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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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16. Abstract

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.

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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, m^2
$\mathcal{A}$	species production function described in equation (5), sec^{-1}
$\mathcal{B}$	enthalpy production function described in equation (6), sec^{-1}
C_p	specific heat at constant pressure
f_i	$= \frac{dy_i}{dt}$
h_i	enthalpy of species i
M	Mach number, $\sqrt{\frac{V^2 M_w}{\gamma RT}}$
M_w	molecular weight
p	pressure of gas mixture, atm
R	universal gas constant
T	temperature, K
t	time
t_o	initial time
V	velocity
w_i	net species production rate, moles/vol-sec
y	general dependent variable
y_o	initial value of dependent variable

γ specific heat ratio, $\dfrac{C_p}{C_p - \dfrac{R}{M_w}}$

ρ density

σ_i concentration, moles of species i 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 arbituary assigned area profile would be

$$\frac{d\sigma_i}{dt} = \frac{w_i}{\rho} \qquad (i = 1, 2, \ldots, N) \tag{1}$$

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

$$\frac{d\rho}{dt} = -p\left[\frac{M^2}{M^2 - 1}\left(\frac{1}{A}\frac{dA}{dt} - \mathcal{A}\right) + \mathcal{A}\right] \tag{3}$$

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

where

$$\mathcal{A} = \frac{RT}{p}\sum_{i=1}^{N} w_i - \mathcal{B} \tag{5}$$

and

$$\mathcal{B} = \frac{1}{p}\left(\frac{\gamma - 1}{\gamma}\right)\sum_{i=1}^{N} h_i w_i \tag{6}$$

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:*

$$\frac{dy_i}{dt} = f_i\left(t, y_i, \ldots, y_N\right) \qquad (i = 1, 2, \ldots, N) \qquad (7)$$

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

*(Here i refers to a particular dependent variable y, and N is the total number of equations in which the variable y changes with the independent variable t. Specifically, y_1, y_2, and y_3 are V, ρ, and T, respectively, and y_4 to y_N are the total number of chemical species.)

a subroutine for the calculation of f_i 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 I.- SUBROUTINES OF PROGRAM OF REFERENCE (2)
AND DESCRIPTION OF ALTERATIONS

Subroutines from program of reference (2)	Alteration performed
GCKP	1. All monitoring of integration removed. 2. Calls for output removed. 3. Problem control yielded to subroutine DRIVES of reference 3 for looping and error treatment coding. 4. Subroutine renamed GPAK.
KINP CIMAGE NAMBLK BLCK INIT OUTP	Minor modifications as to variable initialization and printout scheme setup. In OUTP printing format changed to conserve paper.
COMB SHOK SHOCKS ELEMNT EQLBRM MATRIX GAUSS SPOUT	No changes made.
PRED DERV	Combined and renamed DIFFUN. Internal changes made for updating dependent variables at print location without altering array values for continuation of problem after printing.
PARD	Renamed PEDERV.
THRM CUBS	No changes made.
INTE CASM LESV ERROR PERR AUTO SEARCH	These subroutines completely removed and replaced with subroutines of reference 3. The subroutines used are YOUT COSET YOUTD DECOMP DRIVES SOLVE STIFF

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,

DVAR dependent variable, initially zero but previous value in subsequent steps

V_1 velocity after previous step

V_2 velocity after present step

Present step size is in distance units

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

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 71100_8 as compared with 66700_8 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

data used for the species involved with propane combustion were taken from reference 6 and used in the form of polynomial coefficients presented in reference 7. The computations for the two outputs shown in appendix D were for the stoichiometric combustion of propane and oxygen diluted with argon when subjected to a shock wave traveling at 1.67 km/sec. The calculated results obtained from the computer program of this paper and that from reference 2 are very close at all the printout stations. The comparative time shown at the end of the printout of such program illustrates the advantage of using the Gear solution technique. The computer time required for the calculation using the program of this report was almost an order of magnitude less.

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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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

$$aA + bB \rightleftarrows dD + eE$$

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:

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

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

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):

Columns	Contents	Explanation
1 to 8	Time	Time fundamental variable
	Distance	Distance fundamental variable
11 to 18	Pressure	Pressure is assigned variable
	Area	Area is assigned variable
	(Blank)	Velocity zero (static case)
21 to 23	cgs	Input in internal cgs units

Columns	Contents	Explanation
	(Blank)	Input in internal units cgs
	fps	Input in fps units
	SI	Input in SI units
31 to 33	cgs	Output in cgs units
	(Blank)	Output in cgs units
	fps	Output in fps units
	SI	Output in SI units

(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.

Name	Value	Explanation
HMIN	. . . . .	Minimum step size in cm or sec
	<u>0.0001</u>	cm (if DISTANCE on version card)
	<u>5.0×10^{-8}</u>	Seconds (if TIME on version card)
HMAX	. . . . .	Maximum step size
	<u>0.1000</u>	cm (if DISTANCE version)
	<u>5.0×10^{-5}</u>	Seconds (if TIME version)
HINT	. . . . .	No longer input (assumes value of HMIN initially)
EMAX	<u>0.0001</u>	Maximum error acceptable (becomes EPS in Gear package)

Name	Value	Explanation
ALLM1	TRUE	Third body efficiencies equal to 1. None input
	FALSE	Third body efficiencies to be input. Those not input remain equal to one
ELIM	. . . . .	Deleted
CONC	TRUE	Concentration output as molar concentrations if SI or fps output designated
	FALSE	Mass fractions output if SI or fps output designated
ITPSZ	1	An area or pressure table input
	2	Area or pressure specified by polynomial equation
	3	LSUBM and ETA will be input for area equation
	4	D, VISC, BETA, and ETA will be input for area equation
	5	Zero velocity, no assigned pressure
IPRCOD	1	Distance against area profile given
	2	Distance against pressure profile given
	3	Time against area profile given
	4	Time against pressure profile given
XTB	. . . . .	Array for time or distance portion of profile, must be in correct user units
ATB	. . . . .	Array for area or pressure profile, must be in user units

APPENDIX A

Name	Value	Explanation
NTB	. . . . .	Total entries in area or pressure table, must be less than or equal to 40
CX3	. . . . .	Coefficient of cubed component of pressure/area polynomial equation
CX2	. . . . .	Coefficient of squared component of pressure/area polynomial equation
CX1	. . . . .	Coefficient of pressure/area to the first power in polynomial equation
CX0	. . . . .	Constant term in pressure/area polynomial equation
LSUBM	. . . . .	Characteristic shock tube reaction length for special area equation (see ref. 2)
ETA	. . . . .	Dimensionless exponent in special area equation for boundary layer (see ref. 2)
D	. . . . .	Hydraulic diameter of shock tube
VISC	. . . . .	Viscosity coefficient
BETA	. . . . .	Dimensionless boundary-layer parameter used to calculate LSUBM
END	. . . . .	Changed from reference 2, must always be input
DELP	. . . . .	Deleted (from ref. 2)
PRINT	. . . . .	Deleted (from ref. 2)
APRINT	. . . . .	Deleted (from ref. 2)
NPRNTS	. . . . .	Deleted (from ref. 2)

Name	Value	Explanation
EVSTEP	. . . . .	Deleted (from ref. 2)
DBUGØ	FALSE	Changed, prints output parameters in more concise format
	TRUE	Prints format same as reference 2 with exception of derivatives, increment, and relative error information
PAPS(✓)	FALSE	Program prints at every (5) iterations or number specified by IPRIT
	TRUE	Prints at specific stations specified by END and IDEL or a TPRINT table
IDEL(✓)	. . . . .	Number of increments derived (50 maximum)
IPRIT(✓)	5	Number specifying integration steps between printing
TPRINT(✓)	. . . . .	Table of 50 values for specifying printing location (filled automatically by specifying IDEL)
NPRINT(✓)	. . . . .	Number of values in TPRINT 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

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

Name	Value	Explanation
COMBUS	TRUE	Perform equilibrium combustion calculation
	FALSE	Do not perform equilibrium combustion calculation
SHOCK	TRUE	Perform frozen and equilibrium shock calculations
	FALSE	Do not perform shock calculation
TCON	TRUE	Hold temperature constant
	FALSE	Do not hold temperature constant
RHOCON	TRUE	Hold volume (density) constant
	FALSE	Do not hold volume (density) constant

(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):

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

Card column	FORTRAN format	Content
66 to 73	A8	Name of species to be assigned third body ratio other than unity
74		Not read
75 to 80	F6.3	Efficiency ratio for species in columns 66 to 73

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:

Name	Value	Explanation
Time	. . . . .	Time in seconds
	0.	For default
X	. . . . .	Distance
	0.	For default
MACH	. . . . .	Mach number
	0.	For default
U	. . . . .	Velocity
RHO	. . . . .	Density
T	. . . . .	Temperature
Area	. . . . .	Area for a flow calculation
MDOT	. . . . .	Mass flow rate for a flow calculation
MM Hg	TRUE	Pressure input in mm of mercury
	FALSE	Pressure input in user's choice of input units

Name	Value	Explanation
MOLEF	TRUE	Mole fractions input
	FALSE	Mass fractions input

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.

(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 THRM:

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

APPENDIX A

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 requirements. 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  GPAK(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE4,TAPE7)
C*****************************************************************************
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/COND/DUM1(5),X(28),DUM2(2),NEXT
      COMMON/STCOM1/N,T,H,HMIN,HMAX,EPS,MF,KFLAG,JSTART
      COMMON/CONT/KTCON
      COMMON/UPDT/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 15 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
      NPEDV = 0
      KUP =.FALSE.
      IF(METH .EQ. 1) GO TO 23
      K2=6
      GO TO 24
   23 CONTINUE
      K2=13
   24 CONTINUE
      KTCON=.TRUE.
      CALL DIFFUN(N,T,Y,YDOT,IFN,NPEDV,K2)
      KTCON=.FALSE.

C     PRINT ALL INITIAL CONDITIONS
      CALL OUT2
      IF (NEXT) GO TO 1000


      CALL DRIVES(N,T,TLAST,Y,HMIN,EPS,MF,KFLAG,K2)
      IF(KFLAG .EQ. -4) NEXT = .TRUE.
      IF (NEXT) GO TO 1000



  100 WRITE (6,101)
  101 FORMAT (7HO(GCKP),5X,44HEND OF THIS CASE  -  READ DATA FOR NEXT CA
     *SE)
      GO TO 13

 1000 WRITE (6,1001)
 1001 FORMAT (7HO(GCKP),5X,46HA FATAL ERROR HAS OCCURRED  -  CASE TERMIN
     *ATED)

   13 CONTINUE

      CALL RINP
      GO TO 1

      END
```

APPENDIX B

```
      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              CM**2             *
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     * LDAT (7)   -  FOR TEMPORARY STORAGE OF DATA CARDS    *
C     LOGICAL TAPE UNIT ASSIGNMENTS ARE SPECIFIED IN #NAMBLK#

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


      LOGICAL ALLML,CONC,DBUGO,EXCHR,MOLEF,MMHG,NEXT
      LOGICAL COMBUS,RHOCON,SHOCK,TCON
      LOGICAL PAPS

      INTEGER STOIC

      REAL MDOT,IVAR,M,MW,N,LSUBM,MIXMW,M2,NEW

      DIMENSION ISTOIC(4)
      DIMENSION ISS(25),TBR(3),THMC(7,2)
      DIMENSION SP(4),DSP(4),SPP(2),DSPP(2),SPNM(28),DSPNM(28)
      DIMENSION        LMT(4),SUBS(4),C(25),CX(4)
      DIMENSION CJA(2),FJA(2),SUA(2),CUP1(2),CUP2(2),FUP(2),SUP(2)

      COMMON/LTUS/LTHM,LDAT,NTHRD,NBLANK,NPHOTO
      COMMON/OPTS/VERSI,TIMEV,VERSA,AREAV,TCON,RHOCON,IPRCOD
      COMMON/COND/DVAR,AREA,MDOT,P,IVAR,V,RHO,T,SIGMA(25),LS,LSP3,NEXT
      COMMON/REAC/LSR(4,50),XX(50),RATE(50),LKEQ(50),DLKEQ(50),MM(50),LR
      COMMON/RRAT/A(50),N(50),EACT(50),B(50),M(25,50),ALLML
      COMMON/AFUN/CN(4),ITPSZ,LSUBM,ETA,D,VISC,BETA
      COMMON/SPEC/  SNAM(31),MW(25),W(25),STOIC(25,50),OMEGA(25,50)
      COMMON/STCON1/NO,TO,H,HMIN,HMAX,EMAX,MF,KFLAG,JSTART
      COMMON/TCOF/TC(7,2,25),TLOW,TMID,THI
      COMMON/XVSA/XTB(40),ATB(40),NT,XU,AU(2),CX3,CX2,CX1,CX0
      COMMON/SNMW/DALSP(75),ALMW(75)
      COMMON/KOUT/TITLE(20),UNITI,UNITO,CONC,EXCHR,DELH(50),FPS,SI,DBUGO
      COMMON/GHSC/GRT(25),HRT(25),SR(25),CPR(25),DCPR(25)
      COMMON/NECC/RR,MIXMW,M2,GAMMA,TCPR,R
      COMMON/MISC/TT,PP,CPRO,HRO,ENN,SUMN,ENNL,LLMT(15),BO(15)
      COMMON/INDX/TP,HP,NLM,NS,IQ1,CONVG,KMAT,IMAT
      COMMON/STCS/NSTOIC(4,50),EQUIL(50)
      COMMON/SNOB/CXTB(40),CATB(40),NZ
      COMMON/GJUNK/TLAST
      COMMON/STCOM6/IPRIT,PAPS
      COMMON/PRIN/TPRINT(50),NPRIN,NCO

      EQUIVALENCE (C,SIGMA),(SPNM,DSPNM),(SP,DSP),(SPP,DSPP),(SPT,SP)
      EQUIVALENCE (SPNM,SNAM(4)),(EFFM,SPNM(26)),(BLANK,SPNM(27))
      EQUIVALENCE (HNU,SPNM(28))
      EQUIVALENCE (CX3,CX)

      DATA CU,FU,SU/2HCM,2HFT,2HM /
      DATA CUA/4HCM**,1H2/,FUA/4HFT**,1H2/,SUA/4HM**2,1H /
      DATA CUP1/4HMMHG,1H /,CUP2/3HATM,1H /,FUP/4HLB/F,4HT**2/,SUP/4HN/M
     **,2H*2/
      DATA NEW,CHANGE,REPEAT/3HNEW,4HCHAN,4HREPE/
      DATA TAPEND,CARDS/3HEND,4HCARD/

      NAMELIST/PROB/HMIN,HMAX,EMAX,ALLML,CONC,EXCHR,END,DBUGO,
     * IPRCOD,ITPSZ, XTB,ATB,NTB, CX3,CX2,CX1,CX0, LSUBM,ETA,D,VISC,BETA
     *,COMBUS,SHOCK,TCON,RHOCON,MF
     *,IPRIT
     *,TPRINT,NPRIN,PAPS,IDEL
C    THERMODYNAMIC DATA WILL BE INPUT FROM **UNIT**
      REWIND LTHM
      READ (5,99) UNIT
   99 FORMAT (20A4)
      IF (UNIT .NE. CARDS) GO TO 3

      REWIND LTHM
      READ (5,98) TLOW,TMID,THI
   98 FORMAT (3F10.3)
      WRITE (LTHM,98) TLOW,TMID,THI
    1 READ(5,97)   SPT,(LMT(I),SUBS(I),I=1,4)
   97 FORMAT(A8,16X,4(A2,F3.0))
C     **END** CARD SIGNALS END OF THERMODYNAMIC DATA
      IF(SPT .EQ. TAPEND) GO TO 2
```

APPENDIX B

```
      WRITE(LTHM,97)   SPT,(LMT(I),SUBS(I),I=1,4)
      READ (5,96) ((THMC(K,I),K=1,7),I=1,2)
   96 FORMAT (5E15.8)
      WRITE (LTHM,96) ((THMC(K,I),K=1,7),I=1,2)
      GO TO 1
    2 WRITE(LTHM,97)  SPT
      REWIND LTHM

    3 CALL CIMAGE
C     READ OUTPUT TITLE
      READ (LDAT,99) TITLE
      ACTION = NEW
      GO TO 4

      ENTRY RINP
      NCO = 0
      IDEL = 1
      PAPS=.FALSE.
      NEXT = .FALSE.
      CALL CIMAGE
C     READ NEW OUTPUT TITLE
      READ (LDAT,99) TITLE
C     READ ACTION SWITCH
      READ (LDAT,99) ACTION

      IF (ACTION .NE. NEW) GO TO 9
C     SET STANDARD OPTIONS
    4 CONC = .TRUE.
      EXCHR = .FALSE.
      COMBUS = .FALSE.
      SHOCK = .FALSE.
      TCON = .FALSE.
      RHOCON = .FALSE.
      DBUGO = .FALSE.
      MF=22
      NCO = 0
      IDEL = 1
      PAPS = .FALSE.
      IPRIT = 5
      EMAX = 0.0001
      ITPSZ = 5
      ALLM1 = .TRUE.
      DO 5 I=1,25
      DO 5 J=1,50
    5 M(I,J) = 1.

C     INITIALIZE
      NEXT = .FALSE.
      NLM = 0
      NS = 0
      LS = 0
      LR = 0
      NT = 0
      DO 6 I=1,40
      XTB(I) = 0.
      CXTB(I) = 0.
      ATB(I) = 0.
    6 CATB(I) = 0.
      UNCEND = 0.
      CEND = 0.
      NP = 0
      DO 8 J=1,50
      DO 801 I=1,4
  801 NSTOIC(I,J) = 0
      DO 802 I=1,25
  802 STOIC(I,J) = 0
    8 CONTINUE
      LSUBM = 0.
      ETA = 0.
      D = 0.
      VISC = 0.
      BETA = 0.
      CX3 = 0.
      CX2 = 0.
      CX1 = 0.
      CX0 = 0.
      GO TO 14

    9 IF (ACTION .NE. CHANGE) GO TO 13
C     READ REACTION AND (CHANGED) REACTION RATE
   10 READ(LDAT,95)  (ISTOIC(I),SP(I),I=1,4),TA,TN,TEA
   95 FORMAT(2(I1,1X,A8,1X),2X,2(I1,1X,A8,1X),3X,E11.4,2(2X,F8.4))
C     BLANK CARD SIGNALS END OF CHANGE REACTION LIST
      IF(SP(2) .EQ. BLANK) GO TO 12
C     ADJUST STOICHIOMETRIC COEFFICIENTS
      DO 510 I=1,4
      IF (ISTOIC(I) .NE. 0) GO TO 510
      IF(SP(I).EQ.EFFM.OR.SP(I).EQ.BLANK.OR.SP(I).EQ.HNU)GO TO 510
      ISTOIC(I) = 1
  510 CONTINUE
      ISTOIC(1) = -ISTOIC(1)
      ISTOIC(2) = -ISTOIC(2)
C     SEARCH INPUT REACTION LIST
      DO 11 J=1,LR
      DO 511 I=1,4
      NN = LSR(I,J)
      IF (DSPNM(NN) .NE. DSP(I)  .OR.  NSTOIC(I,J) .NE. ISTOIC(I))
     * GO TO 11
  511 CONTINUE
```

```
      A(J) = TA
      N(J) = TN
      EACT(J) = TEA
      GO TO 10
   11 CONTINUE
C     ERROR MESSAGE - NO MATCH FOUND
      ISTOIC(1) = -ISTOIC(1)
      ISTOIC(2) = -ISTOIC(2)
      WRITE(6,101)  (ISTOIC(I),SP(I),I=1,4)
  101 FORMAT (7HO(KINP),5X,55HTHE INPUT REACTION LIST DOES NOT CONTAIN T
     *HE REACTION  ,I1,1H*,A8,3H + ,I1,1H*,A8,3H = ,I1,1H*,A8,3H + ,
     * I1,1H*,A8)
      NEXT = .TRUE.
      GO TO 10
   12 READ (LDAT,99) ACTION
   13 IF (ACTION .EQ. REPEAT) GO TO 33

   14 LSOLD = LS
      LROLD = LR
C     READ (NEW OR ADDED) REACTION AND REACTION RATE
   15 READ(LDAT,95) (ISTOIC(I),SP(I),I=1,4),TA,TN,TEA
C     BLANK CARD SIGNALS END OF NEW OR ADD REACTION LIST
      IF(SP(2) .EQ. BLANK) GO TO 21
C     ADJUST STOICHIOMETRIC COEFFICIENTS
      DO 515 I=1,4
      IF (ISTOIC(I) .NE. 0) GO TO 515
      IF(SP(I) .EQ. EFFM .OR. SP(I) .EQ. BLANK .OR. SP(I) .EQ. HNU
     * ) GO TO 515
      ISTOIC(I) = 1
  515 CONTINUE
      ISTOIC(1) = -ISTOIC(1)
      ISTOIC(2) = -ISTOIC(2)
      LR = LR + 1
      A(LR) = TA
      N(LR) = TN
      EACT(LR) = TEA
      DO 20 I=1,4
      NSTOIC(I,LR) = ISTOIC(I)
      IF (I .EQ. 2  .OR.  I .EQ. 3) GO TO 215
      IF(SP(I) .EQ. EFFM) GO TO 19
      IF(SP(I) .EQ. BLANK) GO TO 219
      IF(SP(I) .EQ. HNU) GO TO 319
  215 IF (LS .EQ. 0) GO TO 17
C     MATCH INPUT SPECIES AGAINST INPUT SPECIES LIST
      DO 16 II=1,LS
      IF (DSPNM(II) .NE. DSP(I)) GO TO 16
      LSR(I,LR) = II
      STOIC(II,LR) = STOIC(II,LR) + ISTOIC(I)
      GO TO 20
   16 CONTINUE

C     MATCH INPUT SPECIES AGAINST MASTER SPECIES LIST
   17 DO 18 II=1,75
      IF (DALSP(II) .NE. DSP(I)) GO TO 18
      LS = LS + 1
      LSR(I,LR) = LS
      STOIC(LS,LR) = ISTOIC(I)
      SPNM(LS) = SP(I)
      MW(LS) = ALMW(II)
      ISS(LS) = II
      GO TO 20
   18 CONTINUE
C     ERROR MESSAGE - NO MATCH FOUND
      WRITE(6,102) SP(I)
  102 FORMAT (7HO(KINP),5X,54HTHE MASTER SPECIES LIST DOES NOT CONTAIN T
     *HE SPECIES  ,A8)
C ** RUN TERMINATED  -  ERROR IN INPUT REACTION LIST
      STOP

   19 LSR(I,LR) = NTHRD
      GO TO 20

  219 LSR(I,LR) = NBLANK
      GO TO 20

  319 IF (I .EQ. 1) GO TO 320
      ISTOIC(1) = -ISTOIC(1)
      ISTOIC(2) = -ISTOIC(2)
      WRITE(6,106)  (ISTOIC(II),SP(II),II=1,4)
  106 FORMAT (7HO(KINP),5X,42HIMPROPER FORMAT FOR PHOTOCHEMICAL REACTION
     *,2X,I1,1H*,A8,3H + ,I1,1H*,A8,3H = ,I1,1H*,A8,3H + ,I1,1H*,A8)
      STOP
  320 LSR(I,LR) = NPHOTO
   20 CONTINUE
      GO TO 15

   21 IF (ACTION .NE. NEW) GO TO 25
C     READ INERT SPECIES (4 PER CARD)
   22 READ(LDAT,94) (SP(I),I=1,4)
   94 FORMAT(4(A8,8X))
      DO 24 I=1,4
C     BLANK FIELD SIGNALS END OF INERT SPECIES LIST
      IF(SP(1) .EQ. BLANK) GO TO 25
C     SEARCH MASTER SPECIES LIST
      DO 23 II=1,75
      IF (DALSP(II) .NE. DSP(I)) GO TO 23
      LS = LS + 1
      SPNM(LS) = SP(I)
      MW(LS) = ALMW(II)
```

APPENDIX B

```
      ISS(LS) = II
      GO TO 24
   23 CONTINUE
C     ERROR MESSAGE - NO MATCH FOUND
      WRITE(6,102) SP(I)
      NEXT = .TRUE.
      LS = LS + 1
      MW(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) SPT
      IF(SPT .EQ. TAPEND) GO TO 29
      READ (LTHM,96) ((THMC(K,I),K=1,7),I=1,2)
      DO 28 I=LSP,LS
      IF (DSPNM(I) .NE. DSP(I)) GO TO 28
      DO 27 KK=1,2
      DO 27 K=1,7
   27 TC(K,KK,I) = THMC(K,KK)
      II = II + 1
      IF (II .LT. LS) GO TO 26
      GO TO 230
   28 CONTINUE
      GO TO 26
C     ERROR MESSAGE - END OF THERMO TAPE REACHED
   29 WRITE (6,103)
  103 FORMAT (7HO(KINP),5X,42HEND OF THERMO TAPE - NOT ALL SPECIES FOUND
     *)
      NEXT = .TRUE.
  230 REWIND LTHM

   30 LRP = LROLD + 1
C     GET SPECIES ENTHALPY AT REFERENCE T
      TREF = 298.15
      CALL THRM (TREF,0.)

      TRAL = TREF*1.987165
C     COMPUTE HEAT OF REACTION
      DO 32 J=LRP,LR
      DELH(J) = 0.
   80 READ (LDAT,PROB)
      H = HMIN
      IF(.NOT. PAPS) GO TO 1001
      IF(IDEL .EQ. 1) GO TO 1001
      PRINC = END/IDEL
      DO 1000 I=1,IDEL
      TPRINT(I) = PRINC*I
 1000 CONTINUE
      NPRIN = IDEL
 1001 CONTINUE

      IF (.NOT. ALLMI) GO TO 36
      DO 77 I=1,25
      DO 77 J=1,50
   77 M(I,J) = 1.
      GO TO 40
C     READ THIRD BODY RATIOS
   36 READ(LDAT,91)  (ISTOIC(I),SP(I),I=1,4), (SPP(I),TBR(I),I=1,2)
   91 FORMAT(2(II,1X,A8,1X),2X,2(II,1X,A8,1X),2(2X,A8,1X,F6.3))
C     BLANK CARD SIGNALS END OF THIRD BODY RATIO LIST
      IF(SP(2) .EQ. BLANK) GO TO 40
C     ADJUST STOICHIOMETRIC COEFFICIENTS
      DO 536 I=1,4
      IF (ISTOIC(I) .NE. 0) GO TO 536
      IF(SP(I).EQ.EFFM.OR.SP(I).EQ.BLANK.OR.SP(I).EQ.MNU) GO TO 536
      ISTOIC(I) = 1
  536 CONTINUE
      ISTOIC(1) = -ISTOIC(1)
      ISTOIC(2) = -ISTOIC(2)
C     SEARCH INPUT REACTION LIST
      DO 39 J=1,LR
      DO 539 I=1,4
      NN = LSR(I,J)
      IF (DSPNM(NN) .NE. DSP(I)  .OR.  NSTOIC(I,J) .NE. ISTOIC(I))
     * GO TO 39
  539 CONTINUE
      DO 38 I=1,2
      IF(SPP(I) .EQ. BLANK) GO TO 38
C     SEARCH INPUT SPECIES LIST
      DO 37 II=1,LS
      IF (DSPNM(II) .NE. DSPP(I)) GO TO 37
      M(II,J) = TBR(I)
      GO TO 38
      DO 532 I=1,4
      NN = LSR(I,J)
      IF (NN .GT. LS) GO TO 532
      STOC = NSTOIC(I,J)
      DELH(J) = DELH(J) + STOC*HRT(NN)
  532 CONTINUE
   32 DELH(J) = DELH(J)*TRAL

      LSP3 = LS + 3
C     RESET STANDARD OPTIONS
```

```
   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 (LDAT,92) VERSI,VERSA,UNITI,UNITO
   92 FORMAT (4(A4,6X))
      IF (VERSA .EQ. BLANK) VERSA = AREAV

      IF (ACTION .NE. NEW) GO TO 80
C     INITIALIZE STEP SIZE LIMITS
      IF (VERSI .EQ. TIMEV) GO TO 78
      HMIN = 0.0001
      HMAX = 0.1000
      IPRCOD = 2
      GO TO 79
   78 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)  SPP(I)
  104 FORMAT (7HO(KINP),5X,53HTHE INPUT SPECIES LIST DOES NOT CONTAIN TH
     *E SPECIES  ,A8)
      NEXT = .TRUE.
   38 CONTINUE
      GO TO 36
   39 CONTINUE
C     ERROR MESSAGE - NO MATCH FOUND
      ISTOIC(1) = -ISTOIC(1)
      ISTOIC(2) = -ISTOIC(2)
      WRITE(6,101) (ISTOIC(I),SP(I),I=1,4)
      NEXT = .TRUE.
      GO TO 36

C     GET INITIAL CONDITIONS
   40 CALL INIT (ISS,MMHG,MOLEF)


C     CHECK INPUT COMPOSITION
      CSUM = 0.
      DO 47 I=1,LS
   47 CSUM = CSUM + C(I)
      IF (ABS(1.-CSUM) .LE. .001) GO TO 48
      WRITE(6,105) CSUM,(SPNM(I),C(I),I=1,LS)
  105 FORMAT (7HO(KINP),5X,33HINVALID INPUT COMPOSITION  SUM = ,F11.6//
     * (12X,A8,E20.5))
      NEXT = .TRUE.
      RETURN

C     SET INITIAL STEP SIZE

   48 IF(ITPSZ .GT. 2) GO TO 53
      IF (ITPSZ .EQ. 1  .AND.  NTB .EQ. 0) GO TO 53
      IF (NTB .NE. 0) NT = NTB
      NZ = NTB
      CONV = 1.
      CON2 = 1.
      IF (VERSA .NE. AREAV) GO TO 203
      XU = CU
      AU(1) = CUA(1)
      AU(2) = CUA(2)
C     CONVERT AREA PROFILE TO INTERNAL UNITS
      IF (UNITI .NE. FPS) GO TO 201
      XU = FU
      AU(1) = FUA(1)
      AU(2) = FUA(2)
      CONV = 30.48
      GO TO 202
  201 IF (UNITI .NE. SI) GO TO 206
      XU = SU
      AU(1) = SUA(1)
      AU(2) = SUA(2)
      CONV = 100.
  202 CON2 = CONV*CONV
      GO TO 206

  203 XU = CU
      AU(1) = CUP2(1)
      AU(2) = CUP2(2)
C     CONVERT PRESSURE PROFILE TO INTERNAL UNITS
      IF (UNITI .NE. FPS) GO TO 204
      XU = FU
      AU(1) = FUP(1)
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      AU(2) = FUP(2)
      CONV = 30.48
      CON2 = 1./2116.2
      GO TO 205
  204 IF (UNITI .NE. SI) GO TO 205
      XU = SU
      AU(1) = SUP(1)
      AU(2) = SUP(2)
      CONV = 100.
      CON2 = 1./1.01325E+05
  205 IF (.NOT. MMHG) GO TO 206
      AU(1) = CUP1(1)
      AU(2) = CUP1(2)
      CON2 = 1./760.

  206 IF (VERSI .EQ. TIMEV) CONV = 1.
      IF (ITPSZ .EQ. 2) GO TO 208
      DO 207 I=1,NTB
      CXTB(I) = XTB(I)*CONV
  207 CATB(I) = ATB(I)*CON2
      GO TO 53
  208 DO 209 I=1,4
  209 CN(I) = CX(I)*CON2

   53 CONTINUE

   59 IF (ITPSZ .EQ. 1) CALL CUBS (CXTB,CATB,NT)

      IF (UNITI .NE. FPS) GO TO 63
C     CONVERT FROM FPS UNITS TO INTERNAL (CGS) UNITS
      IF (VERSI .NE. TIMEV) GO TO 60
      DVAR = DVAR*30.48
      GO TO 61
   60 IVAR = IVAR*30.48
   61 IF (MMHG) P = P*2.7845
      P = P/2116.2
      AREA = AREA*929.0304
      MDOT = MDOT*453.59237
      V = V*30.48
      RHO = RHO/62.43
      T = T/1.8
      IF(VERSI .EQ. TIMEV) GO TO 68
      CEND = UNCEND*30.48
      GO TO 68
   63 IF (UNITI .NE. SI) GO TO 67
C     CONVERT FROM SI UNITS TO INTERNAL (CGS) UNITS
      IF (VERSI .NE. TIMEV) GO TO 64
      DVAR = DVAR*100.
      GO TO 65
   64 IVAR = IVAR*100.
   65 IF (MMHG) P = P*133.3224
      P = P/1.01325E+05
      AREA = AREA*10000.
      MDOT = MDOT*1000.
      V = V*100.
      RHO = RHO*.001
      IF(VERSI .EQ. TIMEV) GO TO 68
      CEND = UNCEND*100.
      GO TO 68

   67 CEND = UNCEND
      IF (MMHG) P = P/760.

   68 MIXMW = 0.

      IF (.NOT. MOLEF) GO TO 71
C     MOLE FRACTION TO MOLES(I)/MASS(MIXTURE)
      DO 69 I=1,LS
   69 MIXMW = MIXMW + C(I)*MW(I)
      DO 70 I=1,LS
   70 SIGMA(I) = C(I)/MIXMW
      GO TO 73

C     MASS FRACTION TO MOLES(I)/MASS(MIXTURE)
   71 DO 72 I=1,LS
      SIGMA(I) = C(I)/MW(I)
   72 MIXMW = MIXMW + SIGMA(I)
      MIXMW = 1./MIXMW

C     UNIVERSAL GAS CONSTANT IN ATM-CC/MOLE-DEG K
   73 RR = 82.056
C     UNIVERSAL GAS CONSTANT IN ERGS/MOLE-DEG K
      R = 8.3143E+07

      IF (M2 .EQ. 0.  .AND.  .NOT. (COMBUS .OR. SHOCK)) GO TO 81
      CALL THRM (T,1.)
      CPRO = 0.
      DO 74 I=1,LS
   74 CPRO = CPRO + CPR(I)*SIGMA(I)
      GAMMA = CPRO/(CPRO - 1./MIXMW)
      IF (V .NE. 0.) GO TO 81
      V = SQRT(M2*R/MIXMW*GAMMA*T)

   81 IF (P .EQ. 0.) GO TO 82
      RHO = P*MIXMW/(RR*T)
      GO TO 75
   82 IF (RHO .EQ. 0.) GO TO 83
      P = RHO*RR*T/MIXMW
      GO TO 75
```

APPENDIX B

```
   83 IF (IPRCOD .GT. 2) GO TO 84
      X = IVAR
      IF (VERSI .EQ. TIMEV) X = DVAR
      CALL CINP(CATB,CXTB,NT,X,AVAR,DUM1,DUM2)
      GO TO 85
   84 TIME = DVAR
      IF (VERSI .EQ. TIMEV) TIME = IVAR
      CALL CINP(CATB,CXTB,NT,TIME,AVAR,DUM1,DUM2)
   85 IF (VERSA .EQ. AREAV) GO TO 86
      P = AVAR
      GO TO 81
   86 AREA = AVAR
      RHO = MDOT/(AREA*V)
      GO TO 82

   75 IF (MDOT .EQ. 0.) MDOT = RHO*AREA*V
      TO=IVAR
      NO=LSP3
      TLAST=END

      IF (.NOT. (COMBUS .OR. SHOCK)) RETURN
      HRO = 0.
      DO 76 I=1,LS
   76 HRO = HRO + HRT(I)*SIGMA(I)
      HRO = HRO*T
      M2 = V/R*V/T*MIXMW/GAMMA

C     EQUILIBRIUM COMBUSTION
      IF (COMBUS) CALL COMB

C     EQUILIBRIUM AND FROZEN SHOCK
      IF (SHOCK) CALL SHOK

      RETURN
      END



      BLOCK DATA

C     ALPHANUMERIC DATA FOR TESTING AND OUTPUT

      COMMON/LTUS/LTHM,LDAT,NTHRD,NBLANK,NPHOTO
      COMMON/OPTS/DUM1,TIME,DUM2,AREA,DUM(3)
      COMMON/SPEC/SNAM(3),DUM4(25),EFFM,BLANK,HNU,DUM5(25,102)
      COMMON/KOUT/DUM6(74),FPS,SI,DUM7

C     LOGICAL TAPE UNIT ASSIGNMENTS
      DATA LTHM,LDAT/4,7/

C     SPECIES SUBSCRIPTS FOR M,BLANK, AND HNU
      DATA NTHRD,NBLANK,NPHOTO/26,27,28/

C     ALPHANUMERIC DATA
      DATA TIME,AREA/4HTIME,4HAREA/
      DATA SNAM,EFFM,BLANK/1HV,3HRHO,1HT,1HM,1H /
      DATA HNU/3HHNU/
      DATA FPS,SI/3HFPS,2HSI/

      END



      BLOCK DATA

C     SPECIES NAMES AND MOLECULAR WEIGHTS

      COMMON/SNMW/ALSP(75),ALMW(75)

      DATA ALSP/
     * 8HAR      , 8HC6H6    , 8HC6H11   , 8HC6H12   , 8HC2H6CO  ,
     * 8HC2H5CO  , 8HC2H5OH  , 8HCH3CHO  , 8HCH3OH   , 8HCH3CO   ,
     * 8HC2H4OH  , 8HCH2OH   , 8HHNO3    , 8HBR      , 8HBR2     ,
     * 8HC       , 8HC6H13   , 8HC6H14   , 8HCH      , 8HCH2     ,
     * 8HCH3     , 8HCH4     , 8HCN      , 8HCO      , 8HCO2     ,
     * 8HC2H3O   , 8HC2H      , 8HC2H2    , 8HC2H4    , 8HC2N     ,
     * 8HC8H16   , 8HC8H17   , 8HC3H7    , 8HC3H6    , 8HC3H4    ,
     * 8HC2H5    , 8HH       , 8HHCN     , 8HHCL     , 8HHF      ,
     * 8HHO2     , 8HH2      , 8HH2O     , 8HH2O2    , 8HHE      ,
     * 8HN       , 8HC8H18   , 8HC7H14   , 8HC7H15   , 8HNH2     ,
     * 8HNH3     , 8HNO      , 8HNO2     , 8HN2      , 8HN2H4    ,
     * 8HN2O     , 8HN2O4    , 8HC7H16   , 8HO       , 8HOH      ,
     * 8HO2      , 8HHNO     , 8HC2      , 8HXE      , 8HNH      ,
     * 8HHCO     , 8HCH2O    , 8HC9H18   , 8HC2H3    , 8HC3H8    ,
     * 8HC9H19   , 8HC9H20   , 8HC2H6    , 8HO3      , 8HNO3     /

      DATA ALMW/
     * 39.948,    78.114,     83.154,     86.162,     58.081,
     * 57.073,    46.070,     44.054,     32.042,     43.046,
     * 45.062,    31.035,     63.013,     79.909,    159.820,
     * 12.0112,   85.170,     86.170,     13.019,     14.027,
     * 15.035,    16.043,     26.018,     28.011,     44.010,
     * 43.046,    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,     20.006,
```

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     * 33.005,     2.0159,     18.014,     34.014,      4.0026,
     * 14.007,   114.232,     98.189,     99.197,     16.023,
     * 17.031,    30.006,     46.006,     28.013,     32.045,
     * 44.012,    92.009,    100.205,     15.9994,    17.007,
     * 31.997,    31.014,     24.022,    131.300,     15.015,
     * 29.0186,   30.026,    126.243,     27.0463,    44.097,
     *127.251,   128.259,     30.070,     47.9982,    62.0049/

      END



      SUBROUTINE THRM (T,HONLY)

C     THIS ROUTINE CALCULATES (DIMENSIONLESS) THERMODYNAMIC PROPERTIES
C     FROM POLYNOMIAL CURVE FITS

      LOGICAL NEXT

      COMMON/COND/DUM(33),LS,LSP3,NEXT
      COMMON/GHSC/GRT(25),HRT(25),SR(25),CPR(25),DCPR(25)
      COMMON/TCOF/C(7,2,25),TLOW,TMID,THI

      F(T) = A1+T*(A2+T*(A3+T*(A4+T*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*THI) GO TO 2

      WRITE (6,100) T
  100 FORMAT (7HO(THRM),5X,5HERROR,3X,3HT =,F8.2,16H IS OUT OF RANGE)
      NEXT = .TRUE.
      RETURN

    2 WRITE (6,101) T
  101 FORMAT (7HO(THRM),5X,7HWARNING,3X,3HT =,F8.2,16H IS OUT OF RANGE,
     * 4X,28HEXTRAPOLATED VALUES RETURNED)

C     LOCATE PROPER TEMPERATURE RANGE
    3 K = 2
      IF (T .GT. TMID) K = 1

      DO 4 I=1,LS

C     COMPUTE H/(R*T)
      A1 = C(1,K,I) + C(6,K,I)/T
      A2 = C(2,K,I)/2.
      A3 = C(3,K,I)/3.
      A4 = C(4,K,I)/4.
      A5 = C(5,K,I)/5.
    4 HRT(I) = F(T)
      IF (HONLY .EQ. 0.) RETURN

      TPREV = T
      DO 5 I=1,LS

C     COMPUTE G/(R*T)
      A1 = C(1,K,I)*(1.-ALOG(T)) + C(6,K,I)/T - C(7,K,I)
      A2 = -C(2,K,I)/2.
      A3 = -C(3,K,I)/6.
      A4 = -C(4,K,I)/12.
      A5 = -C(5,K,I)/20.
      GRT(I) = F(T)

C     COMPUTE S/R
      A1 = C(1,K,I)*ALOG(T) + C(7,K,I)
      A2 = C(2,K,I)
      A3 = C(3,K,I)/2.
      A4 = C(4,K,I)/3.
      A5 = C(5,K,I)/4.
      SR(I) = F(T)

C     COMPUTE CP/R
      A1 = C(1,K,I)
      A2 = C(2,K,I)
      A3 = C(3,K,I)
      A4 = C(4,K,I)
      A5 = C(5,K,I)
      CPR(I) = F(T)

C     COMPUTE (DCP/DT)/R
      A1 = C(2,K,I)
      A2 = 2.*C(3,K,I)
      A3 = 3.*C(4,K,I)
      A4 = 4.*C(5,K,I)
      A5 = 0.
    5 DCPR(I) = F(T)

      RETURN
      END
```

APPENDIX B

```
      SUBROUTINE CUBS(X,Y,N,XI,YI,DY,D2Y)

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(40),S(40),T(40),U(40),V(40)
      DIMENSION A3(40),A2(40),A1(40),A0(40)

      COMMON/AFUN/C3,C2,C1,C0,ITPSZ,LSUBM,ETA,DIAM,VISC,BETA

      EQUIVALENCE (S,A3),(T,A2),(U,A1),(V,A0)

      G(A) = 1./(1. - A**ETA)
      DG(B) = ETA/LSUBM*TERM**(ETA - 1.)*B*B
      D2G(C,D,E) = C*(ETA - 1. + 2.*ETA*TERM**ETA*D)/E

C     COMPUTE CUBIC SPLINE COEFFICIENTS FROM INPUT TABLE

C     THIS ROUTINE WILL ACCEPT END CONDITIONS OF THE FORM
C      F**(X(1)) = ALPHA1*F**(X(2)) + BETA1*F**(X(3)) + GAMMA1
C      F**(X(N)) = ALPHAN*F**(X(N-1)) + BETAN*F**(X(N-2)) + GAMMAN

C     THE CURRENT END CONDITIONS GIVE A PARABOLIC RUNOUT
C      F**(X(1)) = F**(X(2))
C      F**(X(N)) = F**(X(N-1))

C     CONSTRUCT (TRIDIAGONAL) COEFFICIENT MATRIX
C        S=DIAGONAL,  T=SUPERDIAGONAL,  U=SUBDIAGONAL,  V=CONSTANTS
      DXIM = X(2) - X(1)
      DYIM = Y(2) - Y(1)
      DIM = DYIM/DXIM
      DXI = X(3) - X(2)
      DYI = Y(3) - Y(2)
      DI = DYI/DXI
      BETA1 = 0.
      ALPHA1 = 1.
      GAMMA1 = 0.
      S(2) = (ALPHA1 + 2.)*DXIM + 2.*DXI
      T(2) = BETA1*DXIM + DXI
      V(2) = (DI - DIM) - (GAMMA1/6.)*DXIM
      U(3) = DXI
      NM = N - 1
      DO 2 I=3,NM
      DXIM = DXI
      DYIM = DYI
      DIM = DI
      DXI = X(I+1) - X(I)
      DYI = Y(I+1) - Y(I)
      DI = DYI/DXI
      IF (I .EQ. NM) GO TO 3
      S(I) = 2.*(DXIM + DXI)
      T(I) = DXI
      U(I+1) = T(I)
    2 V(I) = DI - DIM
    3 BETAN = 0.
      ALPHAN = 1.
      GAMMAN = 0.
      S(NM) = 2.*DXIM + (2. + ALPHAN)*DXI
      U(NM) = DXIM + BETAN*DXI
      V(NM) = (DI - DIM) - (GAMMAN/6.)*DXI

      NM2 = N - 2
      DO 4 I=2,NM2
      T(I) = T(I)/S(I)
      V(I) = V(I)/S(I)
      II = I + 1
      S(II) = S(II) - U(II)*T(I)
    4 V(II) = V(II) - U(II)*V(I)
      V(NM) = V(NM)/S(NM)

      D(NM) = V(NM)
      DO 5 J=2,NM2
      I = N - J
    5 D(I) = V(I) - T(I)*D(I+1)
C     GET D(1) AND D(N) FROM END CONDITIONS
      D(1) = ALPHA1*D(2) + BETA1*D(3) + GAMMA1/6.
      D(N) = ALPHAN*D(NM) + BETAN*D(NM2) + GAMMAN/6.

C     COMPUTE CUBIC SPLINE COEFFICIENTS
      DO 6 I=1,NM
      II = I + 1
      DXI = X(II) - X(I)
      DYI = Y(II) - Y(I)
      DI = D(II)
      DIM = D(I)
      A3(I) = (DI - DIM)/DXI
      DI = DI*X(I)
      DIM = DIM*X(II)
      A2(I) = -3.*(DI - DIM)/DXI
      DI = DI*X(I)
      DIM = DIM*X(II)
      B = DYI/DXI - (D(II) - D(I))*DXI
      A1(I) = 3.*(DI - DIM)/DXI + B
      DI = DI*X(I)
      DIM = DIM*X(II)
```

APPENDIX B

```
    6 AO(I) = -(DI - DIM)/DXI + Y(II) - D(II)*DXI*DXI - B*X(II)
      RETURN

      ENTRY CINP
      NM=N-1
      GO TO (7,10,11,11,13),ITPSZ

C     COMPUTE Y, DY/DX, D2Y/DX2 FROM CUBIC SPLINE COEFFICIENTS
    7 DO 8 I=1,NM
      II = I
      IF ((X(I) - XI)*(XI - X(I+1)) .GE. 0.) GO TO 9
    8 CONTINUE
      WRITE (6,100) XI,X(1),X(N)
  100 FORMAT (7HO(CINP),5X,3HXI=,F13.5,17H  IS OUT OF RANGE/10X,5HX(1)=,
     * F13.5,5X,5HX(N)=,F13.5)

    9 YI = ((A3(II)*XI + A2(II))*XI + A1(II))*XI + AO(II)
      DY = (3.*A3(II)*XI + 2.*A2(II))*XI + A1(II)
      D2Y = 6.*A3(II)*XI + 2.*A2(II)
      RETURN

C     COMPUTE Y, DY/DX, D2Y/DX2 FROM INPUT POLYNOMIAL
   10 YI = ((C3*XI + C2)*XI + C1)*XI + C0
      DY = (3.*C3*XI + 2.*C2)*XI + C1
      D2Y = 6.*C3*XI + 2.*C2
      RETURN

C     COMPUTE Y, DY/DX, D2Y/DX2 FROM INPUT SPECIAL FUNCTION
C     EXCEPTIONAL CASE AT X=0
   11 IF (XI .EQ. 0.) GO TO 12
      TERM = XI/LSUBM
      YI = G(TERM)
      DY = DG(YI)
      D2Y = D2G(DY,YI,XI)
      RETURN

   12 YI = 1.

C     FIT A CUBIC THROUGH THE POINTS (0.,Y1),(.05,Y2*),(.05,Y2**), AND
C     (.10,Y3**) IN ORDER TO FIND Y1* AND Y1**
      TERM = .05/LSUBM
      Y2 = G(TERM)
      Y2P = DG(Y2)
      Y2PP = D2G(Y2P,Y2,.05)
      TERM = .10/LSUBM
      Y3 = G(TERM)
      Y3P = DG(Y3)
      Y3PP = D2G(Y3P,Y3,.10)

      DY = (.05*(Y3PP - Y2PP)/(.10 - .05)/2. - Y2PP)*.05 + Y2P
      D2Y = Y2PP - .05*(Y3PP - Y2PP)/(.10 - .05)
      RETURN

C     V=0 CASE - ASSIGNED AREA IS NOT REQUIRED
   13 YI = 1.
      DY = 0.
      D2Y = 0.
      RETURN

      END




      SUBROUTINE INIT (ISS,MMHGS,MOLEFS)

C     READ INITIAL CONDITIONS

      LOGICAL MMHG,MOLEF,MMHGS,MOLEFS

      REAL IVAR,MDOT,M2,MACH
      REAL N,NF,NF2,NF3,NH2,NH3,NO,NO2,N2,N2H4,N2O,N2O4,NE,KR,NH,NOP,NO3

      DIMENSION ISS(25),TINP(75)

      COMMON/LTUS/LTHM,LDAT,NTHRD,NBLANK,NPHOTO
      COMMON/OPTS/VERSI,TIMEV,DUM1(5)
      COMMON/COND/DVAR,AREA,MDOT,P,IVAR,V,RHO,T,CONC(25),LS,DUM2(2)
      COMMON/NECC/DUM3(2),M2,DUM4(3)
      COMMON/FAKE/
     *   AR      ,  C6H6    ,  C6H11   ,  C6H12   ,  C2H6CO  ,
     *   C2H5CO  ,  C2H5OH  ,  CH3CHO  ,  CH3OH   ,  CH3CO   ,
     *   C2H4OH  ,  CH2OH   ,  HNO3    ,  BR      ,  BR2     ,
     *   C          C6H13   ,  C6H14   ,  CH      ,  CH2     ,
     *   CH3     ,  CH4     ,  CN      ,  CO      ,  CO2     ,
     *   C2H3O   ,  C2H     ,  C2H2    ,  C2H4    ,  C2N     ,
     *   C8H16   ,  C8H17   ,  C3H7    ,  C3H6    ,  C3H4    ,
     *   C2H5    ,  H       ,  HCN     ,  HCL     ,  HF      ,
     *   HO2     ,  H2      ,  H2O     ,  H2O2    ,  HE      ,
     *   N       ,  C8H18   ,  C7H14   ,  C7H15   ,  NH2     ,
     *   NH3     ,  NO      ,  NO2     ,  N2      ,  N2H4    ,
     *   N2O     ,  N2O4    ,  C7H16   ,  O       ,  OH      ,
     *   O2      ,  HNO     ,  C2      ,  XE      ,  NH      ,
     *   HCO     ,  CH2O    ,  C9H18   ,  C2H3    ,  C3H8    ,
     *   C9H19   ,  C9H20   ,  C2H6    ,  O3      ,  NO3
```

APPENDIX B

```
      EQUIVALENCE (TINP(1),AR)

      NAMELIST/START/X,AREA,MDOT,P,TIME,V,RHO,T, MACH,   MMHG,MOLEF,
     *   AR      ,   C6H6    ,   C6H11   ,   C6H12   ,   C2H6CO  ,
     *   C2H5CO  ,   C2H5OH  ,   CH3CHO  ,   CH3OH   ,   CH3CO   ,
     *   C2H4OH  ,   CH2OH   ,   HNO3    ,   BR      ,   BR2     ,
     *   C       ,   C6H13   ,   C6H14   ,   CH      ,   CH2     ,
     *   CH3     ,   CH4     ,   CN      ,   CO      ,   CO2     ,
     *   C2H3O   ,   C2H     ,   C2H2    ,   C2H4    ,   C2N     ,
     *   C8H16   ,   C8H17   ,   C3H7    ,   C3H6    ,   C3H4    ,
     *   C2H5    ,   H       ,   HCN     ,   HCL     ,   HF      ,
     *   HO2     ,   H2      ,   H2O     ,   H2O2    ,   HE      ,
     *   N       ,   C8H18   ,   C7H14   ,   C7H15   ,   NH2     ,
     *   NH3     ,   NO      ,   NO2     ,   N2      ,   N2H4    ,
     *   N2O     ,   N2O4    ,   C7H16   ,   O       ,   OH      ,
     *   O2      ,   HNO     ,   C2      ,   XE      ,   NH      ,
     *   HCO     ,   CH2O    ,   C9H18   ,   C2H3    ,   C3H8    ,
     *   C9H19   ,   C9H20   ,   C2H6    ,   O3      ,   NO3

      X = 0.
      TIME = 0.
      MACH = 0.
      DO 1 II=1,75
    1 TINP(II) = 0.
      MMHG = MMHGS
      MOLEF = MOLEFS

      READ (LDAT,START)

      MMHGS = MMHG
      MOLEFS = 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 II=1,LS
      JJ = ISS(II)
    4 CONC(II) = TINP(JJ)

      RETURN
      END
```

```
      SUBROUTINE CIMAGE

C     THIS ROUTINE READS 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 (WORD,CARD)

      DATA FINIS,BLANK/4HFINI,1H /

      READ (5,101) CARD
  101 FORMAT (20A4)
      IF(EOF,5)998,999
  998 STOP
  999 CONTINUE
      REWIND LDAT

      WRITE (6,100)
  100 FORMAT (1H1,56X,18H**  DATA CARDS  **//37X,1H1,9X,1H2,9X,1H3,9X,
     * 1H4,9X,1H5,9X,1H6,9X,1H7,9X,1H8/24X,5HCC  1,8X,8(1H0,9X)//)
      GO TO 2

    1 READ (5,101) CARD
    2 DO 3 I=1,20
      IF (CARD(I) .NE. BLANK) GO TO 4
    3 CONTINUE
      WRITE (6,102)
  102 FORMAT (60X,16H-  BLANK CARD  -)
      GO TO 5
    4 WRITE (6,103) CARD
  103 FORMAT (28X,20A4)
      IF (WORD .EQ. FINIS) GO TO 6
    5 WRITE (LDAT,101) CARD
      GO TO 1

    6 REWIND 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 ALLM1,CONC,DBUGO,EXCHR,NEXT,RHOCON,TCON

      REAL MDOT,IVAR,N,M,MW,MIXMW,M2,MACH,LSUBM

      DIMENSION SPNM(28),PRC(25),PRX(50) ,XXH(50) ,ESP(25)

      COMMON/DERV3/TDERV
      COMMON/LTUS/LTHM,LOAT,NTHRD,NBLANK,NPHOTO
      COMMON/OPTS/VERSI,TIMEV,VERSA,AREAV,TCON,RHOCON,IPRCOD
      COMMON/COND/DVAR,AREA,MDOT,P,IVAR,V,RHO,T,SIGMA(25),LS,LSP3,NEXT
      COMMON/STCOM1/DUM(2),HINT,HMIN,HMAX,EMAX,MF,KFLAG,JSTART
      COMMON/NECC/RR,MIXMW,M2,GAMMA,TCPR,R
      COMMON/KOUT/TITLE(20),UNITI,UNITO,CONC,EXCHR,DELH(50),FPS,SI,DBUGO
      COMMON/REAC/LSR(4,50),XX(50),RATE(50),LKEQ(50),DLKEQ(50),MM(50),LR
      COMMON/RRAT/A(50),N(50),EACT(50),B(50),M(25,50),ALLM1
      COMMON/AFUN/CN(4),ITPSZ,LSUBM,ETA,D,VISC,BETAL
      COMMON/SPEC/SNAM(31),MW(25),W(25),STOIC(25,50),OMEGA(25,50)
      COMMON/XVSA/XTB(40),ATB(40),NTB,XU,AU(2),CX(4)
      COMMON/GHSC/GRT(25),HRT(25),SR(25),CPR(25),DCPR(25)
      COMMON/STCS/NSTOIC(4,50),EQUIL(50)

      EQUIVALENCE (SPNM,SNAM(4))
      EQUIVALENCE (PRX(1),XXH(1))

      ENTRY OUT1

C ** TITLE PAGE
      IF (VERSI .EQ. TIMEV) GO TO 98
      I = 2
      GO TO 99
   98 I = 4
   99 IF (VERSA .EQ. AREAV) I = I - 1
      GO TO (100,200,300,400),I
  100 WRITE (6,101)
  101 FORMAT (1H1,14X,21HDISTANCE-AREA VERSION)
      GO TO 3
  200 WRITE (6,201)
  201 FORMAT (1H1,12X,25HDISTANCE-PRESSURE VERSION)
      GO TO 3
  300 WRITE (6,301)
  301 FORMAT (1H1,16X,17HTIME-AREA VERSION)
      GO TO 3
  400 WRITE (6,401)
  401 FORMAT (1H1,14X,21HTIME-PRESSURE VERSION)
    3 WRITE (6,102) (TITLE(I),I=1,20)
  102 FORMAT(1H+,49X,*GENERAL CHEMICAL KINETICS PROGRAM*,9X,*NASA LANGLE
     LY RESEARCH CENTER*/39X,*LANGLEY VERSION OF LEWIS PROGRAM (TN D-658
     26) USING STIFF ODE*/42X,*SOLUTION TECHNIQUE DEVELOPED BY C.W. GEAR
     3 *//26X,20A4,///5X,*REACTION*,31X,*REACTION*,42X,*REACTION RATE VA
     4RIABLES*/6X,*NUMBER*,78X,1HA,16X,1HN,9X,*ACTIVATION*/119X,*ENERGY*
     5)

C     PRINT REACTION INFORMATION
      DO 6 J=1,LR
      N1 = LSR(1,J)
      N2 = LSR(2,J)
      N3 = LSR(3,J)
      N4 = LSR(4,J)
      NSTOC2 = -NSTOIC(2,J)
      WRITE(6,103) J,NSTOC2,SPNM(N2),NSTOIC(3,J),SPNM(N3),A(J),N(J),
     1EACT(J)
  103 FORMAT(8X,I2,25X,I1,1H*,A8,2X,1H=,2X,I1,1H*,A8,25X,E12.5,5X,
     * F10.4,5X,F10.2)
      IF (N1 .EQ. NBLANK) GO TO 4
      IF (N1 .LE. LS) GO TO 203
      WRITE(6,105)  SPNM(N1)
  105 FORMAT(1H+,21X,A8,2X,1H+)
      GO TO 4
  203 NSTOC1 = -NSTOIC(1,J)
      WRITE(6,204) NSTOC1,SPNM(N1)
  204 FORMAT(1H+,19X,I1,1H*,A8,2X,1H+)
    4 IF (N4 .EQ. NBLANK) GO TO 6
      IF (N4 .LE. LS) GO TO 304
      WRITE(6,104) SPNM(N4)
  104 FORMAT(1H+,61X,1H+,4X,A8)
      GO TO 6
  304 WRITE(6,305) NSTOIC(4,J),SPNM(N4)
  305 FORMAT(1H+,61X,1H+,2X,I1,1H*,A8)

C     CONVERT ACTIVATION ENERGY TO B-FACTOR
    6 B(J) = EACT(J)/1.987165

      IF (.NOT. ALLM1) GO TO 7
      WRITE (6,106)
  106 FORMAT (///51X,29HALL THIRD BODY RATIOS ARE 1.0)
      GO TO 13

    7 WRITE (6,107)
  107 FORMAT (///41X,50HALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWI
     *NG//)
      K = 0
      DO 12 I=1,LS
      DO 12 J=1,LR
```

```
      IF (M(I,J) .EQ. 1.) GO TO 12
      K = K + 1
      IF (K .EQ. 5) K = 1
      GO TO (8,9,10,11),K
    8 WRITE(6,108)  SPNM(I),J,M(I,J)
  108 FORMAT(5X,2HM(,A8,1H,,I2,3H) =,F10.5)
      GO TO 12
    9 WRITE(6,109)  SPNM(I),J,M(I,J)
  109 FORMAT(1H+,36X,2HM(,A8,1H,,I2,3H) =,F10.5)
      GO TO 12
   10 WRITE(6,110)  SPNM(I),J,M(I,J)
  110 FORMAT(1H+,68X,2HM(,A8,1H,,I2,3H) =,F10.5)
      GO TO 12
   11 WRITE(6,111)  SPNM(I),J,M(I,J)
  111 FORMAT(1H+,100X,2HM(,A8,1H,,I2,3H) =,F10.5)
   12 CONTINUE

   13 IF (VERSI .EQ. TIMEV) GO TO 14
      WRITE (6,112) HMIN,HMAX,HINT,EMAX
  112 FORMAT (///56X,20HINTEGRATION CONTROLS//15X,17HMINIMUM STEP SIZE,
     * E14.5,3H CM,33X,17HMAXIMUM STEP SIZE,E14.5,3H CM//15X,17HINITIAL
     *STEP SIZE,E14.5,3H CM,33X,22HMAXIMUM RELATIVE ERROR,F10.5)
      GO TO 15
   14 WRITE (6,113) HMIN,HMAX,HINT,EMAX
  113 FORMAT (///56X,20HINTEGRATION CONTROLS//15X,17HMINIMUM STEP SIZE,
     * E14.5,4H SEC,32X,17HMAXIMUM STEP SIZE,E14.5,4H SEC//15X,17HINITIA
     *L STEP SIZE,E14.5,4H SEC,32X,22HMAXIMUM RELATIVE ERROR,F10.5)

C ** SECOND PAGE
   15 WRITE (6,114)
  114 FORMAT (1H1,50X,31H** ASSIGNED VARIABLE PROFILE **//)
      GO TO (16,18,19,19,20),ITPSZ

   16 GO TO (116,216,316,416),IPRCOD
C     ASSIGNED VARIABLE TABLE
  116 WRITE (6,117) XU,AU
  117 FORMAT (34X,64HTHE AREA IS CALCULATED BY INTERPOLATION FROM THE FO
     *LLOWING TABLE//36X,7HSTATION,10X,17HAXIAL DISTANCE  (,A2,1H),10X,
     * 7HAREA  (,A4,A1,1H))
      GO TO 516
  216 WRITE (6,217) XU,AU
  217 FORMAT (32X,68HTHE PRESSURE IS CALCULATED BY INTERPOLATION FROM TH
     *E FOLLOWING TABLE//36X,7HSTATION,10X,17HAXIAL DISTANCE  (,A2,1H),
     * 9X,11HPRESSURE  (,2A4,1H))
      GO TO 516
  316 WRITE (6,317) AU
  317 FORMAT (34X,64HTHE AREA IS CALCULATED BY INTERPOLATION FROM THE FO
     *LLOWING TABLE//36X,7HSTATION,14X,11HTIME  (SEC),16X,7HAREA  (,A4,
     * A1,1H))
      GO TO 516
  416 WRITE (6,417) AU
  417 FORMAT (32X,68HTHE PRESSURE IS CALCULATED BY INTERPOLATION FROM TH
     *E FOLLOWING TABLE//36X,7HSTATION,14X,11HTIME  (SEC),15X,11HPRESSUR
     *E  (,2A4,1H))
  516 DO 17 I=1,NTB
   17 WRITE (6,616) I,XTB(I),ATB(I)
  616 FORMAT (38X,I2,14X,1PE12.5,15X,E12.5)
      GO TO 21

   18 GO TO (218,318,418,518),IPRCOD
C     ASSIGNED VARIABLE POLYNOMIAL
  218 WRITE (6,219) AU,CX
  219 FORMAT (40X,52HTHE AREA IS CALCULATED FROM THE FOLLOWING POLYNOMIA
     *L//23X,6HAREA (,A4,A1,5H) = (,1PE12.5,9H)X**3 + (,E12.5,9H)X**2 +
     *(,E12.5,6H)X + (,E12.5,1H))
      GO TO 21
  318 WRITE (6,319) AU,CX
  319 FORMAT (38X,56HTHE PRESSURE IS CALCULATED FROM THE FOLLOWING POLYN
     *OMIAL//20X,10HPRESSURE (,2A4,5H) = (,1PE12.5,9H)X**3 + (,E12.5,9H)
     *X**2 + (,E12.5,6H)X + (,E12.5,1H))
      GO TO 21
  418 WRITE (6,419) AU,CX
  419 FORMAT (40X,52HTHE AREA IS CALCULATED FROM THE FOLLOWING POLYNOMIA
     *L//23X,6HAREA (,A4,A1,5H) = (,1PE12.5,9H)T**3 + (,E12.5,9H)T**2 +
     *(,E12.5,6H)T + (,E12.5,1H))
      GO TO 21
  518 WRITE (6,519) AU,CX
  519 FORMAT (38X,56HTHE PRESSURE IS CALCULATED FROM THE FOLLOWING POLYN
     *OMIAL//20X,10HPRESSURE (,2A4,5H) = (,1PE12.5,9H)T**3 + (,E12.5,9H)
     *T**2 + (,E12.5,6H)T + (,E12.5,1H))
      GO TO 21

C     SPECIAL AREA FUNCTION
   19 WRITE (6,118) LSUBM,ETA
  118 FORMAT (41X,50HTHE AREA IS CALCULATED FROM THE FOLLOWING FUNCTION/
     *1/46X,16H1/AREA = 1 - (X/,F10.3,4H)**(,F10.5,1H))
      IF (ITPSZ .EQ. 4) WRITE (6,1118) D,VISC,BETAL
 1118 FORMAT (/6X,20HHYDRAULIC DIAMETER =,F8.4,3H CM,7X,23HVISCOSITY COE
     *FFICIENT =,E12.4,10H GM/CM-SEC,7X,6HBETA =,F7.4)
      GO TO 21

C     ZERO VELOCITY - ASSIGNED VARIABLE NOT REQUIRED
   20 WRITE (6,119)
  119 FORMAT (36X,50HTHIS IS A V=0 PROBLEM - AN ASSIGNED VARIABLE IS NOT
     * REQUIRED)

   21 CONTINUE
```

APPENDIX B

```
  228 IF (RHOCON) WRITE (6,1126)
 1126 FORMAT (///38X,56HTHE VOLUME (DENSITY) WILL BE HELD CONSTANT FOR T
     *HIS CASE)
      IF (TCON) WRITE (6,2126)
 2126 FORMAT (///40X,51HTHE TEMPERATURE WILL BE HELD CONSTANT FOR THIS C
     *ASE)
      RETURN

      ENTRY OUT2

C     INITIAL CONDITIONS
      WRITE (6,127)
  127 FORMAT (1H1,52X,26H**  INITIAL CONDITIONS  **//)
      GO TO 29

      ENTRY OUT3

C     GENERAL OUTPUT
      WRITE (6,128)
  128 FORMAT (1H1)

   29 MACH = SQRT(M2)
      MAX = MAXO(LS,LR)

      TENT = 0.
      CSUM = 0.
      PMLOG = ALOG(P*MIXMW)
C     TOTAL ENTROPY AND MASS FRACTION SUM
      DO 30 I=1,LS
      IF(SIGMA(I) .LE. 0.) GO TO 30
      TENT = TENT + SIGMA(I)*(SR(I) - ALOG(SIGMA(I)) - PMLOG)
   30 CSUM = CSUM + SIGMA(I)*MW(I)
      TENT = TENT*1.987165

      TXXH = 0.
C     ENERGY EXCHANGE RATES
      DO 31 J=1,LR
      XXH(J) = XX(J)*DELH(J)
   31 TXXH = TXXH + XXH(J)

      IF (VERSI .EQ. TIMEV) GO TO 32
      TIME = DVAR
      X = IVAR
      GO TO 33
   32 TIME = IVAR
      X = DVAR

   33 IF (UNITO .NE. FPS) GO TO 48

C     CONVERT FROM INTERNAL (CGS) UNITS TO FPS UNITS
      X = X/30.48
      AREAA = AREA/929.0304
      DOTM = MDOT/453.59237
      PP = P*2116.2
      VV = V/30.48
      RHOO = RHO*62.43
      TT = T*1.8

      WRITE(6,129) TIME,AREAA,X,PP,    VV,    RHOO,
     * TT,DOTM,TENT,     MACH,GAMMA
  129 FORMAT(16X,*TIME*,E14.5,*  SEC*,14X,*AREA*,E14.5,*  SQ FT*,
     1 14X,*AXIAL POSITION*,E14.5,*  FT*///20X,*FLOW PROPERTIES*,45X,
     2 *INTEGRATION INDICATORS*//22X,*PRESSURE*,E22.5,30X,
     3 *STEPS FROM LAST PRINT*,13X/23X,*(LB/FT--2)*/22X,*VELOCITY*,
     4 E22.5,30X,*AVERAGE STEP SIZE*/23X,*(FT/SEC)*/22X,*DENSITY*,
     5 E23.5,30X,*CONTROLLING VARIABLE*/23X,*(LB/FT--3)*/
     6 22X,*TEMPERATURE*,E19.5/23X,*(DEG R)*/22X,*MASS FLOW RATE*,
     7 E16.5/23X,*(LB/SEC)*/22X,*ENTROPY*,E23.5,30X,*RELATIVE ERROR*/
     8  23X,*(BTU/LB/DEG R)*/22X,*MACH NUMBER*,E19.5//22X,*GAMMA*,E25.5)

   34 WRITE (6,131)
  131 FORMAT (//56X,19HCHEMICAL PROPERTIES//)

      CONV = 0.02883
      IF (CONC .OR. EXCHR) GO TO 36

C     PRINT MASS FRACTIONS AND REACTION CONVERSION RATES
      WRITE (6,132)
  132 FORMAT (1X,7HSPECIES,4X,13HMASS FRACTION,3X,13HMOLE FRACTION,3X,
     * 27HNET SPECIES PRODUCTION RATE,5X,8HREACTION,3X,28HNET REACTION C
     *ONVERSION RATE,2X,14HNET RATE/POSI-)
      WRITE (6,133)
  133 FORMAT (50X,16H(MOLE/FT**3/SEC),11X,6HNUMBER,7X,22H(MOLE-FT**3/LB
     **2/SEC),6X,13HTIVE DIR RATE)
      DO 35 J=1,LR
   35 PRX(J) = XX(J)
      CONV = 1./62.43
      GO TO 37

   36 IF (CONC .OR. (.NOT. EXCHR)) GO TO 39

C     PRINT MASS FRACTIONS AND ENERGY EXCHANGE RATES
      WRITE (6,134)
  134 FORMAT (1X,7HSPECIES,4X,13HMASS FRACTION,3X,13HMOLE FRACTION,3X,
     * 27HNET SPECIES PRODUCTION RATE,5X,8HREACTION,5X,24HNET ENERGY EXC
     *HANGE RATE,4X,14HNET RATE/POSI-)
      WRITE (6,135)
```

APPENDIX B

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  135 FORMAT (50X,16H(MOLE/FT**3/SEC),11X,6HNUMBER,8X,21H(BTU-FT**3/LB**
     *2/SEC),6X,13HTIVE DIR RATE)

C     COMPUTE MASS FRACTIONS
   37 DO 38 I=1,LS
   38 PRC(I) = SIGMA(I)*WW(I)
      GO TO 44
   39 IF ((.NOT. CONC) .OR. EXCHR) GO TO 41

C     PRINT MOLAR CONCENTRATIONS AND REACTION CONVERSION RATES
      WRITE (6,136)
  136 FORMAT (1X,7HSPECIES,4X,13HCONCENTRATION,3X,13HMOLE FRACTION,3X,
     * 27HNET SPECIES PRODUCTION RATE,5X,8HREACTION,3X,28HNET REACTION C
     *ONVERSION RATE,2X,14HNET RATE/POSI-)
      WRITE (6,137)
  137 FORMAT (12X,13H(MOLES/FT**3),25X,16H(MOLE/FT**3/SEC),11X,6HNUMBER,
     * 7X,22H(MOLE-FT**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,
     * 27HNET SPECIES PRODUCTION RATE,5X,8HREACTION,5X,24HNET ENERGY EXC
     *HANGE RATE,4X,14HNET RATE/POSI-)
      WRITE (6,139)
  139 FORMAT (12X,13H(MOLES/FT**3),25X,16H(MOLE/FT**3/SEC),11X,6HNUMBER,
     * 8X,21H(BTU-FT**3/LB**2/SEC),6X,13HTIVE DIR RATE)

C     COMPUTE MOLAR CONCENTRATIONS
   42 DO 43 I=1,LS

   43 PRC(I) = SIGMA(I)*RHOO
   44 DO 47 IJ=1,MAX
      IF (IJ .GT. LS  .OR.  IJ .GT. LR) GO TO 45
      FMOL = SIGMA(IJ)*MIXMW
      WW = W(IJ)*62.43
      XXX = PRX(IJ)*CONV
      WRITE(6,140) SPNM(IJ),PRC(IJ),FMOL,WW,IJ,XXX,EQUIL(IJ)
  140 FORMAT(2X,A8,2X,E12.5,E16.5,7X,E16.5,15X,I3,10X,E16.5,7X,E16.5)
      GO TO 47
   45 IF (IJ .GT. LS) GO TO 46
      FMOL = SIGMA(IJ)*MIXMW
      WW = W(IJ)*62.43
      WRITE(6,141) SPNM(IJ),PRC(IJ),FMOL,WW
  141 FORMAT(2X,A8,2X,E12.5,E16.5,7X,E16.5)
      GO TO 47
   46 XXX = PRX(IJ)*CONV
      WRITE (6,142) IJ,XXX,EQUIL(IJ)
  142 FORMAT(78X,I3,10X,E16.5,7X,E16.5)
   47 CONTINUE
      TXXH = TXXH*0.02883
      WRITE (6,143) MIXMW,TXXH,CSUM
  143 FORMAT ( /4X,24HMIXTURE MOLECULAR WEIGHT,F13.5,5X,26HTOTAL ENERGY
     *EXCHANGE RATE,1PE15.5,7X,17HMASS FRACTION SUM,0PF14.8)
      WRITE (6,144)
  144 FORMAT (49X,21H(BTU-FT**3/LB**2/SEC))
      GO TO 78

   48 IF (UNITO .NE. SI) GO TO 63

C     CONVERT FROM INTERNAL (CGS) UNITS TO SI UNITS
      X = X*.01
      AREAA = AREA*.0001
      DOTM = MDOT*0.001
      PP = P*1.01325E+05
      VV = V*.01
      RHOO = RHO*1000.
      TENT = TENT*4184.0

      WRITE(6,145) TIME,AREAA,X,PP,    VV,    RHOO,
     * TT,DOTM,TENT,      MACH,GAMMA
  145 FORMAT(16X,*TIME*,E14.5,*  SEC*,14X,*AREA*,E14.5,*  SQ  M*,
     1 14X,*AXIAL POSITION*,E14.5,*  M *///20X,*FLOW PROPERTIES*,45X,
     2 *INTEGRATION INDICATORS*//22X,*PRESSURE*,E22.5,30X,
     3 *STEPS FROM LAST PRINT*,13X/23X,*(N/M--2  )*/22X,*VELOCITY*,
     4 E22.5,30X,*AVERAGE STEP SIZE*/23X,*(M/SEC )*/22X,*DENSITY*,
     5 E23.5,30X,*CONTROLLING VARIABLE*/23X,*(KG/M--3 )*/
     6 22X,*TEMPERATURE*,E19.5/23X,*(DEG K)*/22X,*MASS FLOW RATE*,
     7 E16.5/23X,*(KG/SEC)*/22X,*ENTROPY*,E23.5,30X,*RELATIVE ERROR*/
     8  23X,*(JOULE/(KG-K))*/22X,*MACH NUMBER*,E19.5//22X,*GAMMA*,E25.5)

   49 WRITE (6,131)

      CONV = 4.1840
      IF (CONC .OR. EXCHR) GO TO 51

C     PRINT MASS FRACTIONS AND REACTION CONVERSION RATES
      WRITE (6,132)
      WRITE (6,146)
  146 FORMAT (50X,15H(MOLE/M**3/SEC),12X,6HNUMBER,7X,21H(MOLE-M**3/KG**2
     */SEC),7X,13HTIVE DIR RATE )
      DO 50 J=1,LR
   50 PRX(J) = XX(J)
      CONV = 0.001
      GO TO 52
```

APPENDIX B

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   51 IF (CONC .OR. (.NOT. EXCHR)) GO TO 54

C     PRINT MASS FRACTIONS AND ENERGY EXCHANGE RATES
      WRITE (6,136)
      WRITE (6,147)
  147 FORMAT (50X,15H(MOLE/M**3/SEC),12X,6HNUMBER,7X,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)*WW(I)
      GO TO 59

   54 IF ((.NOT. CONC) .OR. EXCHR) GO TO 56

C     PRINT MOLAR CONCENTRATIONS AND REACTION CONVERSION RATES
      WRITE (6,136)
      WRITE (6,148)
  148 FORMAT (12X,12H(MOLES/M**3),26X,15H(MOLE/M**3/SEC),12X,6HNUMBER,7X
     *,21H(MOLE-M**3/KG**2/SEC),7X,13HTIVE DIR RATE)
      DO 55 J=1,LR
   55 PRX(J) = XX(J)
      CONV = 0.001
      GO TO 57

C     PRINT MOLAR CONCENTRATIONS AND ENERGY EXCHANGE RATES
   56 WRITE (6,138)
      WRITE (6,149)
  149 FORMAT (12X,12H(MOLES/M**3),26X,15H(MOLE/M**3/SEC),12X,6HNUMBER,7X
     *,22H(JOULE-M**3/KG**2/SEC),6X,13HTIVE DIR RATE)

C     COMPUTE MOLAR CONCENTRATIONS
   57 DO 58 I=1,LS

   58 PRC(I) = SIGMA(I)*RHOO
   59 DO 62 IJ=1,MAX
      IF (IJ .GT. LS .OR. IJ .GT. LR) GO TO 60
      FMOL = SIGMA(IJ)*MIXMW
      WW = W(IJ)*1000.
      XXX = PRX(IJ)*CONV
      WRITE(6,140) SPNM(IJ),PRC(IJ),FMOL,WW,IJ,XXX,EQUIL(IJ)
      GO TO 62
   60 IF (IJ .GT. LS) GO TO 61
      FMOL = SIGMA(IJ)*MIXMW
      WW = W(IJ)*1000.
      WRITE(6,141) SPNM(IJ),PRC(IJ),FMOL,WW
      GO TO 62
   61 XXX = PRX(IJ)*CONV
      WRITE (6,142) IJ,XXX,EQUIL(IJ)
   62 CONTINUE
      TXXH = TXXH*4.1840
      WRITE (6,143) MIXMW,TXXH,CSUM
      WRITE (6,150)
  150 FORMAT (48X,22H(JOULE-M**3/KG**2/SEC))
      GO TO 78

C     PRINT OUTPUT IN INTERNAL (CGS) UNITS
   63 WRITE(6,151) TIME,AREA,X,P,    V,    RHO,
     * T,MDOT,TENT,      MACH,GAMMA
  151 FORMAT(16X,*TIME*,E14.5,*  SEC*,14X,*AREA*,E14.5,*  SQ CM*,
     1 14X,*AXIAL POSITION*,E14.5,*  CM*//20X,*PRESSURE,ATM      =*,
     2 F22.4,20X,*VELOCITY,CM/SEC =*,F22.2//20X,*DENSITY,GM/CC    =*,
     3 E22.5,20X,*TEMPERATURE,K    =*,F22.5//20X,*FLOW RATE,GM/SEC=*,
     4 E22.5,20X,*ENTROPY,CAL/GM-K =*,F22.5//20X,*MACH NUMBER      =*,
     5 F22.5,20X,*GAMMA            =*,F22.5)

   64 WRITE (6,131)
      IF(.NOT. DBUGO) GO TO 700
      IF (CONC .OR. EXCHR) GO TO 66

C     PRINT MASS FRACTIONS AND REACTION CONVERSION RATES
      WRITE (6,132)
      WRITE (6,152)
  152 FORMAT (50X,16H(MOLE/CM**3/SEC),11X,6HNUMBER,7X,22H(MOLE-CM**3/GM*
     **2/SEC),6X,13HTIVE DIR RATE)
      DO 65 J=1,LR
   65 PRX(J) = XX(J)
      GO TO 67
   66 IF (CONC .OR. (.NOT. EXCHR)) GO TO 69

C     PRINT MASS FRACTIONS AND ENERGY EXCHANGE RATES
      WRITE (6,134)
      WRITE (6,153)
  153 FORMAT (50X,16H(MOLE/CM**3/SEC),11X,6HNUMBER,8X,21H(CAL-CM**3/GM**
     *2/SEC),6X,13HTIVE DIR RATE)

C     COMPUTE MASS FRACTIONS
   67 DO 68 I=1,LS
   68 PRC(I) = SIGMA(I)*WW(I)
      GO TO 74

   69 IF ((.NOT. CONC) .OR. EXCHR) GO TO 71

C     PRINT MOLAR CONCENTRATIONS AND REACTION CONVERSION RATES
      WRITE (6,136)
      WRITE (6,154)
  154 FORMAT (12X,13H(MOLES/CM**3),25X,16H(MOLE/CM**3/SEC),11X,6HNUMBER,
     * 7X,22H(MOLE-CM**3/GM**2/SEC),6X,13HTIVE DIR RATE)
      DO 70 J=1,LR
```

APPENDIX B

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   70 PRX(J) = XX(J)
      GO TO 72

C     PRINT MOLAR CONCENTRATIONS AND ENERGY EXCHANGE RATES
   71 WRITE (6,138)
      WRITE (6,155)
  155 FORMAT (12X,13H(MOLES/CM**3),25X,16H(MOLE/CM**3/SEC),11X,6HNUMBER,
     * 8X,21H(CAL-CM**3/GM**2/SEC),6X,13HTIVE DIR 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)*MIXMW
      WRITE(6,140) SPNM(IJ),PRC(IJ),FMOL,W(IJ),IJ,PRX(IJ),EQUIL(IJ)
      GO TO 77
   75 IF (IJ .GT. LS) GO TO 76
      FMOL = SIGMA(IJ)*MIXMW
      WRITE(6,141) SPNM(IJ),PRC(IJ),FMOL,W(IJ)
      GO TO 77
   76 WRITE (6,142) IJ,PRX(IJ), EQUIL(IJ)
   77 CONTINUE
      GO TO 705
  700 CONTINUE
      WRITE(6,701)
  701 FORMAT(1X,*SPECIES*,4X,*MASS FRACTION*,3X,*MOLE FRACTION*,3X,
     1 *MOLAR CONCENTRATION*,3X,*    SIGMA    *,3X,*NET SPECIES PRODUCTI
     2ON RATE*)
      WRITE(6,702)
  702 FORMAT(47X,*(MOLES/CM--3)*,6X,*(MOL(I)/MASS)*,7X,*(MOLES/CC-SEC)*)
      DO 703 I=1,LS
      FMOL = SIGMA(I)*MIXMW
      PRC(I)=SIGMA(I)*RHO
      PRCF = SIGMA(I)*MW(I)
      WRITE(6,704) SPNM(I),PRCF,FMOL,PRC(I),SIGMA(I),W(I)
  704 FORMAT(2X,A8,2X,E12.5,E16.5,7X,E12.5,7X,E12.5,9X,E12.5)
  703 CONTINUE
      PROD = PRC(1)*PRC(3)
      DCOO = PRC(3)*W(1) + PRC(1)*W(3)
      IF(SPNM(1) .NE. 8HCO       ) GO TO 705
      WRITE(6,706) DCOO
  706 FORMAT(3X,* (O)XC(CO) + (CO)XD(O)       = *,E15.5)
  705 CONTINUE
      WRITE (6,2000) PROD
 2000 FORMAT(/3X,60H PRODUCT OF SPECIES 1 AND SPECIES 3 MOLAR CONCENTRAT
     *IONS  =  1PE12.5/ )
      WRITE (6,143) MIXMW,TXXH,CSUM
      WRITE (6,156)
  156 FORMAT (49X,21H(CAL-CM**3/GM**2/SEC))
      WRITE(6,159) TDERV
  159 FORMAT(/5X,*DTEMP/DIVAR  =*,E16.5)

   78 CONTINUE

   82 IF (ABS(1.-CSUM) .LE. .001) RETURN
      WRITE (6,163)
  163 FORMAT (7HO(OUTP),5X,19HINVALID COMPOSITION)
      NEXT = .TRUE.
      RETURN

      END



      SUBROUTINE DIFFUN(NI,TI,Y,YDOT,IFN,NPEDV,K2)

C     PERFORM ALL NECESSARY PRE-DERIVATIVE CALCULATIONS

      LOGICAL ALLM1,TCON,NEXT,RHOCON
      LOGICAL KTCON
      LOGICAL KUP

      INTEGER STOIC

      REAL IVAR,MDOT,LKEQ,MM,N,M,MIXMW,M2
      DIMENSION Y(NI,K2),YDOT(56)

      COMMON/DERV3/TDERV
      COMMON/STCOM8/TPREV,HN1
      COMMON/STCOM9/VOLD
      COMMON/CONT/KTCON
      COMMON/UPDT/KUP
      COMMON/LTUS/LTHM,LDAT,NTHRD,NBLANK,NPHOTO
      COMMON/OPTS/VERSI,TIMEV,VERSA,AREAV,TCON,RHOCON,IPRCOD
      COMMON/COND/DVAR,AREA,MDOT,P,IVAR,V,RHO,T,SIGMA(25),LS,LSP3,NEXT
      COMMON/SPEC/SNAM(31),MW(25),W(25),STOIC(25,50),OMEGA(25,50)
      COMMON/REAC/LSR(4,50),XX(50),RATE(50),LKEQ(50),DLKEQ(50),MM(50),LR
      COMMON/RRAT/A(50),N(50),EACT(50),B(50),M(25,50),ALLM1
      COMMON/GMSC/GRT(25),HRT(25),SR(25),CPR(25),DCPR(25)
      COMMON/NECC/RR,MIXMW,M2,GAMMA,TCPR,R
      COMMON/STCS/NSTOIC(4,50),EQUIL(50)
      COMMON/SNOB/CXTB(40),CATB(40),NZ
      COMMON/DERN/F(28)
```

APPENDIX B

```
      COMMON/SAPS/S1,S2,AA,BB,DTERM
      EQUIVALENCE (DV,F(1))
      D2ADT2(D2) = V*V*D2 + DV/V*DA
      D2ADX2(D2) = (D2/V - DV*DA)/V

      IPHD = 0
      V=Y(1)
      RHO=Y(2)
      T=Y(3)
      DO 200 I=1,LS
      II=I+3
      SIGMA(I)=Y(II)
  200 CONTINUE
      IF(KTCON) GO TO 400
      ENTRY DIFF1
      IF (TCON) GO TO 5
  400 CONTINUE
      MWARN = 0
C     THERMODYNAMIC PROPERTIES
      CALL THRM (T,1.)

      ALOGRT = ALOG(RR*T)
      DO 4 J=1,LR

C     REACTION RATE CONSTANT
      RATE(J) = A(J)*T**N(J)*EXP(-B(J)/T)

C     LN KEQ  AND  D(LN KEQ)/DT
      DELSTC = 0.
      DELG = 0.
      DELH = 0.
      DO 2 I=1,4
      NN = LSP(I,J)
      IF (NN .GT. LS) GO TO 2
      STOC = NSTOIC(I,J)
      DELSTC = DELSTC + STOC
      DELG = DELG + STOC*GRT(NN)
      DELH = DELH + STOC*HRT(NN)
    2 CONTINUE
      LKEQ(J) = -DELG - DELSTC*ALOGRT
      DLKEQ(J) = (DELH - DELSTC)/T
    4 CONTINUE

C     MIXTURE MOLECULAR WEIGHT
    5 DP1 = 0.
      DO 6 I=1,LS
    6 DP1 = DP1 + SIGMA(I)
      SSUM = DP1
      MIXMW = 1./SSUM

C  *******   UPDATE INDEPENDENT AND DEPENDENT VARIABLES
      IF(KUP) GO TO 600
      IVAR = TT
  600 CONTINUE
      IF(VERSI .EQ. TIMEV) GO TO 700
      X = IVAR
      IF(KTCON) TIME = DVAR
      IF((.NOT. KUP) .AND. (.NOT. KTCON)) TIME=DVAR+2.*(TI-TPREV)/(VOLD+
     1Y(1))
      IF(KUP) TIME = DVAR
      GO TO 701
  700 CONTINUE
      TIME = IVAR
      IF(KTCON) X = DVAR
      IF((.NOT. KUP) .AND. (.NOT. KTCON)) X=DVAR+(TI-TPREV)*(VOLD+Y(1))
     1/2.
      IF(KUP) X = DVAR
  701 CONTINUE
C     ASSIGNED VARIABLE
      IF (IPRCOD .GT. 2) GO TO 7
      CALL CINP(CXTB,CATB,NZ,X,AVAR,DA,D2A)
      GO TO 8
    7 CONTINUE
      CALL CINP(CXTB,CATB,NZ,TIME,AVAR,DA,D2A)

C     CALCULATED VARIABLE
    8 IF (VERSA .EQ. AREAV) GO TO 9
      P = AVAR
      IF (V .NE. 0.) AREA = MDOT/(RHO*V)
      GO TO 10
    9 AREA = AVAR
      P = RHO*RR*T/MIXMW
C     MASS FLOW RATE
      MDOT = RHO*AREA*V
   10 DO 20 J=1,LR
      N1 = LSP(1,J)
      N2 = LSP(2,J)
      N3 = LSP(3,J)
      N4 = LSP(4,J)

      IF (N1 .EQ. NPHOTO) GO TO 15
C     THIRD BODY FACTOR
      MM(J) = 0.
      IF (N1 .NE. NTHRD  .AND.  N4 .NE. NTHRD) GO TO 13
      IF (ALLM1) GO TO 12
      DO 11 I=1,LS
   11 MM(J) = MM(J) + M(I,J)*SIGMA(I)
      GO TO 13
```

APPENDIX B

```
   12 MM(J) = SSUM

   13 IF (LKEQ(J) .GT. 0.) GO TO 14
      EXP3 = EXP(-LKEQ(J)/3.)
      EXP1 = RATE(J)*EXP3
      GO TO 15
   14 EXP1 = EXP(ALOG(RATE(J)) - LKEQ(J))
      EXP3 = 1.

C     NET REACTION CONVERSION RATE
   15 SIGMA1 = 0.
      IF (N1 .LE. LS) SIGMA1 = SIGMA(N1)
      SIGMA4 = 0.
      IF (N4 .LE. LS) SIGMA4 = SIGMA(N4)
      NC = -(NSTOIC(1,J) + NSTOIC(2,J)) - 2
      DP1 = POWER(RHO,NC)*RATE(J)*POWER(SIGMA1,-NSTOIC(1,J))*
     * POWER(SIGMA(N2),-NSTOIC(2,J))
      IF (N1 .EQ. NPHOTO) GO TO 18
      NC = (NSTOIC(3,J) + NSTOIC(4,J)) - 2
      DP2 = EXP3*POWER(RHO,NC)*EXP3*POWER(SIGMA(N3),NSTOIC(3,J))*
     * POWER(SIGMA4,NSTOIC(4,J))*EXP1
      XX(J) = DP1 - DP2
      IF (N1 .EQ. NTHRD  .OR.  N4 .EQ. NTHRD) XX(J) = MM(J)*RHO*XX(J)
      IF( XX(J).NE. 0. ) GO TO  29
      EQUIL(J) = 0.
      GO TO 20
   29 IF(XX(J).LT. 0.)  GO TO 30
      EQUIL(J) = XX(J)/DP1
      IF(N1 .EQ. NTHRD .OR. N4 .EQ. NTHRD) EQUIL(J)=EQUIL(J)/(MM(J)*RHO)
      GO TO 20
   30 EQUIL(J) = ABS(XX(J)/DP2)
      IF(N1 .EQ. NTHRD .OR. N4 .EQ. NTHRD) EQUIL(J)=EQUIL(J)/(MM(J)*RHO)
      GO TO 20
   18 XX(J) = DP1
      EQUIL(J) = 1.0
   20 CONTINUE

      RHO2 = RHO*RHO
      TCPR = 0.
      DO 22 I=1,LS

C     TOTAL CP/R
C     NET SPECIES PRODUCTION RATE
      TCPR = TCPR + CPR(I)*SIGMA(I)
      DP1 = 0.
      DO 21 J=1,LR
      STOC = STOIC(I,J)
      OMEGA(I,J) = RHO2*STOC*XX(J)
   21 DP1 = DP1 + OMEGA(I,J)
      W(I) = DP1
   22 CONTINUE

C     GAMMA (FROZEN)
      GAMMA = TCPR/(TCPR - 1./MIXMW)

C     MACH NUMBER SQUARED
      M2 = V/R*V/T*MIXMW/GAMMA

      IF (VERSA .NE. AREAV  .OR.  (M2 .LT. 0.9025 .OR. M2 .GT. 1.1025))
     * GO TO 23
      WMACH = SQRT(M2)
      WRITE (6,101) WMACH
  101 FORMAT (7HO(PRED),5X,7HWARNING,3X,13HMACH NUMBER =,F8.4,19H IS APP
     *ROACHING 1.0)
      MWARN = MWARN + 1
      IF (MWARN .LT. 5) GO TO 23
      WRITE (6,102)
  102 FORMAT (7HO(PRED),5X,24H5 WARNINGS HAVE OCCURRED)
      NEXT = .TRUE.
      RETURN

   23 CONTINUE
C
C     COMPUTE DERIVATIVES WRT THE INDEPENDENT VARIABLE
C


      DPS1 = 0.
      DPS2 = 0.
      DO 1 I=1,3
      F(I) = 0.
    1 CONTINUE

      DENM = RHO
      IF (VERSI .NE. TIMEV) DENM = RHO*V
      DO 50 I=1,LS

C     DSIGMA/DIVAR
      II = I + 3
      F(II) = W(I)/DENM

C     S1 FOR AA
      DPS1 = DPS1 + F(II)
C     S2 FOR BB
   50 DPS2 = DPS2 + HRT(I)*F(II)

      S1 = MIXMW*DPS1
      S2 = MIXMW*DPS2
```

APPENDIX B

```
      GAM1 = GAMMA - 1.
C     BB EQN DERIVATIVES
      BB = GAM1/GAMMA**2

C     AA EQN DERIVATIVES
      AA = S1 - BB

C     DA/DIVAR
      IF (VERSI .EQ. TIMEV  .AND.  IPRCOD .LE. 2) DA = V*DA
      IF (VERSI .NE. TIMEV  .AND.  IPRCOD .GE. 3) DA = DA/V

      IF(VERSA .NE. AREAV) GO TO 51
C     ASSIGNED AREA EQUATIONS
      ED = GAM1*(S2 - S1)
      IF(RHOCON .AND. V .EQ. 0.  .AND. .NOT. TCON) IRHO = 2
      DTERM = DA/AREA - AA
      T1 = 1./(M2 - 1.)
      T2 = M2*T1

C     DV/DIVAR
      F(1) = V*T1*DTERM

C     DRHO/DIVAR
      IF (.NOT. RHOCON) F(2) = -RHO*(T2*DTERM + AA)

C     DT/DIVAR
      IF (.NOT. TCON) F(3) = -T*(GAM1*T2*DTERM + BB)
      IF(IRHO .EQ. 2) F(3) = -T*ED

C     DAREA/DIVAR WRT IVAR
      IF (VERSI .EQ. TIMEV .AND. (IPRCOD .EQ. 1 .AND. V .NE. 0.)) D2A =
     * D2ADT2(D2A)
      IF (VERSI .NE. TIMEV  .AND.  IPRCOD .EQ. 3) D2A = D2ADX2(D2A)

      T3 = (D2A - DA*DA/AREA)/AREA
      GO TO 52
C     ASSIGNED PRESSURE EQUATIONS
   51 DTERM = DA/P
      T2 = -1./GAMMA

C     DV/DIVAR
      IF (V .NE. 0.) F(1) = -DA/(RHO*V)*1.01325E+06

C     DRHO/DIVAR
      IF (.NOT. RHOCON) F(2) = -RHO*(T2*DTERM + AA)

C     DT/DIVAR
      IF (.NOT. TCON) F(3) = -T*(GAM1*T2*DTERM + BB)

C     DP/DIVAR WRT IVAR
      IF (VERSI .EQ. TIMEV  .AND.  IPRCOD .EQ. 2) D2A = D2ADT2(D2A)
      IF (VERSI .NE. TIMEV  .AND.  IPRCOD .EQ. 4) D2A = D2ADX2(D2A)

      T3 = (D2A - DA*DA/P)/P


   52 CONTINUE
      TDERV = F(3)
      IF(KUP) RETURN
      DO 500 I=1,LSP3
      II=I+IEN
      YDOT(II)=F(I)
  500 CONTINUE

      RETURN
      END


      SUBROUTINE PDERV(NO,TO,Y,BETA,NO,NPEDV,K2)

C     COMPUTE ALL MIXED PARTIAL DERIVATIVES

      LOGICAL TCON,RHOCON

      INTEGER STOIC

      REAL LKEQ,MM,N,M,MIXM4,M2
      REAL MMRHO

      DIMENSION PXXRHO(50),PXXT(50),PXXSIG(50,25),PGSIG(25),PM2SIG(25),
     * PS1SIG(25),PS2SIG(25),PAASIG(25),PBBSIG(25)
      DIMENSION BETA(NPEDV,NPEDV),Y(NO,K2)
      COMMON/SAMS/S1,S2,AA,BB,DTERM
      COMMON/LTUS/LTHM,LDAT,NTHPO,NBLANK,NPHOTO
      COMMON/OPTS/VERSI,TIMEV,VERSA,AREAV,TCON,RHOCON,IPRCOD
      COMMON/COND/IVAR,AREA,MDOT,P,IVAR,V,RHO,T,SIGMA(25),LS,LSP3,NEXT
      COMMON/SPEC/SNAM(31),WW(25),W(25),STOIC(25,50),OMEGA(25,50)
      COMMON/REAC/LSR(4,50),XX(50),RATE(50),LKEQ(50),DLKEQ(50),MM(50),LR
      COMMON/RPAT/A(50),N(50),FACT(50),B(50),M(25,50),ALLM1
      COMMON/GHSC/GRT(25),HRT(25),SR(25),CPR(25),DCPR(25)
      COMMON/MECC/PP,MIXM4,M2,GAMMA,TCPR,R
      COMMON/DERN/F(28)
      COMMON/STCS/NSTOIC(4,50),EQUIL(50)
      V=Y(1)
      RHO=Y(2)
      T=Y(3)
      DO 50 I=1,LS
```

APPENDIX B

```
      II=I+3
      SIGMA(I)=Y(II)
   50 CONTINUE
      DO 1 I=1,LSP3
      DO 1 K=1,LSP3
    1 BETA(I,K) = 0.

      IRHO = 0
      IF(RHOCON .AND. V .EQ. 0.  .AND. .NOT. TCON) IRHO = 2
      DO 2 J=1,LR
      DO 2 I=1,LS
    2 PXXSIG(J,I) = 0.

C     XX(J) WRT RHO,T,SIGMA(I)
      DO 9 J=1,LR
      N1 = LSR(1,J)
      N2 = LSR(2,J)
      N3 = LSR(3,J)
      N4 = LSR(4,J)

      IF (N1 .EQ. NPHOTO) GO TO 7
      IF (LKEQ(J) .GT. 0.) GO TO 3
      EXP3 = EXP(-LKEQ(J)/3.)
      EXP1 = RATE(J)*EXP3
      GO TO 4
    3 EXP1 = EXP(ALOG(RATE(J)) - LKEQ(J))
      EXP3 = 1.

    4 SIGMA1 = 0.
      IF (N1 .LE. LS) SIGMA1 = SIGMA(N1)
      SIGMA4 = 0.
      IF (N4 .LE. LS) SIGMA4 = SIGMA(N4)
      NC1 = -(NSTOIC(1,J) + NSTOIC(2,J)) - 2
      C1 = NC1
      NC2 = (NSTOIC(3,J) + NSTOIC(4,J)) - 2
      C2 = NC2
      PXXRHO(J) = C1*POWER(RHO,NC1-1)*RATE(J)*POWER(SIGMA1,-NSTOIC(1,J))
     * *POWER(SIGMA(N2),-NSTOIC(2,J)) - C2*EXP3*POWER(RHO,NC2-1)*EXP3*
     * POWER(SIGMA(N3),NSTOIC(3,J))*POWER(SIGMA4,NSTOIC(4,J))*EXP1
      PXXT(J) = EXP3*POWER(RHO,NC2)*EXP3*POWER(SIGMA(N3),NSTOIC(3,J))*
     * POWER(SIGMA4,NSTOIC(4,J))*EXP1*DLKEQ(J)
      IF (N1 .LE. LS) PXXSIG(J,N1) = FLOAT(-STOIC(N1,J))*POWER(RHO,NC1)*
     * RATE(J)*POWER(SIGMA1,-NSTOIC(1,J)-1)*POWER(SIGMA(N2),-NSTOIC(2,J)
     * )
      PXXSIG(J,N2) = FLOAT(-STOIC(N2,J))*POWER(RHO,NC1)*RATE(J)*
     * POWER(SIGMA1,-NSTOIC(1,J))*POWER(SIGMA(N2),-NSTOIC(2,J)-1)
      PXXSIG(J,N3) = -FLOAT(STOIC(N3,J))*EXP3*POWER(RHO,NC2)*EXP3*
     * POWER(SIGMA(N3),NSTOIC(3,J)-1)*POWER(SIGMA4,NSTOIC(4,J))*EXP1
      IF (N4 .LE. LS) PXXSIG(J,N4) = -FLOAT(STOIC(N4,J))*EXP3*POWER(RHO,
     * NC2)*EXP3*POWER(SIGMA(N3),NSTOIC(3,J)))*POWER(SIGMA4,
     * NSTOIC(4,J)-1)*EXP1
      IF (N1 .EQ. NTHRD) GO TO 8
      IF (N4 .EQ. NTHRD) GO TO 88
      GO TO 9

    7 NC1 = -NSTOIC(2,J) - 2
      C1 = NC1
      PXXRHO(J) = C1*POWER(RHO,NC1-1)*RATE(J)*POWER(SIGMA(N2),
     * -NSTOIC(2,J))
      PXXT(J) = 0.
      PXXSIG(J,N2) = FLOAT(-STOIC(N2,J))*POWER(RHO,NC1)*RATE(J)*
     * POWER(SIGMA(N2),-NSTOIC(2,J)-1)
      GO TO 9

    8 MMRHO = MM(J)*RHO
      PXXRHO(J) = MMRHO*((C1+1.)*POWER(RHO,NC1-1)*RATE(J)*
     * POWER(SIGMA(N2),-NSTOIC(2,J)) - (C2+1.)*EXP3*POWER(RHO,NC2-1)*
     * EXP3*POWER(SIGMA(N3),NSTOIC(3,J))*POWER(SIGMA4,NSTOIC(4,J))*EXP1)
      PXXT(J) = MMRHO*PXXT(J)
      PXXSIG(J,N2) = MMRHO*PXXSIG(J,N2) + XX(J)/MM(J)*M(N2,J)
      PXXSIG(J,N3) = MMRHO*PXXSIG(J,N3) + XX(J)/MM(J)*M(N3,J)
      IF (N4 .LE. LS  .AND.  N4 .NE. N3) PXXSIG(J,N4) = MMRHO*
     * PXXSIG(J,N4) + XX(J)/MM(J)*M(N4,J)
      GO TO 9

   88 MMRHO = MM(J)*RHO
      PXXRHO(J) = MMRHO*((C1+1.)*POWER(RHO,NC1-1)*RATE(J)*
     * POWER(SIGMA1,-NSTOIC(1,J))*POWER(SIGMA(N2),-NSTOIC(2,J)) -
     * (C2+1.)*EXP3*POWER(RHO,NC2-1)*EXP3*POWER(SIGMA(N3),NSTOIC(3,J))*
     * EXP1)
      PXXT(J) = MMRHO*PXXT(J)
      IF (N1 .LE. LS  .AND.  N1 .NE. N2) PXXSIG(J,N1) = MMRHO*
     * PXXSIG(J,N1) + XX(J)/MM(J)*M(N1,J)
      PXXSIG(J,N2) = MMRHO*PXXSIG(J,N2) + XX(J)/MM(J)*M(N2,J)
      PXXSIG(J,N3) = MMRHO*PXXSIG(J,N3) + XX(J)/MM(J)*M(N3,J)
    9 PXXT(J) = PXXT(J) + XX(J)*(N(J) + B(J)/T)/T

      GTGM1 = GAMMA*(GAMMA - 1.)
      PGAMT = 0.
C     GAMMA WRT SIGMA(I)  AND  MACH NUMBER SQUARED WRT SIGMA(I)
      DO 10 I=1,LS
      PGSIG(I) = GTGM1*(MIXMW - CPR(I))/TCPR)
      PM2SIG(I) = -M2*(MIXMW + PGSIG(I))/GAMMA)
   10 PGAMT = PGAMT + SIGMA(I)*DCPR(I)

C     GAMMA WRT T
      PGAMT = -GTGM1/TCPR*PGAMT

C     MACH NUMBER SQUARED WRT V
      PM2V = 2.*V*MIXMW/(GAMMA*R*T)
```

APPENDIX B

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C     MACH NUMBER SQUARED WRT T
      PM2T = -M2*(1./T + PGAMT/GAMMA)

      TERM = RHO
      IF (VERSI .EQ. TIMEV) GO TO 12
      TERM = RHO/V
C     DSIGMA/DIVAR WRT V
      DO 11 II=4,LSP3
   11 BETA(II,1) = -F(III)/V

C     DSIGMA/DIVAR WRT RHO  AND  DSIGMA/DIVAR WRT T
   12 DO 14 II=4,LSP3
      I = II - 3
      DO 13 J=1,LR
      STOC = STOIC(I,J)
      BETA(II,2) = BETA(II,2) + STOC*PXXRHO(J)
   13 BETA(II,3) = BETA(II,3) + STOC*PXXT(J)
      BETA(II,2) = F(III)/RHO + TERM*BETA(II,2)
   14 BETA(II,3) = TERM*BETA(II,3)

C     DSIGMA(I)/DIVAR WRT SIGMA(K)
      DO 16 II=4,LSP3
      I = II - 3
      DO 16 KK=4,LSP3
      K = KK - 3
      DO 15 J=1,LR
      STOC = STOIC(I,J)
   15 BETA(II,KK) = BETA(II,KK) + STOC*PXXSIG(J,K)
   16 BETA(II,KK) = TERM*BETA(II,KK)

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=4,LSP3
      I = II - 3
      PS1V = PS1V + BETA(II,1)
      PS1RHO = PS1RHO + BETA(II,2)
      PS1T = PS1T + BETA(II,3)
      PS2V = PS2V + HRT(I)*BETA(II,1)
      PS2RHO = PS2RHO + HRT(I)*BETA(II,2)
      PS2T = PS2T + HRT(I)*BETA(II,3) + CPR(I)*F(III)/T
      PS1SIG(I) = 0.
      PS2SIG(I) = 0.
      DO 17 KK=4,LSP3
      K = KK - 3
      PS1SIG(I) = PS1SIG(I) + BETA(KK,II)
   17 PS2SIG(I) = PS2SIG(I) + HRT(K)*BETA(KK,II)
      PS1SIG(I) = MIXMW*(PS1SIG(I) - S1)
   18 PS2SIG(I) = MIXMW*(PS2SIG(I) - S2)
      PS1V = MIXMW*PS1V
      PS1RHO = MIXMW*PS1RHO
      PS1T = MIXMW*PS1T
      PS2V = MIXMW*PS2V
      PS2RHO = MIXMW*PS2RHO
      PS2T = MIXMW*PS2T - S2/T

      GM1DG = (GAMMA - 1.)/GAMMA
      S2DG2 = S2/(GAMMA*GAMMA)
C     BB WRT V
      PBBV = GM1DG*PS2V
C     BB WRT RHO
      PBBRHO = GM1DG*PS2RHO
C     BB WRT T
      PBBT = GM1DG*PS2T + S2DG2*PGAMT

C     AA WRT V
      PAAV = PS1V - PBBV
C     AA WRT RHO
      PAARHO = PS1RHO - PBBRHO
C     AA WRT T
      PAAT = PS1T - PBBT

C     BB WRT SIGMA(I)  AND  AA WRT SIGMA(I)
      DO 19 I=1,LS
      PBBSIG(I) = GM1DG*PS2SIG(I) + S2DG2*PGSIG(I)
   19 PAASIG(I) = PS1SIG(I) - PBBSIG(I)

      IF (VERSA .NE. AREAV) GO TO 24
C    ASSIGNED AREA EQUATIONS
      T1 = 1./(M2 - 1.)
      GAM1 = GAMMA - 1.
C     DV/DIVAR WRT V
      BETA(1,1) = T1*(DTERM - F(1)*PM2V - V*PAAV)
C     DV/DIVAR WRT RHO
      BETA(1,2) = -V*T1*PAARHO
C     DV/DIVAR WRT T
      BETA(1,3) = -T1*(V*PAAT + F(1)*PM2T)
C     DV/DIVAR WRT SIGMA(I)
      DO 20 II=4,LSP3
      I = II - 3
   20 BETA(1,II) = -T1*(V*PAASIG(I) + F(1)*PM2SIG(I))

      IF (RHOCON) GO TO 22
C     DRHO/DIVAR WRT V
```

APPENDIX B

```
      BETA(2,1) = RHO*T1*(PAAV + T1*DTERM*PM2V)
C     DPHO/DIVAR WRT RHO
      BETA(2,2) = RHO*T1*PAARHO + F(2)/RHO
C     DPHO/DIVAR WRT T
      BETA(2,3) = RHO*T1*(PAAT + T1*DTERM*PM2T)
C     DPHO/DIVAR WRT SIGMA(I)
      DO 21 II=4,LSP3
      I = II - 3
   21 BETA(2,II) = RHO*T1*(PAASIG(I) + T1*DTERM*PM2SIG(I))

   22 IF(TCON) GO TO 300
C     DT/DIVAR WRT V
      BETA(3,1) = T*(GAM1*T1*(M2*PAAV + T1*DTERM*PM2V) - PBBV)
C     DT/DIVAR WRT RHO
      BETA(3,2) = T*(GAM1*M2*T1*PAARHO - PBBRHO)
C     DT/DIVAR WRT T
      BETA(3,3) = T*(T1*(GAM1*(M2*PAAT + T1*DTERM*PM2T) - M2*DTERM*PGAMT
     * ) - PBBT) + F(3)/T
      IF(IPHO .EQ. 2) BETA(3,3)=BETA(3,3)+T*GAM1* PAAT +T*AA*PGAMT
C     DT/DIVAR WRT SIGMA(I)
      DO 23 II=4,LSP3
      I = II - 3
      BETA(3,II) = T*(T1*(GAM1*(M2*PAASIG(I) + T1*DTERM*PM2SIG(I)) - M2*
     * DTERM*PGSIG(I)) - PBBSIG(I))
      IF(IPHO.EQ.2)BETA(3,II)=BETA(3,II)+GAM1*T*PAASIG(I)+T*AA*PGSIG(I)
   23 CONTINUE

      GO TO 300
C     ASSIGNED PRESSURE EQUATIONS
   24 T1 = 1./(GAMMA*GAMMA)

C     DV/DIVAR WRT V
      IF (V .NE. 0.) BETA(1,1) = -F(1)/V
C     DV/DIVAR WRT RHO
      BETA(1,2) = -F(1)/RHO
C     DV/DIVAR WRT T
      BETA(1,3) = 0.

C     DV/DIVAR WRT SIGMA(I)
      DO 25 II=4,LSP3
   25 BETA(1,II) = 0.

      IF (PHOCON) GO TO 27
C     DPHO/DIVAR WRT V
      BETA(2,1) = -RHO*PAAV
C     DPHO/DIVAR WRT RHO
      BETA(2,2) = F(2)/RHO - RHO*PAARHO
C     DPHO/DIVAR WRT T
      BETA(2,3) = -RHO*(PAAT + T1*DTERM*PGAMT)
C     DPHO/DIVAR WRT SIGMA(I)
      DO 26 II=4,LSP3
      I = II - 3
   26 BETA(2,II) = -RHO*(PAASIG(I) + T1*DTERM*PGSIG(I))

   27 IF(TCON) GO TO 300
C     DT/DIVAR WRT V
      BETA(3,1) = -T*PBBV
C     DT/DIVAR WRT RHO
      BETA(3,2) = -T*PBBRHO
C     DT/DIVAR WRT T
      BETA(3,3) = BB - T*(PBBT - T1*DTERM*PGAMT) + F(3)/T
C     DT/DIVAR WRT SIGMA(I)
      DO 28 II=4,LSP3
      I = II - 3
   28 BETA(3,II) = -T*(PBBSIG(I) - T1*DTERM*PGSIG(I))
  300 CONTINUE
      RETURN
      END

      FUNCTION POWER (X,N)

C     RAISE X TO THE NTH POWER

C     THIS FUNCTION DEFINES 0**0=1 AND 0**N=0 FOR ALL NON-ZERO N

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

      END

      SUBROUTINE COMB

C     EQUILIBRIUM COMBUSTION CALCULATIONS

      LOGICAL TP,HP
```

APPENDIX B

```
      COMMON/COND/DVAR,AREA,MDOT,P,IVAR,V,RHO,T,SIGMA(25),LS,LSP3,NEXT
      COMMON/SPEC/DUM1(3),SPNM(28),DUM2(25,102)
      COMMON/SPECES/EN(25),ENLN(25),DELN(25),A(15,25)
      COMMON/INDX/TP,HP,DUM3(6)
      COMMON/MISC/TT,PP,CPRO,HRO,ENN,DUM4(32)

      TP = .FALSE.
      HP = .TRUE.

      CALL ELEMNT (LS,SPNM,SIGMA)
      ENI = 0.1/FLOAT(LS)
      ENIL = ALOG(ENI)
      DO 3 I=1,LS
      EN(I) = ENI
    3 ENLN(I) = ENIL
      ENN = 0.1

      TT = 3800.
      PP = P
      CALL EQLBRM

      CALL ECOUT

      RETURN
      END




      SUBROUTINE SHOK

C     EQUILIBRIUM AND FROZEN SHOCK CALCULATIONS

      LOGICAL TP,HP,EQL

      REAL MIXMW

      COMMON/COND/DVAR,AREA,MDOT,P,IVAR,V,RHO,T,SIGMA(25),LS,LSP3,NEXT
      COMMON/NECC/RR,MIXMW,M2,GAMMA,TCPR,R
      COMMON/SPEC/DUM1(3),SPNM(28),DUM2(25,102)
      COMMON/SPECES/EN(25),ENLN(25),DELN(25),A(15,25)
      COMMON/POINTS/DLVTP,DLVPT,GAM,WM
      COMMON/INDX/TP,HP,DUM3(6)
      COMMON/MISC/TT,PP,CPRO,HRO,ENN,DUM4(32)

C     INITIALIZE
      TP = .TRUE.
      HP = .FALSE.

C     EQUILIBRIUM SHOCK
      CALL ELEMNT (LS,SPNM,SIGMA)
      GAM = GAMMA
      ENI = 0.1/FLOAT(LS)
      ENIL = ALOG(ENI)
      DO 2 I=1,LS
      EN(I) = ENI
    2 ENLN(I) = ENIL
      ENN = 0.1
      EQL = .TRUE.
      CALL SHOCKS (EQL)
      CALL ESOUT

C     FROZEN SHOCK
      WM = MIXMW
      DLVTP = 1.
      DLVPT = -1.
      GAM = GAMMA
      DO 3 I=1,LS
    3 EN(I) = SIGMA(I)
      EQL = .FALSE.
      CALL SHOCKS (EQL)
      CALL FSOUT

      RETURN
      END


      SUBROUTINE SHOCKS (EQL)

C     SHOCK EQUATIONS


      LOGICAL EQL,NEXT

      REAL MIXMW,M2

      DIMENSION A(2,3),Y(3)

      COMMON/COND/DVAR,AREA,MDOT,P,IVAR,V,RHO,T,DUM1(25),LS,LSP3,NEXT
      COMMON/NECC/RR,MIXMW,M2,DUM2,TCPR,R
      COMMON/GHSC/GRT(25),HRT(25),SR(25),CPR(25),DCPR(25)
      COMMON/SPECES/SIGMA(25),ENLN(25),DELN(25),AAA(15,25)
      COMMON/POINTS/DLVTP,DLVPT,GAMMA,WM
      COMMON/MISC/TT,PP,CPRO,HRO,DUM3(33)
```

APPENDIX B

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C     INITIAL ESTIMATE OF PRESSURE AND TEMPERATURE RATIOS
      P21 = (2.*GAMMA*M2 - GAMMA + 1.)/(GAMMA + 1.)
      T21 = P21*(2./M2 + GAMMA - 1.)/(GAMMA + 1.)
      IF (EQL  .AND.  T*T21 .GT. 2000.) T21 = 0.7*T21 + 600./T

      CONST = MIXMW*V/R*V/T
      P21L = ALOG(P21)
      T21L = ALOG(T21)

C     ITERATE ON PRESSURE AND TEMPERATURE RATIOS
C    *******      ITERATIONS SET AT 99 ARBITRARILY BY AGM    **************
      DO 4 K=1,99
      IF( K .GT. 8) GO TO 8795
      GO TO 8796
 8795 WRITE (6,8797)  K
 8797 FORMAT(16X,I5,* ............. ITERATIONS .................. *)
 8796 CONTINUE
      PP = P21*P
      TT = T21*T
      IF (EQL) CALL EQLBRM
      CALL THRM (TT,1.)
      IF (NEXT) GO TO 5
      TCPR = 0.
      THR = 0.
      DO 2 I=1,LS
      TCPR = TCPR + CPR(I)*SIGMA(I)
    2 THR = THR + HRT(I)*SIGMA(I)
      THR = THR*TT
      RHO12 = T21/P21*MIXMW/WM

      AA = RHO12*CONST
      A(1,1) = -AA*DLVPT - P21
      A(1,2) = -AA*DLVTP
      A(1,3) = P21 - 1. + CONST*(RHO12 - 1.)
      AA = (V*RHO12)**2/R
      A(2,1) = -AA*DLVPT + TT*(DLVTP - 1.)/WM
      A(2,2) = -AA*DLVTP - TT*TCPR
      A(2,3) = THR - HR0 - V*V*(1. - RHO12*RHO12)/(2.*R)

      Y(3) = A(1,1)*A(2,2) - A(1,2)*A(2,1)
      Y(2) = (A(1,1)*A(2,3) - A(2,1)*A(1,3))/Y(3)
      Y(1) = (A(1,3)*A(2,2) - A(2,3)*A(1,2))/Y(3)

      Y1 = ABS(Y(1))
      Y2 = ABS(Y(2))
      IF (Y2 .GT. Y1) Y1 = Y2
      IF (Y1 .LT. 0.5E-04) RETURN
      Y1 = Y1/0.4054652
      IF (Y1 .LE. 1.) GO TO 3
      Y(1) = Y(1)/Y1
      Y(2) = Y(2)/Y1

    3 P21L = P21L + Y(1)
      T21L = T21L + Y(2)
      P21 = EXP(P21L)
      T21 = EXP(T21L)
    4 CONTINUE

    5 IF (.NOT. EQL) GO TO 6
      WRITE (6,100)
  100 FORMAT (9H0(SHOCKS),5X,36HEQUILIBRIUM SHOCK CALCULATION FAILED)
      NEXT = .FALSE.
      RETURN

    6 WRITE (6,101)
  101 FORMAT (9H0(SHOCKS),5X,31HFROZEN SHOCK CALCULATION FAILED)
      NEXT = .TRUE.
      RETURN

      END

      SUBROUTINE ELEMNT (LS,DSPEC,SIGMA)

C     COLLECT ELEMENT DATA FOR EQUILIBRIUM SHOCK OR COMBUSTION


      DIMENSION DSPEC(25),SIGMA(25),LMT(4),SUBS(4)

      COMMON/LTUS/LTHM,LDAT,NTHRO,NBLANK,NPHOTO
      COMMON/SPECES/EN(25),ENLN(25),DELN(25),A(15,25)
      COMMON/MISC/DUML(7),LLMT(15),BO(15)
      COMMON/INDX/TP,HP,NLM,NS,IQ1,DUM2(3)

      EQUIVALENCE (DSP,SP)

      IF (LS .EQ. NS) GO TO 10

C     CONSTRUCT LIST OF ELEMENTS PRESENT
      READ (LTHM,99) DUMMY
      NSP = NS + 1
    2 READ(LTHM,99) SP,(LMT(K),SUBS(K),K=1,4),DUMM1,DUMM2,DUMM3
   99 FORMAT(A8,16X,4(A2,F3.0)/A1/A1/A1)
      DO 8 I=NSP,LS
      IF (DSPEC(I) .NE. DSP) GO TO 8
      DO 3 L=1,15
    3 A(L,I) = 0.
      IF (NLM .NE. 0) GO TO 4
      NLM = 1
```

APPENDIX B

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      LLMT(NLM) = LMT(I)
    4 DO 6 K=1,4
      IF (SUBS(K) .EQ. 0.) GO TO 7
      DO 5 L=1,NLM
      IF (LLMT(L) .NE. LMT(K)) GO TO 5
      A(L,I) = SUBS(K)
      GO TO 6
    5 CONTINUE
      NLM = NLM + 1
      LLMT(NLM) = LMT(K)
      A(NLM,I) = SUBS(K)
    6 CONTINUE
    7 NS = NS + 1
      IF (NS .LT. LS) GO TO 2
      GO TO 9
    8 CONTINUE
      GO TO 2
    9 REWIND LTHM

C     COMPUTE ELEMENT CONCENTRATION IN GM-ATOMS/GM
   10 DO 11 L=1,NLM
      BO(L) = 0.
      DO 11 I=1,LS
   11 BO(L) = BO(L) + A(L,I)*SIGMA(I)
      IQ1 = NLM + 1

      RETURN
      END



      SUBROUTINE EQLBRM

C     CALCULATE EQUILIBRIUM COMPOSITION AND PROPERTIES


      LOGICAL CONVG,ISING,LOGV,TP,NEXT

      DIMENSION PROW(18)

      COMMON/POINTS/DLVTP,DLVPT,GAMMA,WM
      COMMON/SPECES/EN(25),ENLN(25),OELN(25),A(15,25)
      COMMON/MISC/TT,PP,CPRO,HSUBO,ENN,SUMN,ENNL,LLMT(15),BO(15)
      COMMON/INDX/TP,HP,NLM,NS,IQ1,CONVG,KMAT,IMAT
      COMMON/GHSC/GRT(25),HRT(25),SR(25),CPR(25),DCPR(25)
      COMMON/MATX/G(28,28),X(28)
      COMMON/NECC/DUM1(4),CPSUM,DUM2
      COMMON/COND/DUM3(35),NEXT

C     INITIALIZE
      SMALNO = 1.0E-06
      SMNOL = -13.815511
      SIZE = 18.5
      SIZEF = 0.
      CONVG = .FALSE.
      ISING = .FALSE.
      LOGV = .FALSE.
      ITN = 300
      ITNUMB = ITN
      SUMN=ENN
      IAGM = 0
      TLN = ALOG(TT)
      TM = ALOG(PP/ENN)
      ENNL = ALOG(ENN)
      CALL THRM (TT,1.)
      CPSUM = 0.
      DO 2 I=1,NS

C     BEGIN ITERATION
    2 CPSUM = CPSUM + CPR(I)*EN(I)
   43 CALL MATRIX
      NUMB = ITN- (ITNUMB - 1)
      IAGM = IAGM + 1

      IQ2 = IQ1 + 1
      IF (.NOT. CONVG) GO TO 67
      IF (LOGV) GO TO 63
      DO 182 L=1,NLM
  182 PROW(L) = G(IQ1,L)
      GO TO 72

C     LOGV = .TRUE. --- SET UP MATRIX TO SOLVE FOR DLVPT
   63 G(IQ1,IQ2) = ENN
      IQ = IQ1 - 1
      DO 777 I=1,IQ
  777 G(I,IQ2) = G(I,IQ1)
   72 IMAT = IMAT - 1
   67 ITST = IMAT
      CALL GAUSS
      IF (ITST .NE. IMAT) GO TO 774
      IF (.NOT. CONVG) GO TO 85
      IF (LOGV) GO TO 171
      SUM = 0.
      DO 175 L=1,NLM
  175 SUM = SUM + PROW(L)*X(L)
      DLVTP = 1. + (G(IQ2,IQ1) - SUM)/ENN - X(IQ1)
      CCPR = G(IQ2,IQ2)
      DO 176 I=1,IQ1
```

```
  176 CCPR = CCPR - G(IQ2,I)*X(I)
      LOGV = .TRUE.
      GO TO 43

C     SINGULAR MATRIX
  774 IF (.NOT. CONVG) GO TO 871
      WRITE (6,172)
  172 FORMAT (9HO(EQLBRM),5X,26HDERIVATIVE MATRIX SINGULAR)
      GO TO 1171
  871 WRITE (6,74)
   74 FORMAT (9HO(EQLBRM),5X,15HSINGULAR MATRIX)
      IF (ISING) GO TO 873
      ISING = .TRUE.
      DO 970 I=1,NS
      IF (EN(I) .NE. 0.) GO TO 970
      EN(I) = SMALNO
      ENLN(I) = SMNOL
  970 CONTINUE
      WRITE (6,776)
  776 FORMAT (9HO(EQLBRM),5X,7HRESTART)
      GO TO 43

   85 ITNUMB = ITNUMB - 1
C     OBTAIN CORRECTIONS TO THE ESTIMATES
      IF (TP) X(IQ2) = 0.
      DLNT = X(IQ2)
      SUM = X(IQ1)
      DO 101 I=1,NS
      DELN(I) = HRT(I)*DLNT - HRT(I) + (SR(I) - ENLN(I) - TM) + SUM
      DO 99 L=1,NLM
   99 DELN(I) = DELN(I) + A(L,I)*X(L)
  101 CONTINUE
      AMBDA = 1.
      AMBDA1 = 1.
      SUM = ABS(X(IQ1))
      DO 917 I=1,NS
      IF (EN(I) .GT. 0.  .AND.  DELN(I) .GT. SUM) SUM = DELN(I)
      IF (EN(I) .NE. 0.  .OR.  DELN(I) .LE. 0.) GO TO 917
      SUM1 = (-9.212 - ENLN(I) + ENNL)/(DELN(I) - X(IQ1))
      SUM1 = ABS(SUM1)
      IF (SUM1 .LT. AMBDA1) AMBDA1 = SUM1
  917 CONTINUE
      IF (SUM .GT. 2.) AMBDA = 2./SUM
      IF (AMBDA1 .LT. AMBDA) AMBDA = AMBDA1

C     APPLY CORRECTIONS TO ESTIMATES
      SUM = 0.
      DO 113 I=1,NS
      ENLN(I) = ENLN(I) + AMBDA*DELN(I)
      EN(I) = 0.
      IF ((ENLN(I) - ENNL + SIZE) .LE. 0.) GO TO 113
      EN(I) = EXP(ENLN(I))
      SUM = SUM + EN(I)
  113 CONTINUE
      SUMN = SUM
      IF (TP) GO TO 115
      TLN = TLN + AMBDA*DLNT
      TT = EXP(TLN)
      CALL THRM (TT,1.)
      CPSUM = 0.
      DO 3 I=1,NS
    3 CPSUM = CPSUM + CPR(I)*EN(I)
  115 ENNL = ENNL + AMBDA*X(IQ1)
      ENN = EXP(ENNL)
      TM = ALOG(PP/ENN)

C     TEST FOR CONVERGENCE
      IF (ITNUMB .EQ. 0) GO TO 13
      IF (AMBDA .LT. 1.) GO TO 43
      SUM = (ENN - SUMN)/ENN
      SUM = ABS(SUM)
      IF (SUM .GT. 0.5E-05) GO TO 43
      DO 130 I=1,NS
      AA = ABS(DELN(I)/SUMN)*EN(I)
      IF (AA .GT. 0.5E-05) GO TO 43
  130 CONTINUE

   13 CONVG = .TRUE.
      IF (ITNUMB .NE. 0) GO TO 160
      WRITE (6,973) ITN
  973 FORMAT(9HO(EQLBRM),4X,I3,* ITERATIONS - NO CONVERGENCE*)
      GO TO 873
  160 IF (.NOT. (TP .AND. CONVG)) GO TO 143
      CALL THRM (TT,1.)
      CPSUM = 0.
      DO 4 I=1,NS
    4 CPSUM = CPSUM + CPR(I)*EN(I)
  143 ITNUMB = ITN
      GO TO 43

C     CALCULATE EQUILBRIUM PROPERTIES
 1171 DLVPT = -1.
      DLVTP = 1.
      CCPR = CPSUM
      GO TO 199
  171 SUM = 0.
      DO 179 L=1,NLM
```

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  179 SUM = SUM + PROW(L)*X(L)
      DLVPT = -2. + SUM/ENN + X(IQ1)
  199 GAMMA = -1./(DLVPT + DLVTP*DLVTP*ENN/CCPR)
      WM = 1./ENN
      DO 872 I=1,NS
  872 EN(I) = EXP(ENLN(I))
      RETURN
  873 WRITE (6,900)
  900 FORMAT (9HO(EQLBRM),5X,34HEQUILIBRIUM CALCULATIONS ABANDONED)
      NEXT = .TRUE.
      GO TO 171

      END

      SUBROUTINE SPOUT

C     SPECIAL OUTPUT


      LOGICAL FROZ

      REAL MIXMW,M2,MACHI,MACHF,M21,LSUBM

      COMMON/KOUT/DUM1(21),UNITO,DUM2(52),FPS,SI,DBUGO
      COMMON/COND/DVAR,AREA,MDOT,P,TVAR,V,RHO,T,SIGMA(25),LS,LSP3,NEXT
      COMMON/NECC/RR,MIXMW,M2,GAMMAI,TCPR,R
      COMMON/GHSC/GRT(25),HRT(25),SR(25),CPR(25),DCPR(25)
      COMMON/SPEC/DUM3(3),SPNM(28),DUM4(25,102)
      COMMON/AFUN/CX3,CX2,CX1,CX0,ITPSZ,LSUBM,ETA,D,VISC,BETA
      COMMON/MISC/TF,PF,CPRO,HRO,ENN,DUM5(32)
      COMMON/SPECES/EN(25),ENLN(25),DELN(25),A(15,25)
      COMMON/POINTS/DLVTP,DLVPT,GAMMAF,WM

      ENTRY ECOUT
C     EQUILIBRIUM COMBUSTION OUTPUT
      WRITE(6,101)
  101 FORMAT (1H1,50X,30H**  EQUILIBRIUM COMBUSTION  **)
      VI = 0.
      GO TO 2

      ENTRY ESOUT
C     EQUILIBRIUM SHOCK OUTPUT
      WRITE(6,102)
  102 FORMAT (1H1,47X,37H**  EQUILIBRIUM SHOCK CALCULATION  **)

      VI= V
    2 PI= P
      RHOI= RHO
      TI= T
      P21= PF/PI
      T21 = TF/TI
      RHO21 = P21/T21*WM/MIXMW
      FROZ = .FALSE.
      GO TO 3

      ENTRY FSOUT

C     FROZEN SHOCK OUTPUT
      WRITE(6,103)
  103 FORMAT (1H1,49X,32H**  FROZEN SHOCK CALCULATION  **)
      PI=P
      VI= V
      RHOI= RHO
      TI=T
      P21= PF/PI
      T21 = TF/TI
      RHO21= P21/T21
      P= PF
      V= VI/RHO21
      RHO= RHOI*RHO21
      T= TI*T21
      GAMMAF = TCPR/(TCPR - 1./MIXMW)
      FROZ = .TRUE.

    3 CALL THRM (TI,1.)
      PMLOG = ALOG(PI*MIXMW)
      S=0.
      DO 4 I=1,LS
      IF (SIGMA(I) .EQ. 0.) GO TO 4
      S = S + SIGMA(I)*(SR(I) - ALOG(SIGMA(I)) - PMLOG)
    4 CONTINUE
      S = S*1.987165
      MACHI= SQRT(M2)

      VF = VI/RHO21
      RHOF= RHOI*RHO21
      CALL THRM (TF,1.)
      PMLOG = ALOG(PF*WM)
      SF= 0.
      DO 5 I=1,LS
      IF(EN(I) .EQ. 0.) GO TO 5
      SF = SF + EN(I)*(SR(I) - ALOG(EN(I)) - PMLOG)
    5 CONTINUE
      SF = SF*1.987165
      MACHF= SQRT(VF/R*VF/TF*WM/GAMMAF)

      S21= SF/S
      G21= GAMMAF/GAMMAI
```

APPENDIX B

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      IF (VI .EQ. 0.) GO TO 205
      SVI= VI/MACHI
      SVF= VF/MACHF
      V21= VF/VI
      M21= MACHF/MACHI
      SV21= SVF/SVI
      GO TO 305

  205 MACHI = 0.
      SVI = 0.
      SVF = 0.
      V21 = 0.
      M21 = 0.
      SV21 = 0.

  305 IF (.NOT. FROZ  .OR.  ITPSZ .NE. 4) GO TO 405
C     CALCULATE L(M) FOR KINETIC AREA FUNCTION
      PST = 1.
      ROSVST = (GAMMAI/SVI)*1.01325E+06
      LSUBM = (1./PF)*(RHO21/(RHO21-1.))*(ROSVST/(PST*VISC)*MACHI)**((1.
     *-ETA)/ETA)*(3*PI/(4.*BETA))**(1./ETA)

  405 WRITE (6,104)
  104 FORMAT (/41X,13HINITIAL STATE,17X,11HFINAL STATE,17X,19HFINAL/INIT
     *IAL RATIO//)

      IF(UNITO .NE. FPS) GO TO 6
C     CONVERT FROM INTERNAL (CGS) UNITS TO FPS UNITS
      PI= PI*2116.2
      PF= PF*2116.2
      VI= VI/30.48
      VF= VF/30.48
      RHOI= RHOI*62.43
      RHOF= RHOF*62.43
      TI= TI*1.8
      TF= TF*1.8
      SVI= SVI/30.48
      SVF= SVF/30.48
      WRITE(6,105) PI,PF,P21,VI,VF,V21,RHOI,RHOF,RHO21,TI,TF,T21,S,SF,
     * S21,MACHI,MACHF,M21,GAMMAI,GAMMAF,G21,SVI,SVF,SV21
  105 FORMAT (10X,8HPRESSURE,1PE35.5,E29.5,E32.5/11X,10H(LB/FT**2)/10X,
     * 8HVELOCITY,E35.5,E29.5,E32.5/11X,8H(FT/SEC)/10X,7HDENSITY,E36.5,
     * E29.5,E32.5/11X,10H(LB/FT**3)/10X,11HTEMPERATURE,E32.5,E29.5,
     * E32.5/11X,7H(DEG R)/10X,7HENTROPY,E36.5,E29.5,E32.5/11X,14H(BTU/L

     *B/DEG R)/10X,11HMACH NUMBER,E32.5,E29.5,E32.5//10X,5HGAMMA,E38.5,
     * E29.5,E32.5//10X,14HSONIC VELOCITY,E29.5,E29.5,E32.5/11X,8H(FT/SE
     *C))
      GO TO 8

    6 IF (UNITO .NE. SI) GO TO 7
C     CONVERT FROM INTERNAL (CGS) UNITS TO SI UNITS
      PI= PI*1.01325E+05
      PF= PF*1.01325E+05
      VI= VI*0.01
      VF= VF*0.01
      RHOI= RHOI*1000.
      RHOF= RHOF*1000.
      S= S*4184.0
      SF= SF*4184.0
      SVI= SVI*0.01
      SVF= SVF*0.01
      WRITE(6,106) PI,PF,P21,VI,VF,V21,RHOI,RHOF,RHO21,TI,TF,T21,S,SF,
     * S21,MACHI,MACHF,M21,GAMMAI,GAMMAF,G21,SVI,SVF,SV21
  106 FORMAT (10X,8HPRESSURE,1PE35.5,E29.5,E32.5/11X,8H(N/M**2)/10X,8HVE
     *LOCITY,E35.5,E29.5,E32.5/11X,7H(M/SEC)/10X,7HDENSITY,E36.5,E29.5,
     * E32.5/11X,9H(KG/M**2)/10X,11HTEMPERATURE,E32.5,E29.5,E32.5/11X,
     * 7H(DEG K)/10X,7HENTROPY,E36.5,E29.5,E32.5/11X,16H(JOULE/KG/DEG K)
     */10X,11HMACH NUMBER,E32.5,E29.5,E32.5//10X,5HGAMMA,E38.5,E29.5,
     * E32.5//10X,14HSONIC VELOCITY,E29.5,E29.5,E32.5/11X,7H(M/SEC))
      GO TO 8

C     PRINT OUTPUT IN INTERNAL (CGS) UNITS
    7 WRITE(6,107) PI,PF,P21,VI,VF,V21,RHOI,RHOF,RHO21,TI,TF,T21,S,SF,
     * S21,MACHI,MACHF,M21,GAMMAI,GAMMAF,G21,SVI,SVF,SV21
  107 FORMAT (10X,8HPRESSURE,F35.4,F28.4,F32.4/11X,5H(ATM)/10X,8HVELOCIT
     *Y,F33.2,F28.2,F34.4/11X,8H(CM/SEC)/10X,7HDENSITY,1PE36.5,E28.5,
     * 0PF32.4/11X,10H(GM/CM**3)/10X,11HTEMPERATURE,F30.2,F28.2,F34.4/
     * 11X,7H(DEG K)/10X,7HENTROPY,F36.4,F28.4,F32.4/11X,14H(CAL/GM/DEG
     *K)/10X,11HMACH NUMBER,F32.4,F28.4,F32.4//10X,5HGAMMA,F38.4,F28.4,
     * F32.4//10X,14HSONIC VELOCITY,F27.2,F28.2,F34.4/11X,8H(CM/SEC))

    8 WRITE (6,108)
  108 FORMAT (/67X,7HSPECIES,5X,13HMOLE FRACTION)
      DO 9 I=1,LS
      EN(I) = EN(I)*WM
      WRITE(6,109) SPNM(I),EN(I)
  109 FORMAT(68X,A8,E15.5)
    9 CONTINUE
      WRITE(6,110) WM,DLVTP,DLVPT
  110 FORMAT (/10X,24HMIXTURE MOLECULAR WEIGHT,36X,F12.5//10X,22HD(LOG V
     *OLUME)/D(LOG T),E49.4/14X,*AT CONSTANT P*//10X,*D(LOG VOLUME)/D(LO
     *G P)*,E49.4/14X,*AT CONSTANT T*)

      RETURN
      END
```

APPENDIX B

```
      SUBROUTINE MATRIX


      LOGICAL TP,HP,CONVG

      COMMON/SPECES/EN(25),ENLN(25),DELN(25),A(15,25)
      COMMON/MISC/TT,PP,CPRO,HSUBO,ENN,SUMN,ENNL,LLMT(15),BO(15)
      COMMON/INDX/TP,HP, L ,NS,IQ1,CONVG,KMAT,IMAT
      COMMON/GHSC/GRT(25),HRT(25),SR(25),CPR(25),DCPR(25)
      COMMON/MATX/G(28,28),X(28)
      COMMON/NECC/DUM1(4),CPSUM,DUM2


      IQ2 = IQ1 + L
      IQ3 = IQ2 + 1
      KMAT = IQ3
      IF(.NOT.CONVG.AND.TP) KMAT = IQ2
      IMAT = KMAT - 1

C     CLEAR MATRIX STORAGES TO ZERO

      DO 211 I=1,KMAT
      DO 211 K=1,KMAT
      G(I,K) = 0.
  211 CONTINUE
      SSS = 0.
      HSUM = 0.

C     BEGIN SET UP OF ITERATION MATRIX

      KK = L
      TM = ALOG(PP/ENN)
      DO 65  J=1,NS
      H = HRT(J)*EN(J)
      F = (HRT(J) - SR(J) + ENLN(J) + TM)*EN(J)
      SS = H-F
      TERM1 = H
      IF (KMAT .EQ. IQ2) TERM1 = F
      DO 55 I = 1, L

C     CALCULATE THE ELEMENTS  R(I,K)

      IF (A(I,J) .EQ. 0.) GO TO 55
      TERM = A(I,J)*EN(J)
      DO 15  K=I, L
      G(I,K)= G(I,K) + A(K,J)*TERM
   15 CONTINUE

      G(I,IQ1)=G(I,IQ1)+TERM
      G(I,IQ2)=G(I,IQ2)+A(I,J)*TERM1
      IF (CONVG .OR.TP) GO TO 55
      G(I,IQ3)= G(I,IQ3)+A(I,J)*F
   55 CONTINUE
      IF (KMAT .EQ. IQ2) GO TO 64
      IF(CONVG.OR.HP) GO TO 59
      G(IQ2,IQ1) = G(IQ2,IQ1) + SS
      G(IQ2,IQ2) = G(IQ2,IQ2) + HRT(J)*SS
      G(IQ2,IQ3) = G(IQ2,IQ3) + (SR(J) - ENLN(J) - TM)*F
      GO TO 62
   59 G(IQ2,IQ2) = G(IQ2,IQ2) + HRT(J)*H
      IF (CONVG) GO TO 64
      G(IQ2,IQ3) = G(IQ2,IQ3) + HRT(J)*F
   62 G(IQ1,IQ3)=G(IQ1,IQ3)+F
   64 G(IQ1,IQ2)=G(IQ1,IQ2)+TERM1
   65 CONTINUE
      SSS = SSS + G(IQ2,IQ1)
      HSUM = HSUM + G(IQ1,IQ2)
      G(IQ1,IQ1) = SUMN - ENN

C     REFLECT SYMMETRIC PORTIONS OF THE MATRIX

      ISYM = IQ1
      IF(HP.OR.CONVG)ISYM=IQ2
      DO 102 I=1,ISYM
      DO 102 J=I,ISYM
      G(J,I)=G(I,J)
  102 CONTINUE

C     COMPLETE THE RIGHT HAND SIDE

      IF(CONVG)  GO TO 175
      DO 145 I=1,L
  145 G(I,KMAT) = G(I,KMAT) + BO(I) - G(I,IQ1)
      G(IQ1,KMAT) = G(IQ1,KMAT)+ENN-SUMN
C     COMPLETE ENERGY ROW AND TEMPERATURE COLUMN

      IF (KMAT .EQ. IQ2) RETURN
      IF (HP) ENERGY = HSUBO/TT - HSUM
      G(IQ2,IQ3)=G(IQ2,IQ3)+ ENERGY
  175 G(IQ2,IQ2)= G(IQ2,IQ2)+CPSUM

      RETURN
      END
```

APPENDIX B

```
      SUBROUTINE GAUSS

C     SOLVE ANY LINEAR SET OF UP TO 20 EQUATIONS

      DIMENSION COEFX(28)
      COMMON/MATX/G(28,28),X(28)

      COMMON/INDX/TP,HP,NLM,NS,IQ1,CONVG,KMAT,IUSE
      DATA BIGNO/1.E+38/

C     BEGIN ELIMINATION OF NNTH VARIABLE

      IUSE1=IUSE+1
    6 DO 45 NN=1,IUSE
      IF (NN-IUSE) 8,83,8
   83 IF(G(NN,NN))31,23,31

C     SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW

    8 DO 18 I=NN,IUSE
      COEFX(I) = BIGNO
      IF(G(I,NN).EQ.0.)  GO TO 18
      COEFX(I) = 0.
      DO 10 J=NN,IUSE1
      SUM = G(I,J)
      IF(SUM.LT.0.)  SUM=-SUM
      IF(J.NE.NN)  GO TO 9
      Z = SUM
      GO TO 10
    9 IF(SUM.GT.COEFX(I))  COEFX(I)=SUM
   10 CONTINUE
      COEFX(I) = COEFX(I)/Z
   18 CONTINUE
      TEMP = BIGNO
      I=0
   20 DO 22 J=NN,IUSE
      IF (COEFX(J)-TEMP) 87,22,22
   87 TEMP=COEFX(J)
      I=J
   22 CONTINUE
      IF(I) 28,23,28

C     INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH
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(I,J)
      G(I,J)=G(NN,J)
      G(NN,J)=Z
   30 CONTINUE

C     DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH
C     VARIABLE FROM THE REMAINING EQUATIONS

   31 K = NN + 1
      DO 36 J = K, IUSE1
      IF(G(NN,NN).EQ.0.)  GO TO 23
      G(NN,J) = G(NN,J)/G(NN,NN)
   36 CONTINUE
      IF(K-IUSE1) 88,45,88
   88 DO 44 I = K,IUSE
   40 DO 44 J = K, IUSE1
      G(I,J) = G(I,J) - G(I,NN)*G(NN,J)
   44 CONTINUE
   45 CONTINUE

C     BACKSOLVE FOR THE VARIABLES

      K = IUSE
   47 J = K + 1
      X(K) = 0.
      SUM = 0.0
      IF(IUSE - J) 51,48,48
   48 DO 50 I = J,IUSE
      SUM = SUM + G(K,I)*X(I)
   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,NQ,K2)
C *****       PRINT OUT INFORMATION
C
C   IN NAMELIST PROB THE PRINTING VARIABLES ARE
C
C    1 PAPS - SET TRUE IF PRINTING AT SPECIFIC STATIONS DESIRED
C    2 TPRINT - A TABLE OF PRINT STATIONS INPUT 50 VALUES AT MOST
C    3 NPRIN - THE NUMBER OF PRINT STATIONS
```

APPENDIX B

```
C     4 IDEL - INCREMENT FOR AUTOMATIC CALCULATION OF AT MOST 50 PRINT
C              STATIONS.  IDEL NOT INPUT - A TABLE OF TPRINTS MUST BE
C              INPUT IF PAPS = TRUE
C     IF PAPS = FALSE IPRIT INPUT WILL CAUSE PRINTING EVERY IPRIT
C             ITERATIONS
C     END MUST ALWAYS BE SPECIFIED
C  ********************************************************************
      LOGICAL KUP
      LOGICAL TCON,RHOCON
      LOGICAL DVUDT
      REAL IVAR
      DIMENSION Y(NO,K2),YPRINT(28)
      COMMON/PRIN/TPRINT(50),NPRIN,NCO
      COMMON/STCOM1/N,T,H,HMIN,HMAX,EPS1,MF1,KFLAG1,JSTART
      COMMON/COND/DVAR,AREA,MDOT,P,IVAR,V,RHO,Z,SIGMA(25),LS,LSP3,DUM1
      COMMON/UPDT/KUP
      COMMON/STCOM8/TPREV,HN1
      COMMON/STCOM9/VOLD
      COMMON/OPTS/VERSI,TIMEV,DUM2(2),TCON,RHOCON,DUM3
      DVUDT = .FALSE.
      IF(NCO .EQ. 1) GO TO 11
      INT=1
      NCO=1
   11 CONTINUE
      IF((T-H).LT. TPRINT(INT) .AND. TPRINT(INT).LE. T) GO TO 10
      IF(DVUDT) GO TO 13
      ENTRY YOUT1
      IF(RHOCON) GO TO 16
      IF(VERSI .EQ. TIMEV) GO TO 12
      DVAR = DVAR + 2.*(T - TPREV)/(VOLD + Y(1))
      GO TO 16
   12 CONTINUE
      DVAR = DVAR + (T - TPREV)*(VOLD + Y(1))/2.
      GO TO 16

   13 CONTINUE
      IF(RHOCON) GO TO 16
      IF(VERSI .EQ. TIMEV) GO TO 17
      DVAR = DVAR + (T - IVAR)*2./(VOLD + Y(1))
      GO TO 16
   17 CONTINUE
      DVAR = DVAR + (T - IVAR)*((VOLD + Y(1))/2.)
   16 CONTINUE
      RETURN
   10 CONTINUE
      IF(TPRINT(INT) .EQ. T) GO TO 300
      S = (TPRINT(INT) - T)/H
      DO 1 I=1,N
      YPRINT(I) = Y(I)
    1 CONTINUE
      P=1.
      L= NO + 1
      DO 3 J=2,L
      P = P*S
      DO 2 I=1,N
      YPRINT(I) = YPRINT(I) + Y(I,J)*P
    2 CONTINUE
    3 CONTINUE
      V = YPRINT(1)
      RHO = YPRINT(2)
      Z = YPRINT(3)
      DO 200 I=1,LS
      II = I+3
      SIGMA(I) = YPRINT(II)
  200 CONTINUE
      IF(RHOCON) GO TO 15
      IF(VERSI .EQ. TIMEV) GO TO 14
      HOLD1 = TPRINT(INT) - TPREV
      IF(DVUDT) HOLD1 = TPRINT(INT) - IVAR
      DVAR = DVAR + 2.*HOLD1/(V + VOLD)
      GO TO 15
   14 CONTINUE
      HOLD1 = TPRINT(INT) - TPREV
      IF(DVUDT) HOLD1 = TPRINT(INT) - IVAR
      DVAR = DVAR + HOLD1*(V + VOLD)/2.
   15 CONTINUE
      DVUDT = .TRUE.
      VOLD = V
      IVAR = TPRINT(INT)
      KUP =.TRUE.
      CALL DIFF1
      KUP =.FALSE.
      GO TO 400
  300 CONTINUE
      IF(RHOCON) GO TO 400
      IF(VERSI .EQ. TIMEV) GO TO 301
      DVAR = DVAR + 2.*(T - TPREV)/(VOLD + Y(1))
      GO TO 400
  301 DVAR = DVAR + (T - TPREV)*(VOLD + Y(1))/2.
  400 CONTINUE
      CALL OUT3
      INT = INT + 1
      IF(INT .LE. NPRIN) GO TO 11
      RETURN
      END
```

```
      SUBROUTINE YOUTD (Y,NQ)
      DIMENSION Y(28,6)
      WRITE(6,7)
    7 FORMAT(5X,*KFLAG NOT EQUAL TO 0*)
      RETURN
      END



      SUBROUTINE DRIVES(NO,TO,TLAST,Y,HO,EPS,MF,KFLAG,K2)
      LOGICAL PAPS
      COMMON/STCOM1/N,T,H,HMIN,HMAX,EPS1,MF1,KFLAG1,JSTART
      COMMON/STCOM8/TPREV,HN1
      COMMON/STCOM2/YMAX(28)
      COMMON/STCOM3/ERROR(28)
      COMMON/STCOM5/FSAVE(56)
      COMMON/STCOM6/IPRIT,PAPS
      DIMENSION Y(NO,K2),YDOT(56),TNIS4(812)
      DO 9999 I=1,812
      TNIS4(I)=0.
 9999 CONTINUE
      LOUT=6
      IF (EPS.LE.0.) GO TO 400
      IF (NO.LE.0) GO TO 410
      IF((TO-TLAST)*HO.GE.0.) GO TO 420
      N = NO
      T = TO
      H = HO
      HMIN = ABS(HO)
      HMIN = AMIN1(HMIN,.1*HMAX)
      EPS1 = EPS
      MF1 = MF
      JSTART = 0
      KHFLAG = 0
C
      NCOUNT=0
      NIS4 = NO*(NO+1)
   10 CONTINUE
      HN1 = H
      TPREV = T
      CALL STIFF(Y,NO,TNIS4,NIS4,K2)
      NQ = JSTART
C
      KGO = 1 - KFLAG1
      GO TO ( 20,100,200,300),KGO
C  KFLAG1 =   0, -1, -2, -3
C
 20   CONTINUE
      IF(PAPS) GO TO 9998
      CALL YOUT1
      NCOUNT = NCOUNT + 1
      IF(NCOUNT .NE. IPRIT) GO TO 888
      CALL OUT3
      NCOUNT = 0
  888 CONTINUE
      GO TO 9997
 9998 CONTINUE
      CALL YOUT(NO,TLAST,Y,NQ,K2)
 9997 CONTINUE
      IF ((T-TLAST)*H.LT.0.) GO TO 10
C*********************************************************************
C* THE PROBLEM IS FINISHED.  HERE CALL YOUT AND/OR OTHER ROUTINES
C* TO OUTPUT DESIRED FINAL RESULTS.
C*********************************************************************
      CALL OUT3
      GO TO 500
C
 100  WRITE (LOUT,105) T
 105  FORMAT(//30H KFLAG = -1 FROM STIFF AT T = ,E16.8/
     1   38H  ERROR TEST FAILED WITH ABS(H) = HMIN/)
 110  IF (KHFLAG.EQ.10) GO TO 150
      KHFLAG = KHFLAG + 1
      HMIN = HMIN*.1
      H = H*.1
      WRITE (LOUT,115) H
 115  FORMAT(24H  H HAS BEEN REDUCED TO ,E16.8,
     1   26H  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* HMIN HAS BEEN CUT BY 10 ORDERS OF MAGNITUDE WITH NO SUCCESS.
C* AT THIS POINT, OUTPUT INFORMATION NEEDED FOR DEBUGGING.
C*********************************************************************
      CALL YOUTD(Y,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 YOUTD(Y,NQ)

      GO TO 500
C
```

```
 300  WRITE (LOUT,305) T
 305  FORMAT(//30H KFLAG = -3 FROM STIFF AT T = ,E16.8/
     1   45H  CORRECTOR CONVERGENCE COULD NOT BE ACHIEVED/)
      GO TO 110
C
 400  WRITE (LOUT,405)
 405  FORMAT(//26H ILLEGAL INPUT.. EPS.LE.0.//)
      KFLAG = -4
      RETURN
C
 410  WRITE (LOUT,415)
 415  FORMAT(//23H ILLEGAL INPUT.. N.LE.0//)
      KFLAG = -4
      RETURN
C
 420  WRITE (LOUT,425)
 425  FORMAT(//38H ILLEGAL INPUT.. (TO-TLAST)*HO .GE. 0.//)
      KFLAG = -4
      RETURN
C
 500  KFLAG = KFLAG1
      TO = T
      HO = H
      RETURN
C*********************** END OF DRIVES *********************************
      END



      SUBROUTINE STIFF(Y,NO,PW,NIS4,K2)
      DIMENSION PW(NIS4),Y(NO,K2),EL(13),TQ(4)
      COMMON/STCOM1/N,T,H,HMIN,HMAX,EPS,MF,KFLAG,JSTART
      COMMON/STCOM9/VOLD
      COMMON/STCOM2/YMAX(28)
      COMMON/STCOM3/ERROR(28)
      COMMON/STCOM5/FSAVE(56)
      DATA (ANOISE = 1.E-14)
      VOLD = Y(1)
      NPEDV = NO
      KFLAG = 0
      TOLD = T
      IF (JSTART.GT.0) GO TO 200
      IF (JSTART.NE.0) GO TO 120
C***********************************************************************
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.E4 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.
C***********************************************************************
      NSQ = NO*NO
      NSQ1 = NSQ + 1
      NI = NO + 1
      CALL DIFFUN(N,T,Y,FSAVE,0,NPEDV,K2)
      DO 110 I = 1,N
        Y(I,2) = FSAVE(I)*H
        AYI = ABS(Y(I))
        IF (AYI.EQ.0.) AYI = ABS(Y(I,2))
        IF (AYI.EQ.0.) AYI = 1.
 110    YMAX(I) = AYI
      NQ = 1
      L = 2
      RMAX = 1.E4
      EPSJ = SQRT(ANOISE)
      CRATE = 1.
      OLDLO = 1.
      RC = 0.

      MFOLD = 0
      METH = 0
      MITER = 0
      HOLD = H
C***********************************************************************
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 NQ. 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 H 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(0)*H.
C* WHEN RC DIFFERS FROM 1 BY MORE THAN 30 PERCENT, OR THE CALLER HAS
C* CHANGED MITER, IWEVAL IS SET TO MITER TO FORCE THE PARTIALS TO BE
C* UPDATED, IF PARTIALS ARE USED.
C***********************************************************************
 120  IF (MF.EQ.MFOLD) GO TO 150
      MEO = METH
      MIO = MITER
      METH = MF/10
      MITER = MF - 10*METH
      MFOLD = MF
```

```
      IF (MITER.NE.MIO) IWEVAL = MITER
      IF (METH.EQ.MEO) GO TO 150
      IDOUB = L + 1
      IRET = 1
  130 CALL COSET(METH,NQ,EL,TQ,MAXDER)
      RC = RC*EL(1)/OLDLO
      OLDLO = EL(1)
  140 EDN = (TQ(1)*EPS)**2
      E   = (TQ(2)*EPS)**2
      EUP = (TQ(3)*EPS)**2
      BND = (TQ(4)*EPS)**2
      GO TO ( 160 , 170 , 200 ), IRET
  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
      RH = H/HOLD
      H = HOLD
  170 RH = AMAX1(RH,HMIN/ABS(H))
      RH = AMIN1(RH,HMAX/ABS(H),RMAX)
      R1 = 1.
      DO 180 J = 2,L
        R1 = R1*RH
        DO 180 I = 1,N
  180     Y(I,J) = Y(I,J)*R1
      H = H*RH
      RC = RC*RH
      IDOUB = L + 1
      IF (T.NE.TOLD) GO TO 690
C*********************************************************************
C* THIS SECTION COMPUTES THE PREDICTED VALUES BY EFFECTIVELY
C* MULTIPLYING THE Y ARRAY BY THE PASCAL TRIANGLE MATRIX.
C*********************************************************************
  200 IF(ABS(RC-1.).GT.0.3) IWEVAL = MITER
      T = T + H
      DO 210 J1 = 1,NQ
        DO 210 J2 = J1,NQ
          J = NQ - J2 + J1
          DO 210 I = 1,N
  210       Y(I,J) = Y(I,J) + Y(I,J+1)
C*********************************************************************
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 ERROR(I).  IT IS APPROXIMATELY EQUAL TO THE L-TH
C* DERIVATIVE OF Y MULTIPLIED BY H**L/(FACTORIAL(L-1)*EL(L)), AND IS
C* THUS 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* Y VECTOR IS STORED TEMPORARILY IN FSAVE.  THE NORM OF THE
C* ITERATE DIFFERENCE IS STORED IN D.
C*********************************************************************
  220 DO 230 I = 1,N
  230   ERROR(I) = 0.
      M = 0
      CALL DIFFUN(N,T,Y,FSAVE,N,NPEDV,K2)
      IF (IWEVAL.LE.0) GO TO 340
C*********************************************************************
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 MITER = 1 OR 2, THE MATRIX  P = I - L(0)*H*JACOBIAN  IS STORED
C* IN PW AND SUBJECTED TO LU DECOMPOSITION, WITH THE RESULTS ALSO
C* STORED IN PW.  IF MITER = 3, THE MATRIX USED IS  P = I - L(0)*H*D,
C* WHERE D IS A DIAGONAL MATRIX.
C*********************************************************************
      GO TO ( 240 , 260 , 310 ),MITER
  240 CALL PEDERV(N,T,Y,PW,NO,NPEDV,K2)
      R = -EL(1)*H
      DO 250 I = 1,NSQ
  250   PW(I) = PW(I)*R
      GO TO 300
  260 D = 0.
      DO 270 I = 1,N
  270   D = D + FSAVE(I+NO)**2
      RO = ABS(H)*SQRT(D)*1.E03*ANOISE
      J1 = -NO
      DO 290 J = 1,N
        J1 = J1 + NO
        YJ = Y(J)
        R = EPSJ*YMAX(J)
        R = AMAX1(R,RO)
        Y(J) = Y(J) + R
        D = -EL(1)*H/R
      CALL DIFFUN(N,T,Y,FSAVE,0,NPEDV,K2)
        DO 280 I = 1,N
  280     PW(I+J1) = (FSAVE(I) - FSAVE(I+NO))*D
  290   Y(J) = YJ
  300 DO 305 I = 1,N
  305   PW(I*N1-NO) = PW(I*N1-NO) + 1.
      IWEVAL = 0
      RC = 1.
      CALL DECOMP(NO,N,PW,PW(NSQ1),FSAVE,IER)
      IF (IER.NE.0) GO TO 420
      GO TO 360
```

```
 310  R = EL(1)*.1
      DO 320 I = 1,N
 320    PW(I) = Y(I) + R*(FSAVE(I+NO)*H - Y(I,2))
      CALL DIFFUN(N,T,PW,FSAVE,0,NPEDV,K2)
      DO 330 I = 1,N
        RO = PW(I) - Y(I)
        PW(I) = 1.
C*********************************************************************
 410  IF (M.NE.0) CRATE = AMAX1(.9*CRATE,D/D1)
      IF ((D*AMIN1(1.,2.*CRATE)).LE.BND) GO TO 450
      D1 = D
      M = M + 1
      IF (M.EQ.3) GO TO 420
      CALL DIFFUN(N,T,FSAVE,FSAVE,N,NPEDV,K2)
      GO TO 340
C*********************************************************************
C* THE CORRECTOR ITERATION FAILED TO CONVERGE IN 3 TRIES.  IF PARTIALS
C* ARE INVOLVED BUT ARE NOT UP TO DATE, THEY ARE REEVALUATED FOR THE
C* NEXT TRY.  OTHERWISE THE Y ARRAY IS RETRACTED TO ITS VALUES
C* BEFORE PREDICTION, AND H IS REDUCED, IF POSSIBLE.  IF NOT, A
C* NO-CONVERGENCE EXIT IS TAKEN.
C*********************************************************************
 420  IF (IWEVAL.EQ.-1) GO TO 440
      T = TOLD
      RMAX = 2.
      DO 430 J1 = 1,NQ
        DO 430 J2 = J1,NQ
          J = NQ - J2 + J1
          DO 430 I = 1,N
 430        Y(I,J) = Y(I,J) - Y(I,J+1)
      IF (ABS(H).LE.(HMIN*1.00001)) GO TO 680
      RH = .25
      GO TO 170
 440  IWEVAL = MITER
      GO TO 220
C*********************************************************************
C* THE CORRECTOR HAS CONVERGED.  IWEVAL IS SET TO -1 IF PARTIAL
C* DERIVATIVES WERE USED, TO SIGNAL THAT THEY MAY NEED UPDATING ON
C* SUBSEQUENT STEPS.  THE ERROR TEST IS MADE AND CONTROL PASSES TO
C* STATEMENT 500 IF IT FAILS.
C*********************************************************************
 450  D = 0.
      DO 460 I = 1,N
 460    D = D + (ERROR(I)/YMAX(I))**2
      IF (MITER.NE.0) IWEVAL = -1
      IF (D.GT.E) GO TO 500
C*********************************************************************
C* AFTER A SUCCESSFUL STEP, UPDATE THE Y ARRAY AND YMAX.
C* CONSIDER CHANGING H IF IDOUB = 1.  OTHERWISE DECREASE IDOUB BY 1.
C* IF IDOUB IS THEN 1 AND NQ .LT. MAXDER, THEN ERROR IS SAVED FOR

        D = RO - EL(1)*H*(FSAVE(I) - FSAVE(NO+I))
        FSAVE(I) = RO/R
        IF(ABS(RO).EQ.0.) GO TO 330
        IF (D.EQ.0.) GO TO 420
        PW(I) = RO/D
        FSAVE(I) = FSAVE(I)*PW(I)
 330    CONTINUE
      IWEVAL = 0
      RC = 1.
      GO TO 380
 340  IF (MITER.NE.0) GO TO ( 360 , 360 , 400 ), MITER
C*********************************************************************
C* IN THE CASE OF FUNCTIONAL ITERATION, UPDATE Y DIRECTLY FROM
C* THE RESULT OF THE LAST DIFFUN CALL.
C*********************************************************************
      D = 0.
      DO 350 I = 1,N
        R = H*FSAVE(I+NO) - Y(I,2)
        D = D + ( (R-ERROR(I))/YMAX(I) )**2
        FSAVE(I) = Y(I) + EL(1)*R
 350    ERROR(I) = R
      GO TO 410
C*********************************************************************
C* IN THE CASE OF THE CHORD METHOD, COMPUTE THE CORRECTOR ERROR,
C* F 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.
C*********************************************************************
 360  DO 370 I = 1,N
 370    FSAVE(I+NO) = FSAVE(I+NO)*H - Y(I,2) - ERROR(I)
      CALL SOLVE(NO,N,PW,FSAVE(N1),FSAVE,PW(NSQ1))
 380  D = 0.
      DO 390 I = 1,N
        ERROR(I) = ERROR(I) + FSAVE(I)
        D = D + (FSAVE(I)/YMAX(I))**2
 390    FSAVE(I) = Y(I) + EL(1)*ERROR(I)
      GO TO 410
 400  DO 405 I = 1,N
 405    FSAVE(I) = PW(I)*(FSAVE(I+NO)*H - Y(I,2) - ERROR(I))
      GO TO 380
C*********************************************************************
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 CONSIDERED ALSO.  A CHANGE IN H IS MADE ONLY IF IT IS BY A
C* FACTOR OF AT LEAST 1.1.  IF NOT, IDOUB IS SET TO 10 TO PREVENT
C* TESTING FOR THAT MANY STEPS.
```

```
C***********************************************************************
      KFLAG = 0
      DO 470 J = 1,L
        DO 470 I = 1,N
 470      Y(I,J) = Y(I,J) + EL(J)*ERROR(I)
      DO 480 I = 1,N
 480    YMAX(I) = AMAX1(YMAX(I),ABS(Y(I,1)))
      IF (IDOUB.EQ.1) GO TO 520
      IDOUB = IDOUB - 1
      IF (IDOUB.GT.1) GO TO 700
      IF (NQ.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* RESTORE T AND THE Y ARRAY TO THEIR PREVIOUS VALUES, AND PREPARE
C* TO TRY THE STEP AGAIN.  COMPUTE THE OPTIMUM STEP SIZE FOR THIS OR
C* ONE LOWER ORDER.
C***********************************************************************
 500  KFLAG = KFLAG - 1
      T = TOLD
      DO 510 J1 = 1,NQ
        DO 510 J2 = J1,NQ
          J = NQ - J2 + J1
          DO 510 I = 1,N
 510        Y(I,J) = Y(I,J) - Y(I,J+1)
      RMAX = 2.
      IF (ABS(H).LE.(HMIN*1.00001)) GO TO 660
      IF (KFLAG.LE.-3) GO TO 640
      PR3 = 1.E+20
      GO TO 540
C***********************************************************************
C* REGARDLESS OF THE SUCCESS OR FAILURE OF THE STEP, FACTORS
C* PR1, PR2, AND PR3 ARE COMPUTED, BY WHICH H COULD BE DIVIDED
C* AT ORDER NQ - 1, ORDER NQ, OR ORDER NQ + 1, RESPECTIVELY.
C* IN THE CASE OF FAILURE, PR3 = 1.E20 TO AVOID AN ORDER INCREASE.
C* THE SMALLEST OF THESE IS DETERMINED AND THE NEW ORDER CHOSEN
C* ACCORDINGLY.  IF THE ORDER IS TO BE INCREASED, WE COMPUTE ONE
C* ADDITIONAL SCALED DERIVATIVE.
C***********************************************************************
 520  PR3 = 1.E+20
      IF (NQ.EQ.MAXDER) GO TO 540
      D1 = 0.
      DO 530 I = 1,N
 530    D1 = D1 + ((ERROR(I) - Y(I,LMAX))/YMAX(I))**2
      ENQ3 = 0.5/FLOAT(L+1)
      PR3 = ((D1/EUP)**ENQ3)*1.4 + 1.4E-6
 540  ENQ2 = 0.5/FLOAT(L)
      PR2 = ((D/E)**ENQ2)*1.2 + 1.2E-6
      PR1 = 1.E+20
      IF (NQ.EQ.1) GO TO 560
      D = 0.0
      DO 550 I = 1,N
 550    D = D + (Y(I,L)/YMAX(I))**2
      ENQ1 = 0.5/FLOAT(NQ)
      PR1 = ((D/EDN)**ENQ1)*1.3 + 1.3E-6
 560  IF (PR2.LE.PR3) GO TO 570
      IF (PR3.LT.PR1) GO TO 590
 570  IF (PR2.GT.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
      RH = 1./PR3
      IF (RH.LT.1.1) GO TO 610
      DO 600 I = 1,N
 600    Y(I,NEWQ+1) = ERROR(I)*EL(L)/FLOAT(L)
      GO TO 630
 610  IDOUB = 10
      GO TO 700
 620  IF ((KFLAG.EQ.0).AND.(RH.LT.1.1)) GO TO 610
C***********************************************************************
C* IF THERE IS A CHANGE OF ORDER, RESET NQ, L, AND THE COEFFICIENTS.
C* IN ANY CASE H IS RESET ACCORDING TO RH AND THE Y ARRAY IS RESCALED.
C* THEN EXIT FROM 690 IF THE STEP WAS OK, OR REDO THE STEP OTHERWISE.
C***********************************************************************
      IF (NEWQ.EQ.NQ) GO TO 170
 630  NQ = NEWQ
      L = NQ + 1
      IRET = 2
      GO TO 130
C***********************************************************************
C* CONTROL REACHES THIS SECTION IF 3 OR MORE FAILURES HAVE OCCURED.
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
      RH = AMAX1(HMIN/ABS(H),RH)
      H = H*RH
      CALL DIFFUN(N,T,Y,FSAVE,0,NPEDV,K2)
```

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      DO 650 I = 1,N
  650   Y(I,2) = H*FSAVE(I)
      IWEVAL = MITER
      IODUB = 10
      IF (NQ.EQ.1) GO TO 200
      NQ = 1
      L = 2
      IRET = 3
      GO TO 130
C***********************************************************************
C* ALL RETURNS ARE MADE THROUGH THIS SECTION.  H IS SAVED IN HOLD
C* TO ALLOW THE CALLER TO CHANGE H ON THE NEXT STEP.
C***********************************************************************
  660 KFLAG = -1
      GO TO 700
  670 KFLAG = -2
      GO TO 700
  680 KFLAG = -3
      GO TO 700
  690 RMAX = 10.
  700 HOLD = H
      JSTART = NQ
      RETURN
C*********************** END OF STIFF **********************************
      END



      SUBROUTINE COSET(METH,NQ,EL,TQ,MAXDER)
C***********************************************************************
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 TQ, OF LENGTH 3, IS INVOLVED IN ADJUSTING THE STEP SIZE
C* IN RELATION TO TRUNCATION ERROR.  ITS VALUES ARE GIVEN BY THE
C* PERTST ARRAY.
C* THE VECTORS EL AND TQ DEPEND ON METH AND NQ.
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 = 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 PERTST NEED BE GIVEN TO ONLY ABOUT
C* ONE PERCENT ACCURACY.  THE ORDER IN WHICH THE GROUPS APPEAR BELOW
C* IS..  COEFFICIENTS FOR ORDER NQ - 1, COEFFICIENTS FOR ORDER NQ,
C* COEFFICIENTS FOR ORDER NQ + 1.  WITHIN EACH GROUP ARE THE
C* COEFFICIENTS FOR THE ADAMS METHODS, FOLLOWED BY THOSE FOR THE
C* GEAR METHODS.
C***********************************************************************
      DIMENSION PERTST(12,2,3),EL(13),TQ(4)
      DATA (PERTST = 1.,1.,2.,1.,.3158,.07407,.01391,.002182,
     1                .0002945,.00003492,.000003692,.0000003524,
     1              1.,1.,.5,.1667,.04167,1.,1.,1.,1.,1.,1.,1.,
     1              2.,12.,24.,37.89,53.33,70.08,87.97,106.9,
     1                126.7,147.4,168.8,191.0,
     1              2.0,4.5,7.333,10.42,13.7,1.,1.,1.,1.,1.,1.,1.,
     1              12.0,24.0,37.89,53.33,70.08,87.97,106.9,
     1                126.7,147.4,168.8,191.0,1.,
     1              3.0,6.0,9.167,12.5,1.,1.,1.,1.,1.,1.,1.,1.)
      EL(2) = 1.0
      GO TO (1,2),METH
    1 MAXDER = 12
      GO TO (101,102,103,104,105,106,107,108,109,110,111,112),NQ
    2 MAXDER = 5
      GO TO (201,202,203,204,205),NQ
C***********************************************************************
C* THE FOLLOWING COEFFICIENTS SHOULD BE DEFINED TO
C* MACHINE ACCURACY.  FOR EACH ORDER NQ, THEY CAN BE CALCULATED
C* FROM THE GENERATING POLYNOMIAL,
C*       L(T) = EL(1) + EL(2)*T + ... + EL(NQ+1)*T**NQ.
C* FOR THE IMPLICIT ADAMS METHODS, L(T) IS GIVEN BY
C*       DL/DT = (T+1)*(T+2)* ... *(T+NQ-1)/K,     L(-1) = 0,
C* WHERE                   K = FACTORIAL(NQ-1).
C* FOR THE GEAR METHODS,
C*       L(T) = (T+1)*(T+2)* ... *(T+NQ)/K,
C* WHERE         K = FACTORIAL(NQ)*(1 + 1/2 + ... + 1/NQ).
C*
C* THE ORDER IN WHICH THE GROUPS APPEAR BELOW IS..
C* IMPLICIT ADAMS METHODS OF ORDERS 1 TO 12,
C* STIFFLY STABLE GEAR METHODS OF ORDERS 1 TO 5.
C***********************************************************************
  101 EL(1) = 1.0
      GO TO 900
  102 EL(1) = 0.5
      EL(3) = 0.5
      GO TO 900
  103 EL(1) = 4.1666666666667E-01
      EL(3) = 0.75
      EL(4) = 1.6666666666667E-01
      GO TO 900
  104 EL(1) = 0.375
      EL(3) = 9.1666666666667E-01
      EL(4) = 3.3333333333333E-01
      EL(5) = 4.1666666666667E-02
      GO TO 900
  105 EL(1) = 3.4861111111111E-01
      EL(3) = 1.0416666666667
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      EL(4) = 4.8611111111111E-01
      EL(5) = 1.0416666666667E-01
      EL(6) = 8.3333333333333E-03
      GO TO 900
  106 EL(1) = 3.2986111111111E-01
      EL(3) = 1.1416666666667
      EL(4) = 0.625
      EL(5) = 1.7708333333333E-01
      EL(6) = 0.025
      EL(7) = 1.3888888888889E-03
      GO TO 900
  107 EL(1) = 3.1559193121693E-01
      EL(3) = 1.225
      EL(4) = 7.5185185185185E-01
      EL(5) = 2.5520833333333E-01
      EL(6) = 4.8611111111111E-02
      EL(7) = 4.8611111111111E-03
      EL(8) = 1.9841269841270E-04
      GO TO 900
  108 EL(1) = 3.0422453703704E-01
      EL(3) = 1.2964285714286
      EL(4) = 8.6851851851852E-01
      EL(5) = 3.3576388888889E-01
      EL(6) = 7.7777777777778E-02
      EL(7) = 1.0648148148148E-02
      EL(8) = 7.9365079365079E-04
      EL(9) = 2.4801587301587E-05
      GO TO 900
  109 EL(1) = 2.9486800044092E-01
      EL(3) = 1.3589285714286
      EL(4) = 9.7655423280423E-01
      EL(5) = 0.4171875
      EL(6) = 1.1135416666667E-01
      EL(7) = 0.01875
      EL(8) = 1.9345238095238E-03
      EL(9) = 1.1160714285714E-04
      EL(10)= 2.7557319223986E-06
      GO TO 900
  110 EL(1) = 2.8697544642857E-01
      EL(3) = 1.4144841269841
      EL(4) = 1.0772156084656
      EL(5) = 4.9856701940035E-01
      EL(6) = 0.1484375
      EL(7) = 2.9060570987654E-02
      EL(8) = 3.7202380952381E-03
      EL(9) = 2.9968584656085E-04
      EL(10)= 1.3778659611993E-05
      EL(11)= 2.7557319223986E-07
      GO TO 900
  111 EL(1) = 2.8018959644394E-01
      EL(3) = 1.4644841269841
      EL(4) = 1.1715145502646
      EL(5) = 5.7935819033527E-01
      EL(6) = 1.8832286155203E-01
      EL(7) = 4.1430362654321E-02
      EL(8) = 6.2111441798942E-03
      EL(9) = 6.2520667989418E-04
      EL(10)= 4.0417401528513E-05
      EL(11)= 1.5156525573192E-06
      EL(12)= 2.5052108385442E-08
      GO TO 900
  112 EL(1) = 2.7426554003160E-01
      EL(3) = 1.5099386724387
      EL(4) = 1.2602711640212
      EL(5) = 6.5923418209877E-01
      EL(6) = 2.3045800264550E-01
      EL(7) = 5.5697246105232E-02
      EL(8) = 9.4394841269841E-03
      EL(9) = 1.1192749669312E-03
      EL(10)= 9.0939153439153E-05
      EL(11)= 4.8225308641975E-06
      EL(12)= 1.5031265031265E-07
      EL(13)= 2.0876756987868E-09
      GO TO 900
  201 EL(1) = 1.0
      GO TO 900
  202 EL(1) = 6.6666666666667E-01
      EL(3) = 3.3333333333333E-01
      GO TO 900
  203 EL(1) = 5.4545454545455E-01
      EL(3) = EL(1)
      EL(4) = 9.0909090909091E-02
      GO TO 900
  204 EL(1) = 0.48
      EL(3) = 0.7
      EL(4) = 0.2
      EL(5) = 0.02
      GO TO 900
  205 EL(1) = 4.3795620437956E-01
      EL(3) = 8.2116788321168E-01
      EL(4) = 3.1021897810219E-01
      EL(5) = 5.4744525547445E-02
      EL(6) = 3.6496350364964E-03
C*
  900 DO 910 K=1,3
```

```
 910  TQ(K)=PERTST(NQ,METH,K)
      TQ(4) = .5*TQ(2)/FLOAT(NQ+2)
      RETURN
C*********************** END OF COSET **********************************
      END

      SUBROUTINE DECOMP(NDIM, 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                  ON OUTPUT, THE ARRAY WHERE L AND U ARE STORED.
C        IPS       THE ROW PIVOT VECTOR, GIVING THE PERMUTATION MATRIX P.
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 PIVROW
C
C               INITIALIZE IER,IPS,LU,SCALES
C
      IER=0
      DO 5 I = 1, N
         IPS(I) = I
         ROWNRM = 0.0
         DO 2 J = 1, N
            ROWNRM = AMAX1(ROWNRM, ABS(LU(I, J)))
    2    CONTINUE
C
C               TEST FOR MATRIX WITH ZERO ROW.
C
         IF (ROWNRM .EQ. 0.0) GO TO 95
         SCALES(I) = 1.0 / ROWNRM
    5 CONTINUE
C
C               GAUSSIAN ELIMINATION WITH PARTIAL PIVOTING
C
      NM1 = N - 1
      DO 17 K = 1, NM1
         BIG = 0.0
         DO 11 I = K, N
            IP = IPS(I)
            SIZE = ABS(LU(IP, K)) * SCALES(IP)
            IF (SIZE .LE. BIG) GO TO 11
   10          BIG = SIZE
               PIVROW = I
   11    CONTINUE
C
C               TEST FOR ZERO PIVOT
C
         IF (BIG .EQ. 0.0) GO TO 96
C
C               INTERCHANGE ROW IF NECESSARY
C
         IF (PIVROW .EQ. K) GO TO 15
            J = IPS(K)
            IPS(K) = IPS(PIVROW)
            IPS(PIVROW) = J
   15    KP = IPS(K)
         PIVOT = LU(KP, K)
         PIVOT = 1. / PIVOT
         LU(KP, K) = PIVOT
         KP1 = K + 1
         DO 16 I = KP1, N
            IP = IPS(I)
            EM = LU(IP, K) * PIVOT
            LU(IP, K) = EM
            DO 16 J = KP1, N
               LU(IP, J) = LU(IP, J) - EM * LU(KP, J)
   16    CONTINUE
   17 CONTINUE
C
C               TEST FOR LAST PIVOT
C
      IP = IPS(N)
      PIVOT = LU(IP, N)
      IF (PIVOT .EQ. 0.0) GO TO 96
      LU(IP, N) = 1. / PIVOT
      RETURN
C
C               ALL ZERO ELEMENTS IN A ROW
C
   95 IER = 1
      RETURN

C
C               ZERO PIVOT
   96 IER = 2
      RETURN
C
      END
```

APPENDIX B

```
      SUBROUTINE SOLVE(NDIM, N, LU, B, X, IPS)
C
C        LINEAR SYSTEM PACKAGE
C        SOLVE A X = B USING L U FROM SUBROUTINE DECOMP.
C
C        SEE DECOMP FOR DESCRIPTION OF PARAMETERS
C
      DIMENSION B(N),X(N),IPS(N)
      REAL LU(NDIM, N)
C
      NP1 = N + 1
C
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 + LU(IP, J) * X(J)
    2    X(I) = B(IP) - SUM
C
      IP = IPS(N)
      X(N) = X(N) * LU(IP, N)
C
C              BACKWARD SUBSTITUTION - SOLVE U * X = Z, WHERE L * Z = B.
C
      DO 4 IBACK = 2, N
         I = NP1 - IBACK
C              I GOES FROM (N-1) TO 1 BY -1
         IP = IPS(I)
         IP1 = I + 1
         SUM = 0.0
         DO 3 J = IP1, N
    3       SUM = SUM + LU(IP, J) * X(J)
    4    X(I) = (X(I) - SUM) * LU(IP, I)
C
      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 **

          1         2         3         4         5         6         7         8
CC  1     0         0         0         0         0         0         0         0


                    BROMINE DISSOCIATION IN A SHOCK TUBE                    CASE 1
      M       + BR2       =   BR      + BR                6.99E+11    .5      35500.
                                  - BLANK CARD -
    XE
    DISTANCE  AREA
     $PROB    ITPSZ=3,LSUBM=32200.,ETA=0.50, SHOCK=.TRUE.,  END=10.,
          IDEL=20, PAPS=.TRUE.,
                    ALLM1=.FALSE.,   $END
      M       + BR2       =   BR      + BR                          BR2       3.80
                                  - BLANK CARD -
     $START   P=0.1227, MACH=3.2646, T=299.9,  BR2=0.01,XE=0.99,  $END
    FINIS



                                ** DATA CARDS **

          1         2         3         4         5         6         7         8
CC  1     0         0         0         0         0         0         0         0


              METHANE - AIR COMBUSTION (ASSIGNED AREA - TIME INTEGRATION)   CASE 6
                 CH4      =   CH3     +  H                3.00E+14  0.        103000.
        CH4      +  O2       =   CH3     +  HO2              1.00E+13  0.        63000.
        H        +  O2       =   HO2     +  M                1.59E+15  0.        -1000.
        CO       +  O2       =   CO2     +  O                1.60E+13  0.        41000.
        CH3      +  O2       =   CH2O    +  OH               7.50E+10  0.        0.
        H        +  CH4      =   CH3     +  H2               6.90E+13  0.        11800.
        O        +  CH4      =   CH3     +  OH               2.00E+13  0.        9200.
        OH       +  CH4      =   CH3     +  H2O              7.20E+13  0.        5900.
        H        +  O2       =   OH      +  O                1.25E+14  0.        16300.
        O        +  H2       =   OH      +  H                2.96E+13  0.        9800.
        H2       +  OH       =   H2O     +  H                2.10E+13  0.        5100.
        CO       +  OH       =   CO2     +  H                4.20E+11  0.        1000.
        CH3      +  O        =   CH2O    +  H                1.90E+13  0.        0.
        CH2O     +  H        =   HCO     +  H2               1.00E+13  0.        2000.
        CH2O     +  OH       =   HCO     +  H2O              7.00E+10  .70       1000.
        CH2O     +  O        =   HCO     +  OH               4.00E+11  .60       4000.
        HCO      +  O        =   CO      +  OH               1.80E+11  .50       0.
        HCO      +  OH       =   CO      +  H2O              1.10E+11  .50       0.
        HCO      +  H        =   CO      +  H2               1.50E+12  .50       0.
        M        +  HCO      =   H       +  CO               2.00E+13  .50       28600.
        HCO      +  O2       =   CO      +  HO2              1.00E+11  .50       5400.
        HO2      +  HO2      =   H2O2    +  O2               1.80E+12  0.        0.
        H        +  HO2      =   OH      +  OH               7.00E+13  0.        0.
        O        +  HO2      =   OH      +  O2               6.00E+12  0.        0.
        OH       +  HO2      =   H2O     +  O2               6.00E+12  0.        0.
        M        +  H2O2     =   OH      +  OH               1.17E+17  0.        45500.
        H        +  OH       =   H2O     +  M                7.50E+23  -2.60     0.
        M        +  O2       =   O       +  O                2.75E+19  -1.       118700.
        O        +  H2O      =   OH      +  OH               5.75E+13  0.        18000.
                                  - BLANK CARD -
    N2
    TIME      AREA
     $PROB    ITPSZ=1, IPRCOD=1,HMIN=6.25E-10,
          HMAX=1.25E-6,
          EMAX=.0001,
          PAPS=.TRUE.,
          END=2.6615E-4,
          TPPINT=6.35273E-5,1.27C555E-4,1.90582E-4,2.22340E-4,2.54109E-4,
                 2.6615E-4,  NPRIN=6,
          COMBUS=.FALSE.,  ALLM1=.FALSE.,
          XTB=0,5,10,15,20,25,30,35,36,37,38,39,40,40.5,41,42,
          ATB=1000.,1000.45,1002.02,1004.83,1009.24,1016.16,1028.32,1057.02,
              1068.70,1085.55,1112.40,1163.57,1296.59,1371.48,1384.47,
```

```
          1400.45,  NTB=16,
       $END
  H       +  O2       =  HO2      +  M          CH4      5.0     O2       2.0
  H       +  O2       =  HO2      +  M          N2       2.0     H2O      32.5
  H       +  O2       =  HO2      +  M          CO       2.0     CO2      7.5
  H       +  O2       =  HO2      +  M          H2       5.0
  M       +  H2O2     =  OH       +  OH         O2        .78    H2O2     6.6
  M       +  H2O2     =  OH       +  OH         H2O      6.0
  H       +  OH       =  H2O      +  M          N2       1.6     H2O      20.
  H       +  OH       =  H2O      +  M          O2       1.6
                                 -  BLANK CARD  -
 $START   P=1.730,V=157412.62,T=1645.,
          CH4=0.049768, O2=0.199072,  N2=0.75116,
       $END
 FINIS


                              **  DATA CARDS  **

          1         2         3         4         5         6         7         8
CC 1      0         0         0         0         0         0         0         0

       METHANE-AIR COMBUSTION AT CONSTANT  P (ONE UNIMOLECULAR  REACTION)CASE 5
 REPEAT
 DISTANCE  PRESSURE
  $PROB ITPSZ=2, CXO=1.730,HMIN=1.0E-4,HMAX=20., EMAX=.0001,
       COMBUS=.TRUE.,  ALLM1=.FALSE.,
       END=42.,
        PAPS=.TRUE.,
   TPRINT=5.0,10.0,25.0,35.,38.,39.5,40.,40.5,41.,42., NPRIN=10,
       IPRIT=4,  MF=22,
       $END
                                 -  BLANK CARD  -
  $START  AREA=1000.,MACH=2., T=1645.,
          CH4=0.049768, O2=0.199072,  N2=0.75116,
          $END
 FINIS


                              **  DATA CARDS  **

          1         2         3         4         5         6         7         8
CC 1      0         0         0         0         0         0         0         0

       H2-O2 LOW TEMPERATURE  REACTION AT CONSTANT VOLUME  (ADJUSTED RATES) C-8
  H2       +  O2       =  H        +  HO2          1.00E+14  0.       67000.
  H2       +  OH       =  H2O      +  H            2.10E+13  0.       5100.
  H        +  O2       =  OH       +  O            1.25E+14  0.       16300.
  O        +  H2       =  OH       +  H            2.96E+13  0.       9800.
  H        +  O2       =  HO2      +  M            8.50E+14  0.       -1000.
  H        +  HO2      =  OH       +  OH           7.00E+13  0.       0.
  M        +  H2O2     =  OH       +  OH           1.17E+17  0.       45500.
  HO2      +  HO2      =  H2O2     +  O2           1.00E+12  0.       0.
  HO2      +  H2       =  H2O2     +  H            8.50E+12  0.       24000.
  H        +  H2O2     =  H2O      +  OH           3.18E+14  0.       9000.
  OH       +  H2O2     =  H2O      +  HO2          1.00E+13  0.       1800.
  O        +  H2O      =  OH       +  OH           5.75E+13  0.       18000.
                                 -  BLANK CARD  -
                                 -  BLANK CARD  -
 TIME
  $PROB  HMIN=5.0E-5, HMAX=.1,          EMAX=.0003, ALLM1=.FALSE.,
       END=120.,
         RHOCON=.TRUE., TCON=.TRUE., CONC=.FALSE.,
       TPRINT=.75,1.25,5.,10.,20.,30.,40.,50.,55.,60.,65.,75.,85.,95.,
              105.,120.,   NPRIN=16,
       PAPS=.TRUE.,
       $END
  H       +  O2       =  HO2      +  M          H2       5.      O2       2.
  H       +  O2       =  HO2      +  M          H2O      32.5
  M       +  H2O2     =  OH       +  OH         H2O      6.      O2       .78
  M       +  H2O2     =  OH       +  OH         H2O2     6.6     H2       2.3
                                 -  BLANK CARD  -
  $START   MMHG=.TRUE., P=500., T=773.15,  H2=.86, O2=.14,    $END
 FINIS
```

Check Case 1

DISTANCE-AREA VERSION GENERAL CHEMICAL KINETICS PROGRAM NASA LANGLEY RESEARCH CENTER
LANGLEY VERSION OF LEWIS PROGRAM (TN D-6586) USING STIFF ODE
SOLUTION TECHNIQUE DEVELOPED BY C.W. GEAR

BROMINE DISSOCIATION IN A SHOCK TUBE CASE 1

REACTION NUMBER	REACTION	REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	M + 1*BR2 = 1*BR + 1*BR	6.99000E+11	.5000	35500.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(BR2 , 1) = 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 .00010

** ASSIGNED VARIABLE PROFILE **

THE AREA IS CALCULATED FROM THE FOLLOWING FUNCTION

1/AREA = 1 - (X/ 32200.000)**(.50000)

** EQUILIBRIUM SHOCK CALCULATION **

	INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE (ATM)	.1227	1.6130	13.1460
VELOCITY (CM/SEC)	57875.78	18108.11	.3129
DENSITY (GM/CM**3)	65.60921E-05	20.96952E-04	3.1961
TEMPERATURE (DEG K)	299.90	1231.22	4.1054
ENTROPY (CAL/GM/DEG K)	.3421	.3576	1.0451
MACH NUMBER	3.2646	.5171	.1584
GAMMA	1.6586	1.5731	.9485
SONIC VELOCITY (CM/SEC)	17728.29	35015.45	1.9751

SPECIES	MOLE FRACTION
BR2	8.12239E-03
BR	3.71805E-03
XE	9.88160E-01

MIXTURE MOLECULAR WEIGHT 131.34058

D(LOG VOLUME)/D(LOG T) AT CONSTANT P = 1.0161E+00

D(LOG VOLUME)/D(LOG P) AT CONSTANT T = -1.0008E+00

** FROZEN SHOCK CALCULATION **

	INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE (ATM)	.1227	1.6017	13.0535
VELOCITY (CM/SEC)	57875.78	18410.72	.3181
DENSITY (GM/CM**3)	65.60921E-05	20.62485E-04	3.1436
TEMPERATURE (DEG K)	299.90	1245.31	4.1524
ENTROPY (CAL/GM/DEG K)	.3421	.3575	1.0449
MACH NUMBER	3.2646	.5098	.1562
GAMMA	1.6586	1.6577	.9994
SONIC VELOCITY (CM/SEC)	17728.29	36115.84	2.0372

SPECIES	MOLE FRACTION
BR2	1.00000E-02
BR	0.
XE	9.90000E-01

MIXTURE MOLECULAR WEIGHT = 131.58520

D(LOG VOLUME)/D(LOG T) AT CONSTANT P = 1.0000E+00

D(LOG VOLUME)/D(LOG P) AT CONSTANT T = -1.0000E+00

TIME	0.	SEC
AXIAL POSITION	0.	CM
AREA	1.00000E+00	SQ CM

FLOW PROPERTIES

PRESSURE	1.6017	ATM
VELOCITY	18410.72	CM/SEC
TEMPERATURE	1245.31346	K
DENSITY	2.06248E-03	GM/CC
FLOW RATE	3.79718E+01	GM/SEC
ENTROPY	.35751	CAL/GM-K
MACH NUMBER	.50977	
GAMMA	1.65767	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
BR2	1.00000E-02	-3.66695E-05
BR	0.	7.33390E-05
XE	9.90000E-01	0.

MIXTURE MOLECULAR WEIGHT 131.58520

TIME	0.	SEC
AXIAL POSITION	0.	CM
AREA	1.00000E+00	SQ CM

FLOW PROPERTIES

PRESSURE	1.6017	ATM
VELOCITY	18410.72	CM/SEC
TEMPERATURE	1245.31346	K
DENSITY	2.06248E-03	GM/CC
FLOW RATE	3.79718E+01	GM/SEC
ENTROPY	.35751	CAL/GM-K
MACH NUMBER	.50977	
GAMMA	1.65767	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
BR2	1.00000E-02	-3.66695E-05
BR	0.	7.33390E-05
XE	9.90000E-01	0.

MIXTURE MOLECULAR WEIGHT 131.58520

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) 3.97333E+05

MASS FRACTION SUM 1.00000

TIME	2.72633E-05	SEC
AXIAL POSITION	5.00000E-01	CM
AREA	1.00396E+00	SQ CM

FLOW PROPERTIES

PRESSURE	1.6058	ATM
VELOCITY	18301.52	CM/SEC
TEMPERATURE	1245.96881	K
DENSITY	2.06652E-03	GM/CC
FLOW RATE	3.79702E+01	GM/SEC
ENTROPY	.35752	CAL/GM-K
MACH NUMBER	.50659	
GAMMA	1.65772	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
BR2	9.93534E-03	-3.68318E-05
BR	1.28045E-04	7.36637E-05
XE	9.89937E-01	0.

MIXTURE MOLECULAR WEIGHT 131.57678

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) 3.97533E+05

MASS FRACTION SUM 1.00000

TIME	3.31019E-04	SEC
AXIAL POSITION	6.00000E+00	CM
AREA	1.01384E+00	SQ CM

FLOW PROPERTIES

PRESSURE	1.6184	ATM
VELOCITY	17960.51	CM/SEC
TEMPERATURE	1243.66331	K
DENSITY	2.08531E-03	GM/CC
FLOW RATE	3.79716E+01	GM/SEC
ENTROPY	.35756	CAL/GM-K
MACH NUMBER	.49737	
GAMMA	1.65824	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
BR2	9.27260E-03	-3.03577E-05
BR	1.44040E-03	6.07155E-05
XE	9.89287E-01	0.

MIXTURE MOLECULAR WEIGHT 131.49043

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) 3.97333E+05

MASS FRACTION SUM 1.00000

TIME	2.72461E-05	SEC
AXIAL POSITION	5.00000E-01	CM
AREA	1.00396E+00	SQ CM

FLOW PROPERTIES

PRESSURE	1.6053	ATM
VELOCITY	18314.71	CM/SEC
TEMPERATURE	1245.81850	K
DENSITY	2.06614E-03	GM/CC
FLOW RATE	3.79905E+01	GM/SEC
ENTROPY	.35752	CAL/GM-K
MACH NUMBER	.50698	
GAMMA	1.65772	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
BR2	9.93549E-03	-3.67529E-05
BR	1.27737E-04	7.35059E-05
XE	9.89937E-01	0.

MIXTURE MOLECULAR WEIGHT 131.57680

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) 3.96829E+05

MASS FRACTION SUM 1.00000

TIME	3.30791E-04	SEC
AXIAL POSITION	6.00000E+00	CM
AREA	1.01384E+00	SQ CM

FLOW PROPERTIES

PRESSURE	1.6180	ATM
VELOCITY	17972.82	CM/SEC
TEMPERATURE	1243.54007	K
DENSITY	2.08494E-03	GM/CC
FLOW RATE	3.79908E+01	GM/SEC
ENTROPY	.35756	CAL/GM-K
MACH NUMBER	.49773	
GAMMA	1.65823	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
BR2	9.27428E-03	-3.03194E-05
BR	1.43708E-03	6.06389E-05
XE	9.89289E-01	0.

MIXTURE MOLECULAR WEIGHT 131.49065

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) 3.21779E+05

MASS FRACTION SUM 1.00000

TIME	4.42637E-04	SEC
AXIAL POSITION	8.00000E+00	CM
AREA	1.01601E+00	SQ CM

FLOW PROPERTIES

PRESSURE	1.6215	ATM
VELOCITY	17877.85	CM/SEC
TEMPERATURE	1242.69289	K
DENSITY	2.09046E-03	GM/CC
FLOW RATE	3.79714E+01	GM/SEC
ENTROPY	.35756	CAL/GM-K
MACH NUMBER	.49520	
GAMMA	1.65839	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
BR2	9.06919E-03	-2.69612E-05
BR	1.84318E-03	5.39224E-05
XE	9.89088E-01	0.

MIXTURE MOLECULAR WEIGHT 131.46393

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) 2.84373E+05

MASS FRACTION SUM 1.00000

TIME	5.54739E-04	SEC
AXIAL POSITION	1.00000E+01	CM
AREA	1.01794E+00	SQ CM

FLOW PROPERTIES

PRESSURE	1.6241	ATM
VELOCITY	17805.51	CM/SEC
TEMPERATURE	1241.82974	K
DENSITY	2.09498E-03	GM/CC
FLOW RATE	3.79713E+01	GM/SEC
ENTROPY	.35757	CAL/GM-K
MACH NUMBER	.49330	
GAMMA	1.65853	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
BR2	8.89013E-03	-2.34480E-05
BR	2.19775E-03	4.68960E-05
XE	9.88912E-01	0.

MIXTURE MOLECULAR WEIGHT 131.44060

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) 3.21488E+05

MASS FRACTION SUM 1.00000

TIME	4.42332E-04	SEC
AXIAL POSITION	8.00000E+00	CM
AREA	1.01601E+00	SQ CM

FLOW PROPERTIES

PRESSURE	1.6210	ATM
VELOCITY	17890.27	CM/SEC
TEMPERATURE	1242.57201	K
DENSITY	2.09008E-03	GM/CC
FLOW RATE	3.79909E+01	GM/SEC
ENTROPY	.35756	CAL/GM-K
MACH NUMBER	.49557	
GAMMA	1.65839	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
BR2	9.07118E-03	-2.69362E-05
BR	1.83924E-03	5.38724E-05
XE	9.89090E-01	0.

MIXTURE MOLECULAR WEIGHT 131.46419

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) 2.84212E+05

MASS FRACTION SUM 1.00000

TIME	5.54356E-04	SEC
AXIAL POSITION	1.00000E+01	CM
AREA	1.01794E+00	SQ CM

FLOW PROPERTIES

PRESSURE	1.6237	ATM
VELOCITY	17817.93	CM/SEC
TEMPERATURE	1241.71136	K
DENSITY	2.09459E-03	GM/CC
FLOW RATE	3.79909E+01	GM/SEC
ENTROPY	.35757	CAL/GM-K
MACH NUMBER	.49367	
GAMMA	1.65853	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
BR2	8.89233E-03	-2.34354E-05
BR	2.19340E-03	4.68709E-05
XE	9.88914E-01	0.

MIXTURE MOLECULAR WEIGHT 131.44089

```
 TOTAL ENERGY EXCHANGE RATE     2.46251E+05
    (CAL-CM3/GM2/SEC)

 MASS FRACTION SUM                    1.00000

11/28/75  LRC ICOPS INDEPNDT 6600B-131K 01/21/75D
15.53.36.GT05679.
15.53.37.                          LRC COMPUTER COMPLEX
15.53.37.JOB,1,00300,120000,002000.      A4409    R
15.53.37.3274       100681          B-1250
15.53.37.USER.    ALLEN G. MCLAIN                0005
15.53.37.89803N 64730
15.53.37.WAITGO.    PLEASE RUN ON 6600 ONLY
15.55.24.GO.
15.55.24.LINECNT(10000)
15.55.26.FETCH(A4409,,BINARY)
15.55.38.TIME         BG ATTACH
15.56.41.TIME         ED ATTACH
15.56.42.END     FETCH
15.56.42.UPDATE(Q,C=TAPE4,P=BNFILE,D,8)
15.56.49.READING INPUT
15.57.03.UPDATE COMPLETE
15.57.03.UPDATE(Q,P=BNFILE)
15.57.11.READING INPUT
15.57.28.UPDATE COMPLETE
15.57.29.RUN(S,,,COMPILE)
15.58.20.SETINDF.
15.58.21.LGO.
15.59.14.MEMORY   071100 CM
15.59.14.RFL        0000638 O/S CALLS
15.59.14.RFL CPU     29.169650 SEC.
15.59.31.STOP
15.59.32.SPPRINT(OUTPUT,3)
15.59.35.      0000701 O/S CALLS
15.59.35.CPU     36.633872 SEC.
15.59.35.PPU    182.190080 SEC.
15.59.37.COST OF THIS JOB WAS $    10
15.59.37.KWH      2.62      KILOWORD HOURS
17.02.09. GT05679.    7067 LINES PRINTED. LP20
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 TOTAL ENERGY EXCHANGE RATE     2.46209E+05
    (CAL-CM3/GM2/SEC)

 MASS FRACTION SUM                    1.00000

11/04/75  LRC ICOPS INDEPNDT 6600D-131K 01/21/75D
13.48.27.GT05661.
13.48.27.                          LRC COMPUTER COMPLEX
13.48.27.JOB,1,00300,120000,002000.      A4409    R
13.48.27.3274       100681          B-1250
13.48.27.USER.    ALLEN G. MCLAIN                0005
13.48.27.89803N 64730
13.48.28.LINECNT(10000)
13.48.29.FETCH(A4409,,BINARY)
13.48.36.TIME         BG ATTACH
13.49.15.TIME         ED ATTACH
13.49.16.END     FETCH
13.49.16.UPDATE(Q,C=TAPE4,P=BNFILE,D,8)
13.49.20.READING INPUT
13.49.36.UPDATE COMPLETE
13.49.37.UPDATE(Q,P=BNFILE)
13.49.41.READING INPUT
13.49.48.UPDATE COMPLETE
13.49.48.RUN(S,,,COMPILE)
13.50.20.SETINDF.
13.50.21.LGO.
13.50.47.MEMORY   066700 CM
13.50.47.RFL        0000517 O/S CALLS
13.50.47.RFL CPU     27.119152 SEC.
13.51.03.STOP
13.51.05.SPPRINT(OUTPUT,3)
13.51.07.      0000580 O/S CALLS
13.51.07.CPU     35.074925 SEC.
13.51.07.PPU    139.538432 SEC.
13.51.08.COST OF THIS JOB WAS $    10
13.51.08.KWH      2.49      KILOWORD HOURS
14.42.06. GT05661.    6337 LINES PRINTED. LP21
```

Check Case 5

DISTANCE-PRESSURE VERSION GENERAL CHEMICAL KINETICS PROGRAM NASA LANGLEY RESEARCH CENTER
LANGLEY VERSION OF LEWIS PROGRAM (TN D-6586) USING STIFF ODE
SOLUTION TECHNIQUE DEVELOPED BY C.W. GEAR

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

REACTION NUMBER	REACTION	REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1*CH4 = 1*CH3 + 1*H	3.80000E+14	0.0000	103000.00
2	1*CH4 + 1*O2 = 1*CH3 + 1*HO2	1.00000E+13	0.0000	63000.00
3	1*H + 1*O2 = 1*HO2 + M	1.59000E+15	0.0000	-1000.00
4	1*CO + 1*O2 = 1*CO2 + 1*O	1.60000E+13	0.0000	41000.00
5	1*CH3 + 1*O2 = 1*CH2O + 1*OH	7.50000E+10	0.0000	0.00
6	1*H + 1*CH4 = 1*CH3 + 1*H2	6.90000E+13	0.0000	11800.00
7	1*O + 1*CH4 = 1*CH3 + 1*OH	2.00000E+13	0.0000	9200.00
8	1*OH + 1*CH4 = 1*CH3 + 1*H2O	7.20000E+13	0.0000	5900.00
9	1*H + 1*O2 = 1*OH + 1*O	1.25000E+14	0.0000	16300.00
10	1*O + 1*H2 = 1*OH + 1*H	2.96000E+13	0.0000	9800.00
11	1*H2 + 1*OH = 1*H2O + 1*H	2.10000E+13	0.0000	5100.00
12	1*CO + 1*OH = 1*CO2 + 1*H	4.20000E+11	0.0000	1000.00
13	1*CH3 + 1*O = 1*CH2O + 1*H	1.90000E+13	0.0000	0.00
14	1*CH2O + 1*H = 1*HCO + 1*H2	1.00000E+13	0.0000	2000.00
15	1*CH2O + 1*OH = 1*HCO + 1*H2O	7.00000E+10	.7000	1000.00
16	1*CH2O + 1*O = 1*HCO + 1*OH	4.00000E+11	.6000	4000.00
17	1*HCO + 1*O = 1*CO + 1*OH	1.80000E+11	.5000	0.00
18	1*HCO + 1*OH = 1*CO + 1*H2O	1.10000E+11	.5000	0.00
19	1*HCO + 1*H = 1*CO + 1*H2	1.50000E+12	.5000	0.00
20	M + 1*HCO = 1*H + 1*CO + M	2.00000E+13	.5000	28600.00
21	1*HCO + 1*O2 = 1*CO + 1*HO2	1.00000E+11	.5000	5400.00
22	1*HO2 + 1*HO2 = 1*H2O2 + 1*O2	1.80000E+12	0.0000	0.00
23	1*H + 1*HO2 = 1*OH + 1*OH	7.00000E+13	0.0000	0.00
24	1*O + 1*HO2 = 1*OH + 1*O2	6.00000E+12	0.0000	0.00
25	1*OH + 1*HO2 = 1*H2O + 1*O2	6.00000E+12	0.0000	0.00
26	M + 1*H2O2 = 1*OH + 1*OH	1.17000E+17	0.0000	45500.00
27	1*H + 1*OH = 1*H2O + M	7.50000E+23	-2.6000	0.00
28	M + 1*O2 = 1*O + 1*O + M	2.75000E+19	-1.0000	118700.00
29	1*O + 1*H2O = 1*OH + 1*OH	5.75000E+13	0.0000	18000.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(CH4 , 3) =	5.00000	M(O2 , 3) =	2.00000	M(O2 ,26) =	.78000	M(O2 ,27) =	1.60000
M(CO , 3) =	2.00000	M(CO2 , 3) =	3.50000	M(H2 , 3) =	5.00000	M(H2O , 3) =	32.50000
M(H2O ,26) =	6.00000	M(H2O ,27) =	20.00000	M(H2O2 ,26) =	6.60000	M(N2 , 3) =	2.00000
M(N2 ,27) =	1.60000						

INTEGRATION CONTROLS

MINIMUM STEP SIZE 1.00000E-04 CM MAXIMUM STEP SIZE 2.00000E+01 CM

INITIAL STEP SIZE 1.00000E-04 CM MAXIMUM RELATIVE ERROR .00010

** ASSIGNED VARIABLE PROFILE **

THE PRESSURE IS CALCULATED FROM THE FOLLOWING POLYNOMIAL

PRESSURE (ATM) = (0.)X**3 + (0.)X**2 + (0.)X + (17.30000E-01)

** INITIAL CONDITIONS **

TIME	0.	SEC
AXIAL POSITION	0.	CM
AREA	1.00000E+03	SQ CM

FLOW PROPERTIES

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

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CH4	4.97680E-02	-5.08397E-06
CH3	0.	5.08397E-06
H	0.	5.01454E-06
O2	1.99072E-01	-6.95166E-08
HO2	0.	6.94238E-08
CO	0.	0.
CO2	0.	0.
O	0.	1.85618E-10
CH2O	0.	0.
OH	0.	0.
H2	0.	0.
H2O	0.	0.
HCO	0.	0.
H2O2	0.	0.
N2	7.51160E-01	0.

MIXTURE MOLECULAR WEIGHT	28.21038
TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)	4.05133E+06
MASS FRACTION SUM	1.00000

TIME	0.	SEC
AXIAL POSITION	0.	CM
AREA	1.00000E+03	SQ CM

FLOW PROPERTIES

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

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CH4	4.97680E-02	-5.08397E-06
CH3	0.	5.08397E-06
H	0.	5.01454E-06
O2	1.99072E-01	-6.95166E-08
HO2	0.	6.94238E-08
CO	0.	0.
CO2	0.	0.
O	0.	1.85618E-10
CH2O	0.	0.
OH	0.	0.
H2	0.	0.
H2O	0.	0.
HCO	0.	0.
H2O2	0.	0.
N2	7.51160E-01	0.

MIXTURE MOLECULAR WEIGHT	28.21038
TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)	4.05133E+06
MASS FRACTION SUM	1.00000

TIME	1.58818E-04	SEC
AXIAL POSITION	2.50000E+01	CM
AREA	1.01616E+03	SQ CM

FLOW PROPERTIES

PRESSURE	1.7300	ATM
VELOCITY	157412.62	CM/SEC
TEMPERATURE	1671.27618	K
DENSITY	3.55810E-04	GM/CC
FLOW RATE	5.69139E+04	GM/SEC

TIME	1.58818E-04	SEC
AXIAL POSITION	2.50000E+01	CM
AREA	1.01616E+03	SQ CM

FLOW PROPERTIES

PRESSURE	1.7300	ATM
VELOCITY	157412.62	CM/SEC
TEMPERATURE	1671.27618	K
DENSITY	3.55810E-04	GM/CC
FLOW RATE	5.69139E+04	GM/SEC

ENTROPY	2.13913	CAL/GM-K
MACH NUMBER	1.98449	
GAMMA	1.27713	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CH4	4.58362E-02	-8.26286E-04
CH3	3.23902E-04	6.90414E-05
H	1.29214E-06	5.18015E-07
O2	1.95297E-01	-8.03098E-04
HO2	2.62066E-05	1.01757E-05
CO	1.36761E-04	6.13850E-05
CO2	6.82879E-07	3.55534E-07
O	2.29373E-06	7.54473E-07
CH2O	3.46017E-03	6.94937E-04
OH	8.82584E-06	2.01349E-06
H2	6.67891E-05	2.19675E-05
H2O	3.81395E-03	8.25462E-04
HCO	1.26770E-06	5.67747E-07
H2O2	9.35077E-09	6.77905E-09
N2	7.51024E-01	0.

MIXTURE MOLECULAR WEIGHT	28.20528
TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)	-4.05011E+08
MASS FRACTION SUM	1.00000

TIME	2.41404E-04	SEC
AXIAL POSITION	3.80000E+01	CM
AREA	1.11238E+03	SQ CM

FLOW PROPERTIES

PRESSURE	1.7300	ATM
VELOCITY	157412.62	CM/SEC
TEMPERATURE	1818.32068	K
DENSITY	3.25032E-04	GM/CC
FLOW RATE	5.69139E+04	GM/SEC
ENTROPY	2.18611	CAL/GM-K
MACH NUMBER	1.89717	
GAMMA	1.27654	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CH4	2.38726E-02	-1.27531E-02
CH3	4.59133E-03	3.49235E-03
H	1.41780E-04	2.19230E-04
O2	1.72382E-01	-1.35914E-02
HO2	5.89356E-04	2.37251E-04
CO	7.70302E-03	8.30227E-03
CO2	7.94553E-05	1.23370E-04
O	1.09175E-04	1.51401E-04
CH2O	1.30786E-02	6.75894E-04
OH	2.72185E-04	3.96634E-04
H2	2.38766E-03	2.30967E-03
H2O	2.82445E-02	1.67758E-02
HCO	1.28555E-04	1.59223E-04
H2O2	1.41319E-06	1.74458E-07
N2	7.46422E-01	0.

ENTROPY	2.13913	CAL/GM-K
MACH NUMBER	1.98449	
GAMMA	1.27713	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CH4	4.58358E-02	-8.26221E-04
CH3	3.23895E-04	6.89971E-05
H	1.29170E-06	5.37717E-07
O2	1.95297E-01	-8.03047E-04
HO2	2.62163E-05	1.01572E-05
CO	1.36765E-04	6.13672E-05
CO2	6.83191E-07	3.55536E-07
O	2.29206E-06	7.52699E-07
CH2O	3.46056E-03	6.94917E-04
OH	8.82539E-06	2.01842E-06
H2	6.67870E-05	2.19600E-05
H2O	3.81434E-03	8.25414E-04
HCO	1.26755E-06	5.84232E-07
H2O2	9.35293E-09	6.88310E-09
N2	7.51024E-01	0.

MIXTURE MOLECULAR WEIGHT	28.20528
TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)	-4.04996E+08
MASS FRACTION SUM	1.00000

TIME	2.41404E-04	SEC
AXIAL POSITION	3.80000E+01	CM
AREA	1.11243E+03	SQ CM

FLOW PROPERTIES

PRESSURE	1.7300	ATM
VELOCITY	157412.62	CM/SEC
TEMPERATURE	1818.15034	K
DENSITY	3.25017E-04	GM/CC
FLOW RATE	5.69139E+04	GM/SEC
ENTROPY	2.18607	CAL/GM-K
MACH NUMBER	1.89726	
GAMMA	1.27654	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CH4	2.38696E-02	-1.26782E-02
CH3	4.59705E-03	3.43521E-03
H	1.40844E-04	2.48755E-04
O2	1.72374E-01	-1.35319E-02
HO2	5.89292E-04	2.18901E-04
CO	7.70133E-03	8.26889E-03
CO2	7.94765E-05	1.22826E-04
O	1.08509E-04	1.45984E-04
CH2O	1.30898E-02	7.00694E-04
OH	2.70805E-04	4.28220E-04
H2	2.38499E-03	2.29343E-03
H2O	2.82507E-02	1.66864E-02
HCO	1.28145E-04	1.50529E-04
H2O2	1.43660E-06	-2.80371E-07
N2	7.46426E-01	0.

MIXTURE MOLECULAR WEIGHT 28.03244

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) -7.97310E+09

MASS FRACTION SUM 1.00000

TIME	2.50933E-04	SEC
AXIAL POSITION	3.95000E+01	CM
AREA	1.21292E+03	SQ CM

FLOW PROPERTIES

PRESSURE	1.7300	ATM
VELOCITY	157412.62	CM/SEC
TEMPERATURE	1960.59184	K
DENSITY	2.98088E-04	GM/CC
FLOW RATE	5.69139E+04	GM/SEC
ENTROPY	2.23128	CAL/GM-K
MACH NUMBER	1.81528	
GAMMA	1.27872	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CH4	8.31137E-03	-2.30345E-02
CH3	7.99783E-03	9.97817E-04
H	8.20091E-04	2.33859E-03
O2	1.50997E-01	-3.97860E-02
HO2	6.49329E-04	-6.21242E-04
CO	2.24805E-02	3.32716E-02
CO2	5.09655E-04	1.65068E-03
O	6.58033E-04	2.27144E-03
CH2O	9.23084E-03	-1.32438E-02
OH	1.76173E-03	5.98946E-03
H2	5.59512E-03	4.91617E-03
H2O	5.26082E-02	4.88687E-02
HCO	3.72950E-04	3.58210E-04
H2O2	6.04993E-07	-1.25814E-06
N2	7.38107E-01	0.

MIXTURE MOLECULAR WEIGHT 27.72016

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) -3.07243E+10

MASS FRACTION SUM 1.00000

TIME	2.54109E-04	SEC
AXIAL POSITION	4.00000E+01	CM
AREA	1.29715E+03	SQ CM

FLOW PROPERTIES

PRESSURE	1.7300	ATM
VELOCITY	157412.62	CM/SEC
TEMPERATURE	2078.62431	K
DENSITY	2.78732E-04	GM/CC
FLOW RATE	5.69139E+04	GM/SEC
ENTROPY	2.26361	CAL/GM-K
MACH NUMBER	1.75419	
GAMMA	1.28042	

MIXTURE MOLECULAR WEIGHT 28.03260

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) -7.94144E+09

MASS FRACTION SUM 1.00000

TIME	2.50933E-04	SEC
AXIAL POSITION	3.95000E+01	CM
AREA	1.21277E+03	SQ CM

FLOW PROPERTIES

PRESSURE	1.7300	ATM
VELOCITY	157412.62	CM/SEC
TEMPERATURE	1959.49192	K
DENSITY	2.98126E-04	GM/CC
FLOW RATE	5.69139E+04	GM/SEC
ENTROPY	2.23102	CAL/GM-K
MACH NUMBER	1.81583	
GAMMA	1.27873	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CH4	8.32595E-03	-2.27184E-02
CH3	8.00604E-03	8.31825E-04
H	8.10823E-04	2.44013E-03
O2	1.51059E-01	-3.94402E-02
HO2	5.54966E-04	-6.56142E-04
CO	2.24335E-02	3.31149E-02
CO2	5.06834E-04	1.62725E-03
O	6.47805E-04	2.27032E-03
CH2O	9.26052E-03	-1.30184E-02
OH	1.73896E-03	6.13052E-03
H2	5.58413E-03	4.88948E-03
H2O	5.25660E-02	4.92806E-02
HCO	3.72564E-04	1.62834E-04
H2O2	6.14653E-07	-1.28435E-06
N2	7.38142E-01	0.

MIXTURE MOLECULAR WEIGHT 27.72146

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) -3.04127E+10

MASS FRACTION SUM 1.00000

TIME	2.54109E-04	SEC
AXIAL POSITION	4.00000E+01	CM
AREA	1.29673E+03	SQ CM

FLOW PROPERTIES

PRESSURE	1.7300	ATM
VELOCITY	157412.62	CM/SEC
TEMPERATURE	2076.51071	K
DENSITY	2.78824E-04	GM/CC
FLOW RATE	5.69139E+04	GM/SEC
ENTROPY	2.26315	CAL/GM-K
MACH NUMBER	1.75515	
GAMMA	1.28042	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CH4	2.18565E-03	-1.39210E-02
CH3	5.66219E-03	-1.82386E-02
H	2.02896E-03	5.75116E-03
O2	1.33923E-01	-6.47151E-02
HO2	2.82510E-04	-9.40159E-04
CO	3.43716E-02	4.25808E-02
CO2	1.59060E-03	6.64321E-03
O	2.37707E-03	1.15680E-02
CH2O	4.28719E-03	-1.65838E-02
OH	5.43216E-03	1.97430E-02
H2	6.34510E-03	-1.44710E-03
H2O	6.94002E-02	6.11915E-02
HCO	3.83470E-04	-4.80585E-04
H2O2	7.26137E-07	2.52739E-06
N2	7.31730E-01	0.

MIXTURE MOLECULAR WEIGHT	27.48066
TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)	-5.20843E+10
MASS FRACTION SUM	1.00000

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CH4	2.20104E-03	-1.37537E-02
CH3	5.71294E-03	-1.92201E-02
H	2.00954E-03	5.66629E-03
O2	1.34079E-01	-6.43430E-02
HO2	2.86058E-04	-9.50681E-04
CO	3.42891E-02	4.25529E-02
CO2	1.57436E-03	6.55081E-03
O	2.33203E-03	1.15791E-02
CH2O	4.32219E-03	-1.64546E-02
OH	5.36659E-03	1.97101E-02
H2	6.34921E-03	-1.35412E-03
H2O	6.93022E-02	6.07685E-02
HCO	3.85113E-04	-6.75137E-04
H2O2	7.19690E-07	2.53571E-06
N2	7.31790E-01	0.

MIXTURE MOLECULAR WEIGHT	27.48292
TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)	-5.17694E+10
MASS FRACTION SUM	1.00000

Check Case 6

TIME-AREA VERSION GENERAL CHEMICAL KINETICS PROGRAM NASA LANGLEY RESEARCH CENTER
LANGLEY VERSION OF LEWIS PROGRAM (TN D-6586) USING STIFF ODE
SOLUTION TECHNIQUE DEVELOPED BY C.W. GEAR

METHANE - AIR COMBUSTION (ASSIGNED AREA - TIME INTEGRATION) CASE 6

REACTION NUMBER	REACTION	REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1*CH4 = 1*CH3 + 1*H	3.80000E+14	0.0000	103000.00
2	1*CH4 + 1*O2 = 1*CH3 + 1*HO2	1.00000E+13	0.0000	53000.00
3	1*H + 1*O2 = 1*HO2 + M	1.59000E+15	0.0000	-1000.00
4	1*CO + 1*O2 = 1*CO2 + 1*O	1.60000E+13	0.0000	41000.00
5	1*CH3 + 1*O2 = 1*CH2O + 1*OH	7.50000E+10	0.0000	0.00
6	1*H + 1*CH4 = 1*CH3 + 1*H2	6.90000E+13	0.0000	11800.00
7	1*O + 1*CH4 = 1*CH3 + 1*OH	2.00000E+13	0.0000	9200.00
8	1*OH + 1*CH4 = 1*CH3 + 1*H2O	7.20000E+13	0.0000	5900.00
9	1*H + 1*O2 = 1*OH + 1*O	1.25000E+14	0.0000	16300.00
10	1*O + 1*H2 = 1*OH + 1*H	2.96000E+13	0.0000	9800.00
11	1*H2 + 1*OH = 1*H2O + 1*H	2.10000E+13	0.0000	5100.00
12	1*CO + 1*OH = 1*CO2 + 1*H	4.20000E+11	0.0000	1000.00
13	1*CH3 + 1*O = 1*CH2O + 1*H	1.90000E+13	0.0000	0.00
14	1*CH2O + 1*H = 1*HCO + 1*H2	1.00000E+13	0.0000	2000.00
15	1*CH2O + 1*OH = 1*HCO + 1*H2O	7.00000E+10	.7000	1000.00
16	1*CH2O + 1*O = 1*HCO + 1*OH	4.00000E+11	.6000	4000.00
17	1*HCO + 1*O = 1*CO + 1*OH	1.80000E+11	.5000	0.00
18	1*HCO + 1*OH = 1*CO + 1*H2O	1.10000E+11	.5000	0.00
19	1*HCO + 1*H = 1*CO + 1*H2	1.50000E+12	.5000	0.00
20	M + 1*HCO = 1*H + 1*CO	2.00000E+13	.5000	28600.00
21	1*HCO + 1*O2 = 1*CO + 1*HO2	1.00000E+11	.5000	5400.00
22	1*HO2 + 1*HO2 = 1*H2O2 + 1*O2	1.80000E+12	0.0000	0.00
23	1*H + 1*HO2 = 1*OH + 1*OH	7.00000E+13	0.0000	0.00
24	1*O + 1*HO2 = 1*OH + 1*O2	6.00000E+12	0.0000	0.00
25	1*OH + 1*HO2 = 1*H2O + 1*O2	6.00000E+12	0.0000	0.00
26	M + 1*H2O2 = 1*OH + 1*OH	1.17000E+17	0.0000	45500.00
27	1*H + 1*OH = 1*H2O + M	7.50000E+23	-2.6000	0.00
28	M + 1*O2 = 1*O + 1*O	2.75000E+19	-1.0000	118700.00
29	1*O + 1*H2O = 1*OH + 1*OH	5.75000E+13	0.0000	18000.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(CH4	,3) =	5.00000	M(O2	,3) =	2.00000	M(O2	,26) =	.78000	M(O2	,27) =	1.60000
M(CO	,3) =	2.00000	M(CO2	,3) =	7.50000	M(H2	,3) =	5.00000	M(H2O	,3) =	32.50000
M(H2O	,26) =	6.00000	M(H2O	,27) =	20.00000	M(H2O2	,26) =	6.60000	M(N2	,3) =	2.00000
M(N2	,27) =	1.60000									

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

STATION	AXIAL DISTANCE (CM)	AREA (CM**2)
1	0.	10.00000E+02
2	50.00000E-01	10.00450E+02
3	10.00000E+00	10.02020E+02
4	15.00000E+00	10.04830E+02

5	20.00000E+00	10.09240E+02
6	25.00000E+00	10.16160E+02
7	30.00000E+00	10.28320E+02
8	35.00000E+00	10.57020E+02
9	36.00000E+00	10.68700E+02
10	37.00000E+00	10.85550E+02
11	38.00000E+00	11.12400E+02
12	39.00000E+00	11.63570E+02
13	40.00000E+00	12.96590E+02
14	40.50000E+00	13.71480E+02
15	41.00000E+00	13.84470E+02
16	42.00000E+00	14.00450E+02

** INITIAL CONDITIONS **

TIME	0.	SEC
AXIAL POSITION	0.	CM
AREA	1.00000E+03	SQ CM

FLOW PROPERTIES

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

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CH4	4.97680E-02	-5.08397E-06
CH3	0.	5.08397E-06
H	0.	5.01454E-06
O2	1.99072E-01	-6.95166E-08
HO2	0.	6.94238E-08
CO	0.	0.
CO2	0.	0.
O	0.	1.85618E-10
CH2O	0.	0.
OH	0.	0.
H2	0.	0.
H2O	0.	0.
HCO	0.	0.
H2O2	0.	0.
N2	7.51160E-01	0.

MIXTURE MOLECULAR WEIGHT	28.21038
TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)	4.05133E+06
MASS FRACTION SUM	1.00000

TIME	0.	SEC
AXIAL POSITION	0.	CM
AREA	1.00000E+03	SQ CM

FLOW PROPERTIES

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

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CH4	4.97680E-02	-5.08397E-06
CH3	0.	5.08397E-06
H	0.	5.01454E-06
O2	1.99072E-01	-6.95166E-08
HO2	0.	6.94238E-08
CO	0.	0.
CO2	0.	0.
O	0.	1.85619E-10
CH2O	0.	0.
OH	0.	0.
H2	0.	0.
H2O	0.	0.
HCO	0.	0.
H2O2	0.	0.
N2	7.51160E-01	0.

MIXTURE MOLECULAR WEIGHT	28.21038
TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)	4.05133E+06
MASS FRACTION SUM	1.00000

TIME	1.90582E-04	SEC
AXIAL POSITION	3.00002E+01	CM
AREA	1.02832E+03	SQ CM

FLOW PROPERTIES

PRESSURE	1.7300	ATM
VELOCITY	157413.08	CM/SEC
TEMPERATURE	1690.79471	K
DENSITY	3.51600E-04	GM/CC
FLOW RATE	5.69139E+04	GM/SEC
ENTROPY	2.14503	CAL/GM-K
MACH NUMBER	1.97302	
GAMMA	1.27678	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CH4	4.29476E-02	-1.57162E-03
CH3	6.12851E-04	1.85626E-04
H	4.13962E-06	2.21851E-06
O2	1.92442E-01	-1.53425E-03
HO2	7.36425E-05	3.21742E-05
CO	4.44640E-04	2.21395E-04
CO2	2.60643E-06	1.45027E-06
O	5.91879E-06	2.56913E-06
CH2O	5.73320E-03	1.16069E-03
OH	1.77416E-05	6.03174E-06
H2	1.72616E-04	7.46127E-05
H2O	6.72031E-03	1.60801E-03
HCO	4.41962E-06	2.46056E-06
H2O2	6.21163E-08	4.84032E-08
N2	7.50818E-01	0.

MIXTURE MOLECULAR WEIGHT	28.19754	
TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)	-7.76338E+08	
MASS FRACTION SUM	1.00000	

TIME	2.22346E-04	SEC
AXIAL POSITION	3.49996E+01	CM
AREA	1.05702E+03	SQ CM

FLOW PROPERTIES

PRESSURE	1.7300	ATM
VELOCITY	157412.75	CM/SEC
TEMPERATURE	1735.80559	K
DENSITY	3.42056E-04	GM/CC
FLOW RATE	5.69139E+04	GM/SEC
ENTROPY	2.15903	CAL/GM-K
MACH NUMBER	1.94640	
GAMMA	1.27628	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CH4	3.61125E-02	-4.42863E-03

TIME	1.90582E-04	SEC
AXIAL POSITION	3.00002E+01	CM
AREA	1.02832E+03	SQ CM

FLOW PROPERTIES

PRESSURE	1.7300	ATM
VELOCITY	157412.54	CM/SEC
TEMPERATURE	1690.91472	K
DENSITY	3.51602E-04	GM/CC
FLOW RATE	5.69140E+04	GM/SEC
ENTROPY	2.14503	CAL/GM-K
MACH NUMBER	1.97300	
GAMMA	1.27677	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CH4	4.29457E-02	-1.57167E-03
CH3	6.12969E-04	1.85636E-04
H	4.13754E-06	2.37972E-06
O2	1.92440E-01	-1.53433E-03
HO2	7.37145E-05	3.20314E-05
CO	4.44866E-04	2.21333E-04
CO2	2.60940E-06	1.45120E-06
O	5.91731E-06	2.52602E-06
CH2O	5.73476E-03	1.16090E-03
OH	1.77429E-05	6.10140E-06
H2	1.72671E-04	7.45702E-05
H2O	6.72229E-03	1.60915E-03
HCO	4.41808E-06	2.57632E-06
H2O2	6.22105E-08	4.88421E-08
N2	7.50818E-01	0.

MIXTURE MOLECULAR WEIGHT	28.19754	
TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)	-7.76430E+08	
MASS FRACTION SUM	1.00000	

TIME	2.22346E-04	SEC
AXIAL POSITION	3.49995E+01	CM
AREA	1.05702E+03	SQ CM

FLOW PROPERTIES

PRESSURE	1.7302	ATM
VELOCITY	157409.58	CM/SEC
TEMPERATURE	1735.91415	K
DENSITY	3.42068E-04	GM/CC
FLOW RATE	5.69147E+04	GM/SEC
ENTROPY	2.15905	CAL/GM-K
MACH NUMBER	1.94630	
GAMMA	1.27629	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CH4	3.61028E-02	-4.42845E-03

CH3	1.68287E-03	8.61069E-04
H	2.33484E-05	2.02244E-05
O2	1.85538E-01	-4.38417E-03
HO2	2.56585E-04	1.37689E-04
CO	1.97045E-03	1.37821E-03
CO2	1.39392E-05	1.13446E-05
O	2.39028E-05	1.67786E-05
CH2O	9.87690E-03	2.15669E-03
OH	5.91814E-05	3.90672E-05
H2	6.72523E-04	4.42029E-04
H2O	1.38825E-02	4.85736E-03
HCO	2.52987E-05	2.13211E-05
H2O2	5.15245E-07	4.30475E-07
N2	7.49862E-01	0.

MIXTURE MOLECULAR WEIGHT 28.16162

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) -2.26827E+09

MASS FRACTION SUM 1.00000

TIME	2.54109E-04	SEC
AXIAL POSITION	4.00003E+01	CM
AREA	1.29664E+03	SQ CM

FLOW PROPERTIES

PRESSURE	1.7311	ATM
VELOCITY	157368.41	CM/SEC
TEMPERATURE	2078.68636	K
DENSITY	2.78921E-04	GM/CC
FLOW RATE	5.69139E+04	GM/SEC
ENTROPY	2.26347	CAL/GM-K
MACH NUMBER	1.75375	
GAMMA	1.28038	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CH4	2.21248E-03	-1.40216E-02
CH3	5.68544E-03	-1.79905E-02
H	2.01047E-03	5.74350E-03
O2	1.34044E-01	-6.45020E-02
HO2	2.83884E-04	-9.62762E-04
CO	3.43058E-02	4.25487E-02
CO2	1.57981E-03	6.57962E-03
O	2.34793E-03	1.15102E-02
CH2O	4.31781E-03	-1.66320E-02
OH	5.38042E-03	1.97998E-02
H2	6.34734E-03	-1.41261E-03
H2O	6.93203E-02	6.10230E-02
HCO	3.82689E-04	-4.84237E-04
H2O2	7.14304E-07	2.44901E-06
N2	7.31781E-01	0.

MIXTURE MOLECULAR WEIGHT 27.48257

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) -5.16937E+10

MASS FRACTION SUM 1.00000

CH3	1.68382E-03	8.59900E-04
H	2.33357E-05	2.20172E-05
O2	1.85527E-01	-4.38435E-03
HO2	2.57229E-04	1.35795E-04
CO	1.97286E-03	1.37822E-03
CO2	1.39728E-05	1.13644E-05
O	2.38941E-05	1.67628E-05
CH2O	9.88311E-03	2.15736E-03
OH	5.91909E-05	4.03096E-05
H2	6.73051E-04	4.41865E-04
H2O	1.38932E-02	4.85830E-03
HCO	2.52999E-05	2.21093E-05
H2O2	5.18036E-07	4.10711E-07
N2	7.49861E-01	0.

MIXTURE MOLECULAR WEIGHT 28.16158

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) -2.26866E+09

MASS FRACTION SUM 1.00000

TIME	2.54107E-04	SEC
AXIAL POSITION	3.99995E+01	CM
AREA	1.29650E+03	SQ CM

FLOW PROPERTIES

PRESSURE	1.7367	ATM
VELOCITY	157250.54	CM/SEC
TEMPERATURE	2082.84429	K
DENSITY	2.79202E-04	GM/CC
FLOW RATE	5.69225E+04	GM/SEC
ENTROPY	2.26419	CAL/GM-K
MACH NUMBER	1.75350	
GAMMA	1.28040	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CH4	2.10663E-03	-1.35256E-02
CH3	5.58811E-03	-1.87323E-02
H	2.04686E-03	5.79923E-03
O2	1.33606E-01	-6.54159E-02
HO2	2.77554E-04	-9.67421E-04
CO	3.45721E-02	4.26963E-02
CO2	1.61967E-03	6.80391E-03
O	2.41513E-03	1.21893E-02
CH2O	4.20829E-03	-1.65463E-02
OH	5.50839E-03	2.04509E-02
H2	6.33614E-03	-1.65905E-03
H2O	6.97018E-02	6.10606E-02
HCO	3.79407E-04	-6.99053E-04
H2O2	7.27590E-07	2.57139E-06
N2	7.31633E-01	0.

MIXTURE MOLECULAR WEIGHT 27.47702

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) -5.18094E+10

MASS FRACTION SUM 1.00000

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11/19/75  LRC ICOPS INDEPNDT 6400A-131K 01/21/75D
19.33.42.GT05669.
19.33.42.                          LRC COMPUTER COMPLEX
19.33.42.JOB,1,00500,120000,002000.      A4409   R
19.33.42.3274       100681         8-1250
19.33.42.USER.   ALLEN G. MCLAIN                0005
19.33.42.89803N 64730
19.33.42.WAITGO.   PLEASE RUN ON 6400 ONLY
19.34.16.GO.
19.34.16.LINECNT(10000)
19.34.17.FETCH(A4409,,BINARY)
19.34.28.TIME        BG ATTACH
19.38.01.TIME        ED ATTACH
19.38.02.END     FETCH
19.38.03.UPDATE(Q,C=TAPE4,P=BNFILE,D,8)
19.38.10.READING INPUT
19.38.22.UPDATE COMPLETE
19.38.22.UPDATE(Q,P=BNFILE)
19.38.29.READING INPUT
19.38.41.UPDATE COMPLETE
19.38.42.RUN(S,,,COMPILE)
19.39.21.SETINDF.
19.39.23.LGO.
19.39.58.MEMORY  071100 CM
19.39.58.REL       0000565 O/S CALLS
19.39.58.REL CPU     47.072926 SEC.
19.43.33.STOP
19.43.34.SPRINT(OUTPUT,3)
19.43.36.      0000633 O/S CALLS
19.43.36.CPU    217.330763 SEC.
19.43.36.PPU    320.770048 SEC.
19.43.38.COST OF THIS JOB WAS $   14
19.43.38.KWH      3.61      KILOWORD HOURS.
21.16.11. GT05669.    6997 LINES PRINTED. LP23
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11/14/75  LRC ICOPS INDEPNDT 6400A-131K 01/21/75D
20.53.59.GT05664.
20.53.59.                          LRC COMPUTER COMPLEX
20.53.59.JOB,1,00500,120000,002000.      A4409   R
20.53.59.3274       100681         8-1250
20.53.59.USER.   ALLEN G. MCLAIN                0005
20.53.59.89803N 64730
20.53.59.LINECNT(10000)
20.54.00.FETCH(A4409,,BINARY)
20.54.06.TIME        BG ATTACH
20.54.45.TIME        ED ATTACH
20.54.45.END     FETCH
20.54.46.UPDATE(Q,C=TAPE4,P=BNFILE,D,8)
20.54.50.READING INPUT
20.55.00.UPDATE COMPLETE
20.55.00.UPDATE(Q,P=BNFILE)
20.55.04.READING INPUT
20.55.12.UPDATE COMPLETE
20.55.13.RUN(S,,,COMPILE)
20.56.16.SETINDF.
20.56.17.LGO.
20.56.47.MEMORY  066700 CM
20.56.47.REL       0000707 O/S CALLS
20.56.47.REL CPU     46.695533 SEC.
21.03.34.ROLLOUT WAITING ON ALL QUIET.
21.03.34.ROLLOUT INITIATED.
21.03.35.ROLLOUT COMPLETED.  FL  066700
21.07.34.ROLLIN INITIATED.
21.07.34.ROLLIN COMPLETED.
21.20.24.STOP
21.20.25.SPRINT(OUTPUT,3)
21.20.26.      0000776 O/S CALLS
21.20.26.CPU    719.256013 SEC.
21.20.26.PPU    145.596416 SEC.
21.20.27.COST OF THIS JOB WAS $   30
21.20.27.KWH      7.39      KILOWORD HOURS
21.38.23. GT05664.    6829 LINES PRINTED. LP24
```

Check Case 8

TIME-AREA VERSION

GENERAL CHEMICAL KINETICS PROGRAM NASA LANGLEY RESEARCH CENTER
LANGLEY VERSION OF LEWIS PROGRAM (TN D-6586) USING STIFF ODE
SOLUTION TECHNIQUE DEVELOPED BY C.W. GEAR

H2-02 LOW TEMPERATURE REACTION AT CONSTANT VOLUME (ADJUSTED RATES) C-8

REACTION NUMBER	REACTION	REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1*H2 + 1*02 = 1*H + 1*H02	1.00000E+14	0.0000	67000.00
2	1*H2 + 1*OH = 1*H20 + 1*H	2.10000E+13	0.0000	5100.00
3	1*H + 1*02 = 1*OH + 1*O	1.25000E+14	0.0000	16300.00
4	1*O + 1*H2 = 1*OH + 1*H	2.96000E+13	0.0000	9800.00
5	1*H + 1*02 = 1*H02 + M	8.50000E+14	0.0000	-1000.00
6	1*H + 1*H02 = 1*OH + 1*OH	7.00000E+13	0.0000	0.00
7	M + 1*H202 = 1*OH + 1*OH	1.17000E+17	0.0000	45500.00
8	1*H02 + 1*H02 = 1*H202 + 1*02	1.00000E+12	0.0000	0.00
9	1*H02 + 1*H2 = 1*H202 + 1*H	8.50000E+12	0.0000	24000.00
10	1*H + 1*H202 = 1*H20 + 1*OH	3.18000E+14	0.0000	9000.00
11	1*OH + 1*H202 = 1*H20 + 1*H02	1.00000E+13	0.0000	1800.00
12	1*O + 1*H20 = 1*OH + 1*OH	5.75000E+13	0.0000	18000.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2 , 5) = 5.00000	M(H2 , 7) = 2.30000	M(02 , 5) = 2.00000	M(02 , 7) = .78000
M(H20 , 5) = 32.50000	M(H20 , 7) = 6.00000	M(H202 , 7) = 6.60000	

INTEGRATION CONTROLS

MINIMUM STEP SIZE 5.00000E-05 SEC
MAXIMUM STEP SIZE 1.00000E-01 SEC
INITIAL STEP SIZE 5.00000E-05 SEC
MAXIMUM RELATIVE ERROR .00030

** ASSIGNED VARIABLE PROFILE **

THIS IS A V=0 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 **

TIME	0.	SEC
AXIAL POSITION	0.	CM
AREA	1.00000E+00	SQ CM

FLOW PROPERTIES

PRESSURE	.6579	ATM
VELOCITY	0.00	CM/SEC
TEMPERATURE	773.15000	K
DENSITY	6.44320E-05	GM/CC
FLOW RATE	0.	GM/SEC
ENTROPY	6.76838	CAL/GM-K
MACH NUMBER	0.00000	
GAMMA	1.38099	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
H2	8.60000E-01	-1.48936E-16
O2	1.40000E-01	-1.48936E-16
H	0.	1.48936E-16
HO2	0.	1.48936E-16
OH	0.	0.
H2O	0.	0.
O	0.	0.
H2O2	0.	0.

MIXTURE MOLECULAR WEIGHT	6.21325
TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)	2.04835E-03
MASS FRACTION SUM	1.00000

TIME	0.	SEC
AXIAL POSITION	0.	CM
AREA	1.00000E+00	SQ CM

FLOW PROPERTIES

PRESSURE	.6579	ATM
VELOCITY	0.00	CM/SEC
TEMPERATURE	773.15000	K
DENSITY	6.44320E-05	GM/CC
FLOW RATE	0.	GM/SEC
ENTROPY	6.76838	CAL/GM-K
MACH NUMBER	0.00000	
GAMMA	1.38099	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
H2	8.60000E-01	-1.48936E-16
O2	1.40000E-01	-1.48936E-16
H	0.	1.48936E-16
HO2	0.	1.48936E-16
OH	0.	0.
H2O	0.	0.
O	0.	0.
H2O2	0.	0.

MIXTURE MOLECULAR WEIGHT	6.21325
TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)	2.04835E-03
MASS FRACTION SUM	1.00000

TIME	7.50000E-01	SEC
AXIAL POSITION	0.	CM
AREA	1.00000E+00	SQ CM

FLOW PROPERTIES

PRESSURE	.6579	ATM
VELOCITY	0.00	CM/SEC
TEMPERATURE	773.15000	K
DENSITY	6.44320E-05	GM/CC
FLOW RATE	0.	GM/SEC
ENTROPY	6.76838	CAL/GM-K
MACH NUMBER	0.00000	
GAMMA	1.38099	

TIME	7.50000E-01	SEC
AXIAL POSITION	0.	CM
AREA	1.00000E+00	SQ CM

FLOW PROPERTIES

PRESSURE	.6579	ATM
VELOCITY	0.00	CM/SEC
TEMPERATURE	773.15000	K
DENSITY	6.44320E-05	GM/CC
FLOW RATE	0.	GM/SEC
ENTROPY	6.76838	CAL/GM-K
MACH NUMBER	0.00000	
GAMMA	1.38099	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
H2	8.60000E-01	-1.22446E-14
O2	1.40000E-01	-1.23927E-14
H	1.01087E-14	3.80572E-19
HO2	7.15229E-11	2.68112E-15
OH	3.39462E-17	1.37390E-21
H2O	5.00034E-11	2.38470E-15
O	1.01055E-16	3.80825E-21
H2O2	2.00160E-10	8.51919E-15

MIXTURE MOLECULAR WEIGHT 6.21325

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) -9.67218E-02

MASS FRACTION SUM 1.00000

TIME	5.50000E+01	SEC
AXIAL POSITION	0.	CM
AREA	1.00000E+00	SQ CM

FLOW PROPERTIES

PRESSURE	.6444	ATM
VELOCITY	0.00	CM/SEC
TEMPERATURE	773.15000	K
DENSITY	6.44320E-05	GM/CC
FLOW RATE	0.	GM/SEC
ENTROPY	6.72769	CAL/GM-K
MACH NUMBER	0.00000	
GAMMA	1.37565	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
H2	8.37384E-01	-1.29231E-08
O2	1.22014E-01	-6.46021E-09
H	9.27539E-09	-5.38189E-14
HO2	6.91938E-06	5.24911E-14
OH	1.79854E-10	5.00423E-14
H2O	3.93768E-02	1.29259E-08
O	8.29587E-11	-1.05702E-15
H2O2	1.21796E-03	-2.80672E-12

MIXTURE MOLECULAR WEIGHT 6.34317

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) -1.79930E+05

MASS FRACTION SUM 1.00000

TIME	7.50000E+01	SEC
AXIAL POSITION	0.	CM
AREA	1.00000E+00	SQ CM

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
H2	8.60000E-01	-1.41740E-14
O2	1.40000E-01	-1.43218E-14
H	1.17015E-14	4.36892E-19
HO2	8.27395E-11	3.08676E-15
OH	3.97266E-17	4.54205E-21
H2O	6.12251E-11	2.79077E-15
O	1.16977E-16	4.38231E-21
H2O2	2.35896E-10	9.83962E-15

MIXTURE MOLECULAR WEIGHT 6.21325

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) -1.12233E-01

MASS FRACTION SUM 1.00000

TIME	5.50000E+01	SEC
AXIAL POSITION	0.	CM
AREA	1.00000E+00	SQ CM

FLOW PROPERTIES

PRESSURE	.6443	ATM
VELOCITY	0.00	CM/SEC
TEMPERATURE	773.15000	K
DENSITY	6.44320E-05	GM/CC
FLOW RATE	0.	GM/SEC
ENTROPY	6.72737	CAL/GM-K
MACH NUMBER	0.00000	
GAMMA	1.37562	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
H2	8.37240E-01	-1.29193E-08
O2	1.21906E-01	-6.46485E-09
H	9.27814E-09	-6.75857E-12
HO2	6.91917E-06	6.82906E-12
OH	1.79881E-10	1.70275E-12
H2O	3.96297E-02	1.29224E-08
O	8.29234E-11	3.82347E-18
H2O2	1.21758E-03	-4.01829E-12

MIXTURE MOLECULAR WEIGHT 6.34396

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) -1.79944E+05

MASS FRACTION SUM 1.00000

TIME	7.50000E+01	SEC
AXIAL POSITION	0.	CM
AREA	1.00000E+00	SQ CM

FLOW PROPERTIES

PRESSURE	.6362	ATM
VELOCITY	0.00	CM/SEC
TEMPERATURE	773.15000	K
DENSITY	6.44320E-05	GM/CC
FLOW RATE	0.	GM/SEC
ENTROPY	6.69235	CAL/GM-K
MACH NUMBER	0.00000	
GAMMA	1.37253	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
H2	8.22418E-01	-1.27922E-08
O2	1.10740E-01	-6.38249E-09
H	9.33498E-09	-9.88363E-15
HO2	7.00003E-06	-2.54685E-14
OH	1.86848E-10	9.62672E-15
H2O	6.56383E-02	1.28195E-08
O	7.71320E-11	1.27907E-16
H2O2	1.19672E-03	-2.72307E-11

MIXTURE MOLECULAR WEIGHT 6.42463

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) -1.78257E+05

MASS FRACTION SUM 1.00000

TIME	1.20000E+02	SEC
AXIAL POSITION	0.	CM
AREA	1.00000E+00	SQ CM

FLOW PROPERTIES

PRESSURE	.6187	ATM
VELOCITY	0.00	CM/SEC
TEMPERATURE	773.15000	K
DENSITY	6.44320E-05	GM/CC
FLOW RATE	0.	GM/SEC
ENTROPY	6.60429	CAL/GM-K
MACH NUMBER	0.00000	
GAMMA	1.36576	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
H2	7.88884E-01	-1.17385E-08
O2	8.55376E-02	-5.84898E-09
H	9.62950E-09	1.10515E-14
HO2	6.92048E-06	-1.06095E-13
OH	1.90355E-10	4.28070E-14
H2O	1.24502E-01	1.17790E-08
O	6.40247E-11	-2.67377E-15
H2O2	1.06983E-03	-4.04054E-11

MIXTURE MOLECULAR WEIGHT 6.60670

FLOW PROPERTIES

PRESSURE	.6362	ATM
VELOCITY	0.00	CM/SEC
TEMPERATURE	773.15000	K
DENSITY	6.44320E-05	GM/CC
FLOW RATE	0.	GM/SEC
ENTROPY	6.69201	CAL/GM-K
MACH NUMBER	0.00000	
GAMMA	1.37250	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
H2	8.22279E-01	-1.27838E-08
O2	1.10635E-01	-6.38714E-09
H	9.33808E-09	-8.94984E-12
HO2	6.99833E-06	8.91978E-12
OH	1.86891E-10	2.45884E-12
H2O	6.59827E-02	1.28111E-08
O	7.70978E-11	-3.91051E-17
H2O2	1.19593E-03	-2.95627E-11

MIXTURE MOLECULAR WEIGHT 6.42538

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) -1.78225E+05

MASS FRACTION SUM 1.00000

TIME	1.20000E+02	SEC
AXIAL POSITION	0.	CM
AREA	1.00000E+00	SQ CM

FLOW PROPERTIES

PRESSURE	.6187	ATM
VELOCITY	0.00	CM/SEC
TEMPERATURE	773.15000	K
DENSITY	6.44320E-05	GM/CC
FLOW RATE	0.	GM/SEC
ENTROPY	6.60396	CAL/GM-K
MACH NUMBER	0.00000	
GAMMA	1.36574	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
H2	7.88763E-01	-1.17287E-08
O2	8.54473E-02	-5.85031E-09
H	9.63284E-09	-6.19290E-12
HO2	6.91798E-06	6.10812E-12
OH	1.90263E-10	1.96408E-12
H2O	1.24714E-01	1.17692E-08
O	6.39881E-11	-6.87315E-17
H2O2	1.06893E-03	-4.13550E-11

MIXTURE MOLECULAR WEIGHT 6.60736

```
TOTAL ENERGY EXCHANGE RATE   -1.63667E+05
   (CAL-CM3/GM2/SEC)

MASS FRACTION SUM                    .99999

11/19/75  LRC ICOPS INDEPNDT 66000-131K 01/21/75D
17.42.09.GT02854.
17.42.09.                        LRC COMPUTER COMPLEX
17.42.09.JOB,1,00300,120000,002000.      A4409    R
17.42.09.3274       100681         B-1250
17.42.09.USER.   ALLEN G. MCLAIN                0005
17.42.09.89803N 64730
17.42.09.WAITGO.    PLEASE RUN ON 6600 ONLY
17.42.13.GO.
17.42.13.LINECNT(10000)
17.42.14.FETCH(A4409,,BINARY)
17.42.19.TIME        BG ATTACH
17.42.55.TIME        EO ATTACH
17.42.56.END     FETCH
17.42.57.UPDATE(Q,C=TAPE4,P=BNFILE,D,8)
17.43.00.READING INPUT
17.43.09.UPDATE COMPLETE
17.43.10.UPDATE(Q,P=BNFILE)
17.43.13.READING INPUT
17.43.19.UPDATE COMPLETE
17.43.20.RUN(S,,,COMPILE)
17.43.43.SETINDF.
17.43.44.LGO.
17.44.52.MEMORY  071100 CM
17.44.52.REL       0000597 O/S CALLS
17.44.52.REL CPU     27.758539 SEC.
17.45.24.STOP
17.45.25.SPPRINT(OUTPUT,3)
17.45.26.      0000636 O/S CALLS
17.45.26.CPU     46.955029 SEC.
17.45.26.PPU    125.710336 SEC.
17.45.27.COST OF THIS JOB WAS $   11
17.45.27.KWH      2.74      KILOWORD HOURS
20.58.21. GT02854.    6513 LINES PRINTED. LP23
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TOTAL ENERGY EXCHANGE RATE   -1.63589E+05
   (CAL-CM3/GM2/SEC)

MASS FRACTION SUM                    .99999

11/17/75  LRC ICOPS INDEPNDT 66000-131K 01/21/75D
19.56.31.GT05666.
19.56.31.                        LRC COMPUTER COMPLEX
19.56.31.JOB,1,00300,120000,002000.      A4409    R
19.56.31.3274       100681         B-1250
19.56.31.USER.   ALLEN G. MCLAIN                0005
19.56.31.89803N 64730
19.56.31.LINECNT(10000)
19.56.32.FETCH(A4409,,BINARY)
19.56.38.TIME        BG ATTACH
19.58.25.TIME        EO ATTACH
19.58.26.END     FETCH
19.58.27.UPDATE(Q,C=TAPE4,P=BNFILE,D,8)
19.58.31.READING INPUT
19.58.41.UPDATE COMPLETE
19.58.41.UPDATE(Q,P=BNFILE)
19.58.47.READING INPUT
19.58.52.UPDATE COMPLETE
19.58.53.RUN(S,,,COMPILE)
19.59.41.SETINDF.
19.59.43.LGO.
20.00.15.MEMORY  066700 CM
20.00.15.REL       0000539 O/S CALLS
20.00.15.REL CPU     27.098794 SEC.
20.01.30.STOP
20.01.30.SPPRINT(OUTPUT,3)
20.01.32.      0000578 O/S CALLS
20.01.32.CPU     67.082836 SEC.
20.01.32.PPU    204.734464 SEC.
20.01.32.COST OF THIS JOB WAS $   12
20.01.32.KWH      2.99      KILOWORD 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 (TN D-6586) USING STIFF ODE
SOLUTION TECHNIQUE DEVELOPED BY C.W. GEAR

********** PROPANE REACTIONS BY CHINITZ - BAURER 64 RXNS - 31 SPECIES ********

REACTION NUMBER	REACTION	REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1*CO + 1*O2 = 1*O + 1*CO2	1.60000E+13	0.0000	41100.00
2	M + 1*C3H8 = 1*C2H5 + 1*CH3	1.00000E+15	0.0000	28900.00
3	1*OH + 1*H2 = 1*H2O + 1*H	2.20000E+13	0.0000	5150.00
4	1*O + 1*H2 = 1*OH + 1*H	1.80000E+10	1.0000	8900.00
5	1*H + 1*OH = 1*H2O + M	7.50000E+23	-2.6000	0.00
6	1*C + 1*H2O = 1*OH + 1*OH	5.80000E+13	0.0000	19000.00
7	1*H + 1*H = 1*H2 + M	1.00000E+18	-1.0000	0.00
8	1*H2 + 1*O2 = 1*OH + 1*OH	1.70000E+13	0.0000	48200.00
9	1*CO + 1*O = 1*CO2 + M	4.00000E+13	0.0000	0.00
10	1*H + 1*O2 = 1*OH + 1*O	2.20000E+14	0.0000	16800.00
11	1*OH + 1*CO = 1*CO2 + 1*H	5.60000E+11	0.0000	1093.00
12	M + 1*O2 = 1*O + 1*O + M	2.60000E+19	-1.0000	118000.00
13	M + 1*CH4 = 1*CH3 + 1*H	4.00000E+17	0.0000	88421.00
14	1*CH4 + 1*O = 1*OH + 1*CH3	2.00000E+13	0.0000	9220.00
15	1*CH4 + 1*H = 1*CH3 + 1*H2	6.90000E+13	0.0000	11823.00
16	1*CH4 + 1*OH = 1*CH3 + 1*H2O	2.80000E+13	0.0000	4968.00
17	1*CH3 + 1*O = 1*CH2O + 1*H	1.95000E+13	0.0000	2000.00
18	M + 1*CH2O = 1*H2 + 1*CO	2.10000E+16	0.0000	35000.00
19	1*HCO + 1*OH = 1*CO + 1*H2O	2.00000E+13	0.0000	0.00
20	M + 1*HCO = 1*H + 1*CO	2.00000E+12	.5000	28613.00
21	1*CH2O + 1*OH = 1*HCO + 1*H2O	2.00000E+13	0.0000	0.00
22	1*CH3 + 1*O2 = 1*CH2O + 1*OH	1.20000E+12	0.0000	15000.00
23	1*C3H8 + 1*OH = 1*C3H7 + 1*H2O	1.00000E+11	.5000	7200.00
24	1*C3H8 + 1*O = 1*C2H6 + 1*CH2O	1.00000E+12	.5000	0.00
25	1*C3H8 + 1*H = 1*C3H7 + 1*H2	3.60000E+12	.5000	7200.00
26	1*C3H7 + 1*O = 1*C2H6CO + 1*H	8.80000E+11	.5000	0.00
27	1*C3H7 + 1*O = 1*C3H6 + 1*OH	9.80000E+11	.5000	0.00
28	1*C3H7 + 1*OH = 1*C3H6 + 1*H2O	9.80000E+10	.5000	0.00
29	1*C3H7 + 1*O2 = 1*C2H5CO + 1*OH	1.00000E+11	.5000	0.00
30	1*C3H6 + 1*O2 = 1*CH3CHO + 1*CH2O	9.80000E+10	.5000	0.00
31	1*C3H6 + 1*OH = 1*CH3CHO + 1*CH3	8.10000E+10	.5000	1000.00
32	1*C3H6 + 1*O = 1*C3H4 + 1*H2O	8.10000E+11	.5000	0.00
33	1*C3H6 + 1*O = 1*CH2O + 1*C2H4	8.10000E+11	.5000	0.00
34	1*C3H4 + 1*O2 = 1*CH3CO + 1*HCO	1.00000E+11	.5000	0.00
35	1*C2H6 + 1*O = 1*C2H5 + 1*OH	8.90000E+11	.5000	7000.00
36	1*C2H6 + 1*OH = 1*C2H5 + 1*H2O	8.90300E+10	.5000	5500.00
37	1*C2H6 + 1*H = 1*C2H5 + 1*H2	2.00000E+12	0.0000	6200.00
38	1*C2H6CO + 1*OH = 1*C2H5CO + 1*H2O	9.60000E+10	.5000	6700.00
39	1*C2H6CO + 1*H = 1*C2H5CO + 1*H2	3.50000E+12	.5000	10500.00
40	1*C2H5CO + 1*O = 1*C2H5 + 1*CO2	9.00000E+11	.5000	0.00
41	1*C2H5CO + 1*OH = 1*C2H5OH + 1*CO	9.00000E+10	.5000	0.00
42	1*C2H5CO + 1*O2 = 1*C2H4OH + 1*CO2	1.00000E+11	.5000	0.00
43	1*C2H5CO + 1*H = 1*C2H5 + 1*HCO	3.30000E+12	.5000	5300.00
44	1*C2H5OH + 1*H = 1*C2H5 + 1*H2O	3.00000E+12	.5000	4600.00
45	1*C2H4OH + 1*H = 1*C2H5 + 1*OH	3.00000E+12	.5000	9800.00
46	1*C2H5 + 1*O2 = 1*CH3CHO + 1*OH	1.10000E+11	.5000	0.00
47	1*C2H5 + 1*O = 1*C2H4 + 1*OH	8.80000E+11	.5000	0.00
48	1*C2H5 + 1*O = 1*CH3CHO + 1*H	8.80000E+11	.5000	0.00
49	1*C2H5 + 1*OH = 1*C2H4 + 1*H2O	8.90000E+10	.5000	0.00
50	1*CH3CHO + 1*OH = 1*CH3CO + 1*H2O	6.50000E+10	.5000	4000.00
51	1*CH3CHO + 1*H = 1*CH3CO + 1*H2	2.40000E+12	.5000	11000.00
52	1*CH3CO + 1*O = 1*CH3 + 1*CO2	6.10000E+11	.5000	0.00
53	1*CH3CO + 1*O2 = 1*CH2OH + 1*CO2	7.90000E+10	.5000	1500.00
54	1*CH3CO + 1*OH = 1*CH3OH + 1*CO	6.20000E+10	.5000	0.00
55	1*CH3CO + 1*H = 1*CH3 + 1*HCO	2.20000E+12	.5000	5400.00
56	1*CH3OH + 1*H = 1*CH3 + 1*H2O	2.30300E+12	.5000	5300.00
57	1*CH2OH + 1*H = 1*CH3 + 1*OH	2.20000E+12	.5000	10700.00
58	1*C2H4 + 1*O = 1*CH3 + 1*HCO	3.00000E+13	0.0000	0.00
59	1*C2H4 + 1*O = 1*C2H2 + 1*H2O	3.00000E+13	0.0000	0.00
60	1*C2H4 + 1*OH = 1*CH3 + 1*CH2O	1.00000E+11	.5000	7100.00
61	1*C2H2 + 1*O = 1*C2H + 1*OH	3.40300E+15	-.6400	18700.00

62	1*C2H2	+ 1*OH	=	1*C2H	+ 1*H2O	2.20000E+14	0.0000	7000.00
63	1*C2H	+ 1*O2	=	1*CH	+ 1*CO2	1.00000E+14	0.0000	23000.00
64	1*CH	+ 1*O2	=	1*CO	+ 1*OH	8.10000E+13	.5000	0.00

ALL THIRD BODY RATIOS ARE 1.0

INTEGRATION CONTROLS

MINIMUM STEP SIZE 1.00000E-05 CM MAXIMUM STEP SIZE 1.00000E-02 CM

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

** ASSIGNED VARIABLE PROFILE **

THE AREA IS CALCULATED FROM THE FOLLOWING FUNCTION

1/AREA = 1 - (X/ 136.700)**(.50000)

** EQUILIBRIUM SHOCK CALCULATION **

	INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE (ATM)	.0526	1.6543	31.4503
VELOCITY (CM/SEC)	167000.00	52127.85	.3121
DENSITY (GM/CM**3)	84.59816E-06	27.10239E-05	3.2037
TEMPERATURE (DEG K)	300.00	2855.91	9.5197
ENTROPY (CAL/GM/DEG K)	1.1175	1.2897	1.1541
MACH NUMBER	5.2328	.5877	.1123
GAMMA	1.6167	1.2721	.7869
SONIC VELOCITY (CM/SEC)	31913.93	88698.65	2.7793

SPECIES	MOLE FRACTION
CO	1.77123E-02
O2	8.88239E-03
O	4.89909E-03
CO2	1.13792E-02
C3H8	8.87498E-45
C2H5	1.87969E-29
CH3	7.14781E-15
OH	7.72594E-03
H2	5.87368E-03
H2O	2.61112E-02
H	5.88176E-03
CH4	3.09820E-16
CH2O	9.73995E-11
HCO	1.54604E-08
C3H7	1.68281E-43
C2H6	1.42840E-30
C2H6CO	3.11108E-38
C3H6	6.63878E-38
CH3CHO	2.95174E-24
C3H4	1.71713E-32
C2H4	3.13129E-24
CH3CO	2.19280E-22
C2H5CO	1.11779E-36
C2H5OH	1.08320E-31
C2H4OH	7.53468E-30
CH2OH	6.14808E-16
CH3OH	9.98426E-18
C2H2	1.48022E-18
C2H	2.37942E-18
CH	3.59896E-14
AR	9.11534E-01

MIXTURE MOLECULAR WEIGHT	38.39300
D(LOG VOLUME)/D(LOG T) AT CONSTANT P	1.1484E+00
D(LOG VOLUME)/D(LOG P) AT CONSTANT T	-1.0069E+00

** FROZEN SHOCK CALCULATION **

	INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE (ATM)	.0526	1.8090	34.3915
VELOCITY (CM/SEC)	167000.00	41032.16	.2457
DENSITY (GM/CM**3)	84.59816E-06	34.43127E-05	4.0700
TEMPERATURE (DEG K)	300.00	2535.02	8.4501
ENTROPY (CAL/GM/DEG K)	1.1175	1.2342	1.1044
MACH NUMBER	5.2328	.4541	.0868
GAMMA	1.6167	1.5338	.9488
SONIC VELOCITY (CM/SEC)	31913.93	90362.15	2.8314

SPECIES	MOLE FRACTION
CO	0.
O2	5.00000E-02
O	0.
CO2	0.
C3H8	1.00000E-02
C2H5	0.
CH3	0.
OH	0.
H2	0.
H2O	0.
H	0.
CH4	0.
CH2O	0.
HCO	0.
C3H7	0.
C2H6	0.
C2H6CO	0.
C3H6	0.
CH3CHO	0.
C3H4	0.
C2H4	0.
CH3CO	0.
C2H5CO	0.
C2H5OH	0.
C2H4OH	0.
CH2OH	0.
CH3OH	0.
C2H2	0.
C2H	0.
CH	0.
AR	9.40000E-01

MIXTURE MOLECULAR WEIGHT	39.59194
D(LOG VOLUME)/D(LOG T) AT CONSTANT P	1.0000E+00
D(LOG VOLUME)/D(LOG P) AT CONSTANT T	-1.0000E+00

** INITIAL CONDITIONS **

TIME	0.	SEC	TIME	0.	SEC
AXIAL POSITION	0.	CM	AXIAL POSITION	0.	CM
AREA	1.00000E+00	SQ CM	AREA	1.00000E+00	SQ CM

FLOW PROPERTIES

PRESSURE	1.8090	ATM
VELOCITY	41032.16	CM/SEC
TEMPERATURE	2535.01510	K
DENSITY	3.44313E-04	GM/CC
FLOW RATE	1.41279E+01	GM/SEC
ENTROPY	1.23416	CAL/GM-K
MACH NUMBER	.45409	
GAMMA	1.53382	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CO	0.	0.
O2	5.00000E-02	-2.60369E-07
O	0.	5.20739E-07
CO2	0.	0.
C3H8	1.00000E-02	-2.43867E+00
C2H5	0.	2.43867E+00
CH3	0.	2.43867E+00
OH	0.	0.
H2	0.	0.
H2O	0.	0.
H	0.	0.
CH4	0.	0.
CH2O	0.	0.
HCO	0.	0.
C3H7	0.	0.
C2H6	0.	0.
C2H6CO	0.	0.
C3H6	0.	0.
CH3CHO	0.	0.
C3H4	0.	0.
C2H4	0.	0.
CH3CO	0.	0.
C2H5CO	0.	0.
C2H5OH	0.	0.
C2H4OH	0.	0.
CH2OH	0.	0.
CH3OH	0.	0.
C2H2	0.	0.
C2H	0.	0.
CH	0.	0.
AR	9.40000E-01	0.

MIXTURE MOLECULAR WEIGHT	39.59194
TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)	1.76911E+12
MASS FRACTION SUM	1.00000

TIME	1.26166E-06	SEC
AXIAL POSITION	5.00000E-02	CM
AREA	1.01950E+00	SQ CM

FLOW PROPERTIES

PRESSURE	1.8215	ATM
VELOCITY	40146.04	CM/SEC
TEMPERATURE	2518.47982	K
DENSITY	3.45104E-04	GM/CC
FLOW RATE	1.41284E+01	GM/SEC

FLOW PROPERTIES

PRESSURE	1.8090	ATM
VELOCITY	41032.16	CM/SEC
TEMPERATURE	2535.01510	K
DENSITY	3.44313E-04	GM/CC
FLOW RATE	1.41279E+01	GM/SEC
ENTROPY	1.23416	CAL/GM-K
MACH NUMBER	.45409	
GAMMA	1.53382	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CO	0.	0.
O2	5.00000E-02	-2.60369E-07
O	0.	5.20739E-07
CO2	0.	0.
C3H8	1.00000E-02	-2.43867E+00
C2H5	0.	2.43867E+00
CH3	0.	2.43867E+00
OH	0.	0.
H2	0.	0.
H2O	0.	0.
H	0.	0.
CH4	0.	0.
CH2O	0.	0.
HCO	0.	0.
C3H7	0.	0.
C2H6	0.	0.
C2H6CO	0.	0.
C3H6	0.	0.
CH3CHO	0.	0.
C3H4	0.	0.
C2H4	0.	0.
CH3CO	0.	0.
C2H5CO	0.	0.
C2H5OH	0.	0.
C2H4OH	0.	0.
CH2OH	0.	0.
CH3OH	0.	0.
C2H2	0.	0.
C2H	0.	0.
CH	0.	0.
AR	9.40000E-01	0.

MIXTURE MOLECULAR WEIGHT	39.59194
TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)	1.76911E+12
MASS FRACTION SUM	1.00000

TIME	1.26106E-06	SEC
AXIAL POSITION	5.00000E-02	CM
AREA	1.01950E+00	SQ CM

FLOW PROPERTIES

PRESSURE	1.8212	ATM
VELOCITY	40165.24	CM/SEC
TEMPERATURE	2518.32089	K
DENSITY	3.45166E-04	GM/CC
FLOW RATE	1.41340E+01	GM/SEC

ENTROPY	1.24807	CAL/GM-K
MACH NUMBER	.44030	
GAMMA	1.55492	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CO	1.01573E-03	1.28255E-02
O2	4.00427E-02	-2.09274E-02
O	9.90509E-04	4.57039E-03
CO2	3.25137E-04	5.41006E-03
C3H8	1.33706E-06	-3.96484E-05
C2H5	2.83190E-04	-7.22208E-03
CH3	9.69471E-03	-1.04097E-02
OH	4.66332E-03	-1.21282E-02
H2	1.22439E-03	1.25166E-02
H2O	2.32886E-03	1.85570E-02
H	6.45316E-04	9.63802E-04
CH4	7.80494E-05	6.42510E-04
CH2O	7.16399E-06	1.13777E-05
HCO	5.25127E-05	4.51757E-04
C3H7	7.60824E-07	-1.49437E-05
C2H6	4.19672E-05	-5.87205E-06
C2H6CO	4.49935E-06	7.55625E-06
C3H6	9.36581E-06	1.15961E-05
CH3CHO	7.17600E-03	-2.85906E-03
C3H4	9.89596E-07	1.38473E-05
C2H4	5.53151E-04	-1.34729E-03
CH3CO	4.50524E-04	2.16492E-03
C2H5CO	2.80987E-07	1.30143E-06
C2H5OH	5.05896E-07	1.34437E-06
C2H4OH	7.89295E-04	2.26980E-05
CH2OH	6.71647E-04	6.75439E-03
CH3OH	3.21562E-05	4.54611E-04
C2H2	4.30351E-05	4.79219E-04
C2H	3.44361E-05	6.89609E-04
CH	2.60209E-06	7.52362E-05
AR	9.29836E-01	0.

MIXTURE MOLECULAR WEIGHT	39.16384
TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)	-1.83772E+10
MASS FRACTION SUM	1.00000

TIME	1.17788E-05	SEC
AXIAL POSITION	5.00000E-01	CM
AREA	1.06437E+00	SQ CM

FLOW PROPERTIES

PRESSURE	1.7560	ATM
VELOCITY	45051.41	CM/SEC
TEMPERATURE	2804.24800	K
DENSITY	2.94654E-04	GM/CC
FLOW RATE	1.41291E+01	GM/SEC
ENTROPY	1.27983	CAL/GM-K
MACH NUMBER	.46291	
GAMMA	1.56858	

ENTROPY	1.24807	CAL/GM-K
MACH NUMBER	.44053	
GAMMA	1.55492	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CO	1.01431E-03	1.28206E-02
O2	4.00440E-02	-2.08088E-02
O	9.90196E-04	4.57892E-03
CO2	3.24551E-04	5.40660E-03
C3H8	1.33491E-06	-3.93165E-05
C2H5	2.82679E-04	-7.20668E-03
CH3	8.69581E-03	-1.04089E-02
OH	4.66509E-03	-1.21552E-02
H2	1.22303E-03	1.25166E-02
H2O	2.32719E-03	1.85590E-02
H	6.45247E-04	9.60584E-04
CH4	7.79931E-05	6.42437E-04
CH2O	7.16611E-06	1.11430E-05
HCO	5.24862E-05	4.52880E-04
C3H7	7.61687E-07	-1.49716E-05
C2H6	4.19711E-05	-5.95629E-06
C2H6CO	4.49867E-06	7.57230E-06
C3H6	9.36510E-06	1.16203E-05
CH3CHO	7.17721E-03	-2.87137E-03
C3H4	9.87568E-07	1.38643E-05
C2H4	5.53490E-04	-1.35074E-03
CH3CO	4.50378E-04	2.16833E-03
C2H5CO	2.80859E-07	1.30020E-06
C2H5OH	5.06019E-07	1.33715E-06
C2H4OH	7.89420E-04	2.15628E-05
CH2OH	6.70968E-04	6.75375E-03
CH3OH	3.21083E-05	4.54646E-04
C2H2	4.29866E-05	4.80065E-04
C2H	3.43544E-05	6.89235E-04
CH	2.59421E-06	7.50390E-05
AR	9.29837E-01	0.

MIXTURE MOLECULAR WEIGHT	39.16389
TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)	-1.83695E+10
MASS FRACTION SUM	1.00000

TIME	1.17734E-05	SEC
AXIAL POSITION	5.00000E-01	CM
AREA	1.06437E+00	SQ CM

FLOW PROPERTIES

PRESSURE	1.7556	ATM
VELOCITY	45071.84	CM/SEC
TEMPERATURE	2803.98748	K
DENSITY	2.94624E-04	GM/CC
FLOW RATE	1.41341E+01	GM/SEC
ENTROPY	1.27982	CAL/GM-K
MACH NUMBER	.46314	
GAMMA	1.56858	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CO	1.49385E-02	8.28954E-03
O2	1.79184E-02	-1.25790E-02
O	3.29110E-03	2.04344E-03
CO2	7.10253E-03	3.28545E-03
C3H8	2.65612E-09	-1.15644E-08
C2H5	9.77835E-06	-2.65777E-05
CH3	3.11596E-03	-2.66095E-03
OH	6.24316E-03	2.77571E-03
H2	4.65980E-03	3.82439E-04
H2O	2.03182E-02	1.11084E-02
H	2.66794E-03	2.82676E-03
CH4	1.45874E-04	-1.27298E-04
CH2O	3.65746E-06	1.37629E-05
HCO	2.83757E-05	-4.05016E-05
C3H7	1.02414E-09	-3.42272E-09
C2H6	3.87016E-06	-9.90782E-06
C2H6CO	1.59076E-07	-7.61833E-07
C3H6	5.42093E-07	-2.09660E-06
CH3CHO	7.16770E-04	-2.25269E-03
C3H4	1.12776E-06	-1.77523E-06
C2H4	1.13683E-05	-2.82565E-05
CH3CO	1.59629E-04	-3.99399E-04
C2H5CO	3.51151E-08	-1.43905E-07
C2H5OH	1.31075E-07	-3.76987E-07
C2H4OH	5.74001E-05	-2.13048E-04
CH2OH	1.67496E-03	-2.62318E-03
CH3OH	5.03166E-05	-1.26623E-04
C2H2	4.69962E-05	-2.10887E-05
C2H	7.46956E-05	-3.92274E-05
CH	3.02408E-05	-9.67407E-06
AR	9.16729E-01	0.

MIXTURE MOLECULAR WEIGHT	38.61176	
TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)	-9.60711E+09	
MASS FRACTION SUM	1.00000	
TIME	2.27133E-05	SEC
AXIAL POSITION	1.00000E+00	CM
AREA	1.09353E+00	SQ CM

FLOW PROPERTIES

PRESSURE	1.7485	ATM
VELOCITY	45617.61	CM/SEC
TEMPERATURE	2886.87900	K
DENSITY	2.83238E-04	GM/CC
FLOW RATE	1.41291E+01	GM/SEC
ENTROPY	1.28916	CAL/GM-K
MACH NUMBER	.45982	
GAMMA	1.57343	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CO	1.90786E-02	-3.62131E-04
O2	9.71434E-03	-1.01133E-03

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CO	1.49323E-02	8.30954E-03
O2	1.79285E-02	-1.25631E-02
O	3.28895E-03	2.03228E-03
CO2	7.10020E-03	3.28691E-03
C3H8	2.66240E-09	-1.02489E-08
C2H5	9.79473E-06	-2.71036E-05
CH3	3.11898E-03	-2.66081E-03
OH	6.24045E-03	2.76287E-03
H2	4.65922E-03	3.93339E-04
H2O	2.03104E-02	1.11139E-02
H	2.66479E-03	2.84289E-03
CH4	1.46036E-04	-1.27125E-04
CH2O	3.66782E-06	-2.46910E-06
HCO	2.84415E-05	-4.69254E-05
C3H7	1.02627E-09	-3.44145E-09
C2H6	3.87380E-06	-9.90490E-06
C2H6CO	1.58839E-07	-7.59447E-07
C3H6	5.42401E-07	-2.07965E-06
CH3CHO	7.17692E-04	-2.25206E-03
C3H4	1.12931E-06	-1.78721E-06
C2H4	1.13904E-05	-2.83192E-05
CH3CO	1.59935E-04	-4.02625E-04
C2H5CO	3.51127E-08	-1.45279E-07
C2H5OH	1.31332E-07	-3.77019E-07
C2H4OH	5.74418E-05	-2.12801E-04
CH2OH	1.67760E-03	-2.62154E-03
CH3OH	5.04129E-05	-1.26538E-04
C2H2	4.70238E-05	-2.11412E-05
C2H	7.47389E-05	-3.91730E-05
CH	3.02484E-05	-9.68076E-06
AR	9.16736E-01	0.

MIXTURE MOLECULAR WEIGHT	38.61208	
TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)	-9.61537E+09	
MASS FRACTION SUM	1.00000	
TIME	2.27025E-05	SEC
AXIAL POSITION	1.00000E+00	CM
AREA	1.09353E+00	SQ CM

FLOW PROPERTIES

PRESSURE	1.7481	ATM
VELOCITY	45641.05	CM/SEC
TEMPERATURE	2886.69411	K
DENSITY	2.83192E-04	GM/CC
FLOW RATE	1.41341E+01	GM/SEC
ENTROPY	1.28916	CAL/GM-K
MACH NUMBER	.46007	
GAMMA	1.57343	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CO	1.90793E-02	-3.60972E-04
O2	9.71627E-03	-1.00453E-03

O	5.00222E-03	2.69992E-04
CO2	9.70141E-03	9.62992E-04
C3H8	5.30394E-14	-5.13023E-12
C2H5	5.18170E-09	-2.98837E-08
CH3	1.39104E-04	-4.07899E-04
OH	7.91395E-03	1.99179E-04
H2	5.63020E-03	3.49123E-04
H2O	2.60624E-02	6.96146E-05
H	5.61015E-03	6.24785E-04
CH4	7.29652E-06	-2.12464E-05
CH2O	2.05726E-07	-7.31685E-07
HCO	1.03224E-07	-3.93092E-07
C3H7	3.49930E-14	-1.75975E-13
C2H6	1.40720E-08	-6.56428E-08
C2H6CO	2.06446E-12	-1.02754E-11
C3H6	1.67692E-11	-1.82100E-10
CH3CHO	4.06407E-07	-2.56403E-06
C3H4	2.25143E-08	-6.38277E-08
C2H4	7.08069E-09	-4.24136E-08
CH3CO	1.35569E-07	-8.36827E-07
C2H5CO	6.45662E-13	-5.24987E-12
C2H5OH	4.49765E-11	-2.75935E-10
C2H4OH	9.41368E-09	-6.45613E-08
CH2OH	2.96005E-05	-9.44401E-05
CH3OH	2.89407E-07	-9.47310E-07
C2H2	1.96614E-05	-1.17322E-05
C2H	3.10742E-05	-1.80547E-05
CH	1.65338E-05	-8.24040E-06
AR	9.11042E-01	0.

MIXTURE MOLECULAR WEIGHT	38.37227
TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)	-6.32003E+08
MASS FRACTION SUM	1.00000

TIME	3.38104E-05	SEC
AXIAL POSITION	1.50000E+00	CM
AREA	1.11701E+00	SQ CM

FLOW PROPERTIES

PRESSURE	1.7625	ATM
VELOCITY	44507.59	CM/SEC
TEMPERATURE	2899.61106	K
DENSITY	2.84200E-04	GM/CC
FLOW RATE	1.41291E+01	GM/SEC
ENTROPY	1.28943	CAL/GM-K
MACH NUMBER	.44762	
GAMMA	1.57333	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLES/CC-SEC)
CO	1.84453E-02	-2.78212E-04
O2	9.15566E-03	-1.35476E-04
O	5.15490E-03	3.74533E-05
CO2	1.05732E-02	3.12059E-04
C3H8	2.00479E-16	-7.96908E-14
C2H5	2.51005E-12	3.94518E-12
CH3	1.33302E-06	-4.24314E-06
OH	8.03770E-03	4.01636E-05
H2	5.90662E-03	9.32531E-05

O	5.00146E-03	2.70800F-04
CO2	9.69971E-03	9.64127E-04
C3H8	4.08393E-14	-3.50323E-13
C2H5	5.17872E-09	-3.03411E-08
CH3	1.39799E-04	-4.09717E-04
OH	7.91284E-03	1.99736E-04
H2	5.62936E-03	3.49584E-04
H2O	2.60631E-02	7.15334E-05
H	5.60892E-03	6.26475E-04
CH4	7.33540E-06	-2.13473E-05
CH2O	2.06748E-07	-6.02123E-07
HCO	1.03546E-07	-3.97791E-07
C3H7	3.14301E-14	-2.77126E-13
C2H6	1.41193E-08	-6.58328E-08
C2H6CO	1.84554E-12	-1.76119E-11
C3H6	1.53337E-11	-1.40447E-10
CH3CHO	4.06316E-07	-2.56171E-06
C3H4	2.25729E-08	-6.40015E-08
C2H4	7.07387E-09	-4.23396E-08
CH3CO	1.35692E-07	-8.40317E-07
C2H5CO	6.03294E-13	-5.72769E-12
C2H5OH	4.48382E-11	-2.73188E-10
C2H4OH	9.32741E-09	-6.37547E-08
CH2OH	2.97571E-05	-9.48842E-05
CH3OH	2.89709E-07	-9.50132E-07
C2H2	1.96829E-05	-1.17402E-05
C2H	3.11069E-05	-1.80667E-05
CH	1.65454E-05	-8.24131E-06
AR	9.11044E-01	0.

MIXTURE MOLECULAR WEIGHT	38.37232
TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC)	-6.34302E+08
MASS FRACTION SUM	1.00000

TIME	3.37939E-05	SEC
AXIAL POSITION	1.50000E+00	CM
AREA	1.11701E+00	SQ CM

FLOW PROPERTIES

PRESSURE	1.7621	ATM
VELOCITY	44530.45	CM/SEC
TEMPERATURE	2899.44767	K
DENSITY	2.84154E-04	GM/CC
FLOW RATE	1.41341E+01	GM/SEC
ENTROPY	1.28943	CAL/GM-K
MACH NUMBER	.44786	
GAMMA	1.57333	

CHEMICAL PROPERTIES

SPECIES	MOLE FRACTION	NET SPECIES PRODUCTION RAT (MOLES/CC-SEC)
CO	1.84458E-02	-2.78863E-04
O2	9.15610E-03	-1.35799E-04
O	5.15453E-03	3.75375E-05
CO2	1.05727E-02	3.12779E-04
C3H8	1.53734E-19	-1.21523E-18
C2H5	2.15257E-12	-1.06579E-11
CH3	1.34242E-06	-4.27187E-06
OH	8.03688E-03	4.02440E-05
H2	5.90619E-03	9.34522E-05

H2O	2.58055E-02	-1.51774E-04
H	6.01715E-03	1.13959E-04
CH4	6.55913E-08	-2.22497E-07
CH2O	2.08605E-09	-6.13419E-09
HCO	1.77575E-09	-1.16173E-09
C3H7	9.44669E-17	1.06199E-15
C2H6	1.00906E-11	-4.96540E-11
C2H6CO	7.47843E-15	-7.87990E-14
C3H6	3.40000E-14	-9.62055E-13
CH3CHO	6.46282E-11	-4.11778E-10
C3H4	3.65071E-10	-9.37266E-10
C2H4	1.39197E-11	-2.06014E-11
CH3CO	5.67069E-11	-1.29422E-10
C2H5CO	1.37017E-15	2.26949E-14
C2H5OH	2.23918E-14	-1.81285E-13
C2H4OH	4.48695E-12	-3.40338E-11
CH2OH	2.42361E-07	-7.81098E-07
CH3OH	2.39584E-09	-7.66623E-09
C2H2	8.19653E-06	-4.72636E-06
C2H	1.31919E-05	-7.51403E-06
CH	7.45668E-06	-4.10005E-06
AR	9.10873E-01	0.

MIXTURE MOLECULAR WEIGHT 38.36516

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) -8.05479E+07

MASS FRACTION SUM 1.00000

H2O	2.58065E-02	-1.52078E-04
H	6.01676E-03	1.14219E-04
CH4	7.02074E-08	-2.24062E-07
CH2O	2.10054E-09	-6.35214E-09
HCO	1.77555E-08	-1.24021E-09
C3H7	1.20686E-19	-9.74184E-19
C2H6	9.94139E-12	-4.90220E-11
C2H6CO	1.12158E-18	-9.96659E-18
C3H6	7.87116E-16	-2.18709E-15
CH3CHO	3.17357E-11	-1.84939E-10
C3H4	3.66445E-10	-9.91091E-10
C2H4	1.25820E-11	-1.86237E-11
CH3CO	4.98701E-11	-1.68760E-10
C2H5CO	5.50762E-19	-4.17255E-18
C2H5OH	1.59239E-14	-7.92508E-14
C2H4OH	1.76159E-12	-8.87089E-12
CH2OH	2.44018E-07	-7.85865E-07
CH3OH	2.39994E-09	-7.68656E-09
C2H2	8.21127E-06	-4.73248E-06
C2H	1.32152E-05	-7.52343E-06
CH	7.46766E-06	-4.10364E-06
AR	9.10874E-01	0.

MIXTURE MOLECULAR WEIGHT 38.36518

TOTAL ENERGY EXCHANGE RATE (CAL-CM3/GM2/SEC) -8.07790E+07

MASS FRACTION SUM 1.00000

```
11/26/75  LRC ICOPS INDEPNDT 6400A-131K 01/21/75D
20.16.33.GT05681.
20.16.33.                          LRC COMPUTER COMPLEX
20.16.33.JOB,1,01000,165000,002000.      A4409    R
20.16.34.3274       100681         8-1250
20.16.34.USER.    ALLEN G. MCLAIN                0005
20.16.34.89803N 64730
20.16.34.WAITGO.    PLEASE RUN ON 6400 ONLY
20.16.45.GO.
20.16.46.LINECNT(10000)
20.16.46.FETCH(A4409,,BINARY)
20.17.03.TIME         8G ATTACH
20.17.46.TIME         ED ATTACH
20.17.46.END     FETCH
20.17.46.UPDATE(Q,C=TAPE4,P=BNFILE,D,8)
20.17.50.READING INPUT
20.18.00.UPDATE COMPLETE
20.18.00.UPDATE(Q,P=BNFILE)
20.18.04.READING INPUT
20.18.20.UPDATE COMPLETE
20.18.21.RUN(S,,,COMPILE)
20.19.25.SETINDF.
20.19.26.LGO.
20.19.50.MEMORY  135400 CM
20.19.50.RFL       0000822 O/S CALLS
20.19.50.RFL CPU     50.147417 SEC.
20.29.32.STOP
20.29.33.SPPRINT(OUTPUT,3)
20.29.34.      0000892 O/S CALLS
20.29.34.CPU    286.074664 SEC.  <----------
20.29.34.PPU    127.324160 SEC.
20.29.35.COST OF THIS JOB WAS $    27
20.29.35.KWH     6.66      KILOWORD HOURS
21.17.33. GT05681.    8377 LINES PRINTED. LP25
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11/26/75  LRC ICOPS INDEPNDT 6400Z-131K 01/21/75D
01.41.58.GT05682.
01.41.58.                          LRC COMPUTER COMPLEX
01.41.58.JOB,1,02000,145000,002000.      A4409    R
01.41.58.3274       100681         8-1250
01.41.59.USER.    ALLEN G. MCLAIN                0005
01.41.59.89803N 64730
01.41.59.LINECNT(10000)
01.42.01.FETCH(A4409,,BINARY)
01.42.11.TIME         8G ATTACH
01.46.49.TIME         ED ATTACH
01.46.50.END     FETCH
01.46.51.UPDATE(Q,C=TAPE4,P=BNFILE,D,8)
01.46.58.READING INPUT
01.47.08.UPDATE COMPLETE
01.47.09.UPDATE(Q,P=BNFILE)
01.47.16.READING INPUT
01.47.23.UPDATE COMPLETE
01.47.23.RUN(S,,,COMPILE)
01.48.01.SETINDF.
01.48.03.LGO.
01.48.47.MEMORY  133000 CM
01.48.47.RFL       0000568 O/S CALLS
01.48.47.RFL CPU     46.809126 SEC.
02.51.44.STOP
02.51.45.SPPRINT(OUTPUT,3)
02.51.47.      0000638 O/S CALLS
02.51.48.CPU   2554.930635 SEC.  <----------
02.51.48.PPU    199.286784 SEC.
02.51.49.COST OF THIS JOB WAS $  135
02.51.49.KWH     33.82      KILOWORD HOURS
03.35.55. GT05682.    8061 LINES PRINTED. LP25
```

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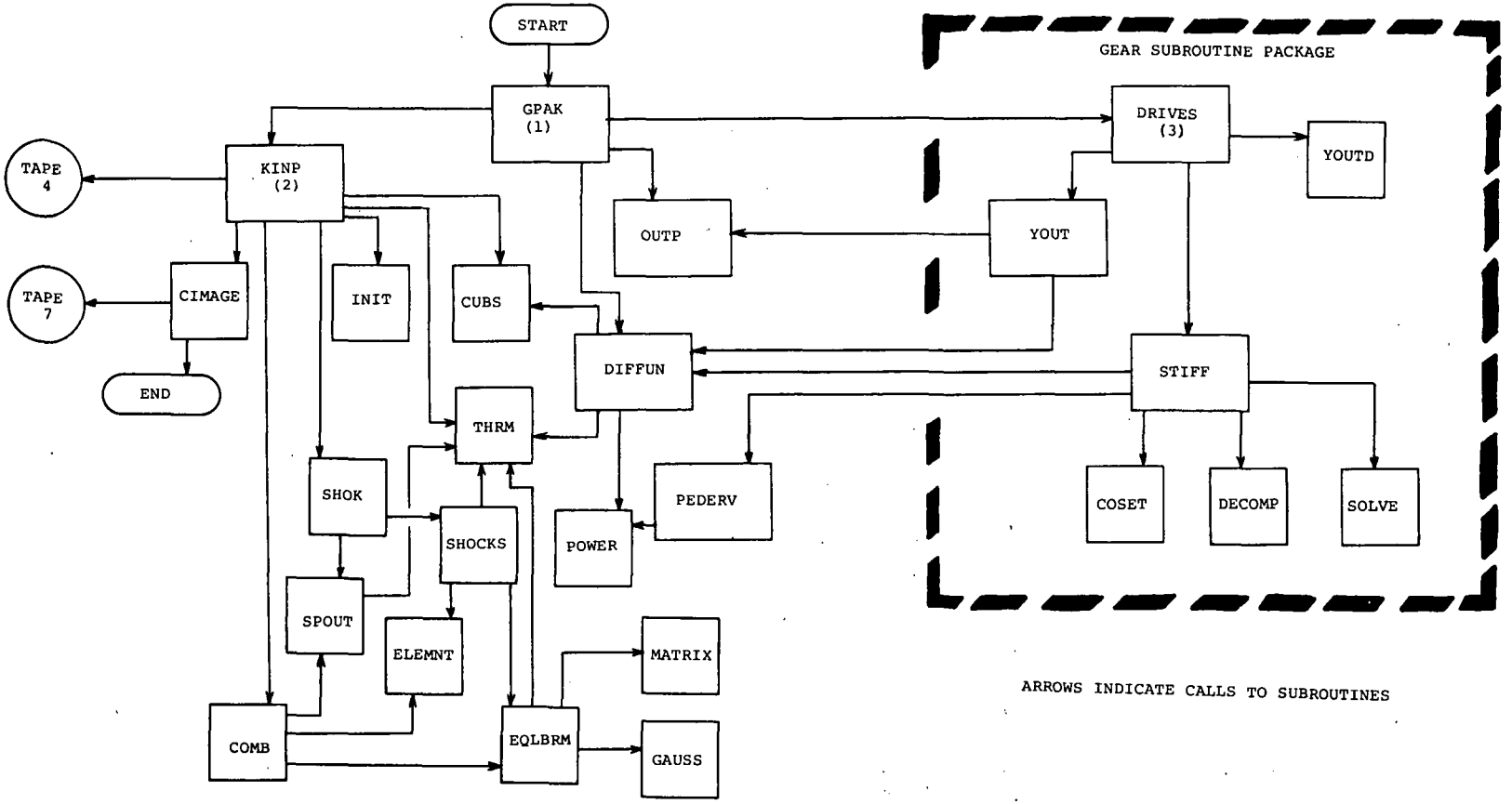

Figure 1.- Overall schematic of the hybrid computer program.

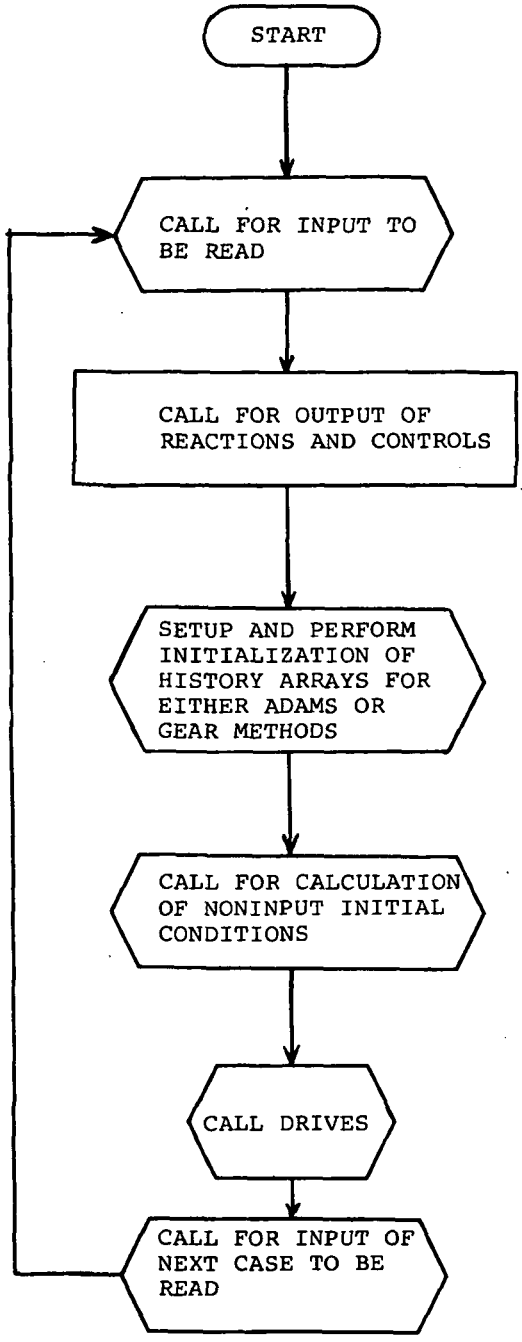

Figure 2.- Flow diagram for main program GPAK.

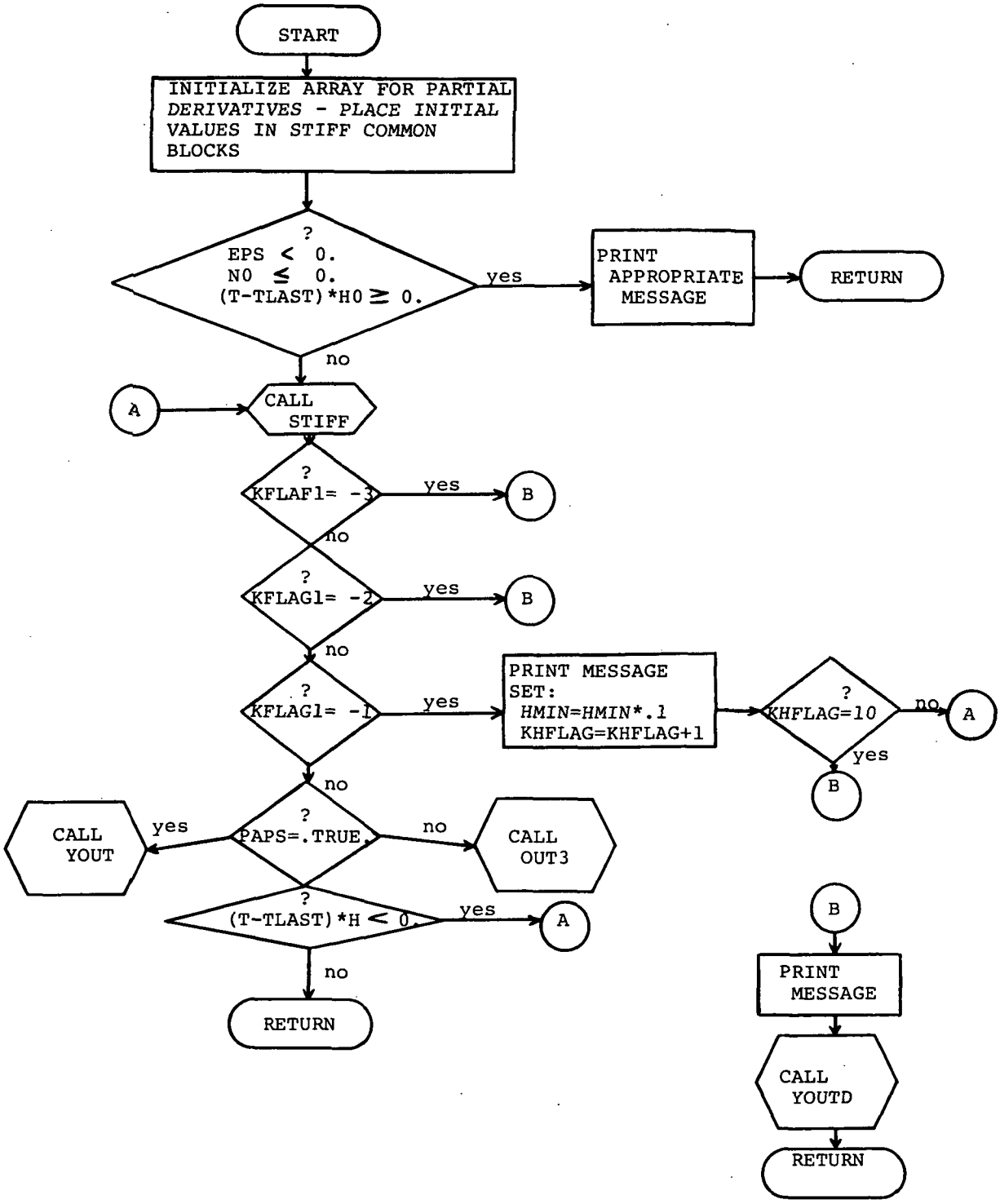

Figure 3.- Flow diagram for subroutine DRIVES.

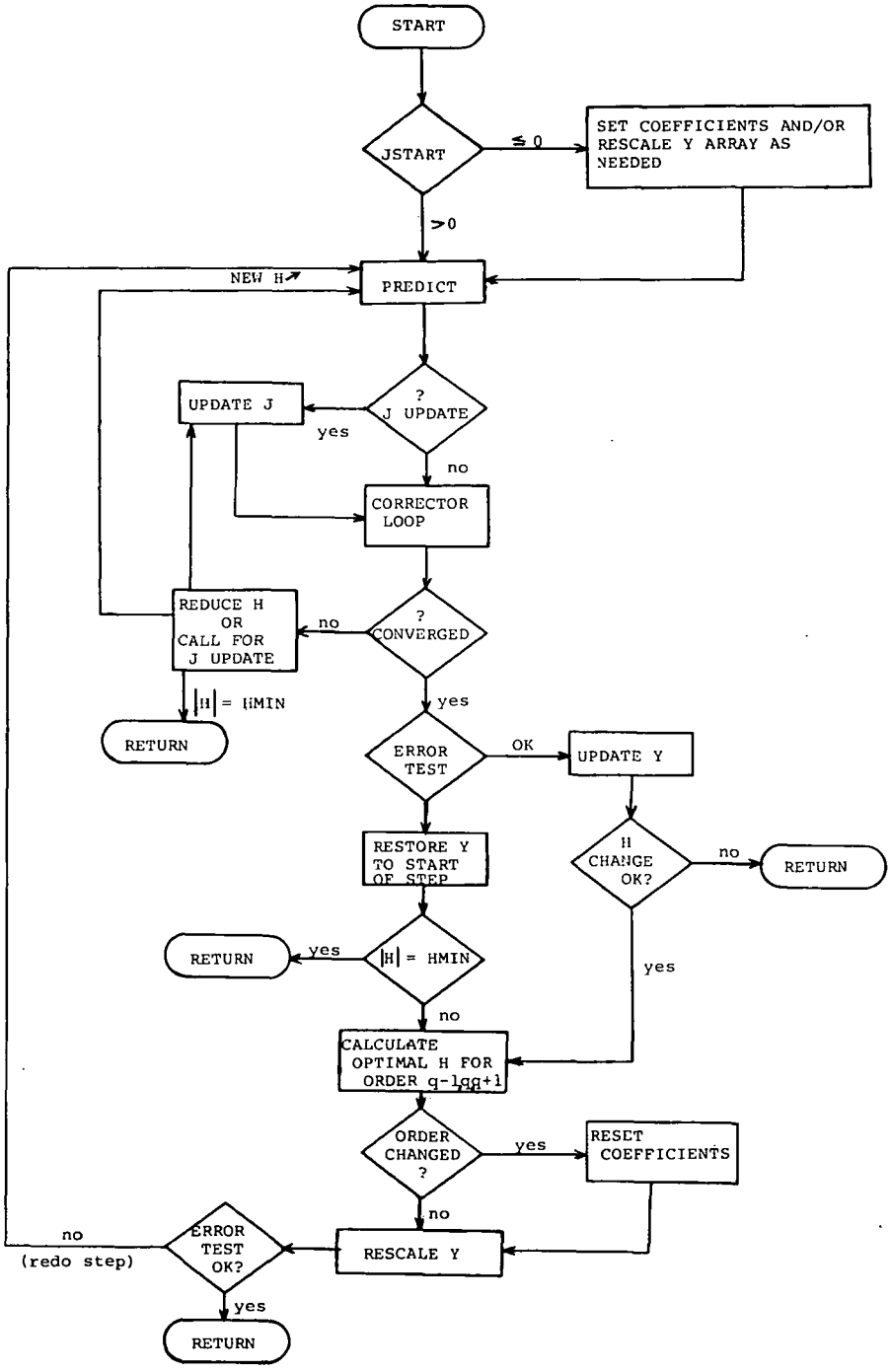

Figure 4.- Flow diagram of subroutine STIFF (from ref. 3).

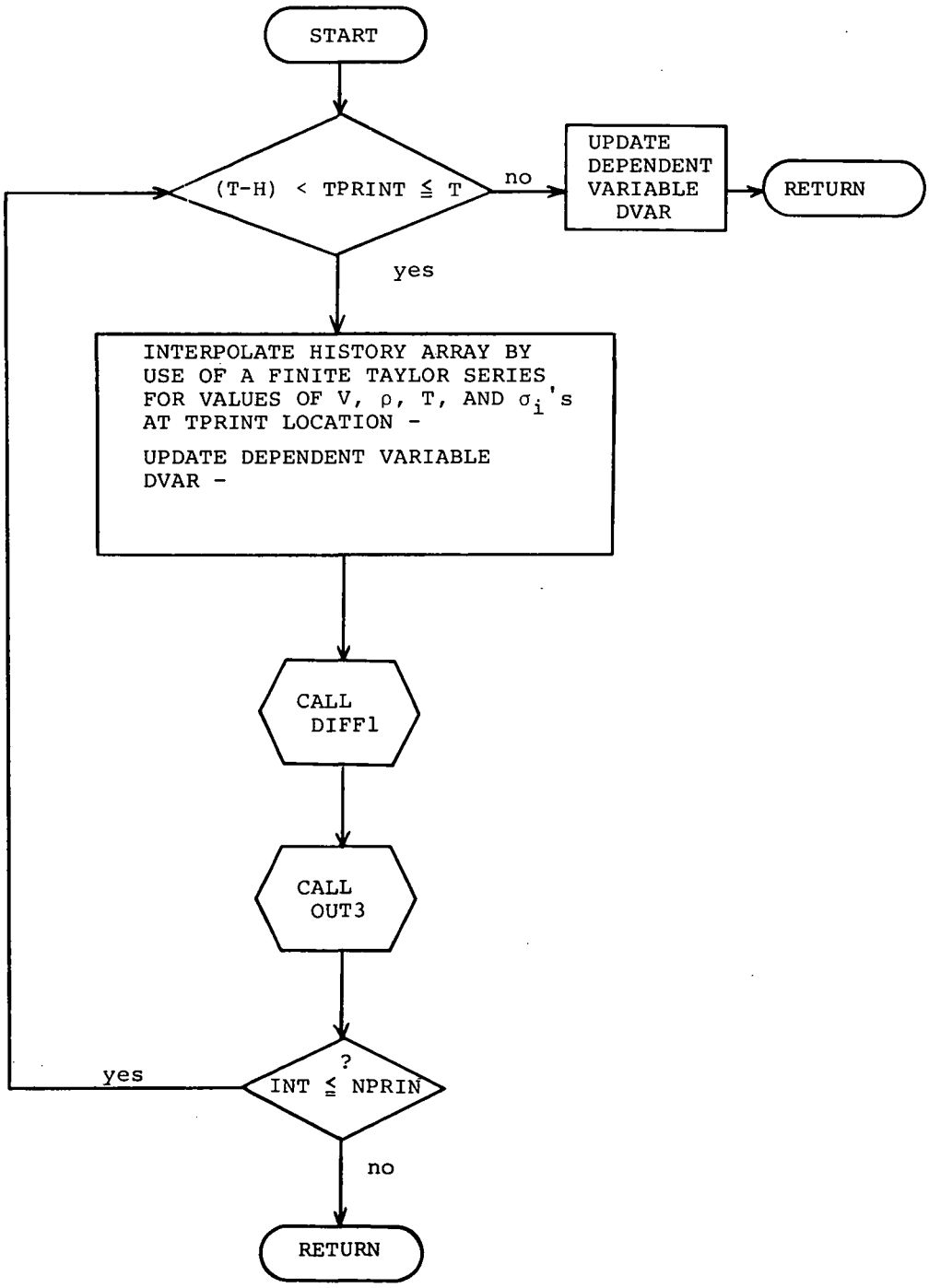

Figure 5.- Flow diagram for subroutine YOUT.

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