species</th>
<th>Mole Fraction</th>
<th>Net Species Production Rate (Moles/CC-SEC)</th>
<th>Mixture Molecular Weight</th>
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<th>Mass Fraction Sum</th>
<th>Time</th>
<th>Axial Position</th>
<th>Area</th>
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<tbody>
<tr>
<td>Br₂</td>
<td>0.00919E-03</td>
<td>-2.6911E-05</td>
<td>131.46393</td>
<td>2.6437E+05</td>
<td>1.00000</td>
<td>5.54E-04</td>
<td>1.0179E+00</td>
<td>5.0CM</td>
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<tr>
<td>Br</td>
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**Flow Properties**

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## Check Case 5

### Methane-Air Combustion at Constant Primary Unimolecular Reaction Case 5

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<td>1<em>CH4 + 1</em>O2 + 1<em>H2O + 1</em>OH</td>
<td>1.1700E+17, 0.0000, 45900.00</td>
<td></td>
</tr>
<tr>
<td>27</td>
<td>1<em>CH4 + 1</em>O2 + 1<em>H2O + 1</em>OH</td>
<td>7.5000E+13, 0.0000, 0.00</td>
<td></td>
</tr>
<tr>
<td>28</td>
<td>1<em>CH4 + 1</em>O2 + 1<em>H2O + 1</em>OH</td>
<td>2.7500E+19, -1.0000, 118700.00</td>
<td></td>
</tr>
<tr>
<td>29</td>
<td>1<em>CH4 + 1</em>O2 + 1<em>H2O + 1</em>OH</td>
<td>5.7500E+13, 0.0000, 16000.00</td>
<td></td>
</tr>
</tbody>
</table>

All third body ratios are 1.0 except the following:

- \( M(\text{CH}_4) = 5.00000 \)
- \( M(\text{O}_2) = 2.00000 \)
- \( M(\text{H}_2) = 5.00000 \)
- \( M(\text{H}_2O) = 2.00000 \)
- \( M(\text{H}_2O) = 2.00000 \)

**Integration Controls**

- Minimum Step Size: 1.0000E-04 CM
- Maximum Step Size: 2.0000E+01 CM
- Initial Step Size: 1.0000E-04 CM
- Maximum Relative Error: 0.00010

**Assigned Variable Profile**

The pressure is calculated from the following polynomial:

\[
\text{Pressure (ATM)} = 0 + 1 \times (0) + 0.5 \times (0) + 0.25 \times (0) + 0.125 \times (0)
\]

\[
= 0 + 0 + 0 + 0 + 0 = 0
\]

\[
= (0.125 \times 17.3 \times 10^0) = 2.1625 \times 10^0
\]
### APPENDIX C

#### INITIAL CONDITIONS

<table>
<thead>
<tr>
<th>TIME</th>
<th>0.0</th>
<th>SEC</th>
</tr>
</thead>
<tbody>
<tr>
<td>AXIAL POSITION</td>
<td>0.0</td>
<td>CM</td>
</tr>
<tr>
<td>AREA</td>
<td>1.0000E+03</td>
<td>50 CM</td>
</tr>
<tr>
<td>TIME</td>
<td>0.0</td>
<td>SEC</td>
</tr>
<tr>
<td>AXIAL POSITION</td>
<td>0.0</td>
<td>CM</td>
</tr>
<tr>
<td>AREA</td>
<td>1.0000E+03</td>
<td>50 CM</td>
</tr>
</tbody>
</table>

### FLOW PROPERTIES

| PRESSURE | 1.7300 | ATM |
| VELOCITY | 157412.62 | CM/SEC |
| TEMPERATURE | 1645.00000 | K |
| DENSITY | 3.61559E-04 | GM/CSC |
| FLOW RATE | 5.69139E+04 | GM/SEC |
| ENTROPY | 2.13077 | CAL/GM-K |
| MACH NUMBER | 2.00000 | |
| GAMMA | 1.27772 | |

### CHEMICAL PROPERTIES

<table>
<thead>
<tr>
<th>SPECIES</th>
<th>MOLE FRACTION</th>
<th>NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH4</td>
<td>4.9768E-02</td>
<td>-5.08397E-06</td>
</tr>
<tr>
<td>CH3</td>
<td>0.00000</td>
<td>5.08397E-06</td>
</tr>
<tr>
<td>H2O</td>
<td>1.9907E-01</td>
<td>-6.95166E-08</td>
</tr>
<tr>
<td>H2</td>
<td>0.00000</td>
<td>6.94238E-08</td>
</tr>
<tr>
<td>CO</td>
<td>0.00000</td>
<td>0.00000</td>
</tr>
<tr>
<td>CO2</td>
<td>0.00000</td>
<td>0.00000</td>
</tr>
<tr>
<td>O</td>
<td>1.8561E-10</td>
<td>0.00000</td>
</tr>
<tr>
<td>CH2=O</td>
<td>0.00000</td>
<td>0.00000</td>
</tr>
<tr>
<td>N2</td>
<td>7.5116E-01</td>
<td>0.00000</td>
</tr>
</tbody>
</table>

**MIXTURE MOLECULAR WEIGHT** 28.21038

**TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)** 4.05133E+06

**MASS FRACTION SUM** 1.00000

### FLOW PROPERTIES

| PRESSURE | 1.7300 | ATM |
| VELOCITY | 157412.62 | CM/SEC |
| TEMPERATURE | 1645.00000 | K |
| DENSITY | 3.61559E-04 | GM/CSC |
| FLOW RATE | 5.69139E+04 | GM/SEC |
| ENTROPY | 2.13077 | CAL/GM-K |
| MACH NUMBER | 2.00000 | |
| GAMMA | 1.27772 | |

**APPENDIX C**
<table>
<thead>
<tr>
<th>Time</th>
<th>2.50933E-04 SEC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Axial Position</td>
<td>3.95000E+01 CM</td>
</tr>
<tr>
<td>Area</td>
<td>1.21777E+03 SQ CM</td>
</tr>
</tbody>
</table>

### Flow Properties

- **Pressure**: 1.7903 ATM
- **Velocity**: 1574.12 CM/SEC
- **Temperature**: 1957.4912 K
- **Density**: 2.98126E-04 GM/CM
- **Flow Rate**: 5.39139E-05 GM/SEC
- **Entropy**: 2.72312E-05 CAL/GM-K
- **Mach Number**: 1.0153
- **Gamma**: 1.27073

### Chemical Properties

- **Species**
  - CH4: 8.31137E-03
  - CH3: 7.99832E-03
  - H: 6.00000E-03
  - O: 1.50977E-01
  - O2: 6.49292E-04
  - CO: 2.46235E-02
  - CO2: 5.96649E-05
  - O3: 6.58033E-04
  - CH2O: 9.28676E-03
  - OH: 1.76173E-03
  - H2: 5.59922E-03
  - H2O: 5.26082E-02
  - H2O2: 3.72952E-04
  - OH2: 6.49897E-07
  - N2: 7.38107E-01

- **Net Species Production Rate (GMOLES/CM-SEC)**
  - CH4: 22.231E-02
  - CH3: 9.47447E-04
  - H: 3.31909E-02
  - O: 2.2142E-04
  - O2: 1.32716E-03
  - CO: 1.5643E-03
  - CO2: 1.65005E-05
  - O3: 4.27214E-03
  - CH2O: 1.12438E-02
  - OH: 5.99845E-03
  - H2: 4.91023E-05
  - H2O: 4.88667E-07
  - H2O2: 3.54210E-04
  - OH2: 1.22914E-06
  - N2: 0.

### Mixture Properties

- **Mixture Molecular Weight**: 27.72146
- **Total Energy Exchange Rate (CAL/CM3/GM2/SEC)**: -3.04127E+10
- **Mass Fraction Sum**: 1.00000

### Flow Properties

- **Pressure**: 1.7903 ATM
- **Velocity**: 1574.12 CM/SEC
- **Temperature**: 1957.4912 K
- **Density**: 2.98126E-04 GM/CM
- **Flow Rate**: 5.39139E-05 GM/SEC
- **Entropy**: 2.72312E-05 CAL/GM-K
- **Mach Number**: 1.0153
- **Gamma**: 1.27073
### Chemical Properties

<table>
<thead>
<tr>
<th>Species</th>
<th>Mole Fraction</th>
<th>Net Species Production Rate (Moles/Sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH4</td>
<td>2.1856E-03</td>
<td>-1.3921E-02</td>
</tr>
<tr>
<td>CH3</td>
<td>5.9219E-03</td>
<td>-1.8238E-02</td>
</tr>
<tr>
<td>H</td>
<td>2.0284E-03</td>
<td>5.7311E-03</td>
</tr>
<tr>
<td>O2</td>
<td>1.3941E-01</td>
<td>-4.4415E-02</td>
</tr>
<tr>
<td>H2O</td>
<td>2.8251E-04</td>
<td>-9.4015E-04</td>
</tr>
<tr>
<td>CO</td>
<td>3.4316E-02</td>
<td>4.2580E-02</td>
</tr>
<tr>
<td>CO2</td>
<td>1.5406E-03</td>
<td>6.0432E-03</td>
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<tr>
<td>O</td>
<td>2.3770E-03</td>
<td>1.1508E-02</td>
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<tr>
<td>CM2O</td>
<td>4.6271E-03</td>
<td>-1.0983E-02</td>
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<tr>
<td>OM</td>
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<tr>
<td>M2</td>
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<td>-1.4471E-03</td>
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<tr>
<td>M2O</td>
<td>6.9400E-02</td>
<td>6.1915E-02</td>
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<tr>
<td>MO2</td>
<td>3.8347E-04</td>
<td>-4.8059E-04</td>
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<td>M2O2</td>
<td>7.1217E-07</td>
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<tr>
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</table>

**Mixture Molecular Weight**: 27.4866

**Total Energy Exchange Rate (Cal/cm³/sec)**: -5.2064E+10

**Mass Fraction Sum**: 1.00000

---

<table>
<thead>
<tr>
<th>Species</th>
<th>Mole Fraction</th>
<th>Net Species Production Rate (Moles/Sec)</th>
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</thead>
<tbody>
<tr>
<td>C4H</td>
<td>2.2010E-03</td>
<td>-1.3755E-02</td>
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<tr>
<td>C3H</td>
<td>4.7129E-03</td>
<td>-1.1325E-02</td>
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<tr>
<td>H</td>
<td>2.0994E-03</td>
<td>5.6662E-03</td>
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<td>N2</td>
<td>1.1469E-01</td>
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<td>2.8695E-04</td>
<td>-9.5068E-04</td>
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<tr>
<td>CO</td>
<td>3.6280E-02</td>
<td>4.2557E-02</td>
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<tr>
<td>CO2</td>
<td>1.5741E-03</td>
<td>6.5509E-03</td>
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<td>O</td>
<td>2.3326E-03</td>
<td>1.1579E-02</td>
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<tr>
<td>C2H2O</td>
<td>4.3229E-03</td>
<td>-1.6651E-02</td>
</tr>
<tr>
<td>OM</td>
<td>5.3665E-03</td>
<td>1.9712E-02</td>
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<tr>
<td>M2</td>
<td>6.3492E-03</td>
<td>-1.3541E-03</td>
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<tr>
<td>M2O</td>
<td>5.9302E-02</td>
<td>6.0765E-02</td>
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<tr>
<td>M2O2</td>
<td>7.1969E-07</td>
<td>-6.7513E-04</td>
</tr>
<tr>
<td>N2</td>
<td>7.3119E-01</td>
<td>2.5357E-06</td>
</tr>
</tbody>
</table>

**Mixture Molecular Weight**: 27.48792

**Total Energy Exchange Rate (Cal/cm³/sec)**: -5.1769E+10

**Mass Fraction Sum**: 1.00000
### Check Case 6

**TIME-AREA VERSION**

**GENERAL CHEMICAL KINETICS PROGRAM**

**NASA LAWSLEY RESEARCH CENTER**

**LANGLEY VERSION OF LEWIS PROGRAM**

**IN D-0986**

**USING STIFF ODE**

**SOLUTION TECHNIQUE DEVELOPED BY C.W. GEAR**

**METHANE - AIR COMBUSTION (ASSIGNED AREA - TIME INTEGRATION)**

**CASE 6**

<table>
<thead>
<tr>
<th>REACTION NUMBER</th>
<th>REACTION</th>
<th>REACTION RATE VARIABLES</th>
<th>A</th>
<th>N</th>
<th>ACTIVATION ENERGY</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1CH4 + 1H2 = 1CH3 + 1H</td>
<td>3.0000E+04</td>
<td>0.0000</td>
<td>100000.00</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>1CH4 + 1H2 = 1CH3 + 1H</td>
<td>1.0000E+13</td>
<td>0.0000</td>
<td>40000.00</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>1.5900E+15</td>
<td>0.0000</td>
<td>-10000.00</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>1.6000E+14</td>
<td>0.0000</td>
<td>-10000.00</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>7.3000E+10</td>
<td>0.0000</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>6.9000E+13</td>
<td>0.0000</td>
<td>118000.00</td>
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</tr>
<tr>
<td>7</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>2.0000E+13</td>
<td>0.0000</td>
<td>92000.00</td>
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</tr>
<tr>
<td>8</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
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<td>0.0000</td>
<td>59000.00</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>1.2500E+14</td>
<td>0.0000</td>
<td>163000.00</td>
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</tr>
<tr>
<td>10</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>2.9000E+13</td>
<td>0.0000</td>
<td>98000.00</td>
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</tr>
<tr>
<td>11</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>2.1000E+13</td>
<td>0.0000</td>
<td>51000.00</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>4.2000E+11</td>
<td>0.0000</td>
<td>10000.00</td>
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</tr>
<tr>
<td>13</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>1.9000E+13</td>
<td>0.0000</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>1.0000E+13</td>
<td>0.0000</td>
<td>2000.00</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>7.0000E+10</td>
<td>0.0000</td>
<td>1000.00</td>
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<tr>
<td>16</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>4.0300E+11</td>
<td>0.0000</td>
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<td></td>
</tr>
<tr>
<td>17</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>1.8000E+11</td>
<td>0.0000</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>1.1000E+11</td>
<td>0.0000</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>4.0000E+12</td>
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<tr>
<td>20</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>2.0000E+13</td>
<td>0.0000</td>
<td>2000.00</td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>1.0000E+11</td>
<td>0.0000</td>
<td>5000.00</td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>1.0000E+12</td>
<td>0.0000</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>23</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>1.5000E+13</td>
<td>0.0000</td>
<td>0.00</td>
<td></td>
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<tr>
<td>24</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>6.0000E+12</td>
<td>0.0000</td>
<td>0.00</td>
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</tr>
<tr>
<td>25</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>6.0000E+12</td>
<td>0.0000</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>26</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>1.1700E+17</td>
<td>0.0030</td>
<td>45500.00</td>
<td></td>
</tr>
<tr>
<td>27</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>7.5000E+23</td>
<td>-2.6000</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>28</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>2.7000E+10</td>
<td>-1.1000</td>
<td>118700.00</td>
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</tr>
<tr>
<td>29</td>
<td>1CH3 + 1H2 = 1CH2 + 1H</td>
<td>5.7500E+13</td>
<td>0.0000</td>
<td>18000.00</td>
<td></td>
</tr>
</tbody>
</table>

**ALL THREE BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING**

| M1CH4 | 31 | 5.0000E04 |
| M1CH4 | 31 | 2.0000E03 |
| M1CO | 31 | 2.0000E00 |
| M1CO | 31 | 1.0000E00 |
| M1CO | 2.00E00 |
| M1CO | 2.00E00 |
| M1CH3 | 2.00E00 |
| M1CH3 | 2.00E00 |
| M1CH3 | 2.00E00 |
| M1CH3 | 2.00E00 |
| M1CH3 | 2.00E00 |

**INTEGRATION CONTROLS**

- **MINIMUM STEP SIZE** 6.25000E-10 SEC
- **MAXIMUM STEP SIZE** 1.25000E-06 SEC
- **INITIAL STEP SIZE** 6.25000E-10 SEC
- **MAXIMUM RELATIVE ERROR** .00010

**ASSIGNED VARIABLE PROFILE**

- THE AREA IS CALCULATED BY INTERPOLATION FROM THE FOLLOWING TABLE

<table>
<thead>
<tr>
<th>STATION</th>
<th>AXIAL DISTANCE (CM)</th>
<th>AREA (CM²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0</td>
<td>10.0000E+02</td>
</tr>
<tr>
<td>2</td>
<td>50.0000E+01</td>
<td>10.0040E+02</td>
</tr>
<tr>
<td>3</td>
<td>100.0000E+00</td>
<td>10.0200E+02</td>
</tr>
<tr>
<td>4</td>
<td>150.0000E+00</td>
<td>10.0480E+02</td>
</tr>
</tbody>
</table>
## APPENDIX C

### INITIAL CONDITIONS

<table>
<thead>
<tr>
<th>TIME (SEC)</th>
<th>AXIAL POSITION (CM)</th>
<th>AREA (SQ CM)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>1.0000 x 0.03</td>
</tr>
</tbody>
</table>

### FLOW PROPERTIES

- **Pressure**: 1.7300 ATM
- **Velocity**: 1574.1262 CM/SEC
- **Temperature**: 4645.0000 K
- **Density**: 3.6159E-04 GM/CC
- **Flow Rate**: 5.69139E+04 GM/SEC
- **Entropy**: 2.12077 CAL/GM-K
- **Mach Number**: 2.00000
- **Gamma**: 1.22772

### CHEMICAL PROPERTIES

<table>
<thead>
<tr>
<th>SPECIES</th>
<th>MOLE FRACTION</th>
<th>NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH₄</td>
<td>4.97680E-02</td>
<td>-5.08397E-06</td>
</tr>
<tr>
<td>CH₃</td>
<td>0</td>
<td>5.08397E-06</td>
</tr>
<tr>
<td>H</td>
<td>0</td>
<td>5.01945E-06</td>
</tr>
<tr>
<td>O₂</td>
<td>1.99072E-01</td>
<td>6.95168E-08</td>
</tr>
<tr>
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#### SPECIES

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### MIXTURE MOLAR WEIGHT

- **Total Energy Exchange Rate (Cal/cm²/sec)**: 4.05133E+06
- **Mass Fraction Sum**: 1.00000

### REFERENCE

- **Pressure**: 1.7300 ATM
- **Velocity**: 1574.1262 CM/SEC
- **Temperature**: 4645.0000 K
- **Density**: 3.6159E-04 GM/CC
- **Flow Rate**: 5.69139E+04 GM/SEC
- **Entropy**: 2.12077 CAL/GM-K
- **Mach Number**: 2.00000
- **Gamma**: 1.22772

### APPENDIX C

- **Pressure**: 1.7300 ATM
- **Velocity**: 1574.1262 CM/SEC
- **Temperature**: 4645.0000 K
- **Density**: 3.6159E-04 GM/CC
- **Flow Rate**: 5.69139E+04 GM/SEC
- **Entropy**: 2.12077 CAL/GM-K
- **Mach Number**: 2.00000
- **Gamma**: 1.22772
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<table>
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<tr>
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<tbody>
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<td>Pressure</td>
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<tr>
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<td>2.1463 kcal/kg</td>
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### Chemical Properties

| Species | Mole Fraction | Net Species Production Rate (Moles/sec)
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**Mixture Molecular Weight**: 27.48257
**Total Energy Exchange Rate** (cal/cm³/gm2/sec): -5.1693E+10
**Mass Fraction Sum**: 1.00000
Check Case 8

**TIME-AREA VERSION**

**GENERAL CHEMICAL KINETICS PROGRAM**

**LANGLEY VERSION OF LEWIS PROGRAM (TN D-6586) USING STIFF ODE**

**SOLUTION TECHNIQUE DEVELOPED BY C.W. GEAR**

**H2-O2 LOW TEMPERATURE REACTION AT CONSTANT VOLUME (ADJUSTED RATES) C-8**

<table>
<thead>
<tr>
<th>REACTION NUMBER</th>
<th>REACTION</th>
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<th>N</th>
<th>ACTIVATION ENERGY</th>
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<td>1H + O2  = 1H + 1H2O2</td>
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<tr>
<td>2</td>
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<td>2.10000E+13</td>
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<tr>
<td>3</td>
<td>1OH + 1H2 = 1H2O + 1H</td>
<td>1.25000E+14</td>
<td>0.0000</td>
<td>16300.00</td>
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<tr>
<td>4</td>
<td>1H + O2  = 1OH2 + 1H</td>
<td>2.96000E+13</td>
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<tr>
<td>5</td>
<td>1H + O2  = 1OH2 + 1H</td>
<td>9.50000E+14</td>
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<tr>
<td>6</td>
<td>1H + 1H2O2 = 1OH + 1OH + 1H2O</td>
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<td>0.00</td>
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<td>7</td>
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<tr>
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<tr>
<td>9</td>
<td>1H + 1H2O2 = 1OH + 1OH + 1H2O</td>
<td>6.50000E+12</td>
<td>0.0000</td>
<td>24000.00</td>
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<td>10</td>
<td>1H + 1H2O2 = 1OH + 1OH + 1H2O</td>
<td>5.16000E+14</td>
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<td>11</td>
<td>1H + 1H2O2 = 1OH + 1OH + 1H2O</td>
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<td>12</td>
<td>1H + 1H2O2 = 1OH + 1OH + 1H2O</td>
<td>5.75000E+13</td>
<td>0.0000</td>
<td>18000.00</td>
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All third body ratios are 1.0 except the following:

\[ \text{M(H2,5)} = 5.00000 \]
\[ \text{M(H2,7)} = 2.30000 \]
\[ \text{M(O2,5)} = 2.00000 \]
\[ \text{M(O2,7)} = 0.78000 \]

**INTEGRATION CONTROLS**

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<th>Minimum Step Size</th>
<th>5.00000E-05 SEC</th>
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<tr>
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<td>5.00000E-05 SEC</td>
</tr>
<tr>
<td>Maximum Step Size</td>
<td>1.00000E-01 SEC</td>
</tr>
<tr>
<td>Maximum Relative Error</td>
<td>.000030</td>
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**ASSIGNED VARIABLE PROFILE**

This is a WHO problem - an assigned variable is not required.

The volume (density) will be held constant for this case.

The temperature will be held constant for this case.
## Initial Conditions

**Flow Properties**

<table>
<thead>
<tr>
<th>TIME (SEC)</th>
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<th>0.0000E+00</th>
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<tbody>
<tr>
<td>AXIAL POSITION (CM)</td>
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<td>0.0000E+00</td>
</tr>
<tr>
<td>AREA (SQ CM)</td>
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<th>TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)</th>
<th>MASS FRACTION SUM</th>
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**Mixture Molecular Weight**: 6.21325

**Total Energy Exchange Rate** (CAL/CM/SEC): -9.67218E-02

**Mass Fraction Sum**: 1.00000

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**Mixture Molecular Weight**: 6.21325

**Total Energy Exchange Rate** (CAL/CM/SEC): -9.67218E-02

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**Mixture Molecular Weight**: 6.21325

**Total Energy Exchange Rate** (CAL/CM/SEC): -9.67218E-02

**Mass Fraction Sum**: 1.00000

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### APPENDIX C

#### FLow Properties

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<td>DENSITY</td>
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#### CHEMICAL PROPERTIES

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**MIXTURE MOLECULAR WEIGHT** 6.42463

**TOTAL ENERGY EXCHANGE RATE** -1.78257E+05 (CAL-CH3/SEC-SEC)

**MASS FRACTION SUM** 1.00000

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**MIXTURE MOLECULAR WEIGHT** 6.42463

**TOTAL ENERGY EXCHANGE RATE** -1.78257E+05 (CAL-CH3/SEC-SEC)

**MASS FRACTION SUM** 1.00000

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**MIXTURE MOLECULAR WEIGHT** 6.42463

**TOTAL ENERGY EXCHANGE RATE** -1.78257E+05 (CAL-CH3/SEC-SEC)

**MASS FRACTION SUM** 1.00000
APPENDIX C

TOTAL ENERGY EXCHANGE RATE  \(-1.63467E+05\)
(CAL-CM3/GR2/SEC)
MASS FRACTION SUM   \(0.9999\)

11/19/75  LRC ICOPS INDEPEND 60000-131K 01/21/75
17.42.09. GT02894.  LRC COMPUTER COMPLEX
17.42.09. LRC COMPUTER COMPLEX
17.42.09. JOB 1: US0300, 120000, 002000, A4409 R
17.42.09. 327A 100681  B-1250
17.42.09. USER: ALLEN G. MCLAIN
17.42.09. 96903M 64750
17.42.09. WAITGO. PLEASE RUN ON 6600 ONLY
17.42.13. GO
17.42.13. LINCNT10000D
17.42.14. FETCH(A4409, BINARY)
17.42.14. TIME BG ATTACH
17.42.59. TIME ED ATTACH
17.42.59. END FETCH
17.42.57. UPDATE(Q, C=TAPE4, P=BFNFILE, D, 9)
17.42.50. READING INPUT
17.42.09. UPDATE COMPLETE
17.42.10. UPDATE(Q, P=BFNFILE)
17.42.13. READING INPUT
17.42.19. UPDATE COMPLETE
17.42.20. RUNS... (COMPLETE)
17.42.43. SETINDF.
17.42.44. LOC.
17.42.52. MEMORY GT1000 CM
17.44.52. A FL 000957 0/5 CALLS
17.44.52. A FL CPU 27.75/654 SEC.
17.45.24. STOP
17.45.25. SPRINT(OUTPUT, 3)
17.45.26. CPU 46.95/624 SEC.
17.45.26. CPU 125.75/536 SEC.
17.45.27. COST OF THIS JOB WAS 11
17.45.27. KWH 2.74 KILOWATT HOURS
20.58.21. GT02894. 6513 LINES PRINTED. LP24

TOTAL ENERGY EXCHANGE RATE  \(-1.63589E+05\)
(CAL-CM3/GR2/SEC)
MASS FRACTION SUM   \(0.9999\)

11/17/75  LRC ICOPS INDEPEND 60000-131K 01/21/75
19.56.31. GT05666. LRC COMPUTER COMPLEX
19.56.31. JDN: 1, 00300, 120000, 002000. A4409 R
19.56.31. 327A 100681  B-1250
19.56.31. USER: ALLEN G. MCLAIN
19.56.31. LINCNT10000D
19.56.32. FETCH(A4409, BINARY)
19.56.32. TIME BG ATTACH
19.58.25. TIME ED ATTACH
19.58.26. END FETCH
19.58.27. UPDATE(Q, C=TAPE4, P=BFNFILE, D, 9)
19.58.31. READING INPUT
19.58.41. UPDATE COMPLETE
19.58.41. UPDATE(Q, P=BFNFILE)
19.58.47. READING INPUT
19.58.52. UPDATE COMPLETE
19.58.53. RUNS... (COMPLETE)
19.59.41. SETINDF.
19.59.43. LOC.
20.00.15. MEMORY GT6000 CM
20.00.15. A FL 000057 0/5 CALLS
20.00.15. A FL CPU 27.75/654 SEC.
20.01.30. STOP
20.01.30. SPRINT(OUTPUT, 3)
20.01.32. 000057A 0/5 CALLS
20.01.32. CPU 67.08/820 SEC.
20.01.32. CPU 204.74/664 SEC.
20.01.32. COST OF THIS JOB WAS 12
20.01.32. KWH 2.94 KILOWATT HOURS
21.05.53. GT05666. 6288 LINES PRINTED. LP24
APPENDIX D

STOICHIOMETRIC PROPANE-OXYGEN-ARGON SHOCK TUBE
COMBUSTION CASE COMPARISON

Comparison of the stoichiometric propane-oxygen-argon shock tube combustion cases is presented in this appendix. The output from the program of this paper is on the left-hand side of each page and the output from the program of NASA TN D-6586 is on the right-hand side.

DISTANCE-AREA VERSION
GENERAL CHEMICAL KINETICS PROGRAM
NASA LANGLEY RESEARCH CENTER
LANGLEY VERSION OF LEWIS PROGRAM ITN 0-65861 USING STIFF ODE
SOLUTION TECHNIQUE DEVELOPED BY C.W. GEAR

********** PROPANE REACTIONS BY CHINITZ - BAUSER 64 RNKS - 31 SPECIES **********

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87
APPENDIX D

62 1*C2H2 + 1*NH = 1*C2H + 1*N2 2.2000E+1 0.00000 7000.00
63 1*C2H + 1*O2 = 1*C* + 1*CO2 1.0000E+14 0.00000 23000.00
64 1*C* + 1*N2 = 1*CO + 1*N* 8.1000E+13 .50000 0.00

ALL THIRD BODY RATIOS ARE 1.0

INTEGRATION CONTROLS

MINIMUM STEP SIZE 1.00000E-05 CM
INITIAL STEP SIZE 1.00000E-05 CM
MAXIMUM STEP SIZE 1.00000E-02 CM
MAXIMUM RELATIVE ERROR .00010

** ASSIGNED VARIABLE PROFILE **

THE AREA IS CALCULATED FROM THE FOLLOWING FUNCTION

1/AREA = 1 - (1/136.7391)**(.530001)

** EQUILIBRIUM SHOCK CALCULATION **

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<th>TEMPERATURE</th>
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SPECIES | MOLE FRACTION
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CO | 1.771236E-02
O2 | 4.88239F-03
O | 4.89906E-03
CO2 | 1.3792E-02
CH3 | 8.87487F-05
C2H5 | 8.7586E-15
CH3 | 7.72594E-03
OH | 5.87368E-03
H2 | 2.61112E-02
H | 5.80176E-03
CH4 | 1.0920E-16
CH2O | 7.3995E-11
HCO | 1.5460E-08
C2H7 | 1.6828E-43
C2H6 | 1.4284E-30
C2H5CO | 3.1110E-38
C3H6 | 6.3378E-38
C3H5CO | 2.9517E-24
C3H4 | 1.7113E-32
C2H4 | 3.1312E-24
CH3CO | 2.1628E-22
C2H5CO | 1.1177E-36
C2H5OH | 1.0832E-31
C2H5CHO | 7.5346E-30
CH2OH | 8.1409E-16
CH3OH | 9.5826E-18
C2H2 | 3.4802E-18
CH | 3.5896E-14
AR | 9.1153E-01

MIXTURE MOLECULAR WEIGHT | 38.39300
DELCG VOLUMES/DELOG T) | 1.1484E+00
AT CONSTANT P | 38.39300
DELCG VOLUMES/DELOG P) | -1.0069E+00
AT CONSTANT T | 38.39300

88
** FROZEN SHOCK CALCULATION **

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** APPENDIX D **

MIXTURE MOLECULAR WEIGHT

39.59194
### APPENDIX D

**Chemical Properties**

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<th>Net Species Production Rate (MOLES/CC-SEC)</th>
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**Mixture Molecular Weight** 39.59194

**Total Energy Exchange Rate** (CAL-CH3/CM2-SEC) 1.6611E+12

**Flow Properties**

| PRESSURE     | 1.0215 ATM |
| VELCEITY     | 50146.84 CM/SEC |
| TEMPERATURE  | 2514.49 K |
| DENSITY      | 3.45194E-04 GM/CC |
| FLOW RATE    | 1.41279E+01 GM/CC |

**Mixture Molecular Weight** 39.59194

**Total Energy Exchange Rate** (CAL-CH3/CM2-SEC) 1.7609E+12

**Flow Properties**

| PRESSURE     | 1.0090 ATM |
| VELCEITY     | 40132.16 CM/SEC |
| TEMPERATURE  | 2535.01 K |
| DENSITY      | 3.44313E-04 GM/CC |
| FLOW RATE    | 1.41279E+01 GM/CC |
### Chemical Properties

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### Mixture Molecular Weight

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<th>FIXED TOTAL ENERGY EXCHANGE RATE (CAL/cm^3/gm/SEC)</th>
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### Flow Properties

| PRESSURE | 1.1560E+00 | ATN |
| TEMPERATURE | 280+280 | K |
| DENSITY | 2.4942E-04 | GM/CM^3 |
| FLOW RATE | 1.2749E+01 | GM/CM^3-SEC |
| ENTROPY | 1.5085 | CAL/GM-K |
| MACH NUMBER | 1.0437E+00 | 50 CM |
| AREA | 1.0643E+00 | 50 CM |

### Flow Properties

| PRESSURE | 1.1560E+00 | ATN |
| TEMPERATURE | 280+280 | K |
| DENSITY | 2.4942E-04 | GM/CM^3 |
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<table>
<thead>
<tr>
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<th>NET SPECIES PRODUCTION RATE (MOLES/SEC-SEC)</th>
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</tr>
<tr>
<td>O2</td>
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<td>2.0328E+03</td>
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**MIXTURE MOLECULAR WEIGHT** 38.61176

**TOTAL ENERGETIC EXCHANGE RATE** -9.6511E+09 (CAL/CM3/GR2/SEC)

**MASS FRACTION SUM** 1.00000

### Flow Properties

**PRESSURE** 1.7401 ATM
**VELOCITY** 45041 CS/SEC
**TEMPERATURE** 2886.4941 K
**DENSITY** 2.8319E+04 CN/MM3
**FLOW RATE** 5.1437E+01 CM3/SEC
**ENTROPY** 0.5597 CAL/MM3/SEC
**MACH NUMBER** 1.57745

---

### Chemical Properties

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<tr>
<th>SPECIES</th>
<th>MOLE FRACTION</th>
<th>NET SPECIES PRODUCTION RATE (MOLES/SEC-SEC)</th>
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<tbody>
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**Flows**

- **Flow Properties**
  - **Pressure**: 1,762 atm
  - **Velocity**: 44,537.2 cm/sec
  - **Temperature**: 289.4612 K
  - **Density**: 2,841.464 g/cm³
  - **Flow Rate**: 1,641.464 g/sec

**Chemical Properties**

- **Species**
  - **Mole Fraction**
  - **Net Species Production Rate**
  - **Mole%CO/CC-SEC**
### APPENDIX D

#### MIXTURE MOLECULAR WEIGHT

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#### TOTAL ENERGY EXCHANGE RATE

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<td>C2H2O: 1.25032E-10</td>
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#### MASS FRACTION SUM

| 1.00003 |

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#### 11/26/75

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#### 11/26/75

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REFERENCES


Figure 1 - Overall schematic of the hybrid computer program.
Figure 2.- Flow diagram for main program GPAK.
Figure 3.- Flow diagram for subroutine DRIVES.
Figure 4. - Flow diagram of subroutine STIFF (from ref. 3).
RETURN

START

\( (T-H) < TPRINT \leq T \) no

yes

INTERPOLATE HISTORY ARRAY BY
USE OF A FINITE TAYLOR SERIES
FOR VALUES OF \( V, \rho, T \) AND \( \sigma_i \)’s
AT TPRINT LOCATION -
UPDATE DEPENDENT VARIABLE
DVAR -

CALL DIFF1

CALL OUT3

yes

? INT \leq NPRIN

no

RETURN

Figure 5.- Flow diagram for subroutine YOUT.
"The aeronautical and space activities of the United States shall be conducted so as to contribute . . . to the expansion of human knowledge of phenomena in the atmosphere and space. The Administration shall provide for the widest practicable and appropriate dissemination of information concerning its activities and the results thereof."
—NATIONAL AERONAUTICS AND SPACE ACT OF 1958

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