NASA
Reference
Publication
1330

March 1994

LSENS, A General Chemical Kinetics and Sensitivity Analysis Code for Homogeneous Gas-Phase Reactions

III. Illustrative Test Problems

David A. Bittker
and Krishnan Radhakrishnan

National Aeronautics and
Space Administration

NASA Reference Publication 1330

1994

LSENS, A General Chemical Kinetics and Sensitivity Analysis Code for Homogeneous Gas-Phase Reactions

III. Illustrative Test Problems

David A. Bittker
Lewis Research Center
Cleveland, Ohio

Krishnan Radhakrishnan
NYMA, Inc.
Lewis Research Center Group
Brook Park, Ohio

National Aeronautics and
Space Administration
Office of Management
Scientific and Technical
Information Program

Preface

LSENS, the Lewis General Chemical Kinetics and Sensitivity Analysis Code, has been developed for homogeneous, gas-phase chemical kinetics computations and contains sensitivity analysis for a variety of problems, including nonisothermal situations. The code is described in a series of three reference publications, which also provide a detailed guide to its use and many illustrative test problems.

LSENS has been designed for accuracy, efficiency, flexibility, and convenience. A variety of chemical reaction models can be considered: static system; steady, one-dimensional, inviscid flow; reaction behind an incident shock wave, including boundary layer correction; and perfectly stirred (highly backmixed) reactor. In addition, the chemical equilibrium state can be computed for the assigned states of temperature and pressure, enthalpy and pressure, temperature and volume, and internal energy and volume. Any reaction problem can be adiabatic, have an assigned heat transfer profile, or for static and flow problems, have an assigned-temperature profile. For static problems either the density is constant or the pressure-versus-time profile is assigned. For flow problems either the pressure or area can be assigned as a function of time or distance. For a static reaction sensitivity coefficients of the dependent variables and their temporal derivatives with respect to the initial values of the dependent variables and/or the three rate coefficient parameters of the chemical reactions can be obtained.

LSENS checks the legality and sufficiency of all input. At the user's option LSENS checks the reaction mechanism for uniqueness and ensures that each reaction satisfies charge and atom balance requirements.

Part I of the series (NASA RP–1328), consisting of chapters 1 to 7, presents the theory and the numerical solution procedures used in LSENS. The ordinary differential equations (ODE's) describing chemical kinetics problems are derived in chapter 2. Chapter 3 describes the numerical integration method and how it is implemented. In chapter 4 the governing ODE's for sensitivity analysis are derived and the solution method and numerical algorithm explained. The governing equations and solution methods for the chemical equilibrium state, equilibrium and frozen thermodynamic states behind an incident shock wave, and perfectly stirred reactor problems are presented in chapters 5 to 7.

Part II of the series (NASA RP–1329), consisting of chapters 8 to 13 and appendixes A to C, describes LSENS, its usage, and how to modify it. Chapter 8 describes the computational capabilities and convenience features built into the code. Chapter 9 presents its structure and description. Chapter 10 lists modifications that may be required to implement LSENS on the user's computer system. Chapter 11 provides a guide to code usage and describes how to prepare the input data files required to execute LSENS. The output information generated by the code is discussed in chapter 12. Example problems illustrating both problem data file construction and code usage are given in chapter 13. These examples supplement chapter 11 by providing additional guidance on preparation of the problem data file.

The partial derivatives required by the numerical solution procedures detailed in chapters 3, 4, and 7 are derived in appendix A. Appendix B shows how to access the system clock for several common computing systems so that execution times can be measured. Appendix C describes the modifications required to change the built-in values for various quantities.

This volume, part III of the series (appendixes D and E), explains the example problems provided with LSENS and presents sample results. Appendix D describes the kinetics test cases. These problems illustrate the various reaction models that can be solved by, and options built into, LSENS. Appendix E describes the kinetics-plus-sensitivity-analysis test cases supplied with the code. The examples in the two appendixes cover a variety of problem types and so should serve as useful models for the structure of the problem data file required to execute the code. Indeed, it is likely that the desired file can be produced by modifying one of the test cases.

Details regarding code availability and procurement can be obtained from COSMIC, 328 East Broad Street, University of Georgia, Athens, GA 30602 (Telephone: 706–542–3265).

Contents

List of Tables vii

Appendix D. Kinetics Test Cases 1
Description of Test Cases 1
Case 1 1
Case 2 1
Case 3 1
Case 4 2
Case 5 2
Case 6 2
Case 7 2
Case 8 2
Case 9 2
Case 10 2
Case 11 3
Case 12 3
Case 13 3
Case 14 3
Case 15 3
Case 16 3
Listing of Results 3

Appendix E. Sensitivity Test Cases 99
Description of Test Cases 99
Case 1 99
Case 2 99
Case 3 99
Case 4 99
Case 5 100
Case 6 100
Case 7 100
Case 8 100
Case 9 100
Listing of Results 100

References 143

List of Tables

Table D.1.—Problem data file for kinetics-only test cases 4

Table D.2.—Selected kinetics test case results 19

Table E.1.—Problem data file for sensitivity analysis test cases 101

Table E.2.—Selected sensitivity test case results 108

Appendix D
Kinetics Test Cases

In this appendix we describe 16 kinetics-only (i.e., no sensitivity analysis) test cases that are provided with the code. These cases were chosen to illustrate both the problem types that can be solved by LSENS and the options built into it. Therefore users can find among them a model problem that can be easily modified to suit their needs. In order to demonstrate the various options for the ACTION switch, all cases were set up in a single data file, which is listed in table D.1. We now describe each problem in some detail, including the source of the chemical mechanism used.

Description of Test Cases

Case 1

The first case illustrates the shock-wave-initiated adiabatic decomposition of pure bromine. It shows the use of the shock kinetics option and the boundary layer correction for area given by Mirels (refs. 1 to 3). The variable SHOCK is set to TRUE in namelist PROB and the boundary layer parameters LSUBM and ETA are also given. The values of pressure, Mach number, and temperature in namelist START are the incident shock conditions. The inert species xenon is listed on the line following the blank line that signals the end of the reaction list. The composition of the initial (unshocked) gas mixture is given as mole fractions following namelist START, and the list is ended with an END line. The rate expression used for the decomposition reaction was measured by Warshay (ref. 4). The namelist SOLVER, which lists the error control parameters EMAX and ATOLSP, is at the end of the data, just before the FINIS card, which ends the case.

Case 2

Test case 2 is a stoichiometric hydrogen-air ignition in supersonic flow through a constant-area duct with heat transfer from the system computed as a linear function of temperature. For this and all other completely new cases the word NEW appears on the ACTION line after the title. The hydrogen-oxygen reaction mechanism is that of Brabbs and Musiak (ref. 5), and the nitrogen-oxygen-hydrogen reactions are from Brabbs et al. (ref. 6). Namelist PROB contains the area profile information (the constant area CX0), the heat transfer equation coefficients HT0 and HT1, and the list of print stations (in centimeters) in the array PRINT. Initial composition is given by the special input, which specifies fuel name and stoichiometry plus equivalence ratio for the fuel–standard air mixture in namelist START. The fuel name, H2, appears in columns 41 and 42 of the integration and assigned variables, units, and fuel name line. Because the standard air contains small percentages of nonreacting carbon dioxide and argon, these species are listed as inert species after the reaction list.

Case 3

This third case is the same problem as case 2 and illustrates the use of the CHANGE and ADD options of the ACTION switch. We have temporarily changed the preexponential factor for the reaction $2HO_2 \rightleftharpoons H_2O_2 + O_2$ and added the reaction of an oxygen atom with H_2O_2 to the mechanism to test the effect of these changes on the computed results. Both the CHANGE and ADD lists end with a blank line. The word REPEAT should not be used after the ADD list because LSENS automatically uses the rest of the mechanism and other data that are unchanged from the previous case. On the integration and assigned variables, units, and fuel name line U.S. customary (FPS) units have been specified for the input of any new data. The only new information that is given in namelist PROB is the print station list (in feet). We have also set the variable EXCHR equal to TRUE to obtain the printout of net energy exchange rates for each reaction instead of the net reaction conversion rates. In namelist START initial temperature and pressure are given in U.S. customary units, and the mass fuel-oxidant ratio is given for the initial mixture. The stoichiometric coefficients of the

fuel are not needed when this ratio is given, but they are saved automatically when the ADD or REPEAT option is used. Comparing the computed results of cases 2 and 3 showed close agreement. Therefore the two changes made in the mechanism for this case were not used in any other test cases.

Case 4

Case 4 is the ignition of a stoichiometric hydrogen-oxygen mixture flowing in a duct whose pressure profile is assigned as a linear function of distance. The flow is subsonic and heat transfer is assigned as a linear function of temperature. The default value of QMREAD is TRUE; it has been set in namelist PROB only for illustrative purposes. The chemical mechanism is the hydrogen-oxygen portion of the mechanism of case 2, and the initial composition is given by the same method used for that case. However, because the oxidant is pure oxygen rather than the standard air, the variables ARAT, NOXRAT, and CRAT are set equal to zero. Output is specified in U.S. customary (FPS) units, but input is in the default (CGS) units. Therefore, the values given in the array PRINT are in centimeters.

Case 5

Case 5 is the static ignition of a methane-oxygen-nitrogen mixture with an assigned pressure profile that increases linearly with time. Heat transfer from the system is given by the Otto cycle correlation option in LSENS. Note that in namelist PROB the logical variable QMREAD must now be set equal to FALSE, and values of the variables BORE, STROKE, TWALL, and RPM are given. The chemical mechanism builds on that of case 2 by adding the oxidation and decomposition reactions of methane and its oxidation products ethane, ethylene, and acetylene, as well as the reactions of carbon monoxide and the formyl (HCO) radical. Also included are reactions of ketene (C_2H_2O), the ketyl (C_2HO) radical, and formaldehyde. All C–H–O reactions were taken from references 7 and 8. Initial mixture composition is given by listing species mole fractions after namelist START.

Case 6

Case 6 is the adiabatic ignition of a methane-oxygen-nitrogen mixture in supersonic flow at a constant assigned pressure of 1.73 atm. A trace amount of CN radical is also present in the oxidant. The chemical mechanism is the same as for case 5. In namelist PROB the logical variable COMBUS has been set equal to TRUE so that the code will perform an assigned-pressure and assigned-enthalpy equilibrium computation, which gives the final conditions that the kinetics computations would approach at long reaction times. With the pressure assigned, LSENS computes a reaction area profile as a function of distance.

Case 7

Case 7 is the same methane-air problem as case 6. However, the area profile computed in case 6 is now assigned as a table of distance and area values, and pressure is computed. We illustrate here the use of the REPEAT option of the ACTION switch. Output is requested at values of the area that are listed in the array APRINT, and COMBUS is set equal to FALSE so that an equilibrium calculation is not performed. Computed results are close to, but not identical to, those of case 6. Small differences arise because area is now computed by interpolation from the table of values at each step.

Case 8

Case 8 is also the same methane-air problem as case 6. Now both the area and temperature profiles computed in case 6 are assigned as tables of values. The REPEAT option is used again to save data from the previous case, including the area-versus-distance table that was used in case 7. Because temperature is assigned as a function of distance in namelist TMPDAT, output is requested at values of temperature, which are assigned in the array TPRINT. Note that only pressure and Mach number are assigned in namelist START.

Case 9

Case 9 is a methane-air reaction in supersonic flow with both temperature and pressure assigned constant values. The REPEAT option is used again so that the chemical mechanism of case 6 is used. The variable COMBUS is set equal to TRUE so that an assigned-pressure and assigned-temperature equilibrium problem will be performed before the kinetic computation. Note that the constant pressure is assigned by setting CX0 in namelist PROB and the assigned constant temperature is given by setting CX0 in namelist TMPDAT.

Case 10

Case 10 is the adiabatic, constant-volume ignition of methanol and oxygen in a static system. The mechanism was obtained by adding to the reactions of case 6 ten reactions involving methanol and CH_2OH taken from reference 9. The variable RHOCON is set equal to TRUE in namelist PROB. The simplified combustion input is used for this rich (fuel-oxygen equivalence ratio, 2.0) mixture. However, very small initial concentrations of three trace species are also read in following namelist START. These additional mole fractions may be read in if their sum does not exceed the code error limit (1.0×10^{-4}) for the deviation of the initial mole fraction

sum from unity. Note also that the starting pressure of 1 atm is written as 760 mm of mercury and the variable MMHG is set equal to TRUE in namelist START.

Case 11

Case 11 illustrates a propane-air perfectly stirred reactor (PSR) combustion process followed by a flow reaction of the products expanding through a diverging nozzle. The reaction mechanism is obtained by adding three propane and propyl radical reactions (ref. 8) to the methane-air mechanism of case 6. We demonstrate, first of all, a typical assigned-mass-flow-rate PSR problem setup in namelist WSPROB and, second, the option to perform an assigned-area flow problem by using the output conditions from the PSR as input conditions for the flow problem. The variables WELSTR and WSFLOW have both been set equal to TRUE in namelist PROB. However, setting only WSFLOW equal to TRUE also tells LSENS to set WELSTR equal to TRUE and perform both problems. Note that the data for the flow problem in namelist PROB include the setting of the logical variable ROCKET equal to TRUE for rocket performance parameter computations. Values of ATHROT and PC must also be given.

Case 12

Case 12 is the high-temperature ionization of air in constant-area subsonic flow. It shows the use of the logical variables DBUGO and ORDER in namelist PROB to obtain the individual net molar formation rates of each species by every reaction in which the species participates. Setting ORDER equal to TRUE is probably more useful, because the net production rates are printed in order of decreasing magnitude and none of the zero rates are printed. The chemical mechanism contains reactions of both neutral and ionic species. Rate expressions for neutral-species reactions are the same as those used for previous test cases. However, the conversion between oxygen atoms and molecular oxygen is written as the recombination process here. The rate expression for it is taken from reference 10, with the preexponential factor increased because the collision partners are N_2 and O_2 instead of argon. Rate expressions for ion-molecule reactions were taken from reference 11.

Case 13

Case 13 is the high-pressure reaction of hydrogen and carbon monoxide in a constant-volume, constant-temperature static system. The variable COMBUS is set equal to TRUE to obtain an assigned-temperature and assigned-volume equilibrium computation. The variables RHOCON and TCON are set equal to TRUE in namelist PROB, and initial temperature and pressure are assigned in namelist START. The chemical mechanism is a small portion of the mechanism of case 6.

Case 14

Case 14 is the photolytic ignition of a stoichiometric hydrogen-oxygen mixture in a constant-volume static system. The variable COMBUS is set equal to TRUE to obtain an assigned-internal-energy and assigned-volume equilibrium computation. The chemical mechanism is that of case 4 with the addition of the photolysis of the H_2 and O_2 molecules. The constant rate coefficients for these reactions were set arbitrarily to give ignition at about 1 s of reaction time.

Case 15

Case 15 is a methane-air ignition reaction in supersonic flow with the area profile assigned as a table of monotonically decreasing values in the array ATB as a function of the increasing XTB values (namelist PROB). The print stations are assigned at values of the area and are given in the array APRINT. Note that they are given in decreasing order, as are the ATB values, and that values different from those in the area table may be given. The first value in the ATB array should not be given in the APRINT array. It will be ignored if present. For this problem initial values of temperature, Mach number, and pressure are set in namelist START.

Case 16

Case 16 is the same as case 15 except for the designation of print stations, and therefore the REPEAT action option has been used. The print stations are listed as values of distance in the array PRINT and are, of course, in increasing order. We have repeated the ATB and XTB arrays in namelist PROB for illustration purposes only. These arrays are saved by use of the REPEAT option and do not have to be listed again unless the user wants to do so.

Listing of Results

The test case file in table D.1 was executed on a Sun SPARCstation 1 computer using the Sun 4.1.3 operating system and the Sun FORTRAN compiler using level 2 optimization except for subroutine KINP, which had to be compiled with no optimization. Sample pages from the output are shown in table D.2. The total execution time for all 16 test cases was approximately 154 s. This time will be significantly shorter for mainframe computers and the current more powerful workstations from Sun and other manufacturers.

TABLE D.1.—PROBLEM DATA FILE FOR KINETICS-ONLY TEST CASES

```
TAPE
  LSENS   BROMINE DISSOCIATION IN A SHOCK TUBE                                CASE 1
   M       +   BR2       =2.0BR                        6.99E+11  0.50       35500.
   THIRDBODY
BR2          3.80     END

XE
DISTANCE  AREA
 &prob  lsubm=32200.0, eta=0.5, shock=.true.,
   print=0.05,2.0,4.0,  &end
 &start  p=0.1227, mach=3.2646, t=299.9,  &end
BR2          0.01
XE           0.99
END
 &solver emax=1.0E-2, atolsp=1.0E-10,  &end
FINIS
  LSENS   HYDROGEN - AIR TEST WITH HEAT TRANSFER          STOICH          CASE 2
NEW
   O       +   H2O       =   OH       +   OH          6.8E+13    0.        18365.
   H       +   O2        =   OH       +   O          1.89E+14   0.         16400.
   O       +   H2        =   OH       +   H          4.20E+14   0.         13750.
   H       +   HO2       =   H2       +   O2         7.28E+13   0.         2126.
   O       +   HO2       =   OH       +   O2          5.0E+13   0.         1000.
   HO2     +   OH        =   H2O      +   O2          8.0E+12   0.         0.
   H       +   HO2       =2.0OH                      1.34E+14   0.         1070.
   H2      +   HO2       =   H2O2     +   H          7.91E+13   0.         25000.
   OH      +   H2O2      =   H2O      +   HO2         6.1E+12   0.         1430.
   HO2     +   HO2       =   H2O2     +   O2          1.8E+12   0.          0.
   H       +   H2O2      =   OH       +   H2O         7.8E+11   0.          0.
   M       +   H2O2      =2.0OH                      1.44E+17   0.         45510.
   THIRDBODY
H2           2.30     O2          .78      H2O         6.0    H2O2         6.6
END
   H2      +   OH        =   H2O      +   H          4.74E+13   0.         6098.
   H       +   O2        =   HO2      +   M          1.46E+15   0.         -1000.
   THIRDBODY
O2           1.30     N2          1.3      H2O         21.3   H2           3.0
END
   M       +   H2O       =   H        +   OH         1.30E+15   0.         105140.
   THIRDBODY
H2           4.00     O2          1.5      H2O         20.0   N2           1.5
END
   H       +   O         =   OH       +   M           7.1E+18   -1.         0.
   M       +   H2        =   H        +   H           2.2E+14   0.          96000.
   THIRDBODY
H2           4.10     O2          2.0      H2O         15.0   N2           2.0
END
   M       +   O2        =   O        +   O          1.80E+18   -1.        118020.
   HO2     +   NO        =   NO2      +   OH         2.09E+12    0.        -477.
   O       +   NO2       =   NO       +   O2          1.0E+13     0.       596.
   NO      +   O         =   NO2      +   M          5.62E+15   0.         -1160.
   NO2     +   H         =   NO       +   OH         3.47E+14   0.          1470.
   NO      +   O         =   N        +   O2           3.8E+9   1.         41370.
   O       +   N2        =   NO       +   N           1.8E+14   0.         76250.
   NO      +   H         =   N        +   OH         2.63E+14   0.         50410.
   M       +   N2O       =   N2       +   O          6.92E+23   -2.5       65000.
   O       +   N2O       =   N2       +   O2          1.0E+14   0.         28020.
   O       +   N2O       =2.0NO                      6.92E+13   0.         26630.
   N       +   NO2       =2.0NO                       4.0E+12   0.         0.
   N2O     +   H         =   N2       +   OH         7.59E+13   0.         15100.
   NO2     +   H2        =   HNO2     +   H           2.4E+13  0.          29000.
   OH      +   NO2       =   HNO3     +   M           3.0E+15  0.          -3800.
   THIRDBODY
O2           0.70     H2          1.4      END
   OH      +   NO        =   HNO2     +   M           5.6E+15  0.          -1700.
   HNO     +   H         =   H2       +   NO          5.0E+12   0.         0.
   H       +   NO        =   HNO      +   M           5.4E+15   0.         -600.
   HNO     +   OH        =   H2O      +   NO          3.6E+13   0.         0.

CO2        AR
DISTANCE  AREA                          H2
 &prob  cx0=2000.0, print=3.048,6.096,7.620,12.19,
   htran=.true., qmread=.true., ht1=5.863, ht0=-42.88,  &end
 &start  p=0.956, t=1559.0, mach=5.0,
   eratio=1.0, scc=0.0, sch=2.0, scox=0.0,  &end
END
 &solver  emax=5.0E-3, atolsp=1.0E-12,  &end
FINIS
  LSENS   HYDROGEN - AIR TEST WITH HEAT TRANSFER     FULL MECHANISM       CASE 3
```

TABLE D.1.—Continued.

```
CHANGE
   HO2      +   HO2      =   H2O2     +   O2          2.0E+12  0.        0.

ADD
   O        +   H2O2     =   OH       +   HO2         8.0E+13   0.       1000.

END
DISTANCE  AREA      FPS                  H2
 &prob  exchr=.true., print=0.1,0.2,0.25,0.4,  &end
 &start  p=2023.09, t=2806.2, mach=5.0,
   flair=0.029163,  &end
END
 &solver  &end
FINIS
  LSENS   HYDROGEN - OXYGEN CASE WITH HEAT TRANSFER                        CASE 4
NEW
   O        +   H2O      =   OH       +   OH          6.8E+13    0.       18365.
   H        +   O2       =   OH       +   O          1.89E+14   0.        16400.
   O        +   H2       =   OH       +   H          4.20E+14   0.        13750.
   H        +   HO2      =   H2       +   O2         7.28E+13   0.        2126.
   O        +   HO2      =   OH       +   O2          5.0E+13   0.        1000.
   HO2      +   OH       =   H2O      +   O2          8.0E+12   0.        0.
   H        +   HO2      =2.0OH                      1.34E+14   0.        1070.
   H2       +   HO2      =   H2O2     +   H          7.91E+13   0.        25000.
   OH       +   H2O2     =   H2O      +   HO2         6.1E+12   0.        1430.
   HO2      +   HO2      =   H2O2     +   O2          1.8E+12   0.         0.
   H        +   H2O2     =   OH       +   H2O         7.8E+11   0.         0.
   M        +   H2O2     =2.0OH                      1.44E+17   0.        45510.
   THIRDBODY
H2          2.30    O2          .78     H2O          6.0    H2O2         6.6
END
   H2       +   OH       =   H2O      +   H          4.74E+13   0.        6098.
   H        +   O2       =   HO2      +   M          1.46E+15   0.        -1000.
   THIRDBODY
O2          1.30    H2          3.0     H2O          21.3   END
   M        +   H2O      =   H        +   OH         1.30E+15   0.        105140.
   THIRDBODY
H2          4.00    O2          1.5     H2O          20.0   END
   H        +   O        =   OH       +   M           7.1E+18   -1.        0.
   M        +   H2       =   H        +   H           2.2E+14   0.         96000.
   THIRDBODY
H2          4.10    O2          2.0     H2O          15.0   END
   M        +   O2       =   O        +   O          1.80E+18   -1.       118020.

END
DISTANCE  PRESSURE            FPS       H2
 &prob  cx0=5.0, cx1=.01, print=10.0,15.0,15.95,
   htran=.true., qmread=.true., ht1=5.863, ht0=-42.88,  &end
 &start  t=1050.0, mach=0.5, area=2000.0, eratio=1.0,
   scc=0.0, sch=2.0, scox=0.0, noxrat=0.0, arat=0.0, crat=0.0,  &end
END
 &solver  emax=5.0E-6, atolsp=1.0E-13,  &end
FINIS
  LSENS   CH4 - O2 - N2 MECH. BATCH RXN. WITH OTTO CYCLE HEAT LOSS         CASE 5
NEW
   M        +   CH4      =   CH3      +   H           2.0E+17   0.        88000.
   H        +   CH4      =   CH3      +   H2         1.26E+14   0.        11900.
   CH4      +   O2       =   CH3      +   HO2        7.94E+13   0.        56000.
   O        +   CH4      =   CH3      +   OH          1.9E+14   0.        11720.
   OH       +   CH4      =   CH3      +   H2O         2.5E+13   0.        5010.
   CH3      +   O2       =   CH3O     +   O           2.4E+13    0.       28680.
   CH3      +   OH       =   CH3O     +   H           6.3E+12   0.         0.
   M        +   CH3O     =   CH2O     +   H           5.0E+13   0.        21000.
   CH3      +   CH3      =   C2H6                     2.4E+14   -.4        0.
   H        +   C2H6     =   C2H5     +   H2         1.32E+14   0.        9700.
   O        +   C2H6     =   C2H5     +   OH         1.13E+14   0.        7850.
   OH       +   C2H6     =   C2H5     +   H2O         8.7E+13   0.        3520.
   M        +   C2H5     =   C2H4     +   H           1.0E+17   0.        31000.
   C2H5     +   O2       =   C2H4     +   HO2         2.0E+12   0.        5000.
   H        +   C2H5     =   C2H4     +   H2          4.8E+13   0.         0.
   CH3      +   CH2      =   C2H4     +   H           2.0E+13   0.         0.
   H        +   C2H4     =   H2       +   C2H3        1.5E+14   0.        10200.
   M        +   C2H4     =   C2H2     +   H2          2.6E+17    0.       79300.
   C2H4     +   OH       =   C2H3     +   H2O         4.8E+12   0.         1230.
   C2H4     +   OH       =   CH3      +   CH2O        2.0E+12   0.         960.
   C2H4     +   O        =   CH3      +   HCO         3.3E+12   0.         1130.
   C2H4     +   O        =   CH2O     +   CH2         2.5E+13   0.        5000.
   M        +   C2H3     =   C2H2     +   H           3.0E+15   0.        32000.
   C2H3     +   O2       =   CH2O     +   HCO        3.98E+12   0.         -250.
   C2H3     +   H        =   C2H2     +   H2          6.0E+12  0.           0.
   C2H3     +   O        =   C2H2O    +   H           3.3E+13  0.           0.
   C2H3     +   OH       =   C2H2     +   H2O         5.0E+12   0.        0.
```

TABLE D.1.—Continued.

```
   C2H3      +   CH2       =   C2H2      +   CH3          3.0E+13    0.        0.
   C2H3      +   C2H       =2.0C2H2                       3.0E+13    0.        0.
   M         +   C2H2      =   C2H       +   H            4.2E+16    0.        107000.
   C2H2      +   O         =   CH2       +   CO           1.6E+14    .0        9890.
   C2H2      +   O         =   C2HO      +   H            4.0E+14    0.0       10660.
   C2H2      +   OH        =   C2H       +   H2O          6.3E+12    0.0       7000.
   C2H2      +   OH        =   C2H2O     +   H            3.2E+11    0.0       200.
   C2H       +   O2        =   C2HO      +   O            5.00E+13   0.        1500.
   C2H       +   OH        =   C2HO      +   H            2.0E+13    0.        0.
   C2HO      +   O2        =2.0CO        +   OH           1.46E+12   0.        2500.
   C2HO      +   O         =2.0CO        +   H            1.202E+12  0.        0.
   C2HO      +   OH        =2.0HCO                        1.0E+13    0.        0.
   C2HO      +   H         =   CH2       +   CO           5.0E+13    0.        0.
   C2HO      +   CH2       =   C2H3      +   CO           3.0E+13    0.        0.
   C2HO      +   CH2       =   CH2O      +   C2H          1.0E+13    0.        2000.
             2.0C2HO       =   C2H2      +2.0CO           1.0E+13    0.        0.
   C2H2O     +   OH        =   CH2O      +   HCO          2.8E+13    0.        0.
   C2H2O     +   OH        =   C2HO      +   H2O          7.5E+12    0.        3000.
   C2H2O     +   H         =   CH3       +   CO           1.13E+13   0.        3428.
   C2H2O     +   H         =   C2HO      +   H2           7.5E+13    0.        8000.
   C2H2O     +   O         =   C2HO      +   OH           5.0E+13    0.        8000.
   C2H2O     +   O         =   CH2O      +   CO           2.0E+13    0.        0.
   M         +   C2H2O     =   CH2       +   CO           2.0E+16    0.        60000.
   C2H       +   O         =   CO        +   CH           5.0E+13    0.        0.
   CH3O      +   O2        =   CH2O      +   HO2          1.0E+13    0.        7170.
   CH3O      +   H         =   CH2O      +   H2           2.0E+13    0.        0.
   M         +   CH2O      =   HCO       +   H            5.0E+16    0.        81000.
   CH2O      +   OH        =   HCO       +   H2O          3.0E+13    0.        1200.
   CH2O      +   H         =   HCO       +   H2           2.5E+13    0.        3990.
   CH2O      +   O         =   HCO       +   OH           3.5E+13    0.        3500.
   CH3       +   CH2O      =   CH4       +   HCO          1.0E+10    0.5       6000.
   CH3       +   HCO       =   CH4       +   CO           3.0E+11    .5        0.
   CH3       +   HO2       =   CH3O      +   OH           2.0E+13    0.        0.
   M         +   CH3       =   CH2       +   H            1.95E+16   0.        91600.
   H         +   CH3       =   H2        +   CH2          2.7E+11    .67       25700.
   O         +   CH3       =   OH        +   CH2          1.9E+11    .68       25700.
   OH        +   CH3       =   H2O       +   CH2          2.7E+11    .67       25700.
   CH        +   CO2       =   HCO       +   CO           3.7E+12    0.        0.
   CH        +   O2        =   HCO       +   O            1.0E+13    0.        0.
   CH2       +   O2        =   CH2O      +   O            5.0E+11    0.5       6960.
   CH2       +   O         =   CH        +   OH           2.0E+11    .7        25800.
   CH2       +   OH        =   CH        +   H2O          5.0E+11    .5        5900.
   CH2       +   H         =   CH        +   H2           3.2E+11    0.7       4970.
   CH2       +   CH2       =   C2H3      +   H            5.0E+12    0.        0.
   CH2       +   CH2       =   C2H2      +   H2           4.0E+13    0.        0.
   HCO       +   O2        =   CO        +   HO2          3.0E+13    0.        0.
   HCO       +   O         =   CO        +   OH           3.0E+13    0.        0.
   HCO       +   OH        =   CO        +   H2O          3.0E+13    0.        0.
   HCO       +   H         =   CO        +   H2           2.0E+13    0.        0.
   M         +   HCO       =   H         +   CO           2.9E+14    0.        15570.
   CO        +   O         =   CO2       +   M            2.4E+15    0.        4100.
   CO        +   O2        =   CO2       +   O            2.5E+12    0.        47690.
   CO        +   OH        =   CO2       +   H            4.17E+11   0.        1000.
   CO        +   HO2       =   CO2       +   OH           5.75E+13   0.        22930.
   O         +   H2O       =   OH        +   OH           6.8E+13    0.        18365.
   H         +   O2        =   OH        +   O            1.89E+14   0.        16400.
   O         +   H2        =   OH        +   H            4.20E+14   0.        13750.
   H         +   HO2       =   H2        +   O2           7.28E+13   0.        2126.
   O         +   HO2       =   OH        +   O2           5.0E+13    0.        1000.
   HO2       +   OH        =   H2O       +   O2           8.0E+12    0.        0.
   H         +   HO2       =2.0OH                         1.34E+14   0.        1070.
   H2        +   HO2       =   H2O2      +   H            7.91E+13   0.        25000.
   OH        +   H2O2      =   H2O       +   HO2          6.1E+12    0.        1430.
   HO2       +   HO2       =   H2O2      +   O2           1.8E+12    0.        0.
   H         +   H2O2      =   OH        +   H2O          7.8E+11    0.        0.
   M         +   H2O2      =2.0OH                         1.44E+17   0.        45510.
   THIRDBODY
H2           2.30    O2          .78     H2O              6.0    H2O2          6.6
END
   H2        +   OH        =   H2O       +   H            4.74E+13   0.        6098.
   H         +   O2        =   HO2       +   M            1.46E+15   0.        -1000.
   THIRDBODY
O2           1.30    N2          1.3     H2O              21.3   CO2           7.0
END
   M         +   H2O       =   H         +   OH           1.30E+15   0.        105140.
   THIRDBODY
H2           4.00    O2          1.5     H2O              20.0   N2            1.5
CO2          4.0     END
   H         +   O         =   OH        +   M            7.1E+18    -1.       0.
   M         +   H2        =   H         +   H            2.2E+14    0.        96000.
   THIRDBODY
H2           4.10    O2          2.0     H2O              15.0   N2            2.0
```

TABLE D.1.—Continued.

```
END
   M        +   O2       =   O        +   O          1.80E+18   -1.       118020.
   CH       +   N2       =   HCN      +   N           1.0E+11   0.        19000.
   CN       +   H2       =   HCN      +   H           6.0E+13   0.        5300.
   O        +   HCN      =   OH       +   CN          1.4E+11  .68        16900.
   OH       +   HCN      =   HNCO     +   H           4.0E+11   0.         2800.
   CN       +   O        =   CO       +   N           1.2E+13   0.           0.
   CN       +   OH       =   NCO      +   H           2.5E+14   0.        6000.
   H2       +   NCO      =   HNCO     +   H           1.0E+14   0.        9000.
   HNCO     +   H        =   NH2      +   CO          1.0E+14   0.        8500.
   CN       +   O2       =   NCO      +   O           3.2E+13   0.        1000.
   CN       +   CO2      =   NCO      +   CO          3.7E+12   0.          0.
   O        +   NCO      =   NO       +   CO          2.0E+13    0.        0.
   N        +   NCO      =   N2       +   CO          1.0E+13    0.        0.
   H        +   NCO      =   NH       +   CO          2.0E+13    0.        0.
   CH       +   NO       =   N        +   HCO         1.6E+13   0.        9940.
   CH       +   NO       =   O        +   HCN         2.0E+12   0.        0.
   NH       +   OH       =   N        +   H2O         5.0E+11   0.5       2000.
   HO2      +   NO       =   NO2      +   OH         2.09E+12    0.      -477.
   O        +   NO2      =   NO       +   O2          1.0E+13     0.      596.
   NO       +   O        =   NO2      +   M          5.62E+15   0.        -1160.
   NO2      +   H        =   NO       +   OH         3.47E+14   0.         1470.
   NO       +   H        =   N        +   OH         2.63E+14   0.        50410.
   NO       +   O        =   N        +   O2           3.8E+9   1.        41370.
   O        +   N2       =   NO       +   N          1.80E+14   0.        76250.
   N        +   NO2      =2.0NO                       4.0E+12   0.        0.
   M        +   N2O      =   N2       +   O          6.92E+23   -2.5      65000.
   O        +   N2O      =   N2       +   O2          1.0E+14   0.        28020.
   O        +   N2O      =2.0NO                      6.92E+13   0.        26630.
   N2O      +   H        =   N2       +   OH         7.59E+13   0.        15100.
   NO2      +   H2       =   HNO2     +   H           2.4E+13  0.        29000.
   OH       +   NO2      =   HNO3     +   M           3.0E+15  0.        -3800.
   THIRDBODY
O2          0.70    H2          1.4      END
   OH       +   NO       =   HNO2     +   M           5.6E+15  0.        -1700.
   HNO      +   H        =   H2       +   NO          5.0E+12   0.        0.
   H        +   NO       =   HNO      +   M           5.4E+15   0.        -600.
   HNO      +   OH       =   H2O      +   NO          3.6E+13   0.        0.

END
TIME      PRESSURE
 &prob  ct0=2.0, ct1=700.0, print=2.5E-4,3.4E-4,3.8E-4,
   htran=.true., qmread=.false., otto=.true., bore=8.5, stroke=7.0,
   twall=1000.0, rpm=2500.0,  &end
 &start  t=1550.0,  &end
CH4       0.1725
O2        0.1725
N2        0.65492
N         0.00001
CH        0.00003
CN        0.00001
CH2       0.00001
END
 &solver  emax=1.0E-4, atolsp=1.0E-13,  &end
FINIS
  LSENS   METHANE  AIR  MECHANISM   CONSTANT PRESSURE FLOW PROBLEM        CASE 6
NEW
   M        +   CH4      =   CH3      +   H           2.0E+17   0.        88000.
   H        +   CH4      =   CH3      +   H2         1.26E+14   0.        11900.
   CH4      +   O2       =   CH3      +   HO2        7.94E+13   0.        56000.
   O        +   CH4      =   CH3      +   OH          1.9E+14   0.        11720.
   OH       +   CH4      =   CH3      +   H2O         2.5E+13   0.        5010.
   CH3      +   O2       =   CH3O     +   O           2.4E+13    0.       28680.
   CH3      +   OH       =   CH3O     +   H           6.3E+12   0.         0.
   M        +   CH3O     =   CH2O     +   H           5.0E+13   0.        21000.
   CH3      +   CH3      =   C2H6                     2.4E+14   -.4       0.
   H        +   C2H6     =   C2H5     +   H2         1.32E+14   0.        9700.
   O        +   C2H6     =   C2H5     +   OH         1.13E+14   0.        7850.
   OH       +   C2H6     =   C2H5     +   H2O         8.7E+13   0.        3520.
   M        +   C2H5     =   C2H4     +   H           1.0E+17   0.        31000.
   C2H5     +   O2       =   C2H4     +   HO2         2.0E+12   0.        5000.
   H        +   C2H5     =   C2H4     +   H2          4.8E+13   0.         0.
   CH3      +   CH2      =   C2H4     +   H           2.0E+13   0.         0.
   H        +   C2H4     =   H2       +   C2H3        1.5E+14   0.        10200.
   M        +   C2H4     =   C2H2     +   H2          2.6E+17    0.       79300.
   C2H4     +   OH       =   C2H3     +   H2O         4.8E+12   0.         1230.
   C2H4     +   OH       =   CH3      +   CH2O        2.0E+12   0.         960.
   C2H4     +   O        =   CH3      +   HCO         3.3E+12   0.         1130.
   C2H4     +   O        =   CH2O     +   CH2         2.5E+13   0.        5000.
   M        +   C2H3     =   C2H2     +   H           3.0E+15   0.        32000.
   C2H3     +   O2       =   CH2O     +   HCO        3.98E+12   0.         -250.
   C2H3     +   H        =   C2H2     +   H2          6.0E+12  0.           0.
```

TABLE D.1.—Continued.

```
   C2H3      +   O        =   C2H2O    +   H          3.3E+13  0.          0.
   C2H3      +   OH       =   C2H2     +   H2O        5.0E+12   0.       0.
   C2H3      +   CH2      =   C2H2     +   CH3        3.0E+13    0.       0.
   C2H3      +   C2H      =2.0C2H2                    3.0E+13   0.        0.
   M         +   C2H2     =   C2H      +   H          4.2E+16   0.       107000.
   C2H2      +   O        =   CH2      +   CO         1.6E+14    .0      9890.
   C2H2      +   O        =   C2HO     +   H          4.0E+14   0.0     10660.
   C2H2      +   OH       =   C2H      +   H2O        6.3E+12   0.0      7000.
   C2H2      +   OH       =   C2H2O    +   H          3.2E+11   0.0      200.
   C2H       +   O2       =   C2HO     +   O         5.00E+13   0.      1500.
   C2H       +   OH       =   C2HO     +   H          2.0E+13    0.       0.
   C2HO      +   O2       =2.0CO       +   OH        1.46E+12   0.      2500.
   C2HO      +   O        =2.0CO       +   H        1.202E+12    0.       0.
   C2HO      +   OH       =2.0HCO                    1.0E+13   0.       0.
   C2HO      +   H        =   CH2      +   CO         5.0E+13    0.       0.
   C2HO      +   CH2      =   C2H3     +   CO         3.0E+13    0.       0.
   C2HO      +   CH2      =   CH2O     +   C2H        1.0E+13   0.      2000.
             2.0C2HO      =   C2H2     +2.0CO         1.0E+13    0.       0.
   C2H2O     +   OH       =   CH2O     +   HCO        2.8E+13    0.       0.
   C2H2O     +   OH       =   C2HO     +   H2O        7.5E+12    0.      3000.
   C2H2O     +   H        =   CH3      +   CO        1.13E+13   0.      3428.
   C2H2O     +   H        =   C2HO     +   H2         7.5E+13   0.      8000.
   C2H2O     +   O        =   C2HO     +   OH         5.0E+13    0.      8000.
   C2H2O     +   O        =   CH2O     +   CO         2.0E+13   0.       0.
   M         +   C2H2O    =   CH2      +   CO         2.0E+16   0.      60000.
   C2H       +   O        =   CO       +   CH         5.0E+13   0.       0.
   CH3O      +   O2       =   CH2O     +   HO2        1.0E+13   0.       7170.
   CH3O      +   H        =   CH2O     +   H2         2.0E+13    0.       0.
   M         +   CH2O     =   HCO      +   H          5.0E+16   0.      81000.
   CH2O      +   OH       =   HCO      +   H2O        3.0E+13    0.      1200.
   CH2O      +   H        =   HCO      +   H2         2.5E+13   0.      3990.
   CH2O      +   O        =   HCO      +   OH         3.5E+13   0.      3510.
   CH3       +   CH2O     =   CH4      +   HCO        1.0E+10   0.5      6000.
   CH3       +   HCO      =   CH4      +   CO         3.0E+11   .5       0.
   CH3       +   HO2      =   CH3O     +   OH         2.0E+13   0.       0.
   M         +   CH3      =   CH2      +   H         1.95E+16    0.      91600.
   H         +   CH3      =   H2       +   CH2        2.7E+11  .67      25700.
   O         +   CH3      =   OH       +   CH2        1.9E+11   .68     25700.
   OH        +   CH3      =   H2O      +   CH2        2.7E+11   .67     25700.
   CH        +   CO2      =   HCO      +   CO         3.7E+12   0.       0.
   CH        +   O2       =   HCO      +   O          1.0E+13   0.       0.
   CH2       +   O2       =   CH2O     +   O          5.0E+11   0.5      6960.
   CH2       +   O        =   CH       +   OH         2.0E+11   .7      25800.
   CH2       +   OH       =   CH       +   H2O        5.0E+11   .5       5900.
   CH2       +   H        =   CH       +   H2         3.2E+11   0.7      4970.
   CH2       +   CH2      =   C2H3     +   H          5.0E+12   0.       0.
   CH2       +   CH2      =   C2H2     +   H2         4.0E+13   0.       0.
   HCO       +   O2       =   CO       +   HO2        3.0E+13   0.       0.
   HCO       +   O        =   CO       +   OH         3.0E+13   0.       0.
   HCO       +   OH       =   CO       +   H2O        3.0E+13    0.       0.
   HCO       +   H        =   CO       +   H2         2.0E+13   0.       0.
   M         +   HCO      =   H        +   CO         2.9E+14   0.      15570.
   CO        +   O        =   CO2      +   M          2.4E+15   0.      4100.
   CO        +   O2       =   CO2      +   O          2.5E+12   0.      47690.
   CO        +   OH       =   CO2      +   H         4.17E+11   0.       1000.
   CO        +   HO2      =   CO2      +   OH        5.75E+13   0.      22930.
   O         +   H2O      =   OH       +   OH         6.8E+13    0.      18365.
   H         +   O2       =   OH       +   O         1.89E+14   0.      16400.
   O         +   H2       =   OH       +   H         4.20E+14   0.      13750.
   H         +   HO2      =   H2       +   O2        7.28E+13   0.      2126.
   O         +   HO2      =   OH       +   O2         5.0E+13   0.      1000.
   HO2       +   OH       =   H2O      +   O2         8.0E+12   0.       0.
   H         +   HO2      =2.0OH                     1.34E+14   0.      1070.
   H2        +   HO2      =   H2O2     +   H          7.91E+13   0.      25000.
   OH        +   H2O2     =   H2O      +   HO2        6.1E+12   0.      1430.
   HO2       +   HO2      =   H2O2     +   O2         1.8E+12   0.       0.
   H         +   H2O2     =   OH       +   H2O        7.8E+11   0.       0.
   M         +   H2O2     =2.0OH                     1.44E+17   0.      45510.
   THIRDBODY
H2           2.30    O2          .78     H2O          6.0    H2O2          6.6
END
   H2        +   OH       =   H2O      +   H          4.74E+13   0.      6098.
   H         +   O2       =   HO2      +   M          1.46E+15   0.      -1000.
   THIRDBODY
O2           1.30    N2          1.3     H2O          21.3   CO2           7.0
END
   M         +   H2O      =   H        +   OH         1.30E+15   0.      105140.
   THIRDBODY
H2           4.00    O2          1.5     H2O          20.0   N2            1.5
CO2          4.0     END
   H         +   O        =   OH       +   M          7.1E+18   -1.       0.
   M         +   H2       =   H        +   H          2.2E+14   0.       96000.
```

TABLE D.1.—Continued.

```
   THIRDBODY
H2          4.10    O2          2.0     H2O          15.0   N2          2.0
END
   M       +   O2      =   O       +   O          1.80E+18   -1.       118020.
   CH      +   N2      =   HCN     +   N           1.0E+11   0.        19000.
   CN      +   H2      =   HCN     +   H           6.0E+13   0.        5300.
   O       +   HCN     =   OH      +   CN          1.4E+11   .68       16900.
   OH      +   HCN     =   HNCO    +   H           4.0E+11   0.         2800.
   CN      +   O       =   CO      +   N           1.2E+13   0.           0.
   CN      +   OH      =   NCO     +   H           2.5E+14   0.        6000.
   H2      +   NCO     =   HNCO    +   H           1.0E+14   0.        9000.
   HNCO    +   H       =   NH2     +   CO          1.0E+14   0.        8500.
   CN      +   O2      =   NCO     +   O           3.2E+13   0.        1000.
   CN      +   CO2     =   NCO     +   CO          3.7E+12   0.         0.
   O       +   NCO     =   NO      +   CO          2.0E+13    0.        0.
   N       +   NCO     =   N2      +   CO          1.0E+13    0.        0.
   H       +   NCO     =   NH      +   CO          2.0E+13    0.        0.
   CH      +   NO      =   N       +   HCO         1.6E+13   0.        9940.
   CH      +   NO      =   O       +   HCN         2.0E+12   0.        0.
   NH      +   OH      =   N       +   H2O         5.0E+11   0.5       2000.
   HO2     +   NO      =   NO2     +   OH         2.09E+12    0.      -477.
   O       +   NO2     =   NO      +   O2          1.0E+13     0.      596.
   NO      +   O       =   NO2     +   M          5.62E+15   0.        -1160.
   NO2     +   H       =   NO      +   OH         3.47E+14   0.         1470.
   NO      +   H       =   N       +   OH         2.63E+14   0.        50410.
   NO      +   O       =   N       +   O2           3.8E+9   1.        41370.
   O       +   N2      =   NO      +   N          1.80E+14   0.        76250.
   N       +   NO2     =2.0NO                      4.0E+12   0.        0.
   M       +   N2O     =   N2      +   O          6.92E+23   -2.5      65000.
   O       +   N2O     =   N2      +   O2          1.0E+14   0.        28020.
   O       +   N2O     =2.0NO                     6.92E+13   0.        26630.
   N2O     +   H       =   N2      +   OH         7.59E+13   0.        15100.
   NO2     +   H2      =   HNO2    +   H           2.4E+13  0.         29000.
   OH      +   NO2     =   HNO3    +   M           3.0E+15  0.         -3800.
   THIRDBODY
O2          0.70    H2          1.4     END
   OH      +   NO      =   HNO2    +   M           5.6E+15  0.         -1700.
   HNO     +   H       =   H2      +   NO          5.0E+12   0.        0.
   H       +   NO      =   HNO     +   M           5.4E+15   0.        -600.
   HNO     +   OH      =   H2O     +   NO          3.6E+13   0.        0.

END
DISTANCE  PRESSURE
 &prob  cx0=1.730, combus=.true., exchr=.true.,
   print=10.0,20.0,25.0,30.0,32.0,34.0,36.0,37.0,38.0,39.0,40.0,41.0,
    42.0,43.0,44.0,45.0,46.0,47.0,48.0,  &end
 &start  area=1000.0, mach=2.0, t=1700.0,  &end
CH4        0.049768
O2         0.199072
N2         0.75116
CN         0.0000001
END
 &solver  emax=1.0E-4, atolsp=1.0E-10,  &end
FINIS
  LSENS   METHANE - AIR WITH AREA PROFILE OF CASE 6                      CASE 7
REPEAT
DISTANCE  AREA
 &prob  pcon=.false., combus=.false.,
   xtb=0.0,10.0,20.0,25.0,30.0,32.0,34.0,36.0,37.0,38.0,39.0,40.0,41.0,
    42.0,43.0,44.0,45.0,46.0,47.0,48.0,
   atb= 1000.00,1000.20,1004.65,1010.85,1023.22,1031.44,1042.92,1059.73,
    1071.45,1087.06,1110.03,1153.75,1284.24,1350.79,1376.81,1397.15,
    1414.00,1428.05,1439.83,1449.81,
   aprint=1023.22,1153.75,1439.83,  &end
 &start  t=1700.0, mach=2.0, p=1.730,  &end
CH4        0.049768
O2         0.199072
N2         0.75116
CN         0.0000001
END
 &solver  emax=5.0E-5, atolsp=1.0E-13,  &end
FINIS
  LSENS   METHANE - AIR WITH AREA AND TEMPERATURE PROFILES OF CASE 6      CASE 8
REPEAT
DISTANCE  AREA
 &prob  tass=.true.,  &end
 &tmpdat  xtb=0.0,15.0,20.0,25.0,30.0,32.0,34.0,36.0,38.0,40.0,41.0,
    42.0,43.0,44.0,45.0,46.0,47.0,48.0,
   tmptb=1700.00,1702.50,1707.74,1718.03,1738.22,1751.43,1769.70,
    1796.16,1838.63,1939.65,2127.05,2225.54,2270.46,2307.71,2339.56,
    2366.73,2389.90,2409.76,
   tprint=1738.22,1939.65,2389.90,  &end
```

TABLE D.1.—Continued.

```
 &start  p=1.730, mach=2.0,  &end
CH4        0.049768
O2         0.199072
N2         0.75116
CN         0.0000001
END
 &solver  emax=1.0E-3, atolsp=1.0E-12, mf=21,  &end
FINIS
  LSENS   METHANE  AIR  MECHANISM   ASSIGNED (CONST.) TEMP. FLOW PROBLEM  CASE 9
REPEAT
DISTANCE  PRESSURE
 &prob  cx0=1.730, combus=.true., exchr=.false.,
   print=25.0,42.0,48.0,  &end
 &tmpdat  cx0=1700.0,  &end
 &start  area=1000.0, mach=2.0,  &end
CH4        0.049768
O2         0.199072
N2         0.75116
CN         0.0000001
END
 &solver  emax=1.0E-4, atolsp=1.0E-13,  &end
FINIS
  LSENS   METHANOL - AIR  COMBUSTION                                        CASE 10
NEW
   M      +   CH3OH    =   CH3      +   OH          3.2E+18   0.        80000.
   O2     +   CH3OH    =   CH2OH    +   HO2         4.0E+13   0.        50900.
   OH     +   CH3OH    =   CH2OH    +   H2O         4.0E+12   0.        2000.
   O      +   CH3OH    =   CH2OH    +   OH          1.6E+12   0.        2300.
   H      +   CH3OH    =   CH2OH    +   H2          3.2E+13   0.        7000.
   H      +   CH3OH    =   CH3      +   H2O         5.0E+12   0.        5300.
   CH3    +   CH3OH    =   CH2OH    +   CH4         2.0E+11   0.        9800.
   HO2    +   CH3OH    =   CH2OH    +   H2O2        6.3E+12   0.        19400.
   M      +   CH2OH    =   CH2O     +   H           2.5E+13   0.        29000.
   O2     +   CH2OH    =   CH2O     +   HO2         1.0E+12   0.        6000.
   M      +   CH4      =   CH3      +   H           2.0E+17   0.        88000.
   H      +   CH4      =   CH3      +   H2         1.26E+14   0.        11900.
   CH4    +   O2       =   CH3      +   HO2        7.94E+13   0.        56000.
   O      +   CH4      =   CH3      +   OH          1.9E+14   0.        11720.
   OH     +   CH4      =   CH3      +   H2O         2.5E+13   0.        5010.
   CH3    +   O2       =   CH3O     +   O           2.4E+13    0.       28680.
   CH3    +   OH       =   CH3O     +   H           6.3E+12   0.         0.
   M      +   CH3O     =   CH2O     +   H           5.0E+13   0.        21000.
   CH3    +   CH3      =   C2H6                     2.4E+14   -.4        0.
   H      +   C2H6     =   C2H5     +   H2         1.32E+14   0.        9700.
   O      +   C2H6     =   C2H5     +   OH         1.13E+14   0.        7850.
   OH     +   C2H6     =   C2H5     +   H2O         8.7E+13   0.        3520.
   M      +   C2H5     =   C2H4     +   H           1.0E+17   0.        31000.
   C2H5   +   O2       =   C2H4     +   HO2         2.0E+12   0.        5000.
   H      +   C2H5     =   C2H4     +   H2          4.8E+13   0.         0.
   CH3    +   CH2      =   C2H4     +   H           2.0E+13   0.         0.
   H      +   C2H4     =   H2       +   C2H3        1.5E+14   0.        10200.
   M      +   C2H4     =   C2H2     +   H2          2.6E+17    0.       79300.
   C2H4   +   OH       =   C2H3     +   H2O         4.8E+12   0.         1230.
   C2H4   +   OH       =   CH3      +   CH2O        2.0E+12   0.         960.
   C2H4   +   O        =   CH3      +   HCO         3.3E+12   0.         1130.
   C2H4   +   O        =   CH2O     +   CH2         2.5E+13   0.        5000.
   M      +   C2H3     =   C2H2     +   H           3.0E+15   0.        32000.
   C2H3   +   O2       =   CH2O     +   HCO        3.98E+12   0.         -250.
   C2H3   +   H        =   C2H2     +   H2          6.0E+12  0.           0.
   C2H3   +   O        =   C2H2O    +   H           3.3E+13  0.           0.
   C2H3   +   OH       =   C2H2     +   H2O         5.0E+12   0.        0.
   C2H3   +   CH2      =   C2H2     +   CH3         3.0E+13    0.        0.
   C2H3   +   C2H      =2.0C2H2                     3.0E+13   0.         0.
   M      +   C2H2     =   C2H      +   H           4.2E+16   0.        107000.
   C2H2   +   O        =   CH2      +   CO          1.6E+14    .0        9890.
   C2H2   +   O        =   C2HO     +   H           4.0E+14   0.0       10660.
   C2H2   +   OH       =   C2H      +   H2O         6.3E+12   0.0        7000.
   C2H2   +   OH       =   C2H2O    +   H           3.2E+11   0.0        200.
   C2H    +   O2       =   C2HO     +   O          5.00E+13   0.        1500.
   C2H    +   OH       =   C2HO     +   H           2.0E+13    0.        0.
   C2HO   +   O2       =2.0CO       +   OH         1.46E+12   0.        2500.
   C2HO   +   O        =2.0CO       +   H         1.202E+12    0.        0.
   C2HO   +   OH       =2.0HCO                      1.0E+13   0.        0.
   C2HO   +   H        =   CH2      +   CO          5.0E+13    0.       0.
   C2HO   +   CH2      =   C2H3     +   CO          3.0E+13    0.        0.
   C2HO   +   CH2      =   CH2O     +   C2H         1.0E+13   0.        2000.
            2.0C2HO    =   C2H2     +2.0CO          1.0E+13    0.        0.
   C2H2O  +   OH       =   CH2O     +   HCO         2.8E+13    0.        0.
   C2H2O  +   OH       =   C2HO     +   H2O         7.5E+12    0.       3000.
   C2H2O  +   H        =   CH3      +   CO         1.13E+13   0.        3428.
   C2H2O  +   H        =   C2HO     +   H2          7.5E+13   0.        8000.
   C2H2O  +   O        =   C2HO     +   OH          5.0E+13    0.       8000.
```

TABLE D.1.—Continued.

```
   C2H2O    +   O       =   CH2O    +   CO        2.0E+13   0.        0.
   M        +   C2H2O   =   CH2     +   CO        2.0E+16   0.        60000.
   C2H      +   O       =   CO      +   CH        5.0E+13   0.        0.
   CH3O     +   O2      =   CH2O    +   HO2       1.0E+13   0.        7170.
   CH3O     +   H       =   CH2O    +   H2        2.0E+13   0.        0.
   M        +   CH2O    =   HCO     +   H         5.0E+16   0.        81000.
   CH2O     +   OH      =   HCO     +   H2O       3.0E+13   0.        1200.
   CH2O     +   H       =   HCO     +   H2        2.5E+13   0.        3990.
   CH2O     +   O       =   HCO     +   OH        3.5E+13   0.        3510.
   CH3      +   CH2O    =   CH4     +   HCO       1.0E+10   0.5       6000.
   CH3      +   HCO     =   CH4     +   CO        3.0E+11   .5        0.
   CH3      +   HO2     =   CH3O    +   OH        2.0E+13   0.        0.
   M        +   CH3     =   CH2     +   H         1.95E+16  0.        91600.
   H        +   CH3     =   H2      +   CH2       2.7E+11   .67       25700.
   O        +   CH3     =   OH      +   CH2       1.9E+11   .68       25700.
   OH       +   CH3     =   H2O     +   CH2       2.7E+11   .67       25700.
   CH       +   CO2     =   HCO     +   CO        3.7E+12   0.        0.
   CH       +   O2      =   HCO     +   O         1.0E+13   0.        0.
   CH2      +   O2      =   CH2O    +   O         5.0E+11   0.5       6960.
   CH2      +   O       =   CH      +   OH        2.0E+11   .7        25800.
   CH2      +   OH      =   CH      +   H2O       5.0E+11   .5        5900.
   CH2      +   H       =   CH      +   H2        3.2E+11   0.7       4970.
   CH2      +   CH2     =   C2H3    +   H         5.0E+12   0.        0.
   CH2      +   CH2     =   C2H2    +   H2        4.0E+13   0.        0.
   HCO      +   O2      =   CO      +   HO2       3.0E+13   0.        0.
   HCO      +   O       =   CO      +   OH        3.0E+13   0.        0.
   HCO      +   OH      =   CO      +   H2O       3.0E+13   0.        0.
   HCO      +   H       =   CO      +   H2        2.0E+13   0.        0.
   M        +   HCO     =   H       +   CO        2.9E+14   0.        15570.
   CO       +   O       =   CO2     +   M         2.4E+15   0.        4100.
   CO       +   O2      =   CO2     +   O         2.5E+12   0.        47690.
   CO       +   OH      =   CO2     +   H         4.17E+11  0.        1000.
   CO       +   HO2     =   CO2     +   OH        5.75E+13  0.        22930.
   O        +   H2O     =   OH      +   OH        6.8E+13   0.        18365.
   H        +   O2      =   OH      +   O         1.89E+14  0.        16400.
   O        +   H2      =   OH      +   H         4.20E+14  0.        13750.
   H        +   HO2     =   H2      +   O2        7.28E+13  0.        2126.
   O        +   HO2     =   OH      +   O2        5.0E+13   0.        1000.
   HO2      +   OH      =   H2O     +   O2        8.0E+12   0.        0.
   H        +   HO2     =2.0OH                    1.34E+14  0.        1070.
   H2       +   HO2     =   H2O2    +   H         7.91E+13  0.        25000.
   OH       +   H2O2    =   H2O     +   HO2       6.1E+12   0.        1430.
   HO2      +   HO2     =   H2O2    +   O2        1.8E+12   0.        0.
   H        +   H2O2    =   OH      +   H2O       7.8E+11   0.        0.
   M        +   H2O2    =2.0OH                    1.44E+17  0.        45510.
   THIRDBODY
H2          2.30    O2          .78     H2O       6.0     H2O2      6.6
END
   H2       +   OH      =   H2O     +   H         4.74E+13  0.        6098.
   H        +   O2      =   HO2     +   M         1.46E+15  0.        -1000.
   THIRDBODY
O2          1.30    N2          1.3     H2O       21.3    CO2       7.0
END
   M        +   H2O     =   H       +   OH        1.30E+15  0.        105140.
   THIRDBODY
H2          4.00    O2          1.5     H2O       20.0    N2        1.5
CO2         4.0     END
   H        +   O       =   OH      +   M         7.1E+18   -1.       0.
   M        +   H2      =   H       +   H         2.2E+14   0.        96000.
   THIRDBODY
H2          4.10    O2          2.0     H2O       15.0    N2        2.0
END
   M        +   O2      =   O       +   O         1.80E+18  -1.       118020.
   CH       +   N2      =   HCN     +   N         1.0E+11   0.        19000.
   CN       +   H2      =   HCN     +   H         6.0E+13   0.        5300.
   O        +   HCN     =   OH      +   CN        1.4E+11   .68       16900.
   OH       +   HCN     =   HNCO    +   H         4.0E+11   0.        2800.
   CN       +   O       =   CO      +   N         1.2E+13   0.        0.
   CN       +   OH      =   NCO     +   H         2.5E+14   0.        6000.
   H2       +   NCO     =   HNCO    +   H         1.0E+14   0.        9000.
   HNCO     +   H       =   NH2     +   CO        1.0E+14   0.        8500.
   CN       +   O2      =   NCO     +   O         3.2E+13   0.        1000.
   CN       +   CO2     =   NCO     +   CO        3.7E+12   0.        0.
   O        +   NCO     =   NO      +   CO        2.0E+13   0.        0.
   N        +   NCO     =   N2      +   CO        1.0E+13   0.        0.
   H        +   NCO     =   NH      +   CO        2.0E+13   0.        0.
   CH       +   NO      =   N       +   HCO       1.6E+13   0.        9940.
   CH       +   NO      =   O       +   HCN       2.0E+12   0.        0.
   NH       +   OH      =   N       +   H2O       5.0E+11   0.5       2000.
   HO2      +   NO      =   NO2     +   OH        2.09E+12  0.        -477.
   O        +   NO2     =   NO      +   O2        1.0E+13   0.        596.
   NO       +   O       =   NO2     +   M         5.62E+15  0.        -1160.
```

TABLE D.1.—Continued.

```
   NO2      +   H        =   NO       +   OH          3.47E+14   0.          1470.
   NO       +   H        =   N        +   OH          2.63E+14   0.         50410.
   NO       +   O        =   N        +   O2            3.8E+9   1.         41370.
   O        +   N2       =   NO       +   N           1.80E+14   0.         76250.
   N        +   NO2      =2.0NO                        4.0E+12   0.         0.
   M        +   N2O      =   N2       +   O           6.92E+23   -2.5       65000.
   O        +   N2O      =   N2       +   O2           1.0E+14   0.         28020.
   O        +   N2O      =2.0NO                       6.92E+13   0.         26630.
   N2O      +   H        =   N2       +   OH          7.59E+13   0.         15100.
   NO2      +   H2       =   HNO2     +   H            2.4E+13  0.         29000.
   OH       +   NO2      =   HNO3     +   M            3.0E+15  0.         -3800.
   THIRDBODY
O2          0.70    H2          1.4      END
   OH       +   NO       =   HNO2     +   M            5.6E+15  0.         -1700.
   HNO      +   H        =   H2       +   NO           5.0E+12   0.         0.
   H        +   NO       =   HNO      +   M            5.4E+15   0.         -600.
   HNO      +   OH       =   H2O      +   NO           3.6E+13   0.         0.

AR
TIME                                        CH3OH
 &prob  rhocon=.true., print=4.0E-4,5.0E-4,6.5E-4,  &end
 &start  t=1300.0, mmhg=.true., p=760.0, eratio=2.0, scc=1.0,
  sch=4.0, scox=1.0,  &end
CN        0.000001
CH        0.00001
N         0.000001
END
 &solver  emax=5.0E-4, atolsp=1.0E-12,  &end
FINIS
  LSENS   PROPANE-AIR WELL-STIRRED REACTOR + ROCKET EXP; EMAX=10-4    CASE 11
NEW
               C3H8     =   C2H5     +   CH3          5.0E+15   0.         83500.
   CH3      +   C3H8     =   CH4      +   C3H7        3.55E+12   0.         10300.
               C3H7     =   C2H4     +   CH3          3.0E+14   0.         33200.
   M        +   CH4      =   CH3      +   H            2.0E+17   0.         88000.
   H        +   CH4      =   CH3      +   H2          1.26E+14   0.         11900.
   CH4      +   O2       =   CH3      +   HO2         7.94E+13   0.         56000.
   O        +   CH4      =   CH3      +   OH           1.9E+14   0.         11720.
   OH       +   CH4      =   CH3      +   H2O          2.5E+13   0.         5010.
   CH3      +   O2       =   CH3O     +   O            2.4E+13    0.        28680.
   CH3      +   OH       =   CH3O     +   H            6.3E+12   0.          0.
   M        +   CH3O     =   CH2O     +   H            5.0E+13   0.         21000.
   CH3      +   CH3      =   C2H6                      2.4E+14   -.4        0.
   H        +   C2H6     =   C2H5     +   H2          1.32E+14   0.         9700.
   O        +   C2H6     =   C2H5     +   OH          1.13E+14   0.         7850.
   OH       +   C2H6     =   C2H5     +   H2O          8.7E+13   0.         3520.
   M        +   C2H5     =   C2H4     +   H            1.0E+17   0.         31000.
   C2H5     +   O2       =   C2H4     +   HO2          2.0E+12   0.         5000.
   H        +   C2H5     =   C2H4     +   H2           4.8E+13   0.          0.
   CH3      +   CH2      =   C2H4     +   H            2.0E+13   0.          0.
   H        +   C2H4     =   H2       +   C2H3         1.5E+14   0.         10200.
   M        +   C2H4     =   C2H2     +   H2           2.6E+17    0.        79300.
   C2H4     +   OH       =   C2H3     +   H2O          4.8E+12   0.          1230.
   C2H4     +   OH       =   CH3      +   CH2O         2.0E+12   0.          960.
   C2H4     +   O        =   CH3      +   HCO          3.3E+12   0.          1130.
   C2H4     +   O        =   CH2O     +   CH2          2.5E+13   0.         5000.
   M        +   C2H3     =   C2H2     +   H            3.0E+15   0.         32000.
   C2H3     +   O2       =   CH2O     +   HCO         3.98E+12   0.          -250.
   C2H3     +   H        =   C2H2     +   H2           6.0E+12  0.            0.
   C2H3     +   O        =   C2H2O    +   H            3.3E+13  0.            0.
   C2H3     +   OH       =   C2H2     +   H2O          5.0E+12   0.         0.
   C2H3     +   CH2      =   C2H2     +   CH3          3.0E+13    0.         0.
   C2H3     +   C2H      =2.0C2H2                      3.0E+13   0.          0.
   M        +   C2H2     =   C2H      +   H            4.2E+16   0.         107000.
   C2H2     +   O        =   CH2      +   CO           1.6E+14    .0        9890.
   C2H2     +   O        =   C2HO     +   H            4.0E+14   0.0        10660.
   C2H2     +   OH       =   C2H      +   H2O          6.3E+12   0.0         7000.
   C2H2     +   OH       =   C2H2O    +   H            3.2E+11   0.0         200.
   C2H      +   O2       =   C2HO     +   O           5.00E+13   0.         1500.
   C2H      +   OH       =   C2HO     +   H            2.0E+13    0.         0.
   C2HO     +   O2       =2.0CO       +   OH          1.46E+12   0.         2500.
   C2HO     +   O        =2.0CO       +   H          1.202E+12    0.         0.
   C2HO     +   OH       =2.0HCO                       1.0E+13   0.         0.
   C2HO     +   H        =   CH2      +   CO           5.0E+13    0.         0.
   C2HO     +   CH2      =   C2H3     +   CO           3.0E+13    0.         0.
   C2HO     +   CH2      =   CH2O     +   C2H          1.0E+13   0.         2000.
            2.0C2HO      =   C2H2     +2.0CO           1.0E+13    0.         0.
   C2H2O    +   OH       =   CH2O     +   HCO          2.8E+13    0.         0.
   C2H2O    +   OH       =   C2HO     +   H2O          7.5E+12    0.         3000.
   C2H2O    +   H        =   CH3      +   CO          1.13E+13   0.         3428.
   C2H2O    +   H        =   C2HO     +   H2           7.5E+13   0.         8000.
   C2H2O    +   O        =   C2HO     +   OH           5.0E+13    0.         8000.
```

TABLE D.1.—Continued.

```
   C2H2O    +   O       =   CH2O    +   CO        2.0E+13   0.        0.
   M        +   C2H2O   =   CH2     +   CO        2.0E+16   0.        60000.
   C2H      +   O       =   CO      +   CH        5.0E+13   0.        0.
   CH3O     +   O2      =   CH2O    +   HO2       1.0E+13   0.        7170.
   CH3O     +   H       =   CH2O    +   H2        2.0E+13    0.       0.
   M        +   CH2O    =   HCO     +   H         5.0E+16   0.        81000.
   CH2O     +   OH      =   HCO     +   H2O       3.0E+13    0.       1200.
   CH2O     +   H       =   HCO     +   H2        2.5E+13   0.        3990.
   CH2O     +   O       =   HCO     +   OH        3.5E+13   0.        3510.
   CH3      +   CH2O    =   CH4     +   HCO       1.0E+10   0.5       6000.
   CH3      +   HCO     =   CH4     +   CO        3.0E+11   .5        0.
   CH3      +   HO2     =   CH3O    +   OH        2.0E+13   0.        0.
   M        +   CH3     =   CH2     +   H        1.95E+16    0.       91600.
   H        +   CH3     =   H2      +   CH2       2.7E+11  .67        25700.
   O        +   CH3     =   OH      +   CH2       1.9E+11   .68       25700.
   OH       +   CH3     =   H2O     +   CH2       2.7E+11   .67       25700.
   CH       +   CO2     =   HCO     +   CO        3.7E+12   0.        0.
   CH       +   O2      =   HCO     +   O         1.0E+13   0.        0.
   CH2      +   O2      =   CH2O    +   O         5.0E+11   0.5       6960.
   CH2      +   O       =   CH      +   OH        2.0E+11   .7        25800.
   CH2      +   OH      =   CH      +   H2O       5.0E+11   .5        5900.
   CH2      +   H       =   CH      +   H2        3.2E+11   0.7       4970.
   CH2      +   CH2     =   C2H3    +   H         5.0E+12   0.        0.
   CH2      +   CH2     =   C2H2    +   H2        4.0E+13   0.        0.
   HCO      +   O2      =   CO      +   HO2       3.0E+13   0.        0.
   HCO      +   O       =   CO      +   OH        3.0E+13   0.        0.
   HCO      +   OH      =   CO      +   H2O       3.0E+13    0.       0.
   HCO      +   H       =   CO      +   H2        2.0E+13   0.        0.
   M        +   HCO     =   H       +   CO        2.9E+14   0.        15570.
   CO       +   O       =   CO2     +   M         2.4E+15   0.        4100.
   CO       +   O2      =   CO2     +   O         2.5E+12   0.        47690.
   CO       +   OH      =   CO2     +   H        4.17E+11   0.        1000.
   CO       +   HO2     =   CO2     +   OH       5.75E+13   0.        22930.
   O        +   H2O     =   OH      +   OH        6.8E+13    0.       18365.
   H        +   O2      =   OH      +   O        1.89E+14   0.        16400.
   O        +   H2      =   OH      +   H        4.20E+14   0.        13750.
   H        +   HO2     =   H2      +   O2       7.28E+13   0.        2126.
   O        +   HO2     =   OH      +   O2        5.0E+13   0.        1000.
   HO2      +   OH      =   H2O     +   O2        8.0E+12              0.
   H        +   HO2     =2.0OH                   1.34E+14   0.        1070.
   H2       +   HO2     =   H2O2    +   H        7.91E+13   0.        25000.
   OH       +   H2O2    =   H2O     +   HO2       6.1E+12   0.        1430.
   HO2      +   HO2     =   H2O2    +   O2        1.8E+12   0.        0.
   H        +   H2O2    =   OH      +   H2O       7.8E+11   0.        0.
   M        +   H2O2    =2.0OH                   1.44E+17   0.        45510.
   THIRDBODY
H2          2.30    O2          .78     H2O       6.0    H2O2        6.6
END
   H2       +   OH      =   H2O     +   H        4.74E+13   0.        6098.
   H        +   O2      =   HO2     +   M        1.46E+15   0.        -1000.
   THIRDBODY
O2          1.30    N2          1.3     H2O       21.3   CO2         7.0
END
   M        +   H2O     =   H       +   OH       1.30E+15   0.        105140.
   THIRDBODY
H2          4.00    O2          1.5     H2O       20.0   N2          1.5
CO2         4.0     END
   H        +   O       =   OH      +   M         7.1E+18   -1.       0.
   M        +   H2      =   H       +   H         2.2E+14   0.        96000.
   THIRDBODY
H2          4.10    O2          2.0     H2O       15.0   N2          2.0
END
   M        +   O2      =   O       +   O        1.80E+18   -1.       118020.
   CH       +   N2      =   HCN     +   N         1.0E+11   0.        19000.
   CN       +   H2      =   HCN     +   H         6.0E+13   0.        5300.
   O        +   HCN     =   OH      +   CN        1.4E+11  .68        16900.
   OH       +   HCN     =   HNCO    +   H         4.0E+11   0.        2800.
   CN       +   O       =   CO      +   N         1.2E+13   0.        0.
   CN       +   OH      =   NCO     +   H         2.5E+14   0.        6000.
   H2       +   NCO     =   HNCO    +   H         1.0E+14   0.        9000.
   HNCO     +   H       =   NH2     +   CO        1.0E+14   0.        8500.
   CN       +   O2      =   NCO     +   O         3.2E+13   0.        1000.
   CN       +   CO2     =   NCO     +   CO        3.7E+12   0.        0.
   O        +   NCO     =   NO      +   CO        2.0E+13    0.       0.
   N        +   NCO     =   N2      +   CO        1.0E+13    0.       0.
   H        +   NCO     =   NH      +   CO        2.0E+13    0.       0.
   CH       +   NO      =   N       +   HCO       1.6E+13   0.        9940.
   CH       +   NO      =   O       +   HCN       2.0E+12   0.        0.
   NH       +   OH      =   N       +   H2O       5.0E+11   0.5       2000.
   HO2      +   NO      =   NO2     +   OH       2.09E+12    0.       -477.
   O        +   NO2     =   NO      +   O2        1.0E+13     0.      596.
   NO       +   O       =   NO2     +   M        5.62E+15   0.        -1160.
```

TABLE D.1.—Continued.

```
   NO2      +   H        =   NO      +   OH          3.47E+14   0.         1470.
   NO       +   H        =   N       +   OH          2.63E+14   0.        50410.
   NO       +   O        =   N       +   O2            3.8E+9   1.        41370.
   O        +   N2       =   NO      +   N           1.80E+14   0.        76250.
   N        +   NO2      =2.0NO                       4.0E+12   0.        0.
   M        +   N2O      =   N2      +   O           6.92E+23   -2.5      65000.
   O        +   N2O      =   N2      +   O2           1.0E+14   0.        28020.
   O        +   N2O      =2.0NO                      6.92E+13   0.        26630.
   N2O      +   H        =   N2      +   OH          7.59E+13   0.        15100.
   NO2      +   H2       =   HNO2    +   H            2.4E+13  0.        29000.
   OH       +   NO2      =   HNO3    +   M            3.0E+15  0.        -3800.
   THIRDBODY
O2          0.70    H2          1.4     END
   OH       +   NO       =   HNO2    +   M            5.6E+15  0.        -1700.
   HNO      +   H        =   H2      +   NO           5.0E+12   0.        0.
   H        +   NO       =   HNO     +   M            5.4E+15   0.        -600.
   HNO      +   OH       =   H2O     +   NO           3.6E+13   0.        0.

AR
DISTANCE  AREA
 &prob  welstr=.true.,  conc=.false., wsflow=.true.,
   cx0=15.0, cx1=20.0, print=0.4,2.0,4.0, rocket=.true., htran= .true.,
   ht1=0.05, ht0=-42.88, pc= 73.5, athrot=2.325,  &end
 &wsprob  dotmax=1600.0, delmd=800.0, mpr=1,  volume=300.0,
   wsrhtr=.true., wsrht1=0.05, wsrht0=-42.88,  &end
 &start  t=614.0, p=5.0, mdot=10.0, molef=.false., x=0.2,  &end
C3H8      0.0873262
N2        0.6892887
O2        0.211232
AR        0.011737
CO2       0.0004162
END
 &solver  emax=1.0E-4, atolsp=1.0E-13,  &end
FINIS
  LSENS   HIGH TEMPERATURE AIR IONIZATION                                  CASE 12
NEW
   N        +   O2       =   NO      +   O            6.4E+09  1.        6250.
   O        +   N2       =   NO      +   N            1.8E+14   0.        76250.
   N        +   O        =   NO      +   M           6.40E+16  -0.5       0.
   THIRDBODY
N2O         2.25    END
   O        +   O        =   O2      +   M            5.7E+13   0.        -1790.
   M        +   N2       =   N       +   N           3.72E+21  -1.6       225000.
   NO       +   O        =   NO2     +   M           5.62E+15   0.        -1160.
   THIRDBODY
N2          1.55    END
   M        +   N2O      =   N2      +   O           6.92E+23   -2.5      65000.
   O        +   N2O      =   N2      +   O2           1.0E+14   0.        28020.
   NO+      +   E        =   N       +   O           1.45E+21  -1.5       0.
   O+       +   E        =   O       +   M           2.00E+26  -2.5       0.
   THIRDBODY
O2          4.50    N           0.03    NO           50.0   O            .03
END
   O2       +   E        =   O2-     +   M           1.52E+21  -1.        1190.
   THIRDBODY
N2          .00002  END
   O2       +   O-       =   O2-     +   O           6.00E+12  0.        0.

END
DISTANCE  AREA
 &prob  cx0=1000.0, dbugo=.true., order=.true.,
   print=0.06,0.50,0.70,  &end
 &start  p=1.6803, v=47002.0, t=4820.0,  &end
N2        0.7905
O2        0.2095
O2-       0.000000001
END
 &solver  emax=1.0E-3, atolsp=1.0E-12,  &end
FINIS
  LSENS   HIGH PRESSURE HYDROGEN - CARBON MONOXIDE REACTION                CASE 13
NEW
   CH3      +   OH       =   CH3O    +   H            6.3E+12   0.        0.
   M        +   CH3O     =   CH2O    +   H            5.0E+13   0.        21000.
   CH3O     +   H        =   CH2O    +   H2           2.0E+13    0.        0.
   CH3      +   HCO      =   CH4     +   CO           3.0E+11   .5        0.
   CH3      +   HO2      =   CH3O    +   OH           2.0E+13   0.        0.
   M            CH4      =   CH3     +   H            2.0E+17   0.        88000.
   H        +   CH4      =   CH3     +   H2          1.26E+14   0.        11900.
   OH       +   CH4      =   CH3     +   H2O          2.5E+13   0.        5010.
   CH2O     +   H        =   HCO     +   H2           2.5E+13   0.        3990.
   CH2O     +   OH       =   HCO     +   H2O          3.0E+13   0.        1200.
   M        +   CH2O     =   H       +   HCO          5.0E+16  0.        81000.
```

TABLE D.1.—Continued.

```
   HCO      +   H        =   CO       +   H2          2.0E+13    0.        0.
   HCO      +   OH       =   CO       +   H2O         3.0E+13   0.        0.
   M        +   HCO      =   H        +   CO          2.9E+14   0.        15570.
   CO       +   OH       =   CO2      +   H          4.17E+11   0.0       1000.
   CO       +   HO2      =   CO2      +   OH         5.75E+13   0.        22930.
   H        +   HO2      =2.00H                      1.34E+14   0.        1070.
   H2       +   HO2      =   H2O2     +   H          7.91E+13   0.        25000.
   OH       +   H2O2     =   H2O      +   HO2         6.1E+12   0.        1430.
   M        +   H2O2     =2.00H                      1.44E+17   0.        45510.
   THIRDBODY
H2          2.30    H2O2        6.6     H2O           6.0    END
   H2       +   OH       =   H2O      +   H          4.74E+13   0.        6098.
   M        +   H2O      =   H        +   OH         1.30E+15   0.        105140.
   THIRDBODY
H2          4.00    CO2         4.0     H2O           20.0   END
   M        +   H2       =   H        +   H           2.2E+14   0.         96000.
   THIRDBODY
H2          4.10    H2O        15.0     END

END
TIME
 &prob  print=1.0,1.E+6,1.E+8,1.E+9, combus=.true.,
   rhocon=.true., tcon=.true.,  &end
 &start  t=1000.0, p=100.0,  &end
H2        0.99
CO        0.01
END
 &solver  emax=1.0E-3, atolsp=1.0E-12,  &end
FINIS
  LSENS   HYDROGEN - OXYGEN LOW TEMPERATURE PHOTOLYTIC IGNITION          CASE 14
NEW
   O        +   H2O      =   OH       +   OH          6.8E+13    0.        18365.
   H        +   O2       =   OH       +   O          1.89E+14   0.        16400.
   O        +   H2       =   OH       +   H          4.20E+14   0.        13750.
   H        +   HO2      =   H2       +   O2         7.28E+13   0.        2126.
   O        +   HO2      =   OH       +   O2          5.0E+13   0.        1000.
   HO2      +   OH       =   H2O      +   O2          8.0E+12              0.
   H        +   HO2      =2.00H                      1.34E+14   0.        1070.
   H2       +   HO2      =   H2O2     +   H          7.91E+13   0.        25000.
   OH       +   H2O2     =   H2O      +   HO2         6.1E+12   0.        1430.
   HO2      +   HO2      =   H2O2     +   O2          1.8E+12   0.         0.
   H        +   H2O2     =   OH       +   H2O         7.8E+11   0.         0.
   M        +   H2O2     =   OH       +   OH         1.44E+17   0.        45510.
   THIRDBODY
H2          2.30    O2           .78     H2O           6.0    H2O2        6.6
END
   H2       +   OH       =   H2O      +   H          4.74E+13   0.        6098.
   H        +   O2       =   HO2      +   M          1.46E+15   0.        -1000.
   THIRDBODY
O2          1.30    H2          3.0     H2O           21.3   END
   M        +   H2O      =   H        +   OH         1.30E+15   0.        105140.
   THIRDBODY
H2          4.00    O2          1.5     H2O           20.0   END
   H        +   O        =   OH       +   M           7.1E+18   -1.        0.
   M        +   H2       =   H        +   H           2.2E+14   0.         96000.
   THIRDBODY
H2          4.10    O2          2.0     H2O           15.0   END
   M        +   O2       =   O        +   O          1.80E+18   -1.       118020.
   HNU      +   H2       >2.0H                          .003   0.          0.
   HNU      +   O2       >2.00                          .005     0.        0.

END
TIME
 &prob  rhocon=.true., iprint=100, combus=.true., end=1.0173,  &end
 &start  t=700.0, p=2.0,  &end
H2        0.667
O2        0.333
END
 &solver  emax=1.0E-6, atolsp=1.0E-11,  &end
FINIS
  LSENS  METHANE AIR MECHAN.; MON. DECR. TABULAR AREA WITH APRINT   CASE 15
NEW
   M        +   CH4      =   CH3      +   H           2.0E+17   0.        88000.
   H        +   CH4      =   CH3      +   H2         1.26E+14   0.        11900.
   CH4      +   O2       =   CH3      +   HO2        7.94E+13   0.        56000.
   O        +   CH4      =   CH3      +   OH          1.9E+14   0.        11720.
   OH       +   CH4      =   CH3      +   H2O         2.5E+13   0.        5010.
   CH3      +   O2       =   CH3O     +   O           2.4E+13    0.       28680.
   CH3      +   OH       =   CH3O     +   H           6.3E+12   0.         0.
   M        +   CH3O     =   CH2O     +   H           5.0E+13   0.        21000.
   CH3      +   CH3      =   C2H6                     2.4E+14   -.4        0.
   H        +   C2H6     =   C2H5     +   H2         1.32E+14   0.        9700.
```

TABLE D.1.—Continued.

O	+	C2H6	=	C2H5	+	OH	1.13E+14	0.	7850.
OH	+	C2H6	=	C2H5	+	H2O	8.7E+13	0.	3520.
M	+	C2H5	=	C2H4	+	H	1.0E+17	0.	31000.
C2H5	+	O2	=	C2H4	+	HO2	2.0E+12	0.	5000.
H	+	C2H5	=	C2H4	+	H2	4.8E+13	0.	0.
CH3	+	CH2	=	C2H4	+	H	2.0E+13	0.	0.
H	+	C2H4	=	H2	+	C2H3	1.5E+14	0.	10200.
M	+	C2H4	=	C2H2	+	H2	2.6E+17	0.	79300.
C2H4	+	OH	=	C2H3	+	H2O	4.8E+12	0.	1230.
C2H4	+	OH	=	CH3	+	CH2O	2.0E+12	0.	960.
C2H4	+	O	=	CH3	+	HCO	3.3E+12	0.	1130.
C2H4	+	O	=	CH2O	+	CH2	2.5E+13	0.	5000.
M	+	C2H3	=	C2H2	+	H	3.0E+15	0.	32000.
C2H3	+	O2	=	CH2O	+	HCO	3.98E+12	0.	-250.
C2H3	+	H	=	C2H2	+	H2	6.0E+12	0.	0.
C2H3	+	O	=	C2H2O	+	H	3.3E+13	0.	0.
C2H3	+	OH	=	C2H2	+	H2O	5.0E+12	0.	0.
C2H3	+	CH2	=	C2H2	+	CH3	3.0E+13	0.	0.
C2H3	+	C2H	=2.0C2H2				3.0E+13	0.	0.
M	+	C2H2	=	C2H	+	H	4.2E+16	0.	107000.
C2H2	+	O	=	CH2	+	CO	1.6E+14	.0	9890.
C2H2	+	O	=	C2HO	+	H	4.0E+14	0.0	10660.
C2H2	+	OH	=	C2H	+	H2O	6.3E+12	0.0	7000.
C2H2	+	OH	=	C2H2O	+	H	3.2E+11	0.0	200.
C2H	+	O2	=	C2HO	+	O	5.00E+13	0.	1500.
C2H	+	OH	=	C2HO	+	H	2.0E+13	0.	0.
C2HO	+	O2	=2.0CO		+	OH	1.46E+12	0.	2500.
C2HO	+	O	=2.0CO		+	H	1.202E+12	0.	0.
C2HO	+	OH	=2.0HCO				1.0E+13	0.	0.
C2HO	+	H	=	CH2	+	CO	5.0E+13	0.	0.
C2HO	+	CH2	=	C2H3	+	CO	3.0E+13	0.	0.
C2HO	+	CH2	=	CH2O	+	C2H	1.0E+13	0.	2000.
	2.0C2HO		=	C2H2	+2.0CO		1.0E+13	0.	0.
C2H2O	+	OH	=	CH2O	+	HCO	2.8E+13	0.	0.
C2H2O	+	OH	=	C2HO	+	H2O	7.5E+12	0.	3000.
C2H2O	+	H	=	CH3	+	CO	1.13E+13	0.	3428.
C2H2O	+	H	=	C2HO	+	H2	7.5E+13	0.	8000.
C2H2O	+	O	=	C2HO	+	OH	5.0E+13	0.	8000.
C2H2O	+	O	=	CH2O	+	CO	2.0E+13	0.	0.
M	+	C2H2O	=	CH2	+	CO	2.0E+16	0.	60000.
C2H	+	O	=	CO	+	CH	5.0E+13	0.	0.
CH3O	+	O2	=	CH2O	+	HO2	1.0E+13	0.	7170.
CH3O	+	H	=	CH2O	+	H2	2.0E+13	0.	0.
M	+	CH2O	=	HCO	+	H	5.0E+16	0.	81000.
CH2O	+	OH	=	HCO	+	H2O	3.0E+13	0.	1200.
CH2O	+	H	=	HCO	+	H2	2.5E+13	0.	3990.
CH2O	+	O	=	HCO	+	OH	3.5E+13	0.	3510.
CH3	+	CH2O	=	CH4	+	HCO	1.0E+10	0.5	6000.
CH3	+	HCO	=	CH4	+	CO	3.0E+11	.5	0.
CH3	+	HO2	=	CH3O	+	OH	2.0E+13	0.	0.
M	+	CH3	=	CH2	+	H	1.95E+16	0.	91600.
H	+	CH3	=	H2	+	CH2	2.7E+11	.67	25700.
O	+	CH3	=	OH	+	CH2	1.9E+11	.68	25700.
OH	+	CH3	=	H2O	+	CH2	2.7E+11	.67	25700.
CH	+	CO2	=	HCO	+	CO	3.7E+12	0.	0.
CH	+	O2	=	HCO	+	O	1.0E+13	0.	0.
CH2	+	O2	=	CH2O	+	O	5.0E+11	0.5	6960.
CH2	+	O	=	CH	+	OH	2.0E+11	.7	25800.
CH2	+	OH	=	CH	+	H2O	5.0E+11	.5	5900.
CH2	+	H	=	CH	+	H2	3.2E+11	0.7	4970.
CH2	+	CH2	=	C2H3	+	H	5.0E+12	0.	0.
CH2	+	CH2	=	C2H2	+	H2	4.0E+13	0.	0.
HCO	+	O2	=	CO	+	HO2	3.0E+13	0.	0.
HCO	+	O	=	CO	+	OH	3.0E+13	0.	0.
HCO	+	OH	=	CO	+	H2O	3.0E+13	0.	0.
HCO	+	H	=	CO	+	H2	2.0E+13	0.	0.
M	+	HCO	=	H	+	CO	2.9E+14	0.	15570.
CO	+	O	=	CO2	+	M	2.4E+15	0.	4100.
CO	+	O2	=	CO2	+	O	2.5E+12	0.	47690.
CO	+	OH	=	CO2	+	H	4.17E+11	0.	1000.
CO	+	HO2	=	CO2	+	OH	5.75E+13	0.	22930.
O	+	H2O	=	OH	+	OH	6.8E+13	0.	18365.
H	+	O2	=	OH	+	O	1.89E+14	0.	16400.
O	+	H2	=	OH	+	H	4.20E+14	0.	13750.
H	+	HO2	=	H2	+	O2	7.28E+13	0.	2126.
O	+	HO2	=	OH	+	O2	5.0E+13	0.	1000.
HO2	+	OH	=	H2O	+	O2	8.0E+12	0.	0.
H	+	HO2	=2.0OH				1.34E+14	0.	1070.
H2	+	HO2	=	H2O2	+	H	7.91E+13	0.	25000.
OH	+	H2O2	=	H2O	+	HO2	6.1E+12	0.	1430.
HO2	+	HO2	=	H2O2	+	O2	1.8E+12	0.	0.
H	+	H2O2	=	OH	+	H2O	7.8E+11	0.	0.

TABLE D.1.—Continued.

```
   M       +   H2O2      =2.0OH                          1.44E+17   0.        45510.
   THIRDBODY
H2          2.30    O2          .78     H2O              6.0    H2O2        6.6
END
   H2      +   OH        =   H2O     +   H               4.74E+13   0.        6098.
   H       +   O2        =   HO2     +   M               1.46E+15   0.        -1000.
   THIRDBODY
O2          1.30    N2          1.3     H2O              21.3   CO2         7.0
END
   M       +   H2O       =   H       +   OH              1.30E+15   0.        105140.
   THIRDBODY
H2          4.00    O2          1.5     H2O              20.0   N2          1.5
CO2         4.0     END
   H       +   O         =   OH      +   M                7.1E+18   -1.        0.
   M       +   H2        =   H       +   H                2.2E+14   0.         96000.
   THIRDBODY
H2          4.10    O2          2.0     H2O              15.0   N2          2.0
END
   M       +   O2        =   O       +   O               1.80E+18   -1.       118020.
   CH      +   N2        =   HCN     +   N                1.0E+11   0.        19000.
   CN      +   H2        =   HCN     +   H                6.0E+13   0.        5300.
   O       +   HCN       =   OH      +   CN               1.4E+11   .68       16900.
   OH      +   HCN       =   HNCO    +   H                4.0E+11   0.         2800.
   CN      +   O         =   CO      +   N                1.2E+13   0.           0.
   CN      +   OH        =   NCO     +   H                2.5E+14   0.        6000.
   H2      +   NCO       =   HNCO    +   H                1.0E+14   0.        9000.
   HNCO    +   H         =   NH2     +   CO               1.0E+14   0.        8500.
   CN      +   O2        =   NCO     +   O                3.2E+13   0.        1000.
   CN      +   CO2       =   NCO     +   CO               3.7E+12   0.         0.
   O       +   NCO       =   NO      +   CO               2.0E+13    0.        0.
   N       +   NCO       =   N2      +   CO               1.0E+13    0.        0.
   H       +   NCO       =   NH      +   CO               2.0E+13    0.        0.
   CH      +   NO        =   N       +   HCO              1.6E+13   0.        9940.
   CH      +   NO        =   O       +   HCN              2.0E+12   0.        0.
   NH      +   OH        =   N       +   H2O              5.0E+11   0.5       2000.
   HO2     +   NO        =   NO2     +   OH              2.09E+12    0.      -477.
   O       +   NO2       =   NO      +   O2               1.0E+13     0.      596.
   NO      +   O         =   NO2     +   M               5.62E+15   0.        -1160.
   NO2     +   H         =   NO      +   OH              3.47E+14   0.         1470.
   NO      +   H         =   N       +   OH              2.63E+14   0.        50410.
   NO      +   O         =   N       +   O2                3.8E+9   1.        41370.
   O       +   N2        =   NO      +   N               1.80E+14   0.        76250.
   N       +   NO2       =2.0NO                           4.0E+12   0.        0.
   M       +   N2O       =   N2      +   O               6.92E+23   -2.5      65000.
   O       +   N2O       =   N2      +   O2               1.0E+14   0.        28020.
   O       +   N2O       =2.0NO                          6.92E+13   0.        26630.
   N2O     +   H         =   N2      +   OH              7.59E+13   0.        15100.
   NO2     +   H2        =   HNO2    +   H                2.4E+13  -0.        29000.
   OH      +   NO2       =   HNO3    +   M                3.0E+15   0.        -3800.
   THIRDBODY
O2          0.70    H2          1.4     END
   OH      +   NO        =   HNO2    +   M                5.6E+15   0.        -1700.
   HNO     +   H         =   H2      +   NO               5.0E+12   0.        0.
   H       +   NO        =   HNO     +   M                5.4E+15   0.        -600.
   HNO     +   OH        =   H2O     +   NO               3.6E+13   0.        0.

END
DISTANCE  AREA
 &prob xtb= 0.0,5.0,10.0,15.0,20.0,25.0,30.0,32.0,34.0,36.0,38.0,40.0,42.0,44.0,
   atb= 1200.0,1180.0,1160.0,1140.0,1120.0,1100.0,1080.0,1060.0,1040.0,1020.0,
   1000.0, 980.0, 960.0, 940.0,
    aprint = 1180.0, 1150., 1110., 950.0,  &end
 &start  t=1600.0, mach=2.0, p=1.730,  &end
CH4         0.049768
O2          0.199072
N2          0.75116
CN          0.0000001
END
 &solver  emax=1.0E-5, atolsp=1.0E-14,  &end
FINIS
LSENS METHANE - AIR WITH TAB. AREA PROFILE OF CASE 15, BUT PRINT ASSIG; CASE 16
REPEAT
DISTANCE  AREA
 &prob xtb= 0.0,5.0,10.0,15.0,20.0,25.0,30.0,32.0,34.0,36.0,38.0,40.0,42.0,44.0,
   atb= 1200.0,1180.0,1160.0,1140.0,1120.0,1100.0,1080.0,1060.0,1040.0,1020.0,
   1000.0, 980.0, 960.0, 940.0,
  print = 5.0, 12.4954, 22.4363, 43.0002,   &end
 &start  t=1600.0, mach=2.0, p=1.730,  &end
CH4         0.049768
O2          0.199072
N2          0.75116
CN          0.0000001
```

TABLE D.1.—Concluded.

```
END
 &solver  emax=1.0E-5, atolsp=1.0E-14,  &end
FINIS
```

TABLE D.2.—SELECTED KINETICS TEST CASE RESULTS

(a) Case 1

```
                                    **  DATA LINES  **
                 1         2         3         4         5         6         7         8
CC  12345678901234567890123456789012345678901234567890123456789012345678901234567890

      LSENS   BROMINE DISSOCIATION IN A SHOCK TUBE                                CASE 1
       M       +   BR2       =2.0BR                      6.99E+11  0.50      35500.
       THIRDBODY
    BR2          3.80    END
                                        -  BLANK LINE  -
    XE
    DISTANCE  AREA
     &prob  lsubm=32200.0, eta=0.5, shock=.true.,
       print=0.05,2.0,4.0,  &end
     &start  p=0.1227, mach=3.2646, t=299.9,  &end
    BR2          0.01
    XE           0.99
    END
     &solver emax=1.0E-2, atolsp=1.0E-10,  &end
    FINIS


*** THE FOLLOWING  2 ELEMENTS CONSIDERED FOR THIS PROBLEM ***

     BR    XE


*** THE FOLLOWING  2 REACTING SPECIES CONSIDERED FOR THIS PROBLEM ***

     BR2       BR


*** THE FOLLOWING  1 INERT SPECIES CONSIDERED FOR THIS PROBLEM ***

     XE


              *** THERMODYNAMIC DATA, MOLECULAR WEIGHT AND HEAT OF FORMATION AT 25 C ***


 BR2                MWT =     159.81799316          H(25 C) =   7.3874E+03 CAL/MOLE
0.44479494E+01   0.10051208E-03  -0.16393816E-07   0.22685621E-11  -0.10236774E-15   0.23659941E+04   0.40888429E+01
0.38469579E+01   0.26111840E-02  -0.40034147E-05   0.28120688E-08  -0.73256201E-12   0.24846985E+04   0.69696984E+01

 BR                 MWT =      79.90899658          H(25 C) =   2.6735E+04 CAL/MOLE
0.20843208E+01   0.71949483E-03  -0.27419924E-06   0.42422649E-10  -0.23791569E-14   0.12858837E+05   0.90838003E+01
0.24611552E+01   0.33319276E-03  -0.10080655E-05   0.12262126E-08  -0.44283511E-12   0.12711920E+05   0.69494734E+01

 XE                 MWT =     131.28999329          H(25 C) =  -2.6311E-13 CAL/MOLE
0.25000000E+01   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  -0.74537500E+03   0.61512742E+01
0.25000000E+01   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  -0.74537500E+03   0.61512742E+01


                                  **  EQUILIBRIUM SHOCK CALCULATION  **
                                INITIAL STATE                FINAL STATE                FINAL/INITIAL RATIO

   PRESSURE                          0.1227                     1.6130                        13.1460
    (ATM)
   VELOCITY                        57877.96                   18108.93                         0.3129
    (CM/SEC)
   DENSITY                        6.56043E-04                2.09678E-03                       3.1961
    (G/CM**3)
   TEMPERATURE                       299.90                    1231.23                         4.1055
    (DEG K)
   ENTHALPY                          0.62802                   36.74173                       58.50399
    (CAL/G)
   INTERNAL ENERGY                  -3.90133                   18.11191                       -4.64249
    (CAL/G)
   SP. HEAT (CP)                     0.03804                    0.04279                        1.12498
    (CAL/G/DEG K)
   ENTROPY                            0.3422                    0.3576                         1.0451
    (CAL/G/DEG K)
   MACH NUMBER                        3.2646                    0.5172                         0.1584

   GAMMA                              1.6586                    1.5471                         0.9328

   SONIC VELOCITY                  17728.96                   35015.99                         1.9751
    (CM/SEC)

                                                        SPECIES     MOLE FRACTION
                                                         BR2         8.11884E-03
                                                         BR          3.72507E-03
                                                         XE          9.88156E-01

   MIXTURE MOLECULAR WEIGHT                                131.33022

   D(LOG VOLUME)/D(LOG T)                                    1.0161
       AT CONSTANT P

   D(LOG VOLUME)/D(LOG P)                                   -1.0008
       AT CONSTANT T


                  COMPUTATIONAL WORK REQUIRED FOR EQUILIBRIUM SHOCK CALCULATION:
                     NO. OF ITERATIONS =      2     CPU TIME =  1.999998E-02 S
```

TABLE D.2.—Continued.

(a) Continued.

** FROZEN SHOCK CALCULATION **

	INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE (ATM)	0.1227	1.6017	13.0535
VELOCITY (CM/SEC)	57877.96	18411.41	0.3181
DENSITY (G/CM**3)	6.56043E-04	2.06233E-03	3.1436
TEMPERATURE (DEG K)	299.90	1245.31	4.1524
ENTHALPY (CAL/G)	0.62802	36.60887	58.29243
INTERNAL ENERGY (CAL/G)	-3.90133	17.80106	-4.56282
SP. HEAT (CP) (CAL/G/DEG K)	0.03804	0.03807	1.00084
ENTROPY (CAL/G/DEG K)	0.3422	0.3575	1.0449
MACH NUMBER	3.2646	0.5098	0.1562
GAMMA	1.6586	1.6577	0.9994
SONIC VELOCITY (CM/SEC)	17728.96	36117.20	2.0372

SPECIES	MOLE FRACTION
BR2	1.00000E-02
BR	0.00000E+00
XE	9.90000E-01

MIXTURE MOLECULAR WEIGHT 131.57527

D(LOG VOLUME)/D(LOG T) AT CONSTANT P 1.0000

D(LOG VOLUME)/D(LOG P) AT CONSTANT T -1.0000

COMPUTATIONAL WORK REQUIRED FOR FROZEN SHOCK CALCULATION:
NO. OF ITERATIONS = 2 CPU TIME = 0.000000E+00 S

DISTANCE-AREA VERSION LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

LSENS BROMINE DISSOCIATION IN A SHOCK TUBE CASE 1

REACTION NUMBER	REACTION	REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	M + 1*BR2 = 2*BR	6.99000E+11	0.5000	35500.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(BR2 , 1) = 3.80000

** NEW INPUT DATA GIVEN IN CGS UNITS ** ** OUTPUT REQUIRED IN CGS UNITS **

** ASSIGNED VARIABLE PROFILE **

THE AREA IS CALCULATED FROM THE FOLLOWING FUNCTION

(SHOCK TUBE CROSS-SECTIONAL AREA)/(AREA) = 1 - (X (CM)/ 32200.000)**(0.50000)

NUMBER OF REACTING SPECIES: 2

NUMBER OF INERT SPECIES: 1

NUMBER OF SPECIES ODE'S REQUIRED FOR THIS CASE: 2

TOTAL NUMBER OF ODE'S REQUIRED FOR THIS CASE: 5

INTEGRATION CONTROLS

INTEGRATION METHOD (MF): 21 MAXIMUM RELATIVE ERROR: 1.00000E-02 SPECIES ABSOLUTE ERROR: 1.00000E-10

MAXIMUM NUMBER OF STEPS ALLOWED FOR THE COMPLETE PROBLEM: 2000

** OUTPUT REQUIRED AT FOLLOWING 3 PRINT STATIONS **

STATION	AXIAL DISTANCE (CM)
1	5.00000E-02
2	2.00000E+00
3	4.00000E+00

TABLE D.2.—Continued.
(a) Continued.

** INITIAL CONDITIONS **

TIME 0.00000E+00 SEC AREA 1.00000E+00 AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES		INTEGRATION INDICATORS	
PRESSURE (ATM)	1.60167	STEPS FROM LAST PRINT	0
VELOCITY (CM/SEC)	18411.41	AVERAGE STEP SIZE	0.00000E+00
DENSITY (G/CM**3)	2.06233E-03	METHOD ORDER	0
TEMPERATURE (DEG K)	1245.31		
MASS FLUX (G/SEC/CM**2)	3.79704E+01	TOTAL NUMBER OF STEPS	0
ENTROPY (CAL/G/DEG K)	0.3575	FUNCT EVALUATIONS	0
MACH NUMBER	0.5098	JACOBIAN EVALUATIONS	0
GAMMA	1.6577		
ENTHALPY (CAL/G)	3.66089E+01		
SP. HEAT (CP) (CAL/G/DEG K)	3.80671E-02		

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
BR2	1.56741E-07	1.00000E-02	-3.66694E-05	1	1.4519E+07	8.62161E+00	1.00000
BR	0.00000E+00	0.00000E+00	7.33389E-05				
XE	1.55174E-05	9.90000E-01	0.00000E+00				

DERIVATIVES (CGS UNITS): T 5.00570E+00 RHO 1.73397E-05 V -5.36590E+02

MIXTURE MOLECULAR WEIGHT 131.57527 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 3.97306E+05 MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 0.860000 S

TIME 2.71785E-06 SEC AREA 1.00125E+00 AXIAL POSITION 5.00000E-02 CM

FLOW PROPERTIES		INTEGRATION INDICATORS	
PRESSURE (ATM)	1.60250	STEPS FROM LAST PRINT	4
VELOCITY (CM/SEC)	18389.24	AVERAGE STEP SIZE	0.14283E-01
DENSITY (G/CM**3)	2.06306E-03	METHOD ORDER	1
TEMPERATURE (DEG K)	1245.51		
MASS FLUX (G/SEC/CM**2)	3.79855E+01	TOTAL NUMBER OF STEPS	4
ENTROPY (CAL/G/DEG K)	0.3575	FUNCT EVALUATIONS	5
MACH NUMBER	0.5091	JACOBIAN EVALUATIONS	2
GAMMA	1.6577		
ENTHALPY (CAL/G)	3.66186E+01		
SP. HEAT (CP) (CAL/G/DEG K)	3.80671E-02		

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
BR2	1.56697E-07	9.99357E-03	-3.67572E-05	1	1.4553E+07	8.63612E+00	0.99999
BR	1.99794E-10	1.27421E-05	7.35144E-05				
XE	1.55229E-05	9.89994E-01	0.00000E+00				

DERIVATIVES (CGS UNITS): T 2.61468E+00 RHO 1.13364E-05 V -3.30484E+02

MIXTURE MOLECULAR WEIGHT 131.57444 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 3.97974E+05 MASS FRACTION SUM 1.00000000

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 1.999998E-02 S UP TO THIS TIME - 1.999998E-02 S

TABLE D.2.—Continued.
(a) Concluded.

```
TIME   2.19540E-04  SEC              AREA   1.01127E+00                    AXIAL POSITION   4.00000E+00  CM

    FLOW PROPERTIES                                                  INTEGRATION INDICATORS

      PRESSURE                 1.61360                                  STEPS FROM LAST PRINT              2
       (ATM)
      VELOCITY             18091.43                                     AVERAGE STEP SIZE             0.14460E+01
       (CM/SEC)
      DENSITY             2.07827E-03                                   METHOD ORDER                       2
       (G/CM**3)
      TEMPERATURE             1244.35
       (DEG K)
      MASS FLUX           3.80227E+01                                   TOTAL NUMBER OF STEPS             10
       (G/SEC/CM**2)
      ENTROPY                  0.3576                                   FUNCT EVALUATIONS                  14
       (CAL/G/DEG K)
      MACH NUMBER              0.5009                                   JACOBIAN EVALUATIONS               5

      GAMMA                    1.6581

      ENTHALPY            3.67484E+01
       (CAL/G)
      SP. HEAT (CP)       3.80723E-02
       (CAL/G/DEG K)

                                          CHEMICAL PROPERTIES

SPECIES    CONCENTRATION   MOLE FRACTION   NET SPECIES PRODUCTION  REACTION   RATE CONST   NET REACTION CONV RATE   NET RATE/POSI-
           (MOLES/CM**3)                   RATE (MOLE/CM**3/SEC)   NUMBER     CGS  UNITS   (MOLE-CM**3/G**2/SEC)    TIVE DIR RATE
 BR2        1.50195E-07     9.50418E-03          -3.32811E-05        1        1.4354E+07        7.70535E+00                0.95156
 BR         1.55159E-08     9.81828E-04           6.65621E-05
 XE         1.56374E-05     9.89514E-01           0.00000E+00

   DERIVATIVES (CGS UNITS): T          -5.00701E-01    RHO          3.10388E-06     V          -5.25083E+01

   MIXTURE MOLECULAR WEIGHT    131.51068     TOTAL ENERGY EXCHANGE RATE    3.55082E+05      MASS FRACTION SUM    1.00000000
                                                (CAL-CM**3/G**2/SEC)

_____________________________________________________________________

   COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP -  0.000000E+00  S     UP TO THIS TIME -  3.000003E-02  S


                 (LSENS)     END OF THIS CASE

                              SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

                                 TOTAL NO. OF STEPS -                        10
                                 TOTAL NO. OF DERIVATIVE EVALUATIONS -       14
                                 TOTAL NO. OF JACOBIAN EVALUATIONS -          5
                                 TOTAL CPU TIME -                     0.030000 S


                                          TOTAL CPU TIME (INCLUDING I/O) REQUIRED =      1.010000 S

                 (LSENS)     READ DATA FOR NEXT CASE
```

TABLE D.2.—Continued.

(b) Case 2

DISTANCE-AREA VERSION LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

LSENS HYDROGEN - AIR TEST WITH HEAT TRANSFER STOICH CASE 2

REACTION NUMBER	REACTION									REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1*O	+	1*H2O	=	2*OH					6.80000E+15	0.0000	18365.00
2	1*H	+	1*O2	=	1*OH	+	1*O			1.89000E+14	0.0000	16400.00
3	1*O	+	1*H2	=	1*OH	+	1*H			4.20000E+14	0.0000	13750.00
4	1*H	+	1*HO2	=	1*H2	+	1*O2			7.28000E+13	0.0000	2126.00
5	1*O	+	1*HO2	=	1*OH	+	1*O2			5.00000E+13	0.0000	1000.00
6	1*HO2	+	1*OH	=	1*H2O	+	1*O2			8.00000E+12	0.0000	0.00
7	1*H	+	1*HO2	=	2*OH					1.34000E+14	0.0000	1070.00
8	1*H2	+	1*HO2	=	1*H2O2	+	1*H			7.91000E+13	0.0000	25000.00
9	1*OH	+	1*H2O2	=	1*H2O	+	1*HO2			6.10000E+12	0.0000	1430.00
10			2*HO2	=	1*H2O2	+	1*O2			1.80000E+12	0.0000	0.00
11	1*H	+	1*H2O2	=	1*OH	+	1*H2O			7.80000E+11	0.0000	0.00
12	M	+	1*H2O2	=	2*OH					1.44000E+17	0.0000	45510.00
13	1*H2	+	1*OH	=	1*H2O	+	1*H			4.74000E+13	0.0000	6098.00
14	1*H	+	1*O2	=	1*HO2	+	M			1.46000E+15	0.0000	-1000.00
15	M	+	1*H2O	=	1*H	+	1*OH			1.30000E+15	0.0000	105140.00
16	1*H	+	1*O	=	1*OH	+	M			7.10000E+18	-1.0000	0.00
17	M	+	1*H2	=	2*H					2.20000E+14	0.0000	96000.00
18	M	+	1*O2	=	2*O					1.80000E+18	-1.0000	118020.00
19	1*HO2	+	1*NO	=	1*NO2	+	1*OH			2.09000E+12	0.0000	-477.00
20	1*O	+	1*NO2	=	1*NO	+	1*O2			1.00000E+13	0.0000	596.00
21	1*NO	+	1*O	=	1*NO2	+	M			5.62000E+15	0.0000	-1160.00
22	1*NO2	+	1*H	=	1*NO	+	1*OH			3.47000E+14	0.0000	1470.00
23	1*NO	+	1*O	=	1*N	+	1*O2			3.80000E+09	1.0000	41370.00
24	1*O	+	1*N2	=	1*NO	+	1*N			1.80000E+14	0.0000	76250.00
25	1*NO	+	1*H	=	1*N	+	1*OH			2.63000E+14	0.0000	50410.00
26	M	+	1*N2O	=	1*N2	+	1*O			6.92000E+23	-2.5000	65000.00
27	1*O	+	1*N2O	=	1*N2	+	1*O2			1.00000E+14	0.0000	28020.00
28	1*O	+	1*N2O	=	2*NO					6.92000E+13	0.0000	26630.00
29	1*N	+	1*NO2	=	2*NO					4.00000E+12	0.0000	0.00
30	1*N2O	+	1*H	=	1*N2	+	1*OH			7.59000E+13	0.0000	15100.00
31	1*NO2	+	1*H2	=	1*HNO2	+	1*H			2.40000E+13	0.0000	29000.00
32	1*OH	+	1*NO2	=	1*HNO3	+	M			3.00000E+15	0.0000	-3800.00
33	1*OH	+	1*NO	=	1*HNO2	+	M			5.60000E+15	0.0000	-1700.00
34	1*HNO	+	1*H	=	1*H2	+	1*NO			5.00000E+12	0.0000	0.00
35	1*H	+	1*NO	=	1*HNO	+	M			5.40000E+15	0.0000	-600.00
36	1*HNO	+	1*OH	=	1*H2O	+	1*NO			3.60000E+13	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2	, 12) =	2.30000	M(O2	, 12) =	0.78000	M(H2O	, 12) =	6.00000	M(H2O2	, 12) =	6.60000
M(O2	, 14) =	1.30000	M(N2	, 14) =	1.30000	M(H2O	, 14) =	21.30000	M(H2	, 14) =	3.00000
M(H2	, 15) =	4.00000	M(O2	, 15) =	1.50000	M(H2O	, 15) =	20.00000	M(N2	, 15) =	1.50000
M(H2	, 17) =	4.10000	M(O2	, 17) =	2.00000	M(H2O	, 17) =	15.00000	M(N2	, 17) =	2.00000
M(O2	, 32) =	0.70000	M(H2	, 32) =	1.40000						

** NEW INPUT DATA GIVEN IN CGS UNITS ** ** OUTPUT REQUIRED IN CGS UNITS **

** ASSIGNED VARIABLE PROFILE **

THE AREA IS CALCULATED FROM THE FOLLOWING POLYNOMIAL

AREA (CM**2) = (0.00000E+00)X**3 + (0.00000E+00)X**2 + (0.00000E+00)X + (2.00000E+03)

THE AREA WILL BE HELD CONSTANT FOR THIS CASE

HEAT TRANSFER CASE: QDOT (CAL/CM-SEC) =

(0.00000E+00)T**4 + (0.00000E+00)T**3 + 0.00000E+00)T**2 + (5.86300E+00)T + (-4.28800E+01)

FUEL-AIR REACTION, FUEL-AIR EQUIVALENCE RATIO = 1.0000 OXYGEN FRACTION IN AIR = 0.2095

NUMBER OF REACTING SPECIES: 16

NUMBER OF INERT SPECIES: 2

NUMBER OF SPECIES ODE'S REQUIRED FOR THIS CASE: 16

TOTAL NUMBER OF ODE'S REQUIRED FOR THIS CASE: 19

INTEGRATION CONTROLS

INTEGRATION METHOD (MF): 21 MAXIMUM RELATIVE ERROR: 5.00000E-03 SPECIES ABSOLUTE ERROR: 1.00000E-12

MAXIMUM NUMBER OF STEPS ALLOWED FOR THE COMPLETE PROBLEM: 2000

** OUTPUT REQUIRED AT FOLLOWING 4 PRINT STATIONS **

STATION	AXIAL DISTANCE (CM)
1	3.04800E+00
2	6.09600E+00
3	7.62000E+00
4	1.21900E+01

TABLE D.2.—Continued.
(b) Continued.

```
                                   ** INITIAL CONDITIONS **

TIME   0.00000E+00  SEC            AREA   2.00000E+03  SQ CM            AXIAL POSITION   0.00000E+00  CM

   FLOW PROPERTIES                                          INTEGRATION INDICATORS

     PRESSURE                 0.95600                        STEPS FROM LAST PRINT              0
      (ATM)
     VELOCITY            450945.64                           AVERAGE STEP SIZE            0.00000E+00
      (CM/SEC)
     DENSITY             1.56988E-04                         METHOD ORDER                       0
      (G/CM**3)
     TEMPERATURE            1559.00
      (DEG K)
     MASS FLOW RATE      1.41586E+05                         TOTAL NUMBER OF STEPS              0
      (G/SEC)
     ENTROPY                 2.6767                         FUNCT EVALUATIONS                  0
      (CAL/G/DEG K)
     MACH NUMBER             5.0000                         JACOBIAN EVALUATIONS               0

     GAMMA                   1.3183

     ENTHALPY            4.54652E+02
      (CAL/G)
     SP. HEAT (CP)       3.91820E-01
      (CAL/G/DEG K)

HEAT LOSS(QDOT/MDOT) =    6.4254E-02  CAL/(G-CM)
```

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSI-TIVE DIR RATE
O	0.00000E+00	0.00000E+00	6.70113E-13	1	1.8113E+11	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	0.00000E+00	2	9.4932E+11	0.00000E+00	0.00000
OH	0.00000E+00	0.00000E+00	0.00000E+00	3	4.9624E+12	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	1.03759E-05	4	3.6652E+13	-4.20984E+02	1.00000
O2	1.10332E-06	1.47639E-01	-1.03753E-05	5	3.6206E+13	0.00000E+00	0.00000
H2	2.20665E-06	2.95278E-01	-1.03756E-05	6	8.0000E+12	0.00000E+00	0.00000
HO2	0.00000E+00	0.00000E+00	1.03753E-05	7	9.4865E+13	0.00000E+00	0.00000
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	8	2.4747E+10	0.00000E+00	0.00000
NO	0.00000E+00	0.00000E+00	0.00000E+00	9	3.8447E+12	0.00000E+00	0.00000
NO2	0.00000E+00	0.00000E+00	0.00000E+00	10	1.8000E+12	0.00000E+00	0.00000
N	0.00000E+00	0.00000E+00	0.00000E+00	11	7.8000E+11	0.00000E+00	0.00000
N2	4.11248E-06	5.50303E-01	-1.26958E-13	12	6.0049E+10	0.00000E+00	0.00000
N2O	0.00000E+00	0.00000E+00	1.26958E-13	13	6.6210E+12	0.00000E+00	0.00000
HNO2	0.00000E+00	0.00000E+00	0.00000E+00	14	2.0162E+15	0.00000E+00	0.00000
HNO3	0.00000E+00	0.00000E+00	0.00000E+00	15	2.3703E+00	0.00000E+00	0.00000
HNO	0.00000E+00	0.00000E+00	0.00000E+00	16	4.5542E+15	0.00000E+00	0.00000
CO2	1.57996E-09	2.11419E-04	0.00000E+00	17	7.6662E+00	1.34051E-02	1.00000
AR	4.90836E-08	6.56802E-03	0.00000E+00	18	3.2937E-02	1.10195E-05	1.00000
				19	2.4379E+12	0.00000E+00	0.00000
				20	8.2499E+12	0.00000E+00	0.00000
				21	8.1724E+15	0.00000E+00	0.00000
				22	2.1590E+14	0.00000E+00	0.00000
				23	9.4003E+06	0.00000E+00	0.00000
				24	3.6821E+03	0.00000E+00	0.00000
				25	2.2552E+07	0.00000E+00	0.00000
				26	5.5707E+06	0.00000E+00	0.00000
				27	1.1803E+10	-5.15143E-06	1.00000
				28	1.2793E+10	0.00000E+00	0.00000
				29	4.0000E+12	0.00000E+00	0.00000
				30	5.8001E+11	0.00000E+00	0.00000
				31	2.0645E+09	0.00000E+00	0.00000
				32	1.0229E+16	0.00000E+00	0.00000
				33	9.6940E+15	0.00000E+00	0.00000
				34	5.0000E+12	0.00000E+00	0.00000
				35	6.5540E+15	0.00000E+00	0.00000
				36	3.6000E+13	0.00000E+00	0.00000

```
DERIVATIVES (CGS UNITS): T          -2.44902E-01    RHO        -7.71706E-10     V          2.21672E+00

MIXTURE MOLECULAR WEIGHT     21.00704     TOTAL ENERGY EXCHANGE RATE    2.21461E+07      MASS FRACTION SUM    1.00000000
                                          (CAL-CM**3/G**2/SEC)

                          CPU TIME FOR INITIALIZATION OF LSENS =     1.210000 S
```

TABLE D.2.—Continued.

(b) Continued.

TIME 1.35672E-05 SEC AREA 2.00000E+03 SQ CM AXIAL POSITION 6.09600E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.32771
VELOCITY (CM/SEC)	445625.60
DENSITY (G/CM**3)	1.58862E-04
TEMPERATURE (DEG K)	2217.16
MASS FLOW RATE (G/SEC)	1.41586E+05
ENTROPY (CAL/G/DEG K)	2.7814
MACH NUMBER	4.2705
GAMMA	1.2858
ENTHALPY (CAL/G)	5.11217E+02
SP. HEAT (CP) (CAL/G/DEG K)	4.10646E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	27
AVERAGE STEP SIZE	0.13164E+00
METHOD ORDER	3
TOTAL NUMBER OF STEPS	72
FUNCT EVALUATIONS	107
JACOBIAN EVALUATIONS	18

HEAT LOSS(QDOT/MDOT) = 9.1509E-02 CAL/(G-CM)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
O	2.00774E-07	2.75114E-02	-6.77700E-03
H2O	1.32763E-06	1.81922E-01	1.27487E-02
OH	2.39442E-07	3.28100E-02	8.54901E-03
H	5.98048E-07	8.19487E-02	-3.43219E-02
O2	2.32416E-07	3.18473E-02	-7.25712E-03
H2	4.86522E-07	6.66666E-02	1.43512E-04
HO2	1.08487E-10	1.48656E-05	-4.01910E-06
H2O2	3.89387E-11	5.33566E-06	-3.79636E-06
HO	1.59973E-11	2.19206E-06	9.07028E-06
NO2	1.35782E-15	1.86058E-10	7.77293E-10
N	3.32950E-13	4.56232E-08	1.19583E-07
N2	4.16156E-06	5.70247E-01	-4.63857E-06
N2O	5.75396E-13	7.88448E-08	3.68849E-08
HNO2	2.12750E-15	2.91525E-10	1.03301E-09
HNO3	3.23871E-20	4.43791E-15	-6.22870E-14
HNO	2.67768E-14	3.66915E-09	1.16987E-08
CO2	1.59882E-09	2.19082E-04	0.00000E+00
AR	4.96696E-08	6.80607E-03	0.00000E+00

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	1.0525E+12	5.09436E+03	0.00046
2	4.5697E+12	7.50542E+04	0.00298
3	1.8531E+13	1.93022E+05	0.00269
4	4.4933E+13	1.11542E+05	0.96560
5	3.9847E+13	3.32109E+04	0.96569
6	8.0000E+12	7.95168E+03	0.96568
7	1.0511E+14	2.60970E+05	0.96580
8	2.7157E+11	-4.62640E+04	0.98787
9	4.4093E+12	1.60926E+03	0.98790
10	1.8000E+12	-1.54158E+00	0.64745
11	7.8000E+11	7.19435E+02	0.99959
12	4.7029E+12	-4.84438E+04	0.31501
13	1.1876E+13	1.22471E+05	0.00223
14	1.8320E+15	3.65639E+05	0.99174
15	5.6249E+04	-3.77492E+05	0.99972
16	3.2023E+15	1.11156E+05	0.99972
17	7.5777E+04	-1.63370E+05	0.99972
18	1.8882E+03	-4.46331E+02	0.99972
19	2.3290E+12	1.11339E-01	0.69518
20	8.7348E+12	8.37342E-02	0.88745
21	7.3127E+15	6.77466E+00	0.99747
22	2.4856E+14	7.10025E+00	0.88779
23	7.0416E+08	-1.36957E+01	0.99350
24	5.4850E+06	1.81586E+02	0.99996
25	2.8246E+09	-1.63152E+02	0.99348
26	1.1707E+09	-3.48602E+01	0.99444
27	1.7299E+11	7.51363E-01	0.94885
28	1.6411E+11	7.51231E-01	1.00000
29	4.0000E+12	7.16014E-08	0.99927
30	2.4650E+12	3.18961E+01	0.94900
31	3.3238E+10	-3.28787E-01	0.99736
32	7.1071E+15	-2.46807E-06	0.00362
33	8.2368E+15	3.69719E-01	0.04052
34	5.0000E+12	3.16912E+00	0.99888
35	6.1878E+15	1.27682E+01	0.74586
36	3.6000E+13	9.13558E+00	0.99888

DERIVATIVES (CGS UNITS): T 1.27427E+02 RHO 3.48122E-07 V -9.76519E+02

MIXTURE MOLECULAR WEIGHT 21.76841 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) -1.12877E+11 MASS FRACTION SUM 1.00000031

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 4.500000E-01 S UP TO THIS TIME - 1.110000E+00 S

TABLE D.2.—Continued.
(b) Concluded.

TIME 2.73051E-05 SEC AREA 2.00000E+03 SQ CM AXIAL POSITION 1.21900E+01 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.57011
VELOCITY (CM/SEC)	442156.36
DENSITY (G/CM**3)	1.60109E-04
TEMPERATURE (DEG K)	2683.01
MASS FLOW RATE (G/SEC)	1.41586E+05
ENTROPY (CAL/G/DEG K)	2.7965
MACH NUMBER	3.9384
GAMMA	1.2685
ENTHALPY (CAL/G)	5.47385E+02
SP. HEAT (CP) (CAL/G/DEG K)	4.18231E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	8
AVERAGE STEP SIZE	0.60182E+00
METHOD ORDER	2
TOTAL NUMBER OF STEPS	82
FUNCT EVALUATIONS	128
JACOBIAN EVALUATIONS	21

HEAT LOSS(QDOT/MDOT) = 1.1080E-01 CAL/(G-CM)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
O	1.37445E-07	1.92722E-02	-3.20044E-03
H2O	1.46834E-06	2.05888E-01	7.35139E-03
OH	2.87650E-07	4.03336E-02	4.53908E-04
H	3.51216E-07	4.92467E-02	-9.33410E-03
O2	1.78006E-07	2.49596E-02	-2.37435E-03
H2	4.62674E-07	6.48751E-02	-2.91830E-03
HO2	1.02125E-10	1.43198E-05	2.51558E-06
H2O2	1.25021E-11	1.75301E-06	5.72723E-06
NO	8.32965E-10	1.16796E-04	1.27179E-04
NO2	1.15525E-13	1.61987E-08	1.75775E-08
N	3.80501E-12	5.33530E-07	3.73859E-07
N2	4.19380E-06	5.88046E-01	-6.39038E-05
N2O	1.44988E-12	2.03299E-07	1.03762E-07
HNO2	2.52785E-14	3.54450E-09	3.44329E-09
HNO3	6.38880E-19	8.95824E-14	9.63872E-13
HNO	3.51863E-13	4.93374E-08	2.65498E-08
CO2	1.61137E-09	2.25942E-04	0.00000E+00
AR	5.00593E-08	7.01920E-03	0.00000E+00

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	2.1705E+12	-6.55786E+03	0.00038
2	8.7211E+12	7.20425E+03	0.00034
3	3.1858E+13	8.78750E+04	0.00111
4	4.8860E+13	4.21963E+04	0.61722
5	4.1449E+13	1.40180E+04	0.61765
6	8.0000E+12	5.66374E+03	0.61780
7	1.0963E+14	9.47669E+06	0.61778
8	7.2737E+11	-8.90178E+03	0.86910
9	4.6649E+12	5.68895E+02	0.86930
10	1.8000E+12	-1.40920E+00	0.65803
11	7.8000E+11	1.26930E+02	0.95004
12	2.8266E+13	-9.82243E+03	0.04524
13	1.5103E+13	1.17231E+05	0.00150
14	1.7612E+15	1.47272E+05	0.87521
15	3.5447E+06	-1.56494E+05	0.95230
16	2.6463E+15	3.38432E+04	0.95229
17	3.3310E+06	-4.01419E+04	0.95223
18	1.6335E+05	-1.61391E+02	0.95227
19	2.2856E+12	1.94614E+00	0.25659
20	8.9424E+12	2.69015E+00	0.48568
21	6.9860E+15	2.01860E+02	0.90720
22	2.6338E+14	2.02541E+02	0.48585
23	4.3505E+09	-1.88724E+02	0.90666
24	1.1071E+08	2.48517E+03	0.99829
25	2.0593E+10	-2.28186E+03	0.90663
26	9.4158E+09	-4.43600E+01	0.92113
27	5.2189E+11	1.60165E+00	0.39478
28	4.6872E+11	3.64335E+00	0.99990
29	4.0000E+12	6.52974E-05	0.95199
30	4.4693E+12	3.50673E+01	0.39499
31	1.0422E+11	-2.11149E+00	0.90668
32	6.1187E+15	3.76002E-05	0.00065
33	7.7031E+15	2.24581E+00	0.00437
34	5.0000E+12	2.24193E+01	0.93011
35	6.0432E+15	1.55674E+02	0.31651
36	3.6000E+13	1.32219E+02	0.93022

DERIVATIVES (CGS UNITS): T 4.69727E+01 RHO 1.23045E-07 V -3.39801E+02

MIXTURE MOLECULAR WEIGHT 22.45008 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) -4.27131E+10 MASS FRACTION SUM 1.00000020

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 1.800001E-01 S UP TO THIS TIME - 1.310000E+00 S

(LSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

TOTAL NO. OF STEPS - 82
TOTAL NO. OF DERIVATIVE EVALUATIONS - 128
TOTAL NO. OF JACOBIAN EVALUATIONS - 21
TOTAL CPU TIME - 1.310000 S

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 3.110000 S

(LSENS) READ DATA FOR NEXT CASE

TABLE D.2.—Continued.

(c) Case 3

DISTANCE-AREA VERSION LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

LSENS HYDROGEN - AIR TEST WITH HEAT TRANSFER FULL MECHANISM CASE 3

REACTION NUMBER	REACTION								REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1*O	+	1*H2O	=	2*OH				6.80000E+15	0.0000	18365.00
2	1*H	+	1*O2	=	1*OH	+	1*O		1.89000E+14	0.0000	16400.00
3	1*O	+	1*H2	=	1*OH	+	1*H		4.20000E+14	0.0000	13750.00
4	1*H	+	1*HO2	=	1*H2	+	1*O2		7.28000E+13	0.0000	2126.00
5	1*O	+	1*HO2	=	1*OH	+	1*O2		5.00000E+13	0.0000	1000.00
6	1*HO2	+	1*OH	=	1*H2O	+	1*O2		8.00000E+12	0.0000	0.00
7	1*H	+	1*HO2	=	2*OH				1.34000E+14	0.0000	1070.00
8	1*H2	+	1*HO2	=	1*H2O2	+	1*H		7.91000E+13	0.0000	25000.00
9	1*OH	+	1*H2O2	=	1*H2O	+	1*HO2		6.10000E+12	0.0000	1430.00
10			2*HO2	=	1*H2O2	+	1*O2		2.00000E+12	0.0000	0.00
11	1*H	+	1*H2O2	=	1*OH	+	1*H2O		7.80000E+11	0.0000	0.00
12	M	+	1*H2O2	=	2*OH				1.44000E+17	0.0000	45510.00
13	1*H2	+	1*OH	=	1*H2O	+	1*H		4.74000E+13	0.0000	6098.00
14	1*H	+	1*O2	=	1*HO2	+	M		1.46000E+15	0.0000	-1000.00
15	M	+	1*H2O	=	1*H	+	1*OH		1.30000E+15	0.0000	105140.00
16	1*H	+	1*O	=	1*OH	+	M		7.10000E+18	-1.0000	0.00
17	M	+	1*H2	=	2*H				2.20000E+14	0.0000	96000.00
18	M	+	1*O2	=	2*O				1.80000E+18	-1.0000	118020.00
19	1*HO2	+	1*NO	=	1*NO2	+	1*OH		2.09000E+12	0.0000	-477.00
20	1*O	+	1*NO2	=	1*NO	+	1*O2		1.00000E+13	0.0000	596.00
21	1*NO	+	1*O	=	1*NO2	+	M		5.62000E+15	0.0000	-1160.00
22	1*NO2	+	1*H	=	1*NO	+	1*OH		3.47000E+14	0.0000	1470.00
23	1*NO	+	1*O	=	1*N	+	1*O2		3.80000E+09	1.0000	41370.00
24	1*O	+	1*N2	=	1*NO	+	1*N		1.80000E+14	0.0000	76250.00
25	1*NO	+	1*H	=	1*N	+	1*OH		2.63000E+14	0.0000	50410.00
26	M	+	1*N2O	=	1*N2	+	1*O		6.92000E+23	-2.5000	65000.00
27	1*O	+	1*N2O	=	1*N2	+	1*O2		1.00000E+14	0.0000	28020.00
28	1*O	+	1*N2O	=	2*NO				6.92000E+13	0.0000	26630.00
29	1*H	+	1*NO2	=	2*NO				4.00000E+12	0.0000	0.00
30	1*N2O	+	1*H	=	1*N2	+	1*OH		7.59000E+13	0.0000	15100.00
31	1*NO2	+	1*H2	=	1*HNO2	+	1*H		2.40000E+13	0.0000	29000.00
32	1*OH	+	1*NO2	=	1*HNO3	+	M		3.00000E+15	0.0000	-3800.00
33	1*OH	+	1*NO	=	1*HNO2	+	M		5.60000E+15	0.0000	-1700.00
34	1*HNO	+	1*H	=	1*H2	+	1*NO		5.00000E+12	0.0000	0.00
35	1*H	+	1*NO	=	1*HNO	+	M		5.40000E+15	0.0000	-600.00
36	1*HNO	+	1*OH	=	1*H2O	+	1*NO		3.60000E+13	0.0000	0.00
37	1*O	+	1*H2O2	=	1*OH	+	1*HO2		8.00000E+13	0.0000	1000.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2	, 12) =	2.30000	M(O2	, 12) =	0.78000	M(H2O	, 12) =	6.00000	M(H2O2	, 12) =	6.60000
M(O2	, 14) =	1.30000	M(N2	, 14) =	1.30000	M(H2O	, 14) =	21.30000	M(H2	, 14) =	3.00000
M(H2	, 15) =	4.00000	M(O2	, 15) =	1.50000	M(H2O	, 15) =	20.00000	M(N2	, 15) =	1.50000
M(H2	, 17) =	4.10000	M(O2	, 17) =	2.00000	M(H2O	, 17) =	15.00000	M(N2	, 17) =	2.00000
M(O2	, 32) =	0.70000	M(H2	, 32) =	1.40000						

** INITIAL CONDITIONS **

TIME 0.00000E+00 SEC AREA 2.00000E+03 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	0.95600
VELOCITY (CM/SEC)	450950.60
DENSITY (G/CM**3)	1.56985E-04
TEMPERATURE (DEG K)	1559.00
MASS FLOW RATE (G/SEC)	1.41585E+05
ENTROPY (CAL/G/DEG K)	2.6768
MACH NUMBER	5.0008
GAMMA	1.3183
ENTHALPY (CAL/G)	4.54661E+02
SP. HEAT (CP) (CAL/G/DEG K)	3.91828E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

HEAT LOSS(QDOT/MDOT) = 6.4255E-02 CAL/(G-CM)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
O	0.00000E+00	0.00000E+00	6.70095E-13
H2O	0.00000E+00	0.00000E+00	0.00000E+00
OH	0.00000E+00	0.00000E+00	0.00000E+00
H	0.00000E+00	0.00000E+00	1.03763E-05
O2	1.10330E-06	1.47636E-01	-1.03756E-05
H2	2.20678E-06	2.95295E-01	-1.03760E-05
HO2	0.00000E+00	0.00000E+00	1.03756E-05
H2O2	0.00000E+00	0.00000E+00	0.00000E+00
NO	0.00000E+00	0.00000E+00	0.00000E+00
NO2	0.00000E+00	0.00000E+00	0.00000E+00
N	0.00000E+00	0.00000E+00	0.00000E+00
N2	4.11238E-06	5.50290E-01	-1.26952E-13
N2O	0.00000E+00	0.00000E+00	1.26952E-13
HNO2	0.00000E+00	0.00000E+00	0.00000E+00
HNO3	0.00000E+00	0.00000E+00	0.00000E+00
HNO	0.00000E+00	0.00000E+00	0.00000E+00
CO2	1.57992E-09	2.11414E-04	0.00000E+00
AR	4.90825E-08	6.56787E-03	0.00000E+00

REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	1.8113E+11	0.00000E+00	0.00000
2	9.4932E+11	0.00000E+00	0.00000
3	4.9624E+12	0.00000E+00	0.00000
4	3.6652E+13	2.21464E+07	1.00000
5	3.6206E+13	0.00000E+00	0.00000
6	8.0000E+12	0.00000E+00	0.00000
7	9.4865E+13	0.00000E+00	0.00000
8	2.4747E+10	0.00000E+00	0.00000
9	3.8447E+12	0.00000E+00	0.00000
10	2.8000E+12	0.00000E+00	0.00000
11	7.8000E+11	0.00000E+00	0.00000
12	6.0049E+10	0.00000E+00	0.00000
13	6.6210E+12	0.00000E+00	0.00000
14	2.0162E+15	0.00000E+00	0.00000
15	2.3703E+00	0.00000E+00	0.00000
16	4.5542E+15	0.00000E+00	0.00000
17	7.6662E+00	1.39704E+03	1.00000
18	3.2937E-02	1.31253E+00	1.00000
19	2.4379E+12	0.00000E+00	0.00000
20	8.2499E+12	0.00000E+00	0.00000
21	8.1724E+15	0.00000E+00	0.00000
22	2.1590E+14	0.00000E+00	0.00000
23	9.4003E+06	0.00000E+00	0.00000
24	3.6821E+03	0.00000E+00	0.00000
25	2.2552E+07	0.00000E+00	0.00000
26	5.5707E+06	0.00000E+00	0.00000
27	1.1803E+10	4.07252E-01	1.00000
28	1.2793E+10	0.00000E+00	0.00000
29	4.0000E+12	0.00000E+00	0.00000
30	5.8001E+11	0.00000E+00	0.00000
31	2.0645E+09	0.00000E+00	0.00000
32	1.0229E+16	0.00000E+00	0.00000
33	9.6940E+15	0.00000E+00	0.00000
34	5.0000E+12	0.00000E+00	0.00000
35	6.5540E+15	0.00000E+00	0.00000
36	3.6000E+13	0.00000E+00	0.00000
37	5.7930E+13	0.00000E+00	0.00000

DERIVATIVES (CGS UNITS): T -2.44900E-01 RHO -7.71685E-10 V 2.21672E+00

MIXTURE MOLECULAR WEIGHT 21.00658 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 2.21478E+07 MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 0.580000 S

TABLE D.2.—Continued.

(c) Continued.

TIME 1.55672E-05 SEC AREA 2.00000E+03 SQ CM AXIAL POSITION 6.09600E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.32893
VELOCITY (CM/SEC)	445612.90
DENSITY (G/CM**3)	1.58865E-04
TEMPERATURE (DEG K)	2219.44
MASS FLOW RATE (G/SEC)	1.41585E+05
ENTROPY (CAL/G/DEG K)	2.7816
MACH NUMBER	4.2686
GAMMA	1.2858
ENTHALPY (CAL/G)	5.11414E+02
SP. HEAT (CP) (CAL/G/DEG K)	4.10698E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	25
AVERAGE STEP SIZE	0.12184E+00
METHOD ORDER	5
TOTAL NUMBER OF STEPS	70
FUNCT EVALUATIONS	109
JACOBIAN EVALUATIONS	19

HEAT LOSS(QDOT/MDOT) = 9.1604E-02 CAL/(G-CM)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
O	2.00450E-07	2.74700E-02	-6.52579E-03
H2O	1.32820E-06	1.82018E-01	1.28361E-02
OH	2.39788E-07	3.28609E-02	8.50641E-03
H	5.96769E-07	8.17821E-02	-3.48516E-02
O2	2.32143E-07	3.18133E-02	-7.40807E-03
H2	4.86645E-07	6.66906E-02	3.39365E-04
NO2	1.11312E-10	1.52564E-05	-4.02841E-06
H2O2	3.44419E-11	4.71997E-06	-9.09783E-07
NO	1.62578E-11	2.22800E-06	9.21933E-06
HO2	1.38234E-15	1.89438E-10	6.93502E-10
N	3.37749E-13	4.62856E-08	1.20388E-07
N2	4.16163E-06	5.70317E-01	-4.71390E-06
H2O	5.76245E-13	7.89695E-08	3.74619E-08
HNO2	2.14756E-15	2.94305E-10	6.82683E-10
HNO3	3.25591E-20	4.46195E-15	9.58168E-15
HNO	2.70663E-14	3.70921E-09	1.17877E-08
CO2	1.59885E-09	2.19109E-04	0.00000E+00
AR	4.96704E-08	6.80691E-03	0.00000E+00

REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	1.0571E+12	4.25857E+07	0.00023
2	4.5872E+12	1.44486E+09	0.00342
3	1.8590E+13	3.34580E+08	0.00249
4	4.4956E+13	-6.01256E+09	0.96601
5	3.9857E+13	-1.72713E+09	0.96609
6	8.0000E+12	-5.52641E+08	0.96609
7	1.0513E+14	-9.08151E+09	0.96621
8	2.7316E+11	-7.75899E+08	0.98583
9	4.4108E+12	-4.84265E+07	0.98586
10	2.0000E+12	4.61206E+04	0.58313
11	7.8000E+11	-4.51744E+07	0.99952
12	4.7530E+12	-3.07344E+09	0.38919
13	1.1893E+13	-1.87286E+09	0.00227
14	1.8316E+15	-1.87997E+10	0.99140
15	5.7642E+04	-4.48379E+10	0.99971
16	3.1990E+15	-1.13196E+10	0.99971
17	7.7490E+04	-1.69212E+10	0.99971
18	1.9388E+03	-5.29303E+07	0.99971
19	2.3287E+12	-5.65088E+02	0.70169
20	8.7360E+12	-3.90309E+03	0.88634
21	7.3108E+15	-5.02902E+05	0.99742
22	2.4864E+14	-2.10028E+05	0.88673
23	7.1170E+08	-4.40001E+05	0.99344
24	5.5833E+06	1.38833E+07	0.99996
25	2.8579E+09	-8.02322E+06	0.99362
26	1.1855E+09	-1.39982E+06	0.99438
27	1.7412E+11	-5.97188E+04	0.94791
28	1.6513E+11	-2.67780E+04	1.00000
29	4.0000E+12	-5.73204E-03	0.99925
30	2.4736E+12	-1.99039E+06	0.94809
31	3.3463E+10	-8.34023E+03	0.99731
32	7.1008E+15	-1.87912E-02	0.00055
33	8.2336E+15	-1.78713E+04	0.03861
34	5.0000E+12	-1.74761E+05	0.99886
35	6.1869E+15	-6.39455E+05	0.74389
36	3.6000E+13	-6.46390E+05	0.99886
37	6.3770E+13	-2.95047E+08	0.98587

DERIVATIVES (CGS UNITS): T 1.28222E+02 RHO 3.50186E-07 V -9.82264E+02

MIXTURE MOLECULAR WEIGHT 21.77113 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) -1.13592E+11 MASS FRACTION SUM 1.00000031

COMPUTER TIME (CPU) REQUIRED, FOR THIS STEP - 4.900002E-01 S UP TO THIS TIME - 1.150000E+00 S

TABLE D.2.—Continued.

(c) Concluded.

TIME 2.73102E-05 SEC AREA 2.00000E+03 SQ CM AXIAL POSITION 1.21920E+01 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.57184
VELOCITY (CM/SEC)	442136.92
DENSITY (G/CM**3)	1.60114E-04
TEMPERATURE (DEG K)	2686.45
MASS FLOW RATE (G/SEC)	1.41585E+05
ENTROPY (CAL/G/DEG K)	2.7966
MACH NUMBER	3.9363
GAMMA	1.2683
ENTHALPY (CAL/G)	5.47634E+02
SP. HEAT (CP) (CAL/G/DEG K)	4.18288E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	7
AVERAGE STEP SIZE	0.66052E+00
METHOD ORDER	2
TOTAL NUMBER OF STEPS	81
FUNCT EVALUATIONS	129
JACOBIAN EVALUATIONS	22

HEAT LOSS(QDOT/MDOT) = 1.1094E-01 CAL/(G-CM)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
O	1.36917E-07	1.92016E-02	-3.09906E-03
H2O	1.46965E-06	2.06108E-01	7.05653E-03
OH	2.87774E-07	4.03582E-02	7.69777E-04
H	3.49652E-07	4.90362E-02	-9.71057E-03
O2	1.77582E-07	2.49046E-02	-2.41684E-03
H2	4.62342E-07	6.48400E-02	-2.57415E-03
HO2	1.03667E-10	1.45386E-05	1.19174E-06
H2O2	1.22152E-11	1.71309E-06	-1.25994E-05
NO	8.47280E-10	1.18825E-04	1.29050E-04
NO2	1.18107E-13	1.65636E-08	2.20897E-08
N	3.86102E-12	5.41480E-07	3.50739E-07
N2	4.19394E-06	5.88169E-01	-6.48330E-05
N2O	1.46727E-12	2.05774E-07	1.03628E-07
HNO2	2.54616E-14	3.57080E-09	6.07427E-09
HNO3	6.47257E-19	9.07731E-14	5.57463E-13
HNO	3.53811E-13	4.96195E-08	2.96754E-08
CO2	1.61142E-09	2.25990E-04	0.00000E+00
AR	5.00609E-08	7.02068E-03	0.00000E+00

REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	2.1801E+12	-9.25500E+07	0.00032
2	8.7555E+12	1.88803E+08	0.00053
3	3.1963E+13	1.55573E+08	0.00106
4	4.8885E+13	-2.24489E+09	0.61744
5	4.1459E+13	-7.19555E+08	0.61785
6	8.0000E+12	-3.88969E+08	0.61797
7	1.0966E+14	-3.25502E+09	0.61805
8	7.3175E+11	-1.63667E+08	0.86281
9	4.6665E+12	-1.87927E+07	0.86300
10	2.0000E+12	5.03511E+04	0.64138
11	7.8000E+11	-8.37399E+06	0.94767
12	2.8576E+13	-6.41412E+08	0.05763
13	1.5125E+13	-1.62137E+09	0.00138
14	1.7608E+15	-7.51326E+09	0.87092
15	3.6355E+06	-1.85008E+10	0.95069
16	2.6429E+15	-3.42377E+09	0.95067
17	3.4086E+06	-4.13239E+09	0.95062
18	1.6783E+05	-1.90176E+07	0.95065
19	2.2853E+12	-9.92867E+03	0.26292
20	8.9436E+12	-1.24722E+05	0.48153
21	6.9840E+15	-1.49241E+07	0.90481
22	2.6348E+14	-5.95953E+06	0.48181
23	4.3996E+09	-6.05406E+06	0.90584
24	1.1276E+08	1.89677E+08	0.99826
25	2.0844E+10	-1.12041E+08	0.90579
26	9.5333E+09	-1.77348E+06	0.91923
27	5.2541E+11	-1.26592E+05	0.38892
28	4.7172E+11	-1.30961E+05	0.99990
29	4.0000E+12	-5.24640E+00	0.95118
30	4.4856E+12	-2.17634E+06	0.38924
31	1.0495E+11	-5.31737E+04	0.90428
32	6.1131E+15	-1.07625E+00	0.00037
33	7.6999E+15	-1.17156E+05	0.00450
34	5.0000E+12	-1.22427E+06	0.92803
35	6.0423E+15	-7.73907E+06	0.31383
36	3.6000E+13	-9.24737E+06	0.92813
37	6.6334E+13	-6.40678E+07	0.86295

DERIVATIVES (CGS UNITS): T 4.66737E+01 RHO 1.22124E-07 V -3.37231E+02

MIXTURE MOLECULAR WEIGHT 22.45486 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) -4.24354E+10 MASS FRACTION SUM 1.00000020

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 1.500001E-01 S UP TO THIS TIME - 1.360001E+00 S

(LSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

TOTAL NO. OF STEPS - 81
TOTAL NO. OF DERIVATIVE EVALUATIONS - 129
TOTAL NO. OF JACOBIAN EVALUATIONS - 22
TOTAL CPU TIME - 1.360001 S

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 2.500000 S

(LSENS) READ DATA FOR NEXT CASE

TABLE D.2.—Continued.

(d) Case 4.

DISTANCE-PRESSURE VERSION LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

LSENS HYDROGEN - OXYGEN CASE WITH HEAT TRANSFER CASE 4

REACTION NUMBER	REACTION									REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1*O	+	1*H2O	=	2*OH					6.80000E+13	0.0000	18365.00
2	1*H	+	1*O2	=	1*OH	+	1*O			1.89000E+14	0.0000	16400.00
3	1*O	+	1*H2	=	1*OH	+	1*H			4.20000E+14	0.0000	13750.00
4	1*H	+	1*HO2	=	1*H2	+	1*O2			7.28000E+13	0.0000	2126.00
5	1*O	+	1*HO2	=	1*OH	+	1*O2			5.00000E+13	0.0000	1000.00
6	1*HO2	+	1*OH	=	1*H2O	+	1*O2			8.00000E+12	0.0000	0.00
7	1*H	+	1*HO2	=	2*OH					1.34000E+14	0.0000	1070.00
8	1*H2	+	1*HO2	=	1*H2O2	+	1*H			7.91000E+13	0.0000	25000.00
9	1*OH	+	1*H2O2	=	1*H2O	+	1*HO2			6.10000E+12	0.0000	1430.00
10			2*HO2	=	1*H2O2	+	1*O2			1.80000E+12	0.0000	0.00
11	1*H	+	1*H2O2	=	1*OH	+	1*H2O			7.80000E+11	0.0000	0.00
12	M	+	1*H2O2	=	2*OH					1.44000E+17	0.0000	45510.00
13	1*H2	+	1*OH	=	1*H2O	+	1*H			4.74000E+13	0.0000	6098.00
14	1*H	+	1*O2	=	1*HO2	+	M			1.46000E+15	0.0000	-1000.00
15	M	+	1*H2O	=	1*H	+	1*OH			1.30000E+15	0.0000	105140.00
16	1*H	+	1*O	=	1*OH	+	M			7.10000E+18	-1.0000	0.00
17	M	+	1*H2	=	2*H					2.20000E+14	0.0000	96000.00
18	M	+	1*O2	=	2*O					1.80000E+18	-1.0000	118020.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2 , 12) =	2.30000	M(O2 , 12) =	0.78000	M(H2O , 12) =	6.00000	M(H2O2 , 12) =	6.60000
M(O2 , 14) =	1.30000	M(H2 , 14) =	3.00000	M(H2O , 14) =	21.30000	M(H2 , 15) =	4.00000
M(O2 , 15) =	1.50000	M(H2O , 15) =	20.00000	M(H2 , 17) =	4.10000	M(O2 , 17) =	2.00000
M(H2O , 17) =	15.00000						

** INITIAL CONDITIONS **

TIME 0.00000E+00 SEC AREA 2.15280E+00 SQ FT AXIAL POSITION 0.00000E+00 FT

FLOW PROPERTIES

PRESSURE (LB/FT**2)	1.05810E+04
VELOCITY (FT/SEC)	1.62598E+03
DENSITY (LB/FT**3)	4.35122E-02
TEMPERATURE (DEG R)	1890.00
MASS FLOW RATE (LB/SEC)	1.52297E+02
ENTROPY (BTU/LB/DEG R)	3.68867E+00
MACH NUMBER	5.00000E-01
GAMMA	1.35148E+00
ENTHALPY (BTU/LB)	8.22027E+02
SP. HEAT (CP) (BTU/LB/DEG R)	6.36196E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

HEAT LOSS(QDOT/MDOT) = 4.8552E+00 BTU/(LB-FT)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/FT**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/FT**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-FT**3/LB**2/SEC)	NET RATE/POSITIVE DIR RATE
O	0.00000E+00	0.00000E+00	6.54229E-17	1	1.0232E+10	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	0.00000E+00	2	7.2933E+10	0.00000E+00	0.00000
OH	0.00000E+00	0.00000E+00	0.00000E+00	3	5.7715E+11	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	3.55695E-05	4	2.6280E+13	-1.87869E-02	1.00000
O2	1.20765E-03	3.33333E-01	-3.55695E-05	5	3.0962E+13	0.00000E+00	0.00000
H2	2.41531E-03	6.66667E-01	-3.55695E-05	6	8.0000E+12	0.00000E+00	0.00000
HO2	0.00000E+00	0.00000E+00	3.55695E-05	7	8.0240E+13	0.00000E+00	0.00000
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	8	4.9501E+08	0.00000E+00	0.00000
				9	3.0739E+12	0.00000E+00	0.00000
				10	1.8000E+12	0.00000E+00	0.00000
				11	7.8000E+11	0.00000E+00	0.00000
				12	4.8505E+07	0.00000E+00	0.00000
				13	2.5499E+12	0.00000E+00	0.00000
				14	2.3577E+15	0.00000E+00	0.00000
				15	1.6976E-07	0.00000E+00	0.00000
				16	6.7619E+15	0.00000E+00	0.00000
				17	2.2947E-06	5.77599E-10	1.00000
				18	4.6675E-10	1.72773E-14	1.00000

DERIVATIVES (FPS UNITS): T 2.22574E+01 RHO 2.14009E-03 V -2.93352E+02

MIXTURE MOLECULAR WEIGHT 12.01013 TOTAL ENERGY EXCHANGE RATE 1.77867E+03 MASS FRACTION SUM 1.00000000

(BTU-FT**3/LB**2/SEC)

CPU TIME FOR INITIALIZATION OF LSENS = 0.900000 S

TABLE D.2.—Continued.
(d) Continued.

TIME 2.08104E-04 SEC AREA 2.25905E+00 SQ FT AXIAL POSITION 3.28100E-01 FT

FLOW PROPERTIES

PRESSURE (LB/FT**2)	1.07926E+04
VELOCITY (FT/SEC)	1.52749E+03
DENSITY (LB/FT**3)	4.41395E-02
TEMPERATURE (DEG R)	1900.90
MASS FLOW RATE (LB/SEC)	1.52297E+02
ENTROPY (BTU/LB/DEG R)	3.68915E+00
MACH NUMBER	4.68508E-01
GAMMA	1.35101E+00
ENTHALPY (BTU/LB)	8.26637E+02
SP. HEAT (CP) (BTU/LB/DEG R)	6.36664E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	101
AVERAGE STEP SIZE	0.99075E-01
METHOD ORDER	2
TOTAL NUMBER OF STEPS	101
FUNCT EVALUATIONS	129
JACOBIAN EVALUATIONS	17

HEAT LOSS(QDOT/MDOT) = 4.8834E+00 BTU/(LB-FT)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/FT**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/FT**3/SEC)
O	2.35957E-10	6.42196E-08	4.86527E-06
H2O	7.32071E-07	1.99245E-04	1.96657E-02
OH	1.93035E-10	5.25377E-08	4.78803E-06
H	3.74249E-09	1.01858E-06	7.72885E-05
O2	1.22390E-03	3.33105E-01	-2.54053E-02
H2	2.44879E-03	6.66479E-01	-3.22992E-02
HO2	3.86994E-07	1.05327E-04	5.95029E-03
H2O2	4.05418E-07	1.10341E-04	9.61734E-03

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-FT**3/LB**2/SEC)	NET RATE/POSITIVE DIR RATE
1	1.0762E+10	1.42394E-05	0.93166
2	7.6296E+10	2.87317E+00	1.00000
3	5.9938E+11	2.84734E+00	1.00000
4	2.6434E+13	2.92939E-01	0.93068
5	3.1047E+13	2.33083E-02	1.00000
6	8.0000E+12	4.91341E-03	1.00000
7	8.0477E+13	9.58268E-01	1.00000
8	5.3022E+08	3.94675E+00	0.95538
9	3.0860E+12	1.98468E-03	0.99955
10	1.8000E+12	2.20947E+00	0.99691
11	7.8000E+11	9.72995E-03	1.00000
12	5.4969E+07	1.20822E+00	1.00000
13	2.5930E+12	1.00771E+01	0.99998
14	2.3513E+15	1.26972E+01	0.99984
15	2.2664E-07	-7.21735E-05	1.00000
16	6.7231E+15	2.87269E-06	1.00000
17	2.9877E-06	-6.86190E-05	0.99999
18	6.4193E-10	-2.43644E-09	0.99999

DERIVATIVES (FPS UNITS): T 8.43709E+01 RHO 8.54923E-04 V -3.07830E+02

MIXTURE MOLECULAR WEIGHT 12.01328 TOTAL ENERGY EXCHANGE RATE (BTU-FT**3/LB**2/SEC) -1.33268E+06 MASS FRACTION SUM 1.00000000

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 6.099997E-01 S UP TO THIS TIME - 6.099997E-01 S

TABLE D.2.—Continued.
(d) Concluded.

TIME 3.38532E-04 SEC AREA 2.57048E+00 SQ FT AXIAL POSITION 5.23319E-01 FT

FLOW PROPERTIES

PRESSURE (LB/FT**2)	1.09185E+04
VELOCITY (FT/SEC)	1.46571E+03
DENSITY (LB/FT**3)	4.04266E-02
TEMPERATURE (DEG R)	2117.59
MASS FLOW RATE (LB/SEC)	1.52297E+02
ENTROPY (BTU/LB/DEG R)	3.75331E+00
MACH NUMBER	4.29328E-01
GAMMA	1.34109E+00
ENTHALPY (BTU/LB)	8.29365E+02
SP. HEAT (CP) (BTU/LB/DEG R)	6.44879E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	81
AVERAGE STEP SIZE	0.11319E-01
METHOD ORDER	4
TOTAL NUMBER OF STEPS	241
FUNCT EVALUATIONS	324
JACOBIAN EVALUATIONS	34

HEAT LOSS(QDOT/MDOT) = 5.4439E+00 BTU/(LB-FT)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/FT**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/FT**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-FT**3/LB**2/SEC)	NET RATE/POSITIVE DIR RATE
O	1.50296E-07	4.50428E-05	2.78407E-01	1	2.6351E+10	-4.21688E-01	0.16951
H2O	5.32254E-05	1.59514E-02	3.25414E+01	2	1.6974E+11	4.09029E+03	0.99887
OH	2.64514E-07	7.92732E-05	4.90561E-01	3	1.1719E+12	3.76604E+03	0.99818
H	2.25878E-06	6.76943E-04	4.09676E+00	4	2.9321E+13	2.07131E+03	0.99985
O2	1.08970E-03	3.26576E-01	-1.55385E+01	5	3.2599E+13	1.53250E+02	1.00000
H2	2.18564E-03	6.55024E-01	-3.36171E+01	6	8.0000E+12	6.61902E+01	1.00000
HO2	3.19142E-06	9.56450E-04	2.02588E-01	7	8.4787E+13	5.99043E+03	1.00000
H2O2	2.30550E-06	6.90946E-04	-1.31927E+00	8	1.7942E+09	-8.56699E+02	0.87476
				9	3.3088E+12	1.97733E+01	0.99981
				10	1.8000E+12	1.79476E+02	0.99884
				11	7.8000E+11	3.98113E+01	1.00000
				12	5.0566E+08	7.04241E+01	0.99132
				13	3.4909E+12	1.97505E+04	0.99849
				14	2.2394E+15	7.88762E+03	0.99997
				15	3.8180E-05	-3.46610E+01	1.00000
				16	6.0352E+15	1.07327E+00	1.00000
				17	3.2231E-04	-1.89787E+01	1.00000
				18	1.8191E-07	-9.26897E-04	1.00000

DERIVATIVES (FPS UNITS): T 7.77921E+04 RHO -1.37638E+00 V -3.50268E+02

MIXTURE MOLECULAR WEIGHT 12.11563 TOTAL ENERGY EXCHANGE RATE -1.76542E+09 (BTU-FT**3/LB**2/SEC) MASS FRACTION SUM 1.00000001

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 5.100002E-01 S UP TO THIS TIME - 1.490000E+00 S

(LSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

TOTAL NO. OF STEPS -	241
TOTAL NO. OF DERIVATIVE EVALUATIONS -	324
TOTAL NO. OF JACOBIAN EVALUATIONS -	34
TOTAL CPU TIME -	1.490000 S

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 2.640000 S

(LSENS) READ DATA FOR NEXT CASE

TABLE D.2.—Continued.

(e) Case 5

TIME-PRESSURE VERSION LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

LSENS CH4 - O2 - N2 MECH. BATCH RXN. WITH OTTO CYCLE HEAT LOSS CASE 5

REACTION NUMBER	REACTION							REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	M	+	1*CH4	=	1*CH3	+	1*H	2.00000E+17	0.0000	88000.00
2	1*H	+	1*CH4	=	1*CH3	+	1*H2	1.26000E+14	0.0000	11900.00
3	1*CH4	+	1*O2	=	1*CH3	+	1*HO2	7.94000E+13	0.0000	56000.00
4	1*O	+	1*CH4	=	1*CH3	+	1*OH	1.90000E+14	0.0000	11720.00
5	1*OH	+	1*CH4	=	1*CH3	+	1*H2O	2.50000E+13	0.0000	5010.00
6	1*CH3	+	1*O2	=	1*CH3O	+	1*O	2.40000E+13	0.0000	28680.00
7	1*CH3	+	1*OH	=	1*CH3O	+	1*H	6.30000E+12	0.0000	0.00
8	M	+	1*CH3O	=	1*CH2O	+	1*H	5.00000E+13	0.0000	21000.00
9			2*CH3	=	1*C2H6			2.40000E+14	-0.4000	0.00
10	1*H	+	1*C2H6	=	1*C2H5	+	1*H2	1.32000E+14	0.0000	9700.00
11	1*O	+	1*C2H6	=	1*C2H5	+	1*OH	1.13000E+14	0.0000	7850.00
12	1*OH	+	1*C2H6	=	1*C2H5	+	1*H2O	8.70000E+13	0.0000	3520.00
13	M	+	1*C2H5	=	1*C2H4	+	1*H	1.00000E+17	0.0000	31000.00
14	1*C2H5	+	1*O2	=	1*C2H4	+	1*HO2	2.00000E+12	0.0000	5000.00
15	1*H	+	1*C2H5	=	1*C2H4	+	1*H2	4.80000E+13	0.0000	0.00
16	1*CH3	+	1*CH2	=	1*C2H4	+	1*H	2.00000E+13	0.0000	0.00
17	1*H	+	1*C2H4	=	1*H2	+	1*C2H3	1.50000E+14	0.0000	10200.00
18	M	+	1*C2H4	=	1*C2H2	+	1*H2	2.60000E+17	0.0000	79300.00
19	1*C2H4	+	1*OH	=	1*C2H3	+	1*H2O	4.80000E+12	0.0000	1230.00
20	1*C2H4	+	1*OH	=	1*CH3	+	1*CH2O	2.00000E+12	0.0000	960.00
21	1*C2H4	+	1*O	=	1*CH3	+	1*HCO	3.30000E+12	0.0000	1130.00
22	1*C2H4	+	1*O	=	1*CH2O	+	1*CH2	2.50000E+13	0.0000	5000.00
23	M	+	1*C2H3	=	1*C2H2	+	1*H	3.00000E+15	0.0000	32000.00
24	1*C2H3	+	1*O2	=	1*CH2O	+	1*HCO	3.98000E+12	0.0000	-250.00
25	1*C2H3	+	1*H	=	1*C2H2	+	1*H2	6.00000E+12	0.0000	0.00
26	1*C2H3	+	1*O	=	1*C2H2O	+	1*H	3.30000E+13	0.0000	0.00
27	1*C2H3	+	1*OH	=	1*C2H2	+	1*H2O	5.00000E+12	0.0000	0.00
28	1*C2H3	+	1*CH2	=	1*C2H2	+	1*CH3	3.00000E+13	0.0000	0.00
29	1*C2H3	+	1*C2H	=	2*C2H2			3.00000E+13	0.0000	0.00
30	M	+	1*C2H2	=	1*C2H	+	1*H	4.20000E+16	0.0000	107000.00
31	1*C2H2	+	1*O	=	1*CH2	+	1*CO	1.60000E+14	0.0000	9890.00
32	1*C2H2	+	1*O	=	1*C2HO	+	1*H	4.00000E+14	0.0000	10660.00
33	1*C2H2	+	1*OH	=	1*C2H	+	1*H2O	6.30000E+12	0.0000	7000.00
34	1*C2H2	+	1*OH	=	1*C2H2O	+	1*H	3.20000E+11	0.0000	200.00
35	1*C2H	+	1*O2	=	1*C2HO	+	1*O	5.00000E+13	0.0000	1500.00
36	1*C2H	+	1*OH	=	1*C2HO	+	1*H	2.00000E+13	0.0000	0.00
37	1*C2HO	+	1*O2	=	2*CO	+	1*OH	1.46000E+12	0.0000	2500.00
38	1*C2HO	+	1*O	=	2*CO	+	1*H	1.20200E+12	0.0000	0.00
39	1*C2HO	+	1*OH	=	2*HCO			1.00000E+13	0.0000	0.00
40	1*C2HO	+	1*H	=	1*CH2	+	1*CO	5.00000E+13	0.0000	0.00
41	1*C2HO	+	1*CH2	=	1*C2H3	+	1*CO	3.00000E+13	0.0000	0.00
42	1*C2HO	+	1*CH2	=	1*CH2O	+	1*C2H	1.00000E+13	0.0000	2000.00
43			2*C2HO	=	1*C2H2	+	2*CO	1.00000E+13	0.0000	0.00
44	1*C2H2O	+	1*OH	=	1*CH2O	+	1*HCO	2.80000E+13	0.0000	0.00
45	1*C2H2O	+	1*OH	=	1*C2HO	+	1*H2O	7.50000E+12	0.0000	3000.00
46	1*C2H2O	+	1*H	=	1*CH3	+	1*CO	1.13000E+13	0.0000	3428.00
47	1*C2H2O	+	1*H	=	1*C2HO	+	1*H2	7.50000E+13	0.0000	8000.00
48	1*C2H2O	+	1*O	=	1*C2HO	+	1*OH	5.00000E+13	0.0000	8000.00
49	1*C2H2O	+	1*O	=	1*CH2O	+	1*CO	2.00000E+13	0.0000	0.00
50	M	+	1*C2H2O	=	1*CH2	+	1*CO	2.00000E+16	0.0000	60000.00
51	1*C2H	+	1*O	=	1*CO	+	1*CH	5.00000E+13	0.0000	0.00
52	1*CH3O	+	1*O2	=	1*CH2O	+	1*HO2	1.00000E+13	0.0000	7170.00
53	1*CH3O	+	1*H	=	1*CH2O	+	1*H2	2.00000E+13	0.0000	0.00
54	M	+	1*CH2O	=	1*HCO	+	1*H	5.00000E+16	0.0000	81000.00
55	1*CH2O	+	1*OH	=	1*HCO	+	1*H2O	3.00000E+13	0.0000	1200.00
56	1*CH2O	+	1*H	=	1*HCO	+	1*H2	2.50000E+13	0.0000	3990.00
57	1*CH2O	+	1*O	=	1*HCO	+	1*OH	3.50000E+13	0.0000	3500.00
58	1*CH3	+	1*CH2O	=	1*CH4	+	1*HCO	1.00000E+10	0.5000	6000.00
59	1*CH3	+	1*HCO	=	1*CH4	+	1*CO	3.00000E+11	0.5000	0.00
60	1*CH3	+	1*HO2	=	1*CH3O	+	1*OH	2.00000E+13	0.0000	0.00
61	M	+	1*CH3	=	1*CH2	+	1*H	1.95000E+16	0.0000	91600.00
62	1*H	+	1*CH3	=	1*H2	+	1*CH2	2.70000E+11	0.6700	25700.00
63	1*O	+	1*CH3	=	1*OH	+	1*CH2	1.90000E+11	0.6800	25700.00
64	1*OH	+	1*CH3	=	1*H2O	+	1*CH2	2.70000E+11	0.6700	25700.00
65	1*CH	+	1*CO2	=	1*HCO	+	1*CO	3.70000E+12	0.0000	0.00
66	1*CH	+	1*O2	=	1*HCO	+	1*O	1.00000E+13	0.0000	0.00
67	1*CH2	+	1*O2	=	1*CH2O	+	1*O	5.00000E+11	0.5000	6960.00
68	1*CH2	+	1*O	=	1*CH	+	1*OH	2.00000E+11	0.7000	25800.00
69	1*CH2	+	1*OH	=	1*CH	+	1*H2O	5.00000E+11	0.5000	5900.00
70	1*CH2	+	1*H	=	1*CH	+	1*H2	3.20000E+11	0.7000	4970.00
71			2*CH2	=	1*C2H3	+	1*H	5.00000E+12	0.0000	0.00
72			2*CH2	=	1*C2H2	+	1*H2	4.00000E+13	0.0000	0.00
73	1*HCO	+	1*O2	=	1*CO	+	1*HO2	3.00000E+13	0.0000	0.00
74	1*HCO	+	1*O	=	1*CO	+	1*OH	3.00000E+13	0.0000	0.00
75	1*HCO	+	1*OH	=	1*CO	+	1*H2O	3.00000E+13	0.0000	0.00
76	1*HCO	+	1*H	=	1*CO	+	1*H2	2.00000E+13	0.0000	0.00
77	M	+	1*HCO	=	1*H	+	1*CO	2.90000E+14	0.0000	15570.00
78	1*CO	+	1*O	=	1*CO2	+	M	2.40000E+15	0.0000	4100.00
79	1*CO	+	1*O2	=	1*CO2	+	1*O	2.50000E+12	0.0000	47690.00
80	1*CO	+	1*OH	=	1*CO2	+	1*H	4.17000E+11	0.0000	1000.00
81	1*CO	+	1*HO2	=	1*CO2	+	1*OH	5.75000E+13	0.0000	22930.00
82	1*O	+	1*H2O	=	2*OH			6.80000E+13	0.0000	18365.00
83	1*H	+	1*O2	=	1*OH	+	1*O	1.89000E+14	0.0000	16400.00
84	1*O	+	1*H2	=	1*OH	+	1*H	4.20000E+14	0.0000	13750.00
85	1*H	+	1*HO2	=	1*H2	+	1*O2	7.28000E+13	0.0000	2126.00
86	1*O	+	1*HO2	=	1*OH	+	1*O2	5.00000E+13	0.0000	1000.00
87	1*HO2	+	1*OH	=	1*H2O	+	1*O2	8.00000E+12	0.0000	0.00
88	1*H	+	1*HO2	=	2*OH			1.34000E+14	0.0000	1070.00
89	1*H2	+	1*HO2	=	1*H2O2	+	1*H	7.91000E+13	0.0000	25000.00
90	1*OH	+	1*H2O2	=	1*H2O	+	1*HO2	6.10000E+12	0.0000	1430.00
91			2*HO2	=	1*H2O2	+	1*O2	1.80000E+12	0.0000	0.00
92	1*H	+	1*H2O2	=	1*OH	+	1*H2O	7.80000E+11	0.0000	0.00
93	M	+	1*H2O2	=	2*OH			1.44000E+17	0.0000	45510.00
94	1*H2	+	1*OH	=	1*H2O	+	1*H	4.74000E+13	0.0000	6098.00
95	1*H	+	1*O2	=	1*HO2	+	M	1.46000E+15	0.0000	-1000.00
96	M	+	1*H2O	=	1*H	+	1*OH	1.50000E+15	0.0000	105140.00
97	1*H	+	1*O	=	1*OH	+	M	7.10000E+18	-1.0000	0.00
98	M	+	1*H2	=	2*H			2.20000E+14	0.0000	96000.00
99	M	+	1*O2	=	2*O			1.80000E+18	-1.0000	118020.00
100	1*CH	+	1*N2	=	1*HCN	+	1*N	1.00000E+11	0.0000	19000.00
101	1*CN	+	1*H2	=	1*HCN	+	1*H	6.00000E+13	0.0000	5300.00
102	1*O	+	1*HCN	=	1*OH	+	1*CN	1.40000E+11	0.6800	16900.00
103	1*OH	+	1*HCN	=	1*HNCO	+	1*H	4.00000E+11	0.0000	2800.00
104	1*CH	+	1*O	=	1*CO	+	1*N	1.20000E+13	0.0000	0.00
105	1*CH	+	1*OH	=	1*HCO	+	1*N	2.50000E+14	0.0000	6000.00
106	1*NH2	+	1*HCO	=	1*HNCO	+	1*H	1.00000E+14	0.0000	9000.00
107	1*HNCO	+	1*H	=	1*NH2	+	1*CO	1.00000E+14	0.0000	8500.00
108	1*CH	+	1*O2	=	1*HCO	+	1*O	3.20000E+13	0.0000	1000.00
109	1*CN	+	1*CO2	=	1*NCO	+	1*CO	3.70000E+12	0.0000	0.00
110	1*O	+	1*NCO	=	1*NO	+	1*CO	2.00000E+13	0.0000	0.00

TABLE D.2.—Continued.

(e) Continued.

111	1*N	+	1*NCO	=	1*N2	+	1*CO	1.00000E+13	0.0000	0.00
112	1*H	+	1*NCO	=	1*NH	+	1*CO	2.00000E+13	0.0000	0.00
113	1*CH	+	1*NO	=	1*N	+	1*HCO	1.60000E+13	0.0000	9940.00
114	1*CH	+	1*NO	=	1*O	+	1*HCN	2.00000E+12	0.0000	0.00
115	1*NH	+	1*OH	=	1*N	+	1*H2O	5.00000E+11	0.5000	2000.00
116	1*HO2	+	1*NO	=	1*NO2	+	1*OH	2.09000E+12	0.0000	-477.00
117	1*O	+	1*NO2	=	1*NO	+	1*O2	1.00000E+13	0.0000	596.00
118	1*NO	+	1*O	=	1*NO2	+	M	5.62000E+15	0.0000	-1160.00
119	1*NO2	+	1*H	=	1*NO	+	1*OH	3.47000E+14	0.0000	1470.00
120	1*NO	+	1*H	=	1*N	+	1*OH	2.63000E+14	0.0000	50410.00
121	1*NO	+	1*O	=	1*N	+	1*O2	3.80000E+09	1.0000	41370.00
122	1*O	+	1*N2	=	1*NO	+	1*N	1.80000E+14	0.0000	76250.00
123	1*N	+	1*NO2	=	2*NO			4.00000E+12	0.0000	0.00
124	M	+	1*N2O	=	1*N2	+	1*O	6.92000E+23	-2.5000	65000.00
125	1*O	+	1*N2O	=	1*N2	+	1*O2	1.00000E+14	0.0000	28020.00
126	1*O	+	1*N2O	=	2*NO			6.92000E+13	0.0000	26630.00
127	1*H2O	+	1*H	=	1*N2	+	1*OH	7.59000E+13	0.0000	15100.00
128	1*NO2	+	1*H2	=	1*HNO2	+	1*H	2.40000E+13	0.0000	29000.00
129	1*OH	+	1*NO2	=	1*HNO3	+	M	3.00000E+15	0.0000	-3800.00
130	1*OH	+	1*NO	=	1*HNO2	+	M	5.60000E+15	0.0000	-1700.00
131	1*HNO	+	1*H	=	1*H2	+	1*NO	5.00000E+12	0.0000	0.00
132	1*H	+	1*NO	=	1*HNO	+	M	5.40000E+15	0.0000	-600.00
133	1*HNO	+	1*OH	=	1*H2O	+	1*NO	3.60000E+13	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2	, 93) =	2.30000	M(O2	, 93) =	0.78000	M(H2O	, 93) =	6.00000	M(H2O2	, 93) =	6.60000
M(O2	, 95) =	1.30000	M(N2	, 95) =	1.30000	M(H2O	, 95) =	21.30000	M(CO2	, 95) =	7.00000
M(H2	, 96) =	4.00000	M(O2	, 96) =	1.50000	M(H2O	, 96) =	20.00000	M(N2	, 96) =	1.50000
M(CO2	, 96) =	4.00000	M(H2	, 98) =	4.10000	M(O2	, 98) =	2.00000	M(H2O	, 98) =	15.00000
M(N2	, 98) =	2.00000	M(O2	,129) =	0.70000	M(H2	,129) =	1.40000			

TRANSPORT PROPERTY COEFFICIENTS

H2	0.687200E+00	-0.617320E+00	-0.111490E+03	0.577240E+00	VISC
H2	0.116129E+01	0.469043E+03	-0.551496E+05	-0.149041E+01	COND
CH4	0.600440E+00	-0.817476E+02	0.165196E+04	0.154710E+01	VISC
CH4	0.853201E+00	-0.288931E+03	0.193692E+05	0.355349E+00	COND
C2H2	0.579032E+00	-0.152664E+03	0.628889E+04	0.177748E+01	VISC
C2H2	0.666734E+00	-0.330498E+03	0.165066E+05	0.118596E+01	COND
C2H4	0.578808E+00	-0.148526E+03	0.598107E+04	0.175623E+01	VISC
C2H4	0.674458E+00	-0.506382E+03	0.309615E+05	0.150224E+01	COND
NO	0.646504E+00	0.388567E+01	-0.858737E+04	0.165204E+01	VISC
NO	0.614175E+00	-0.260319E+03	0.360173E+05	0.110633E+01	COND
N2	0.633933E+00	-0.119153E+02	-0.471490E+04	0.166605E+01	VISC
N2	0.686393E+00	-0.161885E+03	0.236277E+05	0.482688E+00	COND
O	0.763927E+00	0.569723E+02	-0.345462E+04	0.822320E+00	VISC
O	0.776744E+00	0.803466E+02	-0.349619E+04	-0.481407E-01	COND
H	0.860209E+00	0.498177E+02	-0.542523E+04	-0.102874E+01	VISC
H	0.869708E+00	0.670316E+02	-0.828927E+04	0.891354E+00	COND
H2O	0.756380E+00	-0.301892E+03	0.187539E+05	0.987951E+00	VISC
H2O	0.123241E+01	-0.163667E+03	0.141541E+05	-0.291285E+01	COND
NO2	0.603384E+00	-0.988315E+02	-0.969625E+03	0.200464E+01	VISC
NO2	0.504502E+00	-0.475725E+03	0.415525E+05	0.201241E+01	COND
OH	0.597497E+00	-0.365001E+03	0.351359E+05	0.217217E+01	VISC
OH	0.812287E+00	-0.264930E+03	0.343595E+05	0.105187E+00	COND
CO	0.779825E+00	0.193974E+03	-0.317845E+05	0.436375E+00	VISC
CO	0.800546E+00	-0.237400E+02	0.804541E+04	-0.468414E+00	COND
CO2	0.440370E+00	-0.288400E+03	0.193120E+05	0.324659E+01	VISC
CO2	0.603518E+00	-0.438483E+03	0.322949E+05	0.134025E+01	COND
O2	0.659260E+00	0.941422E+00	-0.711780E+04	0.164432E+01	VISC
O2	0.478050E+00	-0.452958E+03	0.579015E+05	0.228192E+01	COND

TABLE D.2.—Continued.

(e) Continued.

** INITIAL CONDITIONS **

TIME 0.00000E+00 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	2.00000
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	4.18827E-04
TEMPERATURE (DEG K)	1550.00
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	2.2819
MACH NUMBER	0.0000
GAMMA	1.2285
ENTHALPY (CAL/G)	3.15126E+02
SP. HEAT (CP) (CAL/G/DEG K)	4.01086E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

HEAT LOSS(QDOT/TOTMAS) = 3.3606E+02 CAL/(G-SEC)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	2.71255E-06	1.72500E-01	-1.07574E-05
CH3	0.00000E+00	0.00000E+00	1.07574E-05
H	0.00000E+00	0.00000E+00	3.45795E-06
H2	0.00000E+00	0.00000E+00	9.89090E-07
O2	2.71255E-06	1.72500E-01	-2.40723E-02
HO2	0.00000E+00	0.00000E+00	7.42305E-06
O	0.00000E+00	0.00000E+00	2.40649E-02
OH	0.00000E+00	0.00000E+00	0.00000E+00
H2O	0.00000E+00	0.00000E+00	0.00000E+00
CH3O	0.00000E+00	0.00000E+00	0.00000E+00
CH2O	0.00000E+00	0.00000E+00	8.76480E-04
C2H6	0.00000E+00	0.00000E+00	0.00000E+00
C2H5	0.00000E+00	0.00000E+00	0.00000E+00
C2H4	0.00000E+00	0.00000E+00	0.00000E+00
CH2	1.57249E-10	1.00000E-05	-8.78705E-04
C2H3	0.00000E+00	0.00000E+00	1.23636E-07
C2H2	0.00000E+00	0.00000E+00	9.89090E-07
HCO	0.00000E+00	0.00000E+00	1.27964E-02
C2H2O	0.00000E+00	0.00000E+00	0.00000E+00
C2H	0.00000E+00	0.00000E+00	0.00000E+00
CO	0.00000E+00	0.00000E+00	0.00000E+00
C2HO	0.00000E+00	0.00000E+00	0.00000E+00
CN	4.71747E-10	3.00000E-05	-1.27974E-02
CO2	0.00000E+00	0.00000E+00	0.00000E+00
H2O2	0.00000E+00	0.00000E+00	0.00000E+00
N2	1.02986E-05	6.54920E-01	-1.01739E-06
HCN	0.00000E+00	0.00000E+00	1.01739E-06
N	1.57249E-10	1.00000E-05	-5.25625E-04
CN	1.57249E-10	1.00000E-05	-9.86541E-03
HNCO	0.00000E+00	0.00000E+00	0.00000E+00
NCO	0.00000E+00	0.00000E+00	9.86541E-03
NH2	0.00000E+00	0.00000E+00	0.00000E+00
NO	0.00000E+00	0.00000E+00	5.26643E-04
NH	0.00000E+00	0.00000E+00	0.00000E+00
HO2	0.00000E+00	0.00000E+00	0.00000E+00
N2O	0.00000E+00	0.00000E+00	6.36740E-13
HNO2	0.00000E+00	0.00000E+00	0.00000E+00
HNO3	0.00000E+00	0.00000E+00	0.00000E+00
HNO	0.00000E+00	0.00000E+00	0.00000E+00

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	7.8170E+04	1.90081E+01	1.00000
2	2.6453E+12	0.00000E+00	0.00000
3	1.0089E+06	4.23169E+01	1.00000
4	4.2290E+12	0.00000E+00	0.00000
5	4.9151E+12	0.00000E+00	0.00000
6	2.1694E+09	0.00000E+00	0.00000
7	6.3000E+12	0.00000E+00	0.00000
8	5.4698E+10	0.00000E+00	0.00000
9	1.2708E+13	0.00000E+00	0.00000
10	5.6608E+12	0.00000E+00	0.00000
11	8.8355E+12	0.00000E+00	0.00000
12	2.7746E+13	0.00000E+00	0.00000
13	4.2560E+12	0.00000E+00	0.00000
14	3.9449E+11	0.00000E+00	0.00000
15	4.8000E+13	0.00000E+00	0.00000
16	2.0000E+13	0.00000E+00	0.00000
17	5.4688E+12	0.00000E+00	0.00000
18	1.7127E+06	0.00000E+00	0.00000
19	3.2197E+12	0.00000E+00	0.00000
20	1.4644E+12	0.00000E+00	0.00000
21	2.2866E+12	0.00000E+00	0.00000
22	4.9311E+12	0.00000E+00	0.00000
23	9.2284E+10	0.00000E+00	0.00000
24	4.3165E+12	0.00000E+00	0.00000
25	6.0000E+12	0.00000E+00	0.00000
26	3.3000E+13	0.00000E+00	0.00000
27	5.0000E+12	0.00000E+00	0.00000
28	3.0000E+13	0.00000E+00	0.00000
29	3.0000E+13	0.00000E+00	0.00000
30	3.4377E+01	0.00000E+00	0.00000
31	6.4511E+12	0.00000E+00	0.00000
32	1.2560E+13	0.00000E+00	0.00000
33	6.4914E+11	0.00000E+00	0.00000
34	2.9988E+11	0.00000E+00	0.00000
35	3.0723E+13	0.00000E+00	0.00000
36	2.0000E+13	0.00000E+00	0.00000
37	6.4842E+11	0.00000E+00	0.00000
38	1.2020E+12	0.00000E+00	0.00000
39	1.0000E+13	0.00000E+00	0.00000
40	5.0000E+13	0.00000E+00	0.00000
41	3.0000E+13	0.00000E+00	0.00000
42	5.2240E+12	0.00000E+00	0.00000
43	1.0000E+13	0.00000E+00	0.00000
44	2.8000E+13	0.00000E+00	0.00000
45	2.8318E+12	0.00000E+00	0.00000
46	3.7131E+12	0.00000E+00	0.00000
47	5.5855E+12	0.00000E+00	0.00000
48	3.7237E+12	0.00000E+00	0.00000
49	2.0000E+13	0.00000E+00	0.00000
50	6.9349E+07	0.00000E+00	0.00000
51	5.0000E+13	0.00000E+00	0.00000
52	9.7506E+11	0.00000E+00	0.00000
53	2.0000E+13	0.00000E+00	0.00000
54	1.8966E+05	0.00000E+00	0.00000
55	2.0320E+13	0.00000E+00	0.00000
56	6.8446E+12	0.00000E+00	0.00000
57	1.1235E+13	0.00000E+00	0.00000
58	5.6126E+10	0.00000E+00	0.00000
59	1.1811E+13	0.00000E+00	0.00000
60	2.0000E+13	0.00000E+00	0.00000
61	2.3684E+03	0.00000E+00	0.00000
62	8.8143E+09	0.00000E+00	0.00000
63	6.6755E+09	0.00000E+00	0.00000
64	8.8143E+09	0.00000E+00	0.00000
65	3.7000E+12	0.00000E+00	0.00000
66	1.0000E+13	7.29487E+04	1.00000
67	2.0548E+12	4.99659E+03	1.00000
68	7.8789E+09	0.00000E+00	0.00000
69	2.8989E+12	0.00000E+00	0.00000
70	1.0905E+13	0.00000E+00	0.00000
71	5.0000E+12	7.04819E-01	1.00000
72	4.0000E+13	5.63855E+00	1.00000
73	3.0000E+13	0.00000E+00	0.00000
74	3.0000E+13	0.00000E+00	0.00000
75	3.0000E+13	0.00000E+00	0.00000
76	2.0000E+13	0.00000E+00	0.00000
77	1.8494E+12	0.00000E+00	0.00000
78	6.3403E+14	0.00000E+00	0.00000
79	4.7169E+05	0.00000E+00	0.00000
80	3.0140E+11	0.00000E+00	0.00000
81	3.3616E+10	0.00000E+00	0.00000
82	1.7500E+11	0.00000E+00	0.00000

TABLE D.2.—Continued.

(e) Continued.

83	9.2059E+11	0.00000E+00	0.00000
84	4.8362E+12	0.00000E+00	0.00000
85	3.6506E+13	0.00000E+00	0.00000
86	3.6139E+13	0.00000E+00	0.00000
87	8.0000E+12	0.00000E+00	0.00000
88	9.4675E+13	0.00000E+00	0.00000
89	2.3615E+10	0.00000E+00	0.00000
90	3.8344E+12	0.00000E+00	0.00000
91	1.8000E+12	0.00000E+00	0.00000
92	7.8000E+11	0.00000E+00	0.00000
93	5.5139E+10	0.00000E+00	0.00000
94	6.5458E+12	0.00000E+00	0.00000
95	2.0200E+15	0.00000E+00	0.00000
96	1.9463E+00	0.00000E+00	0.00000
97	4.5806E+15	0.00000E+00	0.00000
98	6.4038E+00	0.00000E+00	0.00000
99	2.6554E-02	6.45704E-06	1.00000
100	2.0941E+08	5.79989E+00	1.00000
101	1.0736E+13	0.00000E+00	0.00000
102	8.5636E+10	0.00000E+00	0.00000
103	1.6116E+11	0.00000E+00	0.00000
104	1.2000E+13	0.00000E+00	0.00000
105	3.5640E+13	0.00000E+00	0.00000
106	5.3827E+12	0.00000E+00	0.00000
107	6.3314E+12	0.00000E+00	0.00000
108	2.3129E+13	5.62402E+04	1.00000
109	3.7000E+12	0.00000E+00	0.00000
110	2.0000E+13	0.00000E+00	0.00000
111	1.0000E+13	0.00000E+00	0.00000
112	2.0000E+13	0.00000E+00	0.00000
113	6.3472E+11	0.00000E+00	0.00000
114	2.0000E+12	0.00000E+00	0.00000
115	1.0283E+13	0.00000E+00	0.00000
116	2.4401E+12	0.00000E+00	0.00000
117	8.2407E+12	0.00000E+00	0.00000
118	8.1902E+15	0.00000E+00	0.00000
119	2.1531E+14	0.00000E+00	0.00000
120	2.0519E+07	0.00000E+00	0.00000
121	8.6487E+06	-3.00226E+03	1.00000
122	3.1918E+03	0.00000E+00	0.00000
123	4.0000E+12	0.00000E+00	0.00000
124	5.0056E+06	0.00000E+00	0.00000
125	1.1199E+10	-3.62989E-06	1.00000
126	1.2170E+10	0.00000E+00	0.00000
127	5.6382E+11	0.00000E+00	0.00000
128	1.9553E+09	0.00000E+00	0.00000
129	1.0302E+16	0.00000E+00	0.00000
130	9.7250E+15	0.00000E+00	0.00000
131	5.0000E+12	0.00000E+00	0.00000
132	6.5614E+15	0.00000E+00	0.00000
133	3.6000E+13	0.00000E+00	0.00000

DERIVATIVES (CGS UNITS), T 6.22257E+06 RHO -1.53490E+00

MIXTURE MOLECULAR WEIGHT 26.63461 TOTAL ENERGY EXCHANGE RATE -6.00627E+09 (CAL-CM**3/G**2/SEC) MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 2.360001 S

REYNOLDS NUMBER = 3.8301E+03 PRANDTL NUMBER = 0.722 HEAT TRANSFER COEFF = 5.43804E-04

REYNOLDS NUMBER = 3.8295E+03 PRANDTL NUMBER = 0.722 HEAT TRANSFER COEFF = 5.43781E-04

REYNOLDS NUMBER = 3.8290E+03 PRANDTL NUMBER = 0.722 HEAT TRANSFER COEFF = 5.43757E-04

REYNOLDS NUMBER = 3.8289E+03 PRANDTL NUMBER = 0.722 HEAT TRANSFER COEFF = 5.43748E-04

REYNOLDS NUMBER = 3.8290E+03 PRANDTL NUMBER = 0.722 HEAT TRANSFER COEFF = 5.43774E-04

REYNOLDS NUMBER = 3.8296E+03 PRANDTL NUMBER = 0.722 HEAT TRANSFER COEFF = 5.43875E-04

REYNOLDS NUMBER = 3.8302E+03 PRANDTL NUMBER = 0.722 HEAT TRANSFER COEFF = 5.43971E-04

REYNOLDS NUMBER = 3.8315E+03 PRANDTL NUMBER = 0.722 HEAT TRANSFER COEFF = 5.44174E-04

REYNOLDS NUMBER = 3.8435E+03 PRANDTL NUMBER = 0.722 HEAT TRANSFER COEFF = 5.46018E-04

REYNOLDS NUMBER = 3.9190E+03 PRANDTL NUMBER = 0.722 HEAT TRANSFER COEFF = 5.57572E-04

TIME 2.50000E-04 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	2.17500
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	4.46455E-04
TEMPERATURE (DEG K)	1581.40
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	2.2856
MACH NUMBER	0.0000
GAMMA	1.2273
ENTHALPY (CAL/G)	3.24834E+02
SP. HEAT (CP) (CAL/G/DEG K)	4.02837E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	177
AVERAGE STEP SIZE	0.14198E-05
METHOD ORDER	4
TOTAL NUMBER OF STEPS	177
FUNCT EVALUATIONS	211
JACOBIAN EVALUATIONS	27

HEAT LOSS(QDOT/TOTMAS) = 3.5278E+02 CAL/(G-SEC)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
CH4	2.85311E-06	1.70224E-01	-2.52423E-04	1	1.3786E+05	3.24282E+01	0.98045
CH3	4.30681E-09	2.56956E-04	1.60071E-05	2	2.8562E+12	1.73561E+02	0.93111
H	4.55929E-12	2.72019E-07	2.18857E-08	3	1.4475E+06	4.89553E+01	0.82341
H2	4.84210E-09	2.88893E-04	3.45887E-05	4	4.5609E+12	2.23457E+02	0.99983

TABLE D.2.—Continued.

(e) Continued.

O2	2.86938E-06	1.71195E-01	-1.50269E-04
HO2	1.15893E-09	6.91451E-05	1.34298E-06
O	3.42336E-12	2.04247E-07	1.47194E-08
OH	1.11965E-11	6.68014E-07	5.29820E-08
H2O	2.34793E-08	1.40084E-03	1.68188E-04
CH3O	3.25482E-11	1.94191E-06	1.45999E-07
CH2O	1.67694E-08	1.00051E-03	1.19800E-04
C2H6	8.12846E-09	4.84966E-04	5.01102E-05
C2H5	3.50933E-14	2.09376E-09	2.90382E-10
C2H4	2.55090E-10	1.52194E-05	3.40857E-06
CH2	8.88046E-16	5.29832E-11	1.40189E-11
C2H3	1.12477E-15	6.71066E-11	2.06752E-11
C2H2	8.61795E-13	5.14170E-08	1.42724E-08
HCO	7.80929E-14	4.65923E-09	8.29057E-10
C2H2O	7.68740E-15	4.58651E-10	1.16384E-10
C2H	7.35539E-20	4.38842E-15	2.24083E-15
CO	1.14765E-09	6.84719E-05	9.33697E-06
C2HO	2.44409E-17	1.45821E-12	5.21570E-13
CH	2.66284E-21	1.58872E-16	6.36807E-17
CO2	1.97891E-11	1.18067E-06	7.17669E-08
H2O2	2.13958E-12	1.27653E-07	2.90198E-09
N2	1.09779E-05	6.54971E-01	-1.65843E-11
HCN	4.80586E-14	2.86731E-09	5.57553E-11
N	3.03433E-17	1.81036E-12	1.55584E-13
CN	2.13920E-16	1.27630E-11	-8.30707E-12
HNCO	1.53401E-10	9.15229E-06	3.18111E-07
NCO	1.17063E-11	6.98429E-07	-3.24701E-07
NH2	3.78526E-13	2.25839E-08	4.67378E-09
NO	1.08959E-10	6.50081E-06	-1.66719E-07
NH	9.91090E-13	5.91311E-08	9.50676E-10
NO2	5.94447E-11	3.54663E-06	1.67635E-07
N2O	2.60224E-15	1.55256E-10	1.64957E-11
HNO2	1.92629E-16	1.14928E-11	1.49045E-12
HNO3	3.58837E-18	2.14092E-13	1.95458E-14
HNO	4.36919E-16	2.60677E-11	8.83195E-13

5	5.0764E+12	8.09378E+02	0.99482
6	2.6100E+09	1.61769E+02	0.99969
7	6.3000E+12	-1.19526E+01	0.88691
8	6.2629E+10	1.71413E+02	1.00000
9	1.2606E+13	2.66781E+02	0.22741
10	6.0261E+12	1.12042E+00	0.99999
11	9.2942E+12	1.29753E+00	1.00000
12	2.8383E+13	1.29596E+01	1.00000
13	5.1976E+12	1.51884E+01	0.99023
14	4.0741E+11	1.87688E-01	0.91190
15	4.8000E+13	3.72064E-05	0.96563
16	2.0000E+13	3.83611E-04	0.99960
17	5.8405E+12	3.40765E-02	0.99992
18	2.8558E+06	6.12585E-02	1.00000
19	3.2453E+12	4.65023E-02	0.99999
20	1.4735E+12	-1.89858E+00	0.98900
21	2.3033E+12	1.00911E-02	1.00000
22	5.0926E+12	2.23108E-02	0.99996
23	1.1343E+11	1.06944E-02	0.99683
24	4.3096E+12	6.97796E-02	1.00000
25	6.0000E+12	1.52647E-07	0.98885
26	3.3000E+13	6.37491E-07	1.00000
27	5.0000E+12	3.15643E-07	0.99916
28	3.0000E+13	-8.94469E-09	0.98347
29	3.0000E+13	-3.78078E-15	0.23291
30	6.8529E+01	4.95406E-09	0.99757
31	6.8758E+12	1.01771E-04	1.00000
32	1.3454E+13	1.99137E-04	1.00000
33	6.7911E+11	3.28545E-05	0.99936
34	3.0027E+11	1.45351E-05	0.99994
35	3.1022E+13	3.28480E-05	1.00000
36	2.0000E+13	8.24984E-11	0.99835
37	6.5895E+11	2.31849E-04	1.00000
38	1.2020E+12	5.04569E-10	1.00000
39	1.0000E+13	1.37213E-08	0.99943
40	5.0000E+13	2.34844E-08	0.84014
41	3.0000E+13	3.26669E-12	0.99997
42	5.2918E+12	-1.21985E-11	0.95489
43	1.0000E+13	2.99696E-14	1.00000
44	2.8000E+13	-4.95879E-04	0.97620
45	2.8871E+12	1.22344E-06	0.98133
46	3.7960E+12	-1.43264E-04	0.99536
47	5.8812E+12	7.77150E-07	0.75149
48	3.9208E+12	5.17343E-07	0.99938
49	2.0000E+13	2.64062E-06	1.00000
50	1.0210E+08	6.52580E-05	0.98871
51	5.0000E+13	6.31646E-11	1.00000
52	1.0212E+12	4.78484E+02	1.00000
53	2.0000E+13	1.48901E-02	1.00000
54	3.1973E+05	4.50864E-01	1.00000
55	2.0478E+13	1.92897E+01	1.00000
56	7.0230E+12	2.69389E+00	1.00000
57	1.1491E+13	3.30966E+00	1.00000
58	5.8928E+10	2.13510E+01	0.99995
59	1.1930E+13	2.01204E-02	0.99950
60	2.0000E+13	5.00828E+02	1.00000
61	4.2750E+03	1.54813E-03	0.99995
62	1.0544E+10	1.03850E-03	0.99982
63	7.9867E+09	5.90774E-04	1.00000
64	1.0544E+10	2.55073E-03	0.99999
65	3.7000E+12	7.88303E-13	0.80589
66	1.0000E+13	3.83334E-07	1.00000
67	2.1708E+12	2.77517E-02	1.00000
68	9.4364E+09	1.43926E-10	1.00000
69	3.0417E+12	1.51722E-07	0.99994
70	1.1419E+13	2.31764E-07	0.99918
71	5.0000E+12	1.97793E-11	0.99983
72	4.0000E+13	1.58261E-10	1.00000
73	3.0000E+13	3.37231E+01	0.99991
74	3.0000E+13	4.02375E-05	1.00000
75	3.0000E+13	1.31601E-04	1.00000
76	2.0000E+13	3.57247E-05	0.99997
77	2.0447E+12	1.34269E+01	0.99999
78	6.5102E+14	2.15077E-04	0.99999
79	6.4149E+05	1.05983E-02	1.00000
80	3.0334E+11	1.95405E-02	0.99922
81	3.8971E+10	2.60052E-01	1.00000
82	1.9700E+11	7.67928E-02	0.96665
83	1.0233E+12	6.71583E+01	0.99996
84	5.2845E+12	4.38374E-01	0.99749
85	3.7010E+13	5.98353E-01	0.60987
86	3.6372E+13	7.23273E-01	0.99902
87	8.0000E+12	5.05542E-01	0.97069
88	9.5330E+13	2.52715E+00	1.00000
89	2.7745E+10	7.79485E-01	0.99790
90	3.8699E+12	-1.62040E-02	0.97210
91	1.8000E+12	1.21193E+01	0.99918
92	7.8000E+11	3.81738E-05	1.00000
93	7.3942E+10	1.29004E+01	1.00000
94	6.8083E+12	1.71270E+00	0.92488
95	2.0070E+15	-2.26033E+01	0.88915
96	3.8337E+00	-3.03366E-05	0.73560
97	4.4897E+15	5.84064E-06	0.99118
98	1.1892E+01	6.40088E-06	0.71586
99	5.5705E-02	1.33869E-05	0.99600
100	2.3670E+08	3.46777E-11	0.99894
101	1.1109E+13	5.76083E-05	0.99784
102	9.6806E+10	-1.29648E-08	0.13960
103	1.6410E+11	-2.22104E-04	0.99801
104	1.2000E+13	4.40890E-08	1.00000
105	3.7046E+13	-3.06725E-04	0.99855
106	5.7043E+12	1.61964E+00	0.99843
107	6.6881E+12	2.34484E-02	0.99918
108	2.3278E+13	6.99404E-02	0.97565
109	3.7000E+12	-6.96497E-02	1.00000
110	2.0000E+13	4.02112E-03	1.00000
111	1.0000E+13	1.78208E-08	1.00000
112	2.0000E+13	5.35532E-03	0.99999
113	6.7673E+11	9.84929E-13	0.99986
114	2.0000E+12	2.90544E-12	0.99800
115	1.0522E+13	5.85767E-04	0.99998
116	2.4326E+12	1.53201E+00	0.99409
117	8.2724E+12	7.06890E-03	0.83660
118	8.1292E+15	-3.84982E-01	0.99934
119	2.1736E+14	2.95548E-01	0.99999
120	2.8399E+07	2.95437E-09	0.04174
121	1.1521E+07	-5.85441E-04	0.99996
122	5.2184E+03	4.61519E-07	0.46907
123	4.0000E+12	3.61974E-08	0.99999
124	7.2362E+06	-7.54880E-05	0.97945

TABLE D.2.—Continued.

(e) Continued.

125	1.3417E+10	-7.29295E-06	0.99992
126	1.4449E+10	4.92204E-10	0.76218
127	6.2148E+11	2.11138E-08	0.57076
128	2.3573E+09	3.40413E-03	0.99999
129	1.0053E+16	9.80617E-08	0.00018
130	9.6190E+15	-3.39665E-03	0.77489
131	5.0000E+12	-1.29143E-07	0.72101
132	6.5360E+15	4.94748E-06	0.01812
133	3.6000E+13	6.45631E-07	0.73072

DERIVATIVES (CGS UNITS): T 1.44692E+05 RHO 1.02827E-01

MIXTURE MOLECULAR WEIGHT 26.63670 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) -4.61382E+07 MASS FRACTION SUM 1.00000000

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 1.356000E+01 S UP TO THIS TIME - 1.356000E+01 S

TIME 3.80000E-04 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	2.26600
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	4.58842E-04
TEMPERATURE (DEG K)	1603.00
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	2.2899
MACH NUMBER	0.0000
GAMMA	1.2265
ENTHALPY (CAL/G)	3.29654E+02
SP. HEAT (CP) (CAL/G/DEG K)	4.03946E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	4
AVERAGE STEP SIZE	0.95497E-05
METHOD ORDER	4
TOTAL NUMBER OF STEPS	190
FUNCT EVALUATIONS	232
JACOBIAN EVALUATIONS	28

HEAT LOSS(QDOT/TOTMAS) = 3.6518E+02 CAL/(G-SEC)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	2.88586E-06	1.67520E-01	-4.82629E-04
CH3	7.16096E-09	4.15684E-04	2.72195E-05
H	9.44129E-12	5.48054E-07	5.68900E-08
H2	1.16588E-08	6.76774E-04	7.26359E-05
O2	2.92036E-06	1.69523E-01	-3.06580E-04
HO2	1.43687E-09	8.34084E-05	2.52978E-06
O	6.31264E-12	3.66440E-07	3.04531E-08
OH	2.16486E-11	1.25667E-06	1.14853E-07
H2O	5.64924E-08	3.27930E-03	3.50123E-04
CH3O	6.07057E-11	3.52388E-06	2.95168E-07
CH2O	3.87673E-08	2.25038E-03	2.17101E-04
C2H6	1.70146E-08	9.87676E-04	8.49566E-05
C2H5	1.25432E-13	7.28117E-09	1.18897E-09
C2H4	1.24779E-09	7.24325E-05	1.38887E-05
CH2	6.72284E-15	3.90251E-10	1.03560E-10
C2H3	1.07956E-14	6.26667E-10	1.84743E-10
C2H2	7.07630E-12	4.10769E-07	1.09221E-07
HCO	3.19879E-13	1.85685E-08	3.40938E-09
C2H2O	6.54205E-14	3.79757E-09	1.07426E-09
C2H	1.17378E-18	6.81363E-14	2.84774E-14
CO	3.97024E-09	2.30467E-04	3.98261E-05
C2HO	3.78074E-16	2.19466E-11	7.84855E-12
CH	4.11860E-20	2.39079E-15	9.16900E-16
CO2	3.89344E-11	2.26008E-06	2.81059E-07
H2O2	2.79110E-12	1.62020E-07	6.54427E-09
N2	1.12825E-05	6.54932E-01	-3.44228E-11
HCN	5.93685E-14	3.44625E-09	1.07598E-10
N	5.78177E-17	3.35624E-12	2.79034E-13
CN	2.89114E-18	1.67826E-13	1.69649E-12
HNCO	1.68587E-10	9.78622E-06	-9.01295E-09
NCO	4.82385E-14	2.80018E-09	-2.09922E-09
NH2	1.36719E-12	7.93636E-08	1.09877E-08
NO	9.79850E-11	5.68789E-06	-4.13025E-08
NH	1.03340E-12	5.99872E-08	-2.29972E-10
NO2	7.51410E-11	4.36183E-06	4.15427E-08
N2O	5.84091E-15	3.39056E-10	3.40858E-11
HNO2	4.76105E-16	2.76372E-11	2.74619E-12
HNO3	7.23725E-18	4.20112E-13	1.10586E-14
HNO	6.53848E-16	3.79550E-11	2.52944E-12

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	2.0103E+05	4.54497E+01	0.95745
2	3.0057E+12	3.37791E+02	0.86841
3	1.8402E+06	5.29514E+01	0.71882
4	4.7959E+12	4.14859E+02	0.99971
5	5.1866E+12	1.52173E+03	0.98872
6	2.9514E+09	2.92999E+02	0.99944
7	6.3000E+12	-4.18674E+01	0.90025
8	6.8528E+10	3.40390E+02	1.00000
9	1.2538E+13	4.63634E+02	0.15182
10	6.2819E+12	4.79305E+00	0.99998
11	9.6122E+12	4.90377E+00	1.00000
12	2.8814E+13	5.04120E+01	1.00000
13	5.9362E+12	5.94914E+01	0.97645
14	4.1623E+11	6.11498E-01	0.84438
15	4.8000E+13	2.50331E-04	0.92717
16	2.0000E+13	4.57137E-03	0.99958
17	6.1016E+12	3.41357E-01	0.99982
18	4.0118E+06	4.09607E-01	1.00000
19	3.2625E+12	4.18585E-01	0.99998
20	1.4796E+12	-7.31149E+00	0.97469
21	2.3145E+12	8.65920E-02	1.00000
22	5.2029E+12	1.94643E-01	0.99992
23	1.3011E+11	1.14396E-01	0.99538
24	4.3049E+12	6.44649E-01	1.00000
25	6.0000E+12	2.86320E-06	0.98571
26	3.3000E+13	1.06818E-05	1.00000
27	5.0000E+12	5.54353E-06	0.99878
28	3.0000E+13	-1.44198E-07	0.93308
29	3.0000E+13	3.40441E-13	0.18854
30	1.0840E+02	6.24103E-08	0.99431
31	7.1735E+12	1.52204E-03	1.00000
32	1.4083E+13	2.98803E-03	1.00000
33	6.9980E+11	5.08423E-04	0.99849
34	3.0053E+11	2.18656E-04	0.99993
35	3.1222E+13	5.08346E-04	1.00000
36	2.0000E+13	2.40882E-09	0.99789
37	6.6605E+11	3.49296E-03	1.00000
38	1.2020E+12	1.36259E-08	1.00000
39	1.0000E+13	3.88617E-07	0.99964
40	5.0000E+13	7.23664E-07	0.85366
41	3.0000E+13	3.62176E-10	0.99999
42	5.3373E+12	-4.43154E-10	0.87306
43	1.0000E+13	6.78932E-12	1.00000
44	2.8000E+13	-4.71936E-03	0.96162
45	2.9245E+12	1.87676E-05	0.95359
46	3.8522E+12	-9.16916E-04	0.98782
47	6.0863E+12	8.27268E-06	0.46331
48	4.0575E+12	7.94950E-06	0.99880
49	2.0000E+13	3.92308E-05	1.00000
50	1.5205E+08	6.88898E-04	0.97461
51	5.0000E+13	1.75971E-09	1.00000
52	1.0531E+12	8.86733E+02	1.00000
53	2.0000E+13	5.44458E-02	1.00000
54	4.5244E+05	1.43520E+00	1.00000
55	2.0583E+13	-8.20509E+01	1.00000
56	7.1441E+12	1.24199E+01	0.99999
57	1.1665E+13	1.35592E+01	1.00000
58	6.0875E+10	8.02643E+01	0.99994
59	1.2011E+13	1.30633E-01	0.99962
60	2.0000E+13	9.77447E+02	1.00000

TABLE D.2.—Continued.

(e) Concluded.

61	6.3306E+03	3.70820E-03	0.99969
62	1.1879E+10	3.81096E-03	0.99904
63	8.9994E+09	1.93227E-03	1.00000
64	1.1879E+10	8.74606E-03	0.99992
65	3.7000E+12	2.48042E-11	0.88017
66	1.0000E+13	5.71294E-06	1.00000
67	2.2518E+12	2.09983E-01	1.00000
68	1.0640E+10	2.14481E-09	1.00000
69	3.1408E+12	2.17081E-06	0.99983
70	1.1776E+13	3.54322E-06	0.99802
71	5.0000E+12	1.07329E-09	0.99992
72	4.0000E+13	8.58696E-09	1.00000
73	3.0000E+13	1.33098E+02	0.99989
74	3.0000E+13	2.87734E-04	1.00000
75	3.0000E+13	9.86753E-04	1.00000
76	2.0000E+13	2.86879E-04	0.99995
77	2.1858E+12	5.72099E+01	0.99998
78	6.6256E+14	1.35873E-03	1.00000
79	7.8698E+05	4.33403E-02	1.00000
80	3.0465E+11	1.24306E-01	0.99948
81	4.2996E+10	1.16503E+00	1.00000
82	2.1314E+11	3.51582E-01	0.97386
83	1.0978E+12	1.43758E+02	0.99994
84	5.6053E+12	1.95506E+00	0.99776
85	3.7349E+13	1.28029E+00	0.53200
86	3.6528E+13	1.57210E+00	0.99895
87	8.0000E+12	1.13456E+00	0.95988
88	9.5769E+13	6.17087E+00	1.00000
89	3.0883E+10	2.45305E+00	0.99826
90	3.8937E+12	-5.39477E-02	0.97971
91	1.8000E+12	1.76372E+01	0.99919
92	7.8000E+11	9.76281E-05	1.00000
93	8.9868E+10	2.01130E+01	0.99999
94	6.9886E+12	7.65984E+00	0.91428
95	1.9984E+15	-3.32238E+01	0.84868
96	6.0163E+00	-1.13822E-04	0.73488
97	4.4292E+15	2.14502E-05	0.99307
98	1.7945E+01	2.16902E-05	0.67666
99	9.1136E-02	2.16023E-05	0.99195
100	2.5679E+08	5.66673E-10	0.99985
101	1.1365E+13	1.48680E-06	0.81714
102	1.0504E+11	1.84693E-07	0.98774
103	1.6608E+11	-5.09767E-04	0.99802
104	1.2000E+13	1.04024E-09	1.00000
105	3.8011E+13	-2.76070E-06	0.99592
106	5.9286E+12	9.88959E-03	0.62446
107	6.9362E+12	5.21894E-02	0.99524
108	2.3378E+13	9.24716E-04	0.98632
109	3.7000E+12	-9.31316E-04	1.00000
110	2.0000E+13	2.89274E-05	1.00000
111	1.0000E+13	1.32473E-10	1.00000
112	2.0000E+13	4.29779E-05	0.99338
113	7.0618E+11	1.35350E-11	0.99990
114	2.0000E+12	3.83195E-11	0.99956
115	1.0685E+13	1.13530E-03	0.99995
116	2.4276E+12	1.60201E+00	0.98681
117	8.2936E+12	1.71995E-02	0.92047
118	8.0889E+15	-6.39344E-01	0.99936
119	2.1873E+14	7.37043E-01	1.00000
120	3.5248E+07	-8.45191E-08	0.35304
121	1.3944E+07	-1.13540E-03	0.99996
122	7.2356E+03	1.59753E-06	0.65265
123	4.0000E+12	8.25412E-08	1.00000
124	9.2424E+06	-1.50490E-04	0.97148
125	1.5129E+10	-1.15446E-05	0.99977
126	1.6196E+10	2.68156E-09	0.94538
127	6.6303E+11	1.31456E-07	0.75694
128	2.6693E+09	1.11070E-02	0.99999
129	9.8902E+15	5.25262E-08	0.00004
130	9.5491E+15	-1.10940E-02	0.87002
131	5.0000E+12	-3.19520E-07	0.68548
132	6.5192E+15	1.34555E-05	0.02727
133	3.6000E+13	1.76069E-06	0.72745

```
DERIVATIVES (CGS UNITS): T          1.94923E+05    RHO          8.54162E-02

MIXTURE MOLECULAR WEIGHT     26.63512     TOTAL ENERGY EXCHANGE RATE   -9.14644E+07      MASS FRACTION SUM    1.00000000
                                                (CAL-CM**3/G**2/SEC)


COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP -  2.699986E-01  S     UP TO THIS TIME -  1.477000E+01  S


          (LSENS)     END OF THIS CASE


                SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

                   TOTAL NO. OF STEPS -                    190
                   TOTAL NO. OF DERIVATIVE EVALUATIONS -   232
                   TOTAL NO. OF JACOBIAN EVALUATIONS -      28
                   TOTAL CPU TIME -                 14.769997 S


                          TOTAL CPU TIME (INCLUDING I/O) REQUIRED =     18.459999 S


          (LSENS)     READ DATA FOR NEXT CASE
```

TABLE D.2.—Continued.

(f) Case 6

DISTANCE-PRESSURE VERSION LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

LSENS METHANE AIR MECHANISM CONSTANT PRESSURE FLOW PROBLEM CASE 6

REACTION NUMBER	REACTION							REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	M	+	1*CH4	=	1*CH3	+	1*H	2.00000E+17	0.0000	88000.00
2	1*H	+	1*CH4	=	1*CH3	+	1*H2	1.26000E+14	0.0000	11900.00
3	1*CH4	+	1*O2	=	1*CH3	+	1*HO2	7.94000E+13	0.0000	56000.00
4	1*O	+	1*CH4	=	1*CH3	+	1*OH	1.90000E+14	0.0000	11720.00
5	1*OH	+	1*CH4	=	1*CH3	+	1*H2O	2.50000E+13	0.0000	5010.00
6	1*CH3	+	1*O2	=	1*CH3O	+	1*O	2.40000E+13	0.0000	28680.00
7	1*CH3	+	1*OH	=	1*CH3O	+	1*H	6.30000E+12	0.0000	0.00
8	M	+	1*CH3O	=	1*CH2O	+	1*H	5.00000E+13	0.0000	21000.00
9			2*CH3	=	1*C2H6			2.40000E+14	-0.4000	0.00
10	1*H	+	1*C2H6	=	1*C2H5	+	1*H2	1.32000E+14	0.0000	9700.00
11	1*O	+	1*C2H6	=	1*C2H5	+	1*OH	1.13000E+14	0.0000	7850.00
12	1*OH	+	1*C2H6	=	1*C2H5	+	1*H2O	8.70000E+13	0.0000	3520.00
13	M	+	1*C2H5	=	1*C2H4	+	1*H	1.00000E+17	0.0000	31000.00
14	1*C2H5	+	1*O2	=	1*C2H4	+	1*HO2	2.00000E+12	0.0000	5000.00
15	1*H	+	1*C2H5	=	1*C2H4	+	1*H2	4.80000E+13	0.0000	0.00
16	1*CH3	+	1*CH2	=	1*C2H4	+	1*H	2.00000E+13	0.0000	0.00
17	1*H	+	1*C2H4	=	1*H2	+	1*C2H3	1.50000E+14	0.0000	10200.00
18	M	+	1*C2H4	=	1*C2H2	+	1*H2	2.60000E+17	0.0000	79300.00
19	1*C2H4	+	1*OH	=	1*C2H3	+	1*H2O	4.80000E+12	0.0000	1230.00
20	1*C2H4	+	1*HO2	=	1*CH3	+	1*CH2O	2.00000E+12	0.0000	960.00
21	1*C2H4	+	1*O	=	1*CH3	+	1*HCO	3.30000E+12	0.0000	1130.00
22	1*C2H4	+	1*O	=	1*CH2O	+	1*CH2	2.50000E+13	0.0000	5000.00
23	M	+	1*C2H3	=	1*C2H2	+	1*H	3.00000E+15	0.0000	32000.00
24	1*C2H3	+	1*O2	=	1*CH2O	+	1*HCO	3.98000E+12	0.0000	-250.00
25	1*C2H3	+	1*H	=	1*C2H2	+	1*H2	6.00000E+12	0.0000	0.00
26	1*C2H3	+	1*O	=	1*C2H2O	+	1*H	3.30000E+13	0.0000	0.00
27	1*C2H3	+	1*OH	=	1*C2H2	+	1*H2O	5.00000E+12	0.0000	0.00
28	1*C2H3	+	1*CH2	=	1*C2H2	+	1*CH3	3.00000E+13	0.0000	0.00
29	1*C2H3	+	1*C2H	=	2*C2H2			3.00000E+13	0.0000	0.00
30	M	+	1*C2H2	=	1*C2H	+	1*H	4.20000E+16	0.0000	107000.00
31	1*C2H2	+	1*O	=	1*CH2	+	1*CO	1.60000E+14	0.0000	9890.00
32	1*C2H2	+	1*O	=	1*C2HO	+	1*H	4.00000E+14	0.0000	10660.00
33	1*C2H2	+	1*OH	=	1*C2H	+	1*H2O	6.30000E+12	0.0000	7000.00
34	1*C2H2	+	1*OH	=	1*C2H2O	+	1*H	3.20000E+11	0.0000	200.00
35	1*C2H	+	1*O2	=	1*C2HO	+	1*O	5.00000E+13	0.0000	1500.00
36	1*C2H	+	1*OH	=	1*C2HO	+	1*H	2.00000E+13	0.0000	0.00
37	1*C2HO	+	1*O2	=	2*CO	+	1*OH	1.46000E+12	0.0000	2500.00
38	1*C2HO	+	1*O	=	2*CO	+	1*H	1.20200E+12	0.0000	0.00
39	1*C2HO	+	1*OH	=	2*HCO			1.00000E+13	0.0000	0.00
40	1*C2HO	+	1*H	=	1*CH2	+	1*CO	5.00000E+13	0.0000	0.00
41	1*C2HO	+	1*CH2	=	1*C2H3	+	1*CO	3.00000E+13	0.0000	0.00
42	1*C2HO	+	1*CH2	=	1*CH2O	+	1*C2H	1.00000E+13	0.0000	2000.00
43			2*C2HO	=	1*C2H2	+	2*CO	1.00000E+13	0.0000	0.00
44	1*C2H2O	+	1*OH	=	1*CH2O	+	1*HCO	2.80000E+13	0.0000	0.00
45	1*C2H2O	+	1*OH	=	1*C2HO	+	1*H2O	7.50000E+12	0.0000	3000.00
46	1*C2H2O	+	1*H	=	1*CH3	+	1*CO	1.13000E+13	0.0000	3428.00
47	1*C2H2O	+	1*H	=	1*C2HO	+	1*H2	7.50000E+13	0.0000	8000.00
48	1*C2H2O	+	1*O	=	1*C2HO	+	1*OH	5.00000E+13	0.0000	8000.00
49	1*C2H2O	+	1*O	=	1*CH2O	+	1*CO	2.00000E+13	0.0000	0.00
50	M	+	1*C2H2O	=	1*CH2	+	1*CO	2.00000E+16	0.0000	60000.00
51	1*C2H	+	1*O	=	1*CO	+	1*CH	5.00000E+13	0.0000	0.00
52	1*CH3O	+	1*O2	=	1*CH2O	+	1*HO2	1.00000E+13	0.0000	7170.00
53	1*CH3O	+	1*H	=	1*CH2O	+	1*H2	2.00000E+13	0.0000	0.00
54	M	+	1*CH2O	=	1*HCO	+	1*H	5.00000E+16	0.0000	81000.00
55	1*CH2O	+	1*OH	=	1*HCO	+	1*H2O	3.00000E+13	0.0000	1200.00
56	1*CH2O	+	1*H	=	1*HCO	+	1*H2	2.50000E+13	0.0000	3990.00
57	1*CH2O	+	1*O	=	1*HCO	+	1*OH	3.50000E+13	0.0000	3510.00
58	1*CH3	+	1*CH2O	=	1*CH4	+	1*HCO	1.00000E+10	0.5000	6000.00
59	1*CH3	+	1*HCO	=	1*CH4	+	1*CO	3.00000E+11	0.5000	0.00
60	1*CH3	+	1*HO2	=	1*CH3O	+	1*OH	2.00000E+13	0.0000	0.00
61	M	+	1*CH3	=	1*CH2	+	1*H	1.95000E+16	0.0000	91600.00
62	1*H	+	1*CH3	=	1*H2	+	1*CH2	2.70000E+11	0.6700	25700.00
63	1*O	+	1*CH3	=	1*OH	+	1*CH2	1.90000E+11	0.6800	25700.00
64	1*OH	+	1*CH3	=	1*H2O	+	1*CH2	2.70000E+11	0.6700	25700.00
65	1*CH	+	1*CO2	=	1*HCO	+	1*CO	3.70000E+12	0.0000	0.00
66	1*CH	+	1*O2	=	1*HCO	+	1*O	1.00000E+13	0.0000	0.00
67	1*CH2	+	1*O2	=	1*CH2O	+	1*O	5.00000E+11	0.5000	6960.00
68	1*CH2	+	1*O	=	1*CH	+	1*OH	2.00000E+11	0.7000	25800.00
69	1*CH2	+	1*OH	=	1*CH	+	1*H2O	5.00000E+11	0.5000	5900.00
70	1*CH2	+	1*H	=	1*CH	+	1*H2	3.20000E+11	0.7000	4970.00
71			2*CH2	=	1*C2H3	+	1*H	5.00000E+12	0.0000	0.00
72			2*CH2	=	1*C2H2	+	1*H2	4.00000E+13	0.0000	0.00
73	1*HCO	+	1*O2	=	1*CO	+	1*HO2	3.00000E+13	0.0000	0.00
74	1*HCO	+	1*O	=	1*CO	+	1*OH	3.00000E+13	0.0000	0.00
75	1*HCO	+	1*OH	=	1*CO	+	1*H2O	3.00000E+13	0.0000	0.00
76	1*HCO	+	1*H	=	1*CO	+	1*H2	2.00000E+13	0.0000	0.00
77	M	+	1*HCO	=	1*H	+	1*CO	2.90000E+14	0.0000	15570.00
78	1*CO	+	1*O	=	1*CO2	+	M	2.40000E+15	0.0000	4100.00
79	1*CO	+	1*O2	=	1*CO2	+	1*O	2.50000E+12	0.0000	47690.00
80	1*CO	+	1*OH	=	1*CO2	+	1*H	4.17000E+11	0.0000	1000.00
81	1*CO	+	1*HO2	=	1*CO2	+	1*OH	5.75000E+13	0.0000	22930.00
82	1*O	+	1*H2O	=	2*OH			6.80000E+13	0.0000	18365.00
83	1*H	+	1*O2	=	1*OH	+	1*O	1.89000E+14	0.0000	16400.00
84	1*O	+	1*H2	=	1*OH	+	1*H	4.20000E+14	0.0000	13750.00
85	1*H	+	1*HO2	=	1*H2	+	1*O2	7.28000E+13	0.0000	2126.00
86	1*O	+	1*HO2	=	1*OH	+	1*O2	5.00000E+13	0.0000	1000.00
87	1*HO2	+	1*OH	=	1*H2O	+	1*O2	8.00000E+12	0.0000	0.00
88	1*H	+	1*HO2	=	2*OH			1.34000E+14	0.0000	1070.00
89	1*H2	+	1*HO2	=	1*H2O2	+	1*H	7.91000E+13	0.0000	25000.00
90	1*OH	+	1*H2O2	=	1*H2O	+	1*HO2	6.10000E+12	0.0000	1430.00
91			2*HO2	=	1*H2O2	+	1*O2	1.80000E+12	0.0000	0.00
92	1*H	+	1*H2O2	=	1*OH	+	1*H2O	7.80000E+11	0.0000	0.00
93	M	+	1*H2O2	=	2*OH			1.44000E+17	0.0000	45510.00
94	1*H2	+	1*OH	=	1*H2O	+	1*H	4.74000E+13	0.0000	6098.00
95	1*H	+	1*O2	=	1*HO2	+	M	1.46000E+15	0.0000	-1000.00
96	M	+	1*H2O	=	1*H	+	1*OH	1.30000E+15	0.0000	105140.00
97	1*H	+	1*O	=	1*OH	+	M	7.10000E+18	-1.0000	0.00
98	M	+	1*H2	=	2*H			2.20000E+14	0.0000	96000.00
99	M	+	1*O2	=	2*O			1.80000E+18	-1.0000	118020.00
100	1*CH	+	1*N2	=	1*HCN	+	1*N	1.00000E+11	0.0000	19000.00
101	1*CN	+	1*H2	=	1*HCN	+	1*H	6.00000E+13	0.0000	5300.00
102	1*O	+	1*HCN	=	1*OH	+	1*CN	1.40000E+11	0.6800	16900.00

TABLE D.2.—Continued.

(f) Continued.

103	1*OH	+	1*HCN	=	1*HNCO	+	1*H	4.00000E+11	0.0000	2800.00
104	1*CN	+	1*O	=	1*CO	+	1*N	1.20000E+13	0.0000	0.00
105	1*CN	+	1*OH	=	1*NCO	+	1*H	2.50000E+14	0.0000	6000.00
106	1*H2	+	1*NCO	=	1*HNCO	+	1*H	1.00000E+14	0.0000	9000.00
107	1*HNCO	+	1*H	=	1*NH2	+	1*CO	1.00000E+14	0.0000	8500.00
108	1*CN	+	1*O2	=	1*NCO	+	1*O	3.20000E+13	0.0000	1000.00
109	1*CN	+	1*CO2	=	1*NCO	+	1*CO	3.70000E+12	0.0000	0.00
110	1*O	+	1*NCO	=	1*NO	+	1*CO	2.00000E+13	0.0000	0.00
111	1*N	+	1*NCO	=	1*N2	+	1*CO	1.00000E+13	0.0000	0.00
112	1*H	+	1*NCO	=	1*NH	+	1*CO	2.00000E+13	0.0000	0.00
113	1*CH	+	1*NO	=	1*N	+	1*HCO	1.60000E+13	0.0000	9940.00
114	1*CH	+	1*NO	=	1*O	+	1*HCN	2.00000E+12	0.0000	0.00
115	1*NH	+	1*OH	=	1*N	+	1*H2O	5.00000E+11	0.5000	2000.00
116	1*HO2	+	1*NO	=	1*NO2	+	1*OH	2.09000E+12	0.0000	-477.00
117	1*O	+	1*NO2	=	1*NO	+	1*O2	1.00000E+13	0.0000	596.00
118	1*NO	+	1*O	=	1*NO2	+	M	5.62000E+15	0.0000	-1160.00
119	1*NO2	+	1*H	=	1*NO	+	1*OH	3.47000E+14	0.0000	1470.00
120	1*NO	+	1*H	=	1*N	+	1*OH	2.63000E+14	0.0000	50410.00
121	1*NO	+	1*O	=	1*N	+	1*O2	3.80000E+09	1.0000	41370.00
122	1*O	+	1*N2	=	1*NO	+	1*N	1.80000E+14	0.0000	76250.00
123	1*N	+	1*NO2	=	2*NO			4.00000E+12	0.0000	0.00
124	M	+	1*N2O	=	1*N2	+	1*O	6.92000E+23	-2.5000	65000.00
125	1*O	+	1*N2O	=	1*N2	+	1*O2	1.00000E+14	0.0000	28020.00
126	1*O	+	1*N2O	=	2*NO			6.92000E+13	0.0000	26630.00
127	1*N2O	+	1*H	=	1*N2	+	1*OH	7.59000E+13	0.0000	15100.00
128	1*NO2	+	1*H2	=	1*HNO2	+	1*H	2.40000E+13	0.0000	29000.00
129	1*OH	+	1*NO2	=	1*HNO3	+	M	3.00000E+15	0.0000	-3800.00
130	1*OH	+	1*NO	=	1*HNO2	+	M	5.60000E+15	0.0000	-1700.00
131	1*HNO	+	1*H	=	1*H2	+	1*NO	5.00000E+12	0.0000	0.00
132	1*H	+	1*NO	=	1*HNO	+	M	5.40000E+15	0.0000	-600.00
133	1*HNO	+	1*OH	=	1*H2O	+	1*NO	3.60000E+13	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2 , 93) =	2.30000	M(O2 , 93) =	0.78000	M(H2O , 93) =	6.00000	M(H2O2 , 93) =	6.60000
M(O2 , 95) =	1.30000	M(N2 , 95) =	1.30000	M(H2O , 95) =	21.30000	M(CO2 , 95) =	7.00000
M(H2 , 96) =	4.00000	M(O2 , 96) =	1.50000	M(H2O , 96) =	20.00000	M(N2 , 96) =	1.50000
M(CO2 , 96) =	4.00000	M(H2 , 98) =	4.10000	M(O2 , 98) =	2.00000	M(H2O , 98) =	15.00000
M(N2 , 98) =	2.00000	M(O2 ,129) =	0.70000	M(H2 ,129) =	1.40000		

** EQUILIBRIUM CALCULATION **

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED ENTHALPY AND PRESSURE

	INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE (ATM)	1.7300	1.7300	1.0000
VELOCITY (CM/SEC)	0.00	0.00	1.0000
DENSITY (G/CM**3)	3.49869E-04	2.30793E-04	0.6597
TEMPERATURE (DEG K)	1700.00	2553.11	1.5018
ENTHALPY (CAL/G)	379.22696	379.22711	1.00000
INTERNAL ENERGY (CAL/G)	259.48010	197.69731	0.76190
SP. HEAT (CP) (CAL/G/DEG K)	0.32691	0.54085	1.65441
ENTROPY (CAL/G/DEG K)	2.1420	2.3097	1.0783
MACH NUMBER	0.0000	0.0000	1.0000
GAMMA	1.2746	1.1514	0.9033
SONIC VELOCITY (CM/SEC)	79913.95	94814.24	1.1865

SPECIES	MOLE FRACTION
CH4	2.79483E-10
CH3	2.79483E-10
H	1.00214E-03
H2	1.76022E-03
O2	8.94256E-02
HO2	1.55944E-05
O	4.23158E-03
OH	1.15976E-02
H2O	9.05405E-02
CH3O	2.79483E-10
CH2O	2.79483E-10
C2H6	2.79483E-10
C2H5	2.79483E-10
C2H4	2.79483E-10
CH2	2.79483E-10
C2H3	2.79483E-10
C2H2	2.79483E-10
HCO	2.79483E-10
C2H2O	2.79483E-10
C2H	2.79483E-10
CO	5.35472E-03
C2HO	2.79483E-10
CH	2.79483E-10
CO2	4.39498E-02
H2O2	2.72872E-07
N2	7.36205E-01
HCN	2.79483E-10

TABLE D.2.—Continued.
(f) Continued.

N	3.06077E-07
CN	2.79483E-10
HNCO	2.79483E-10
NCO	2.79483E-10
NH2	2.79483E-10
NO	1.59036E-02
NH	4.66032E-08
NO2	1.16681E-05
N2O	1.13359E-06
HNO2	2.41994E-07
HNO3	2.79483E-10
HNO	3.58947E-07

MIXTURE MOLECULAR WEIGHT	27.94827
D(LOG VOLUME)/D(LOG T) AT CONSTANT P	1.0999
D(LOG VOLUME)/D(LOG P) AT CONSTANT T	-1.0039

COMPUTATIONAL WORK REQUIRED FOR EQUILIBRIUM CALCULATION:
NO. OF ITERATIONS = 15 CPU TIME = 7.999992E-02 S

** INITIAL CONDITIONS **

TIME 0.00000E+00 SEC AREA 1.00000E+03 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.73000
VELOCITY (CM/SEC)	159827.88
DENSITY (G/CM**3)	3.49869E-04
TEMPERATURE (DEG K)	1700.00
MASS FLOW RATE (G/SEC)	5.59188E+04
ENTROPY (CAL/G/DEG K)	2.1420
MACH NUMBER	2.0000
GAMMA	1.2746
ENTHALPY (CAL/G)	3.79227E+02
SP. HEAT (CP) (CAL/G/DEG K)	3.26913E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
CH4	6.17216E-07	4.97680E-02	-1.50903E-05	1	9.7244E+05	6.37423E+06	1.00000
CH3	0.00000E+00	0.00000E+00	1.50903E-05	2	3.7198E+12	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	7.44369E-06	3	5.0180E+06	3.32443E+06	1.00000
H2	0.00000E+00	0.00000E+00	0.00000E+00	4	5.9162E+12	0.00000E+00	0.00000
O2	2.46886E-06	1.99072E-01	-8.05210E-05	5	5.6736E+12	0.00000E+00	0.00000
HO2	0.00000E+00	0.00000E+00	7.64658E-06	6	4.9334E+09	0.00000E+00	0.00000
O	0.00000E+00	0.00000E+00	7.28745E-05	7	6.3000E+12	0.00000E+00	0.00000
OH	0.00000E+00	0.00000E+00	0.00000E+00	8	9.9825E+10	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	0.00000E+00	9	1.2247E+13	0.00000E+00	0.00000
CH3O	0.00000E+00	0.00000E+00	0.00000E+00	10	7.4740E+12	0.00000E+00	0.00000
CH2O	0.00000E+00	0.00000E+00	0.00000E+00	11	1.1064E+13	0.00000E+00	0.00000
C2H6	0.00000E+00	0.00000E+00	0.00000E+00	12	3.0690E+13	0.00000E+00	0.00000
C2H5	0.00000E+00	0.00000E+00	0.00000E+00	13	1.0344E+13	0.00000E+00	0.00000
C2H4	0.00000E+00	0.00000E+00	0.00000E+00	14	4.5524E+11	0.00000E+00	0.00000
CH2	0.00000E+00	0.00000E+00	0.00000E+00	15	4.8000E+13	0.00000E+00	0.00000
C2H3	0.00000E+00	0.00000E+00	0.00000E+00	16	2.0000E+13	0.00000E+00	0.00000
C2H2	0.00000E+00	0.00000E+00	0.00000E+00	17	7.3247E+12	0.00000E+00	0.00000
HCO	0.00000E+00	0.00000E+00	0.00000E+00	18	1.6606E+07	0.00000E+00	0.00000
C2H2O	0.00000E+00	0.00000E+00	0.00000E+00	19	3.3351E+12	0.00000E+00	0.00000
C2H	0.00000E+00	0.00000E+00	0.00000E+00	20	1.5053E+12	0.00000E+00	0.00000
CO	0.00000E+00	0.00000E+00	0.00000E+00	21	2.3618E+12	0.00000E+00	0.00000
C2HO	0.00000E+00	0.00000E+00	0.00000E+00	22	5.6904E+12	0.00000E+00	0.00000
CH	0.00000E+00	0.00000E+00	0.00000E+00	23	2.3080E+11	0.00000E+00	0.00000
CO2	0.00000E+00	0.00000E+00	0.00000E+00	24	4.2857E+12	0.00000E+00	0.00000
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	25	6.0000E+12	0.00000E+00	0.00000

TABLE D.2.—Continued.

(f) Continued.

N2	9.31578E-06	7.51160E-01	-1.20855E-11
HCN	0.00000E+00	0.00000E+00	0.00000E+00
N	0.00000E+00	0.00000E+00	0.00000E+00
CN	1.24019E-12	1.00000E-07	-7.28744E-05
HNCO	0.00000E+00	0.00000E+00	0.00000E+00
NCO	0.00000E+00	0.00000E+00	7.28744E-05
NH2	0.00000E+00	0.00000E+00	0.00000E+00
NO	0.00000E+00	0.00000E+00	0.00000E+00
NH	0.00000E+00	0.00000E+00	0.00000E+00
NO2	0.00000E+00	0.00000E+00	0.00000E+00
N2O	0.00000E+00	0.00000E+00	1.20855E-11
HNO2	0.00000E+00	0.00000E+00	0.00000E+00
HNO3	0.00000E+00	0.00000E+00	0.00000E+00
HNO	0.00000E+00	0.00000E+00	0.00000E+00

26	3.3000E+13	0.00000E+00	0.00000
27	5.0000E+12	0.00000E+00	0.00000
28	3.0000E+13	0.00000E+00	0.00000
29	3.0000E+13	0.00000E+00	0.00000
30	7.3700E+02	0.00000E+00	0.00000
31	8.5640E+12	0.00000E+00	0.00000
32	1.7046E+13	0.00000E+00	0.00000
33	7.9329E+11	0.00000E+00	0.00000
34	3.0160E+13	0.00000E+00	0.00000
35	3.2072E+13	0.00000E+00	0.00000
36	2.0000E+13	0.00000E+00	0.00000
37	6.9656E+11	0.00000E+00	0.00000
38	1.2020E+12	0.00000E+00	0.00000
39	1.0000E+13	0.00000E+00	0.00000
40	5.0000E+13	0.00000E+00	0.00000
41	3.0000E+13	0.00000E+00	0.00000
42	5.5320E+12	0.00000E+00	0.00000
43	1.0000E+13	0.00000E+00	0.00000
44	2.8000E+13	0.00000E+00	0.00000
45	3.0859E+12	0.00000E+00	0.00000
46	4.0962E+12	0.00000E+00	0.00000
47	7.0241E+12	0.00000E+00	0.00000
48	4.6827E+12	0.00000E+00	0.00000
49	2.0000E+13	0.00000E+00	0.00000
50	3.8682E+08	0.00000E+00	0.00000
51	5.0000E+13	0.00000E+00	0.00000
52	1.1974E+12	0.00000E+00	0.00000
53	2.0000E+13	0.00000E+00	0.00000
54	1.9307E+06	0.00000E+00	0.00000
55	2.1031E+13	0.00000E+00	0.00000
56	7.6735E+12	0.00000E+00	0.00000
57	1.2383E+13	0.00000E+00	0.00000
58	6.9803E+10	0.00000E+00	0.00000
59	1.2369E+13	0.00000E+00	0.00000
60	2.0000E+13	0.00000E+00	0.00000
61	3.2663E+04	0.00000E+00	0.00000
62	1.9580E+10	0.00000E+00	0.00000
63	1.4842E+10	0.00000E+00	0.00000
64	1.9580E+10	0.00000E+00	0.00000
65	3.7000E+12	0.00000E+00	0.00000
66	1.0000E+13	0.00000E+00	0.00000
67	2.6268E+12	0.00000E+00	0.00000
68	1.7601E+10	0.00000E+00	0.00000
69	3.5950E+12	0.00000E+00	0.00000
70	1.3413E+13	0.00000E+00	0.00000
71	5.0000E+12	0.00000E+00	0.00000
72	4.0000E+13	0.00000E+00	0.00000
73	3.0000E+13	0.00000E+00	0.00000
74	3.0000E+13	0.00000E+00	0.00000
75	3.0000E+13	0.00000E+00	0.00000
76	2.0000E+13	0.00000E+00	0.00000
77	2.8889E+12	0.00000E+00	0.00000
78	7.1305E+14	0.00000E+00	0.00000
79	1.8492E+06	0.00000E+00	0.00000
80	3.1015E+11	0.00000E+00	0.00000
81	6.4836E+10	0.00000E+00	0.00000
82	2.9616E+11	0.00000E+00	0.00000
83	1.4726E+12	0.00000E+00	0.00000
84	7.1708E+12	0.00000E+00	0.00000
85	3.8799E+13	0.00000E+00	0.00000
86	3.7189E+13	0.00000E+00	0.00000
87	8.0000E+12	0.00000E+00	0.00000
88	9.7622E+13	0.00000E+00	0.00000
89	4.8329E+10	0.00000E+00	0.00000
90	3.9948E+12	0.00000E+00	0.00000
91	1.8000E+12	0.00000E+00	0.00000
92	7.8000E+11	0.00000E+00	0.00000
93	2.0307E+11	0.00000E+00	0.00000
94	7.7952E+12	0.00000E+00	0.00000
95	1.9630E+15	0.00000E+00	0.00000
96	3.9562E+01	0.00000E+00	0.00000
97	4.1765E+15	0.00000E+00	0.00000
98	1.0018E+02	0.00000E+00	0.00000
99	7.1175E-01	2.12050E+01	1.00000
100	3.6090E+08	0.00000E+00	0.00000
101	1.2497E+13	0.00000E+00	0.00000
102	1.4798E+11	0.00000E+00	0.00000
103	1.7462E+11	0.00000E+00	0.00000
104	1.2000E+13	0.00000E+00	0.00000
105	4.2324E+13	0.00000E+00	0.00000
106	6.9658E+12	0.00000E+00	0.00000
107	8.0770E+12	0.00000E+00	0.00000
108	2.3801E+13	-3.77764E+06	1.00000
109	3.7000E+12	0.00000E+00	0.00000
110	2.0000E+13	0.00000E+00	0.00000
111	1.0000E+13	0.00000E+00	0.00000
112	2.0000E+13	0.00000E+00	0.00000
113	8.4381E+11	0.00000E+00	0.00000
114	2.0000E+12	0.00000E+00	0.00000
115	1.1405E+13	0.00000E+00	0.00000
116	2.4070E+12	0.00000E+00	0.00000
117	8.3826E+12	0.00000E+00	0.00000
118	7.9225E+15	0.00000E+00	0.00000
119	2.2457E+14	0.00000E+00	0.00000
120	8.6958E+07	0.00000E+00	0.00000
121	3.1028E+07	0.00000E+00	0.00000
122	2.8358E+04	0.00000E+00	0.00000
123	4.0000E+12	0.00000E+00	0.00000
124	2.5566E+07	0.00000E+00	0.00000
125	2.4991E+10	7.80528E+00	1.00000
126	2.6097E+10	0.00000E+00	0.00000
127	8.6897E+11	0.00000E+00	0.00000
128	4.4875E+09	0.00000E+00	0.00000
129	9.2394E+15	0.00000E+00	0.00000
130	9.2627E+15	0.00000E+00	0.00000
131	5.0000E+12	0.00000E+00	0.00000
132	6.4495E+15	0.00000E+00	0.00000
133	3.6000E+13	0.00000E+00	0.00000

DERIVATIVES (CGS UNITS): T -5.12217E-02 RHO 9.22781E-09 V 0.00000E+00

MIXTURE MOLECULAR WEIGHT 28.21102 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 5.92105E+06 MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 2.340000 S

TABLE D.2.—Continued.

(f) Continued.

TIME 2.94066E-04 SEC AREA 1.43983E+03 SQ CM AXIAL POSITION 4.70000E+01 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.73000
VELOCITY (CM/SEC)	159827.88
DENSITY (G/CM**3)	2.42993E-04
TEMPERATURE (DEG K)	2389.90
MASS FLOW RATE (G/SEC)	5.59188E+04
ENTROPY (CAL/G/DEG K)	2.3063
MACH NUMBER	1.6673
GAMMA	1.2738
ENTHALPY (CAL/G)	3.79227E+02
SP. HEAT (CP) (CAL/G/DEG K)	3.35630E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	4
AVERAGE STEP SIZE	0.26316E+00
METHOD ORDER	3
TOTAL NUMBER OF STEPS	187
FUNCT EVALUATIONS	284
JACOBIAN EVALUATIONS	36

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	5.73493E-11	6.50081E-06	-5.57743E-06
CH3	1.12913E-09	1.27992E-04	-1.14166E-04
H	4.22012E-08	4.78370E-03	-5.23454E-04
H2	3.80903E-08	4.31771E-03	-2.30715E-04
O2	8.62787E-07	9.78009E-02	-1.05454E-03
HO2	1.73505E-10	1.96676E-05	-5.68861E-07
O	1.08953E-07	1.23503E-02	-8.58925E-04
OH	1.48846E-07	1.68724E-02	-1.29853E-04
H2O	7.21783E-07	8.18173E-02	7.43665E-04
CH3O	6.20209E-12	7.03035E-07	-5.27733E-07
CH2O	1.76259E-11	1.99798E-06	-1.53116E-06
C2H6	7.14414E-14	8.09821E-09	6.99064E-08
C2H5	5.84465E-16	6.62517E-11	2.64853E-09
C2H4	3.33358E-13	3.77876E-08	-7.66669E-08
CH2	1.01723E-11	1.15308E-06	-9.92644E-07
C2H3	1.09283E-14	1.23877E-09	-1.52066E-09
C2H2	5.96399E-14	6.76045E-09	-1.78284E-08
HCO	1.07672E-12	1.22051E-07	-9.31583E-08
C2H2O	1.72493E-14	1.95529E-09	-2.85693E-09
C2H	3.48576E-16	3.95126E-11	-1.06144E-10
CO	1.31702E-07	1.49291E-02	-2.08396E-03
C2HO	7.64025E-14	8.66057E-09	-2.00198E-08
CH	2.13301E-12	2.41787E-07	-2.17147E-07
CO2	2.95745E-07	3.35241E-02	2.20719E-03
H2O2	9.95871E-12	1.12886E-06	-1.64267E-07
N2	6.46972E-06	7.33373E-01	-1.37072E-05
HCN	3.49320E-13	3.95970E-08	-2.72924E-08
N	1.05796E-12	1.19924E-07	1.50385E-08
CN	2.25860E-15	2.56023E-10	-1.71786E-10
HNCO	5.03698E-14	5.70965E-09	-1.34140E-09
NCO	1.49889E-14	1.69906E-09	-9.42490E-10
NH2	2.28458E-12	2.58967E-07	9.42576E-09
NO	6.27721E-10	7.11550E-05	2.73613E-05
NH	6.72476E-14	7.62282E-09	1.25351E-09
NO2	4.16756E-13	4.72411E-08	1.92319E-08
N2O	6.52489E-12	7.39626E-07	1.75917E-08
HNO2	2.64396E-14	2.99705E-09	7.54600E-10
HNO3	3.08559E-18	3.49766E-13	9.69517E-14
HNO	8.95348E-14	1.01492E-08	1.93741E-09

REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	1.7933E+09	-5.21884E+07	0.97006
2	1.0284E+13	4.49564E+04	0.17311
3	6.0086E+08	-7.63059E+04	0.74010
4	1.6106E+13	7.44685E+05	0.17599
5	8.7054E+12	-3.18369E+06	0.17575
6	5.7214E+10	1.16487E+06	0.04310
7	6.3000E+12	8.81381E+06	0.04144
8	6.0059E+11	1.14117E+07	1.00000
9	1.0687E+13	-1.11000E+06	0.05364
10	1.7121E+13	-5.38423E+03	0.99996
11	2.1638E+13	-1.22440E+04	0.99996
12	4.1460E+13	-1.58056E+05	0.99996
13	1.4626E+14	4.30442E+05	0.87082
14	6.9790E+11	-7.57558E+01	0.98512
15	4.8000E+13	-1.30923E+03	0.99680
16	2.0000E+13	-2.43183E+05	0.99901
17	1.7512E+13	-1.02700E+04	0.99919
18	1.4561E+10	3.02366E+04	1.00000
19	3.7048E+12	-5.43564E+04	0.99920
20	1.6340E+12	-2.00195E+04	0.99198
21	2.6012E+12	-4.29343E+04	1.00000
22	8.7238E+12	-3.97272E+04	0.99997
23	3.5547E+12	2.55864E+05	0.99838
24	4.1951E+12	-5.32165E+04	1.00000
25	6.0000E+12	-2.81409E+03	0.99996
26	3.3000E+13	-5.38937E+04	1.00000
27	5.0000E+12	-1.03387E+04	0.99996
28	3.0000E+13	-3.66434E+00	0.99083
29	3.0000E+13	-1.60559E-04	0.99921
30	6.8926E+06	-8.11258E+00	0.50947
31	1.9939E+13	-1.04814E+05	0.99911
32	4.2387E+13	-1.07208E+05	0.99317
33	1.4428E+12	1.64036E+03	0.94969
34	3.0680E+11	-1.03891E+03	0.98766
35	3.6459E+13	-5.01001E+03	0.86440
36	2.0000E+13	-7.28677E+02	0.86416
37	8.6245E+11	-7.89664E+04	1.00000
38	1.2020E+12	-1.67395E+04	1.00000
39	1.0000E+13	-5.20369E+04	1.00000
40	5.0000E+13	-5.85659E+04	0.86955
41	3.0000E+13	-3.75628E+01	0.99998
42	6.5630E+12	-2.52975E+00	0.99994
43	1.0000E+13	-7.47799E-02	1.00000
44	2.8000E+13	-1.85277E+04	0.99986
45	3.9877E+12	-1.33179E+03	0.44621
46	5.4903E+12	3.41117E+04	0.93977
47	1.3915E+13	-1.67974E+02	0.44444
48	9.2767E+12	-4.43695E+01	0.44637
49	2.0000E+13	-6.51035E+04	1.00000
50	6.5191E+10	-2.50437E+04	0.65841
51	5.0000E+13	-2.35233E+03	0.99877
52	2.2096E+12	-6.22748E+06	1.00000
53	2.0000E+13	-7.42049E+06	1.00000
54	1.9577E+09	4.61331E+05	0.99203
55	2.3302E+13	-3.00312E+07	0.99980
56	1.0791E+13	-1.90304E+06	0.99980
57	1.6714E+13	-6.59553E+06	0.99980
58	1.3820E+11	-6.80754E+02	0.99976
59	1.4666E+13	-2.69003E+04	0.99494
60	2.0000E+13	-1.16626E+06	0.79507
61	8.1933E+07	1.24817E+06	0.82368
62	2.2115E+11	9.64434E+05	0.99563
63	1.6821E+11	2.54523E+06	0.99565
64	2.2115E+11	-6.00556E+06	0.99565
65	3.7000E+12	-2.52867E+06	1.00000
66	1.0000E+13	-2.24556E+07	1.00000
67	5.6453E+12	-5.07638E+07	0.99999
68	2.0256E+11	-2.07294E+03	0.93058
69	7.0570E+12	-2.94060E+06	0.93056
70	2.6033E+13	-4.31821E+05	0.93034
71	5.0000E+12	-6.17280E+02	0.99982
72	4.0000E+13	-9.14860E+03	1.00000
73	3.0000E+13	-1.68075E+07	0.98053
74	3.0000E+13	-5.16700E+06	0.99583
75	3.0000E+13	-8.42740E+06	0.99583
76	2.0000E+13	-1.36283E+06	0.99582
77	1.0929E+13	2.23351E+07	0.83103
78	1.0122E+15	-2.71328E+08	0.98304
79	1.0885E+08	-5.31123E+05	0.31387
80	3.3782E+11	-8.71384E+08	0.31268
81	4.6002E+11	-8.93220E+06	0.85306
82	1.4226E+12	9.64819E+06	0.00030
83	5.9803E+12	1.07360E+08	0.00174
84	2.3219E+13	1.06120E+07	0.00348
85	4.6528E+13	-2.38281E+08	0.78509
86	4.0506E+13	-5.17051E+08	0.78584
87	8.0000E+12	-1.85899E+08	0.78578

TABLE D.2.—Continued.
(f) Concluded.

88	1.0697E+14	-3.54242E+08	0.78621
89	4.0925E+11	-6.49419E+06	0.88170
90	4.5140E+12	-3.40183E+06	0.88207
91	1.8000E+12	2.51645E+04	0.44952
92	7.8000E+11	-3.68001E+05	0.97479
93	9.9219E+12	-2.27774E+07	0.02117
94	1.3126E+13	-6.02175E+07	0.00318
95	1.8022E+15	-1.39278E+09	0.88480
96	3.1562E+05	-4.94529E+08	0.97532
97	2.9708E+15	-2.03708E+08	0.97533
98	3.6600E+05	-2.55654E+07	0.97524
99	1.2142E+04	-7.35703E+06	0.97529
100	1.8302E+09	1.40111E+03	1.00000
101	1.9655E+13	5.62600E+03	0.90930
102	7.9062E+11	9.94915E+03	0.90961
103	2.2182E+11	-2.55132E+03	0.94545
104	1.2000E+13	-3.84964E+03	0.99974
105	7.0673E+13	-5.09117E+03	0.54738
106	1.5031E+13	4.91817E+02	0.24735
107	1.6699E+13	-1.40636E+03	0.26554
108	2.5924E+13	-2.97597E+03	0.54817
109	3.7000E+12	2.47680E+01	0.34147
110	2.0000E+13	-5.65642E+04	0.99999
111	1.0000E+13	-4.73399E-01	0.99312
112	2.0000E+13	-7.62823E+03	0.99938
113	1.9730E+12	-1.80925E+03	1.00000
114	2.0000E+12	-3.26283E+03	0.99980
115	1.6042E+13	-6.77672E+03	0.07093
116	2.3108E+12	-2.15031E+02	0.01046
117	8.8206E+12	-2.44031E+05	0.78358
118	7.1749E+15	-4.75353E+06	0.88581
119	2.5463E+14	-1.73284E+06	0.78395
120	6.4580E+09	-6.92211E+06	0.98015
121	1.4962E+09	-2.71002E+06	0.98019
122	1.9161E+07	1.71804E+07	0.99833
123	4.0000E+12	-2.30557E+00	0.99571
124	2.8189E+09	-7.21704E+05	0.86767
125	2.7393E+11	-2.12044E+05	0.81324
126	2.5402E+11	-1.08361E+05	0.99999
127	3.1578E+12	-7.46260E+05	0.81357
128	5.3486E+10	-2.79425E+03	0.88529
129	6.6776E+15	-8.12716E-02	0.00003
130	8.0103E+15	-6.17291E+03	0.00111
131	5.0000E+12	-1.68412E+04	0.96268
132	6.1272E+15	-4.04360E+05	0.33665
133	3.6000E+13	-5.45158E+05	0.96280

```
DERIVATIVES (CGS UNITS): T          2.14117E+01    RHO        -1.82533E-06    V          0.00000E+00

MIXTURE MOLECULAR WEIGHT     27.54436     TOTAL ENERGY EXCHANGE RATE   -4.71681E+09      MASS FRACTION SUM    1.00000003
                                                (CAL-CM**3/G**2/SEC)


COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP -  3.800011E-01  S     UP TO THIS TIME -  1.247001E+01  S


(LSENS)     END OF THIS CASE


                SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

                   TOTAL NO. OF STEPS -                    190
                   TOTAL NO. OF DERIVATIVE EVALUATIONS -   289
                   TOTAL NO. OF JACOBIAN EVALUATIONS -      37
                   TOTAL CPU TIME -                 12.710009 S


                                TOTAL CPU TIME (INCLUDING I/O) REQUIRED =     21.950001 S


(LSENS)     READ DATA FOR NEXT CASE


                                  **  DATA LINES  **
              1         2         3         4         5         6         7         8
CC  12345678901234567890123456789012345678901234567890123456789012345678901234567890

     LSENS   METHANE - AIR WITH AREA PROFILE OF CASE 6                        CASE 7
    REPEAT
    DISTANCE  AREA
     &prob  pcon=.false., combus=.false.,
       xtb=0.0,10.0,20.0,25.0,30.0,32.0,34.0,36.0,37.0,38.0,39.0,40.0,41.0,
        42.0,43.0,44.0,45.0,46.0,47.0,48.0,
       atb= 1000.00,1000.20,1004.65,1010.85,1023.22,1031.44,1042.92,1059.73,
        1071.45,1087.06,1110.03,1153.75,1284.24,1350.79,1376.81,1397.15,
        1414.00,1428.05,1439.83,1449.81,
       aprint=1023.22,1153.75,1439.83,  &end
     &start  t=1700.0, mach=2.0, p=1.730,  &end
    CH4          0.049768
    O2           0.199072
    N2           0.75116
    CN           0.0000001
    END
     &solver  emax=5.0E-5, atolsp=1.0E-13,  &end
    FINIS
```

TABLE D.2.—Continued.

(g) Case 7

** INITIAL CONDITIONS **

TIME 0.00000E+00 SEC AREA 1.00000E+03 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.73000
VELOCITY (CM/SEC)	159827.88
DENSITY (G/CM**3)	3.49869E-04
TEMPERATURE (DEG K)	1700.00
MASS FLOW RATE (G/SEC)	5.59188E+04
ENTROPY (CAL/G/DEG K)	2.1420
MACH NUMBER	2.0000
GAMMA	1.2746
ENTHALPY (CAL/G)	3.79227E+02
SP. HEAT (CP) (CAL/G/DEG K)	3.26913E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	6.17216E-07	4.97680E-02	-1.50903E-05
CH3	0.00000E+00	0.00000E+00	1.50903E-05
H	0.00000E+00	0.00000E+00	7.44369E-06
H2	0.00000E+00	0.00000E+00	0.00000E+00
O2	2.46886E-06	1.99072E-01	-8.05210E-05
HO2	0.00000E+00	0.00000E+00	7.64658E-06
O	0.00000E+00	0.00000E+00	7.28745E-05
OH	0.00000E+00	0.00000E+00	0.00000E+00
H2O	0.00000E+00	0.00000E+00	0.00000E+00
CH3O	0.00000E+00	0.00000E+00	0.00000E+00
CH2O	0.00000E+00	0.00000E+00	0.00000E+00
C2H6	0.00000E+00	0.00000E+00	0.00000E+00
C2H5	0.00000E+00	0.00000E+00	0.00000E+00
C2H4	0.00000E+00	0.00000E+00	0.00000E+00
CH2	0.00000E+00	0.00000E+00	0.00000E+00
C2H3	0.00000E+00	0.00000E+00	0.00000E+00
C2H2	0.00000E+00	0.00000E+00	0.00000E+00
HCO	0.00000E+00	0.00000E+00	0.00000E+00
C2H2O	0.00000E+00	0.00000E+00	0.00000E+00
C2H	0.00000E+00	0.00000E+00	0.00000E+00
CO	0.00000E+00	0.00000E+00	0.00000E+00
C2HO	0.00000E+00	0.00000E+00	0.00000E+00
CH	0.00000E+00	0.00000E+00	0.00000E+00
CO2	0.00000E+00	0.00000E+00	0.00000E+00
H2O2	0.00000E+00	0.00000E+00	0.00000E+00
N2	9.31578E-06	7.51160E-01	-1.20855E-11
HCN	0.00000E+00	0.00000E+00	0.00000E+00
N	0.00000E+00	0.00000E+00	0.00000E+00
CN	1.24019E-12	1.00000E-07	-7.28744E-05
HNCO	0.00000E+00	0.00000E+00	0.00000E+00
NCO	0.00000E+00	0.00000E+00	7.28744E-05
NH2	0.00000E+00	0.00000E+00	0.00000E+00
NO	0.00000E+00	0.00000E+00	0.00000E+00
NH	0.00000E+00	0.00000E+00	0.00000E+00
NO2	0.00000E+00	0.00000E+00	0.00000E+00
N2O	0.00000E+00	0.00000E+00	1.20855E-11
HNO2	0.00000E+00	0.00000E+00	0.00000E+00
HNO3	0.00000E+00	0.00000E+00	0.00000E+00
HNO	0.00000E+00	0.00000E+00	0.00000E+00

REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	9.7244E+05	6.37423E+06	1.00000
2	3.7198E+12	0.00000E+00	0.00000
3	5.0180E+06	3.32443E+06	1.00000
4	5.9162E+12	0.00000E+00	0.00000
5	5.6736E+12	0.00000E+00	0.00000
6	4.9334E+09	0.00000E+00	0.00000
7	6.3000E+12	0.00000E+00	0.00000
8	9.9825E+10	0.00000E+00	0.00000
9	1.2247E+13	0.00000E+00	0.00000
10	7.4740E+12	0.00000E+00	0.00000
11	1.1064E+13	0.00000E+00	0.00000
12	3.0690E+13	0.00000E+00	0.00000
13	1.0344E+13	0.00000E+00	0.00000
14	4.5524E+11	0.00000E+00	0.00000
15	4.8000E+13	0.00000E+00	0.00000
16	2.0000E+13	0.00000E+00	0.00000
17	7.3247E+12	0.00000E+00	0.00000
18	1.6606E+07	0.00000E+00	0.00000
19	3.3351E+12	0.00000E+00	0.00000
20	1.5053E+12	0.00000E+00	0.00000
21	2.3618E+12	0.00000E+00	0.00000
22	5.6904E+12	0.00000E+00	0.00000
23	2.3080E+11	0.00000E+00	0.00000
24	4.2857E+12	0.00000E+00	0.00000
25	6.0000E+12	0.00000E+00	0.00000
26	3.3000E+13	0.00000E+00	0.00000
27	5.0000E+12	0.00000E+00	0.00000
28	3.0000E+13	0.00000E+00	0.00000
29	3.0000E+13	0.00000E+00	0.00000
30	7.3700E+02	0.00000E+00	0.00000
31	8.5640E+12	0.00000E+00	0.00000
32	1.7046E+13	0.00000E+00	0.00000
33	7.9329E+11	0.00000E+00	0.00000
34	3.0160E+11	0.00000E+00	0.00000
35	3.2072E+13	0.00000E+00	0.00000
36	2.0000E+13	0.00000E+00	0.00000
37	6.9656E+11	0.00000E+00	0.00000
38	1.2020E+12	0.00000E+00	0.00000
39	1.0000E+13	0.00000E+00	0.00000
40	5.0000E+13	0.00000E+00	0.00000
41	3.0000E+13	0.00000E+00	0.00000
42	5.5320E+12	0.00000E+00	0.00000
43	1.0000E+13	0.00000E+00	0.00000
44	2.8000E+13	0.00000E+00	0.00000
45	3.0359E+12	0.00000E+00	0.00000
46	4.0962E+12	0.00000E+00	0.00000
47	7.0241E+12	0.00000E+00	0.00000
48	4.6827E+12	0.00000E+00	0.00000
49	2.0000E+13	0.00000E+00	0.00000
50	3.8682E+08	0.00000E+00	0.00000
51	5.0000E+13	0.00000E+00	0.00000
52	1.1974E+12	0.00000E+00	0.00000
53	2.0000E+13	0.00000E+00	0.00000
54	1.9307E+06	0.00000E+00	0.00000
55	2.1031E+13	0.00000E+00	0.00000
56	7.6735E+12	0.00000E+00	0.00000
57	1.2383E+13	0.00000E+00	0.00000
58	6.9803E+10	0.00000E+00	0.00000
59	1.2369E+13	0.00000E+00	0.00000
60	2.0000E+13	0.00000E+00	0.00000
61	3.2663E+04	0.00000E+00	0.00000
62	1.9580E+10	0.00000E+00	0.00000
63	1.4842E+10	0.00000E+00	0.00000
64	1.9580E+10	0.00000E+00	0.00000
65	3.7000E+12	0.00000E+00	0.00000
66	1.0000E+13	0.00000E+00	0.00000
67	2.6268E+12	0.00000E+00	0.00000
68	1.7601E+10	0.00000E+00	0.00000
69	3.5950E+12	0.00000E+00	0.00000
70	1.3413E+13	0.00000E+00	0.00000
71	5.0000E+12	0.00000E+00	0.00000
72	4.0000E+13	0.00000E+00	0.00000
73	3.0000E+13	0.00000E+00	0.00000
74	3.0000E+13	0.00000E+00	0.00000
75	3.0000E+13	0.00000E+00	0.00000

TABLE D.2.—Continued.

(g) Continued.

76	2.0000E+13	0.00000E+00	0.00000
77	2.8889E+12	0.00000E+00	0.00000
78	7.1305E+14	0.00000E+00	0.00000
79	1.8492E+06	0.00000E+00	0.00000
80	3.1015E+11	0.00000E+00	0.00000
81	6.4836E+10	0.00000E+00	0.00000
82	2.9616E+11	0.00000E+00	0.00000
83	1.4726E+12	0.00000E+00	0.00000
84	7.1708E+12	0.00000E+00	0.00000
85	3.8799E+13	0.00000E+00	0.00000
86	3.7189E+13	0.00000E+00	0.00000
87	8.0000E+12	0.00000E+00	0.00000
88	9.7622E+13	0.00000E+00	0.00000
89	4.8329E+10	0.00000E+00	0.00000
90	3.9948E+12	0.00000E+00	0.00000
91	1.8000E+12	0.00000E+00	0.00000
92	7.8000E+11	0.00000E+00	0.00000
93	2.0307E+11	0.00000E+00	0.00000
94	7.7952E+12	0.00000E+00	0.00000
95	1.9630E+15	0.00000E+00	0.00000
96	3.9562E+01	0.00000E+00	0.00000
97	4.1765E+15	0.00000E+00	0.00000
98	1.0018E+02	0.00000E+00	0.00000
99	7.1175E-01	2.12050E+01	1.00000
100	3.6090E+08	0.00000E+00	0.00000
101	1.2497E+13	0.00000E+00	0.00000
102	1.4798E+11	0.00000E+00	0.00000
103	1.7462E+11	0.00000E+00	0.00000
104	1.2000E+13	0.00000E+00	0.00000
105	4.2324E+13	0.00000E+00	0.00000
106	6.9658E+12	0.00000E+00	0.00000
107	8.0770E+12	0.00000E+00	0.00000
108	2.3801E+13	-3.77764E+06	1.00000
109	3.7000E+12	0.00000E+00	0.00000
110	2.0000E+13	0.00000E+00	0.00000
111	1.0000E+13	0.00000E+00	0.00000
112	2.0000E+13	0.00000E+00	0.00000
113	8.4381E+11	0.00000E+00	0.00000
114	2.0000E+12	0.00000E+00	0.00000
115	1.1405E+13	0.00000E+00	0.00000
116	2.4070E+12	0.00000E+00	0.00000
117	8.3826E+12	0.00000E+00	0.00000
118	7.9225E+15	0.00000E+00	0.00000
119	2.2457E+14	0.00000E+00	0.00000
120	8.6958E+07	0.00000E+00	0.00000
121	3.1028E+07	0.00000E+00	0.00000
122	2.8358E+04	0.00000E+00	0.00000
123	4.0000E+12	0.00000E+00	0.00000
124	2.5566E+07	0.00000E+00	0.00000
125	2.4991E+10	7.80528E+00	1.00000
126	2.6097E+10	0.00000E+00	0.00000
127	8.6897E+11	0.00000E+00	0.00000
128	4.4875E+09	0.00000E+00	0.00000
129	9.2394E+15	0.00000E+00	0.00000
130	9.2627E+15	0.00000E+00	0.00000
131	5.0000E+12	0.00000E+00	0.00000
132	6.4495E+15	0.00000E+00	0.00000
133	3.6000E+13	0.00000E+00	0.00000

DERIVATIVES (CGS UNITS): T 7.80578E-03 RHO 5.34600E-08 V -5.05156E+00

MIXTURE MOLECULAR WEIGHT 28.21102 TOTAL ENERGY EXCHANGE RATE 5.92105E+06 (CAL-CM**3/G**2/SEC) MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 1.070000 S

TABLE D.2.—Continued.

(g) Continued.

TIME 2.94080E-04 SEC AREA 1.43983E+03 SQ CM AXIAL POSITION 4.70000E+01 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.73125
VELOCITY (CM/SEC)	159765.65
DENSITY (G/CM**3)	2.43084E-04
TEMPERATURE (DEG K)	2390.72
MASS FLOW RATE (G/SEC)	5.59179E+04
ENTROPY (CAL/G/DEG K)	2.3063
MACH NUMBER	1.6664
GAMMA	1.2738
ENTHALPY (CAL/G)	3.79465E+02
SP. HEAT (CP) (CAL/G/DEG K)	3.35641E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	171
AVERAGE STEP SIZE	0.41227E-01
METHOD ORDER	4
TOTAL NUMBER OF STEPS	353
FUNCT EVALUATIONS	500
JACOBIAN EVALUATIONS	55

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	5.70493E-11	6.46442E-06	-5.56527E-06
CH3	1.12286E-09	1.27235E-04	-1.13689E-04
H	4.21831E-08	4.77989E-03	-5.23517E-04
H2	3.80956E-08	4.31672E-03	-2.31095E-04
D2	8.63035E-07	9.77931E-02	-1.05168E-03
HO2	1.73619E-10	1.96733E-05	-5.66640E-07
O	1.08967E-07	1.23473E-02	-8.59825E-04
OH	1.48973E-07	1.68806E-02	-1.31377E-04
H2O	7.22054E-07	8.18181E-02	7.44332E-04
CH3O	6.18167E-12	7.00464E-07	-5.26294E-07
CH2O	1.75679E-11	1.99067E-06	-1.52189E-06
C2H6	7.07055E-14	8.01186E-09	-1.90424E-08
C2H5	5.79157E-16	6.56260E-11	7.31591E-11
C2H4	3.29110E-13	3.72925E-08	-7.09441E-08
CH2	1.01311E-11	1.14798E-06	-9.85971E-07
C2H3	1.07964E-14	1.22338E-09	-2.48748E-09
C2H2	5.82564E-14	6.60121E-09	-1.21744E-08
HCO	1.07281E-12	1.21563E-07	-9.27399E-08
C2H2O	1.70385E-14	1.93069E-09	-2.55950E-09
C2H	3.39526E-16	3.84728E-11	-6.59282E-11
CO	1.31666E-07	1.49194E-02	-2.08052E-03
C2HO	7.37796E-14	8.36019E-09	-1.44817E-08
CH	2.12511E-12	2.40803E-07	-2.15627E-07
CO2	2.95949E-07	3.35349E-02	2.20339E-03
H2O2	9.94278E-12	1.12665E-06	-1.63298E-07
N2	6.47215E-06	7.33378E-01	-1.37893E-05
HCN	3.48809E-13	3.95245E-08	-2.73224E-08
N	1.06319E-12	1.20473E-07	1.50510E-08
CN	2.25791E-15	2.55851E-10	-1.71466E-10
HNCO	5.04079E-14	5.71187E-09	-1.34537E-09
NCO	1.49924E-14	1.69884E-09	-9.46275E-10
NH2	2.28551E-12	2.58978E-07	9.41418E-09
NO	6.32259E-10	7.16432E-05	2.75254E-05
NH	6.76764E-14	7.66862E-09	1.26142E-09
NO2	4.20064E-13	4.75987E-08	1.93621E-08
N2O	6.53480E-12	7.40478E-07	1.76058E-08
HNO2	2.65700E-14	3.01073E-09	7.54597E-10
HNO3	3.10331E-18	3.51645E-13	9.60823E-14
HNO	8.99356E-14	1.01909E-08	1.93850E-09

REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	1.8048E+09	-5.17899E+07	0.96982
2	1.0293E+13	4.46211E+04	0.17278
3	6.0330E+08	-7.57979E+04	0.73913
4	1.6120E+13	7.39534E+05	0.17566
5	8.7086E+12	-3.16252E+06	0.17541
6	5.7333E+10	1.16335E+06	0.04321
7	6.3000E+12	8.79239E+06	0.04156
8	6.0150E+11	1.13871E+07	1.00000
9	1.0686E+13	-9.64762E+05	0.04718
10	1.7133E+13	-5.32624E+03	0.99996
11	2.1650E+13	-1.21172E+04	0.99996
12	4.1470E+13	-1.56484E+05	0.99996
13	1.4659E+14	4.27759E+05	0.87169
14	6.9815E+11	-7.50631E+01	0.98515
15	4.8000E+13	-1.29580E+03	0.99680
16	2.0000E+13	-2.40673E+05	0.99901
17	1.7525E+13	-1.01347E+04	0.99919
18	1.4645E+10	3.00121E+04	1.00000
19	3.7051E+12	-5.36740E+04	0.99919
20	1.6341E+12	-1.97671E+04	0.99195
21	2.6014E+12	-4.23644E+04	1.00000
22	8.7269E+12	-3.92109E+04	0.99996
23	3.5630E+12	2.53274E+05	0.99841
24	4.1950E+12	-5.25494E+04	1.00000
25	6.0000E+12	-2.77687E+03	0.99996
26	3.3000E+13	-5.32106E+04	1.00000
27	5.0000E+12	-1.02150E+04	0.99996
28	3.0000E+13	-3.60306E+00	0.99090
29	3.0000E+13	-1.54389E-04	0.99921
30	6.9464E+06	-7.79094E+00	0.50338
31	1.9953E+13	-1.02390E+05	0.99909
32	4.2420E+13	-1.04745E+05	0.99324
33	1.4435E+12	1.60360E+03	0.94988
34	3.0681E+11	-1.01478E+03	0.98752
35	3.6462E+13	-4.88309E+03	0.86526
36	2.0000E+13	-7.10544E+02	0.86503
37	8.6261E+11	-7.62362E+04	1.00000
38	1.2020E+12	-1.61568E+04	1.00000
39	1.0000E+13	-5.02556E+04	1.00000
40	5.0000E+13	-5.62043E+04	0.86517
41	3.0000E+13	-3.60992E+01	0.99998
42	6.5640E+12	-2.43154E+00	0.99994
43	1.0000E+13	-6.96815E-02	1.00000
44	2.8000E+13	-1.83031E+04	0.99986
45	3.9885E+12	-1.35077E+03	0.45802
46	5.4917E+12	3.60106E+04	0.96035
47	1.3925E+13	-1.70244E+02	0.45629
48	9.2820E+12	-4.49845E+01	0.45818
49	2.0000E+13	-6.42681E+04	1.00000
50	6.5476E+10	-2.49452E+04	0.65940
51	5.0000E+13	-2.28976E+03	0.99876
52	2.2108E+12	-6.20734E+06	1.00000
53	2.0000E+13	-7.38735E+06	1.00000
54	1.9692E+09	4.62373E+05	0.99209
55	2.3304E+13	-2.99380E+07	0.99980
56	1.0794E+13	-1.89509E+06	0.99980
57	1.6719E+13	-6.57142E+06	0.99980
58	1.3828E+11	-6.74653E+02	0.99976
59	1.4669E+13	-2.66371E+04	0.99489
60	2.0000E+13	-1.15848E+06	0.79425
61	8.2479E+07	1.25085E+06	0.82486
62	2.2161E+11	9.59954E+05	0.99563
63	1.6856E+11	2.53483E+06	0.99564
64	2.2161E+11	-5.98533E+06	0.99564
65	3.7000E+12	-2.51915E+06	1.00000
66	1.0000E+13	-2.23620E+07	1.00000
67	5.6491E+12	-5.05691E+07	0.99999
68	2.0299E+11	-2.06745E+03	0.93050
69	7.0612E+12	-2.93049E+06	0.93048
70	2.6049E+13	-4.29786E+05	0.93026
71	5.0000E+12	-6.11830E+02	0.99982
72	4.0000E+13	-9.06783E+03	1.00000
73	3.0000E+13	-1.67365E+07	0.98041
74	3.0000E+13	-5.14479E+06	0.99579
75	3.0000E+13	-8.39724E+06	0.99579
76	2.0000E+13	-1.35621E+06	0.99577
77	1.0941E+13	2.22615E+07	0.83069
78	1.0125E+15	-2.71219E+08	0.98288

TABLE D.2.—Continued.

(g) Concluded

79	1.0922E+08	-5.31228E+05	0.31308
80	3.3785E+11	-8.69108E+08	0.31190
81	4.6079E+11	-8.93559E+06	0.85228
82	1.4245E+12	9.41893E+06	0.00029
83	5.9875E+12	1.06652E+08	0.00172
84	2.3242E+13	1.05930E+07	0.00348
85	4.6535E+13	-2.37923E+08	0.78420
86	4.0509E+13	-5.16523E+08	0.78495
87	8.0000E+12	-1.85830E+08	0.78489
88	1.0698E+14	-3.53684E+08	0.78532
89	4.1000E+11	-6.47435E+06	0.88118
90	4.5145E+12	-3.39511E+06	0.88156
91	1.8000E+12	2.51669E+04	0.44940
92	7.8000E+11	-3.66899E+05	0.97457
93	9.9547E+12	-2.27140E+07	0.02108
94	1.3132E+13	-6.02479E+07	0.00318
95	1.8021E+15	-1.39117E+09	0.88429
96	3.1804E+05	-4.93960E+08	0.97511
97	2.9698E+15	-2.03454E+08	0.97512
98	3.6856E+05	-2.55127E+07	0.97503
99	1.2242E+04	-7.35218E+06	0.97507
100	1.8327E+09	1.39732E+03	1.00000
101	1.9663E+13	5.61968E+03	0.90925
102	7.9177E+11	9.94238E+03	0.90956
103	2.2187E+11	-2.54811E+03	0.94536
104	1.2000E+13	-3.84606E+03	0.99974
105	7.0704E+13	-5.08990E+03	0.54712
106	1.5040E+13	4.93186E+02	0.24782
107	1.6710E+13	-1.40358E+03	0.26496
108	2.5926E+13	-2.97245E+03	0.54790
109	3.7000E+12	2.47856E+01	0.34184
110	2.0000E+13	-5.65425E+04	0.99999
111	1.0000E+13	-4.75469E-01	0.99306
112	2.0000E+13	-7.62101E+03	0.99937
113	1.9745E+12	-1.81552E+03	1.00000
114	2.0000E+12	-3.27179E+03	0.99980
115	1.6047E+13	-6.76546E+03	0.07033
116	2.3107E+12	-1.92250E+02	0.00929
117	8.8210E+12	-2.45625E+05	0.78294
118	7.1743E+15	-4.78280E+06	0.88517
119	2.5465E+14	-1.74329E+06	0.78331
120	6.4816E+09	-6.95800E+06	0.98006
121	1.5012E+09	-2.72471E+06	0.98010
122	1.9267E+07	1.72713E+07	0.99832
123	4.0000E+12	-2.33353E+00	0.99568
124	2.8298E+09	-7.22372E+05	0.86721
125	2.7449E+11	-2.12419E+05	0.81230
126	2.5451E+11	-1.08668E+05	0.99999
127	3.1613E+12	-7.46464E+05	0.81262
128	5.3598E+10	-2.80283E+03	0.88464
129	6.6758E+15	-8.04826E-02	0.00003
130	8.0093E+15	-6.18944E+03	0.00110
131	5.0000E+12	-1.68918E+04	0.96240
132	6.1269E+15	-4.06066E+05	0.33593
133	3.6000E+13	-5.47495E+05	0.96252

```
DERIVATIVES (CGS UNITS): T          2.13842E+01    RHO        -1.82919E-06    V          1.22400E+00

MIXTURE MOLECULAR WEIGHT     27.54458     TOTAL ENERGY EXCHANGE RATE   -4.71024E+09      MASS FRACTION SUM    1.00000003
                                               (CAL-CM**3/G**2/SEC)


COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP -  1.128000E+01  S     UP TO THIS TIME -  2.184000E+01  S

            (LSENS)     END OF THIS CASE

                  SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

                     TOTAL NO. OF STEPS -                    353
                     TOTAL NO. OF DERIVATIVE EVALUATIONS -   500
                     TOTAL NO. OF JACOBIAN EVALUATIONS -      55
                     TOTAL CPU TIME -                 21.840000 S


                          TOTAL CPU TIME (INCLUDING I/O) REQUIRED =     24.139996 S

            (LSENS)     READ DATA FOR NEXT CASE
```

TABLE D.2.—Continued.

(h) Case 8

```
                                   ** DATA LINES **
                         1         2         3         4         5         6         7         8
CC  12345678901234567890123456789012345678901234567890123456789012345678901234567890123456789 0

     LSENS   METHANE - AIR WITH AREA AND TEMPERATURE PROFILES OF CASE 6      CASE 8
    REPEAT
    DISTANCE  AREA
     &prob  tass=.true.,  &end
     &tmpdat  xtb=0.0,15.0,20.0,25.0,30.0,32.0,34.0,36.0,38.0,40.0,41.0,
       42.0,43.0,44.0,45.0,46.0,47.0,48.0,
      tmptb=1700.00,1702.50,1707.74,1718.03,1738.22,1751.43,1769.70,
       1796.16,1838.63,1939.65,2127.05,2225.54,2270.46,2307.71,2339.56,
       2366.73,2389.90,2409.76,
      tprint=1738.22,1939.65,2389.90,  &end
     &start  p=1.730, mach=2.0,  &end
    CH4          0.049768
    O2           0.199072
    N2           0.75116
    CN           0.0000001
    END
     &solver  emax=1.0E-3, atolsp=1.0E-12, mf=21,  &end
    FINIS
```

DISTANCE-AREA VERSION LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

LSENS METHANE - AIR WITH AREA AND TEMPERATURE PROFILES OF CASE 6 CASE 8

REACTION NUMBER	REACTION							REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	M	+	1*CH4	=	1*CH3	+	1*H	2.00000E+17	0.0000	88000.00
2	1*H	+	1*CH4	=	1*CH3	+	1*H2	1.26000E+14	0.0000	11900.00
3	1*CH4	+	1*O2	=	1*CH3	+	1*HO2	7.94000E+13	0.0000	56000.00
4	1*O	+	1*CH4	=	1*CH3	+	1*OH	1.90000E+14	0.0000	11720.00
5	1*OH	+	1*CH4	=	1*CH3	+	1*H2O	2.50000E+13	0.0000	5010.00
6	1*CH3	+	1*O2	=	1*CH3O	+	1*O	2.40000E+13	0.0000	28680.00
7	1*CH3	+	1*OH	=	1*CH3O	+	1*H	6.30000E+12	0.0000	0.00
8	M	+	1*CH3O	=	1*CH2O	+	1*H	5.00000E+13	0.0000	21000.00
9			2*CH3	=	1*C2H6			2.40000E+14	-0.4000	0.00
10	1*H	+	1*C2H6	=	1*C2H5	+	1*H2	1.32000E+14	0.0000	9700.00
11	1*O	+	1*C2H6	=	1*C2H5	+	1*OH	1.13000E+14	0.0000	7850.00
12	1*OH	+	1*C2H6	=	1*C2H5	+	1*H2O	8.70000E+15	0.0000	3520.00
13	M	+	1*C2H5	=	1*C2H4	+	1*H	1.00000E+17	0.0000	31000.00
14	1*C2H5	+	1*O2	=	1*C2H4	+	1*HO2	2.00000E+12	0.0000	5000.00
15	1*H	+	1*C2H5	=	1*C2H4	+	1*H2	4.80000E+13	0.0000	0.00
16	1*CH3	+	1*CH2	=	1*C2H4	+	1*H	2.00000E+13	0.0000	0.00
17	1*H	+	1*C2H4	=	1*H2	+	1*C2H3	1.50000E+14	0.0000	10200.00
18	M	+	1*C2H4	=	1*C2H2	+	1*H2	2.60000E+17	0.0000	79300.00
19	1*C2H4	+	1*OH	=	1*C2H3	+	1*H2O	4.80000E+12	0.0000	1230.00
20	1*C2H4	+	1*OH	=	1*CH3	+	1*CH2O	2.00000E+12	0.0000	960.00
21	1*C2H4	+	1*O	=	1*CH3	+	1*HCO	3.30000E+12	0.0000	1130.00
22	1*C2H4	+	1*O	=	1*CH2O	+	1*CH2	2.50000E+13	0.0000	5000.00
23	M	+	1*C2H3	=	1*C2H2	+	1*H	3.00000E+15	0.0000	32000.00
24	1*C2H3	+	1*O2	=	1*CH2O	+	1*HCO	3.98000E+12	0.0000	-250.00
25	1*C2H3	+	1*H	=	1*C2H2	+	1*H2	6.00000E+12	0.0000	0.00
26	1*C2H3	+	1*O	=	1*C2H2O	+	1*H	3.30000E+13	0.0000	0.00
27	1*C2H3	+	1*OH	=	1*C2H2	+	1*H2O	5.00000E+12	0.0000	0.00
28	1*C2H3	+	1*CH2	=	1*C2H2	+	1*CH3	3.00000E+13	0.0000	0.00
29	1*C2H3	+	1*C2H	=	2*C2H2			3.00000E+13	0.0000	0.00
30	M	+	1*C2H2	=	1*C2H	+	1*H	4.20000E+16	0.0000	107000.00
31	1*C2H2	+	1*O	=	1*CH2	+	1*CO	1.60000E+14	0.0000	9890.00
32	1*C2H2	+	1*O	=	1*C2HO	+	1*H	4.00000E+14	0.0000	10660.00
33	1*C2H2	+	1*OH	=	1*C2H	+	1*H2O	6.30000E+12	0.0000	7000.00
34	1*C2H2	+	1*OH	=	1*C2H2O	+	1*H	3.20000E+11	0.0000	200.00
35	1*C2H	+	1*O2	=	1*C2HO	+	1*O	5.00000E+13	0.0000	1500.00
36	1*C2H	+	1*OH	=	1*C2HO	+	1*H	2.00000E+13	0.0000	0.00
37	1*C2HO	+	1*O2	=	2*CO	+	1*OH	1.46000E+12	0.0000	2500.00
38	1*C2HO	+	1*O	=	2*CO	+	1*H	1.20200E+12	0.0000	0.00
39	1*C2HO	+	1*OH	=	2*HCO			1.00000E+13	0.0000	0.00
40	1*C2HO	+	1*H	=	1*CH2	+	1*CO	5.00000E+13	0.0000	0.00
41	1*C2HO	+	1*CH2	=	1*C2H3	+	1*CO	3.00000E+13	0.0000	0.00
42	1*C2HO	+	1*CH2	=	1*CH2O	+	1*C2H	1.00000E+13	0.0000	2000.00
43			2*C2HO	=	1*C2H2	+	2*CO	1.00000E+13	0.0000	0.00
44	1*C2H2O	+	1*OH	=	1*CH2O	+	1*HCO	2.80000E+13	0.0000	0.00
45	1*C2H2O	+	1*OH	=	1*C2HO	+	1*H2O	7.50000E+12	0.0000	3000.00
46	1*C2H2O	+	1*H	=	1*CH3	+	1*CO	1.13000E+13	0.0000	3428.00
47	1*C2H2O	+	1*H	=	1*C2HO	+	1*H2	7.50000E+13	0.0000	8000.00
48	1*C2H2O	+	1*O	=	1*C2HO	+	1*OH	5.00000E+13	0.0000	8000.00
49	1*C2H2O	+	1*O	=	1*CH2O	+	1*CO	2.00000E+13	0.0000	0.00
50	M	+	1*C2H2O	=	1*CH2	+	1*CO	2.00000E+16	0.0000	60000.00
51	1*C2H	+	1*O	=	1*CO	+	1*CH	5.00000E+13	0.0000	0.00
52	1*CH3O	+	1*O2	=	1*CH2O	+	1*HO2	1.00000E+13	0.0000	7170.00
53	1*CH3O	+	1*H	=	1*CH2O	+	1*H2	2.00000E+13	0.0000	0.00
54	M	+	1*CH2O	=	1*HCO	+	1*H	5.00000E+16	0.0000	81000.00
55	1*CH2O	+	1*OH	=	1*HCO	+	1*H2O	3.00000E+13	0.0000	1200.00
56	1*CH2O	+	1*H	=	1*HCO	+	1*H2	2.50000E+13	0.0000	3990.00
57	1*CH2O	+	1*O	=	1*HCO	+	1*OH	3.50000E+13	0.0000	3510.00
58	1*CH3	+	1*CH2O	=	1*CH4	+	1*HCO	1.00000E+10	0.5000	6000.00
59	1*CH3	+	1*HCO	=	1*CH4	+	1*CO	3.00000E+11	0.5000	0.00
60	1*CH3	+	1*HO2	=	1*CH3O	+	1*OH	2.00000E+13	0.0000	0.00
61	M	+	1*CH3	=	1*CH2	+	1*H	1.95000E+16	0.0000	91600.00
62	1*H	+	1*CH3	=	1*H2	+	1*CH2	2.70000E+11	0.6700	25700.00
63	1*O	+	1*CH3	=	1*OH	+	1*CH2	1.90000E+11	0.6800	25700.00
64	1*OH	+	1*CH3	=	1*H2O	+	1*CH2	2.70000E+11	0.6700	25700.00
65	1*CH	+	1*CO2	=	1*HCO	+	1*CO	3.70000E+12	0.0000	0.00
66	1*CH	+	1*O2	=	1*HCO	+	1*O	1.00000E+13	0.0000	0.00
67	1*CH2	+	1*O2	=	1*CH2O	+	1*O	5.00000E+11	0.5000	6960.00
68	1*CH2	+	1*O	=	1*CH	+	1*OH	2.00000E+11	0.7000	25800.00
69	1*CH2	+	1*OH	=	1*CH	+	1*H2O	5.00000E+11	0.5000	5900.00
70	1*CH2	+	1*H	=	1*CH	+	1*H2	3.20000E+11	0.7000	4970.00
71			2*CH2	=	1*C2H3	+	1*H	5.00000E+12	0.0000	0.00
72			2*CH2	=	1*C2H2	+	1*H2	4.00000E+13	0.0000	0.00
73	1*HCO	+	1*O2	=	1*CO	+	1*HO2	3.00000E+13	0.0000	0.00
74	1*HCO	+	1*O	=	1*CO	+	1*OH	3.00000E+13	0.0000	0.00
75	1*HCO	+	1*OH	=	1*CO	+	1*H2O	3.00000E+13	0.0000	0.00
76	1*HCO	+	1*H	=	1*CO	+	1*H2	2.00000E+13	0.0000	0.00

TABLE D.2.—Continued.

(h) Continued.

77	M	+	1*HCO	=	1*H	+	1*CO	2.90000E+14	0.0000	15570.00
78	1*CO	+	1*O	=	1*CO2	+	M	2.40000E+15	0.0000	4100.00
79	1*CO	+	1*O2	=	1*CO2	+	1*O	2.50000E+12	0.0000	47690.00
80	1*CO	+	1*OH	=	1*CO2	+	1*H	4.17000E+11	0.0000	1000.00
81	1*CO	+	1*HO2	=	1*CO2	+	1*OH	5.75000E+13	0.0000	22930.00
82	1*O	+	1*H2O	=	2*OH			6.80000E+13	0.0000	18365.00
83	1*H	+	1*O2	=	1*OH	+	1*O	1.89000E+14	0.0000	16400.00
84	1*O	+	1*H2	=	1*OH	+	1*H	4.20000E+14	0.0000	13750.00
85	1*H	+	1*HO2	=	1*H2	+	1*O2	7.28000E+13	0.0000	2126.00
86	1*O	+	1*HO2	=	1*OH	+	1*O2	5.00000E+13	0.0000	1000.00
87	1*HO2	+	1*OH	=	1*H2O	+	1*O2	8.00000E+12	0.0000	0.00
88	1*H	+	1*HO2	=	2*OH			1.34000E+14	0.0000	1070.00
89	1*H2	+	1*HO2	=	1*H2O2	+	1*H	7.91000E+13	0.0000	25000.00
90	1*OH	+	1*H2O2	=	1*H2O	+	1*HO2	6.10000E+12	0.0000	1430.00
91			2*HO2	=	1*H2O2	+	1*O2	1.80000E+12	0.0000	0.00
92	1*H	+	1*H2O2	=	1*OH	+	1*H2O	7.80000E+11	0.0000	0.00
93	M	+	1*H2O2	=	2*OH			1.44000E+17	0.0000	45510.00
94	1*H2	+	1*OH	=	1*H2O	+	1*H	4.74000E+13	0.0000	6098.00
95	1*H	+	1*O2	=	1*HO2	+	M	1.46000E+15	0.0000	-1000.00
96	M	+	1*H2O	=	1*H	+	1*OH	1.50000E+15	0.0000	105140.00
97	1*H	+	1*O	=	1*OH	+	M	7.10000E+18	-1.0000	0.00
98	M	+	1*H2	=	2*H			2.20000E+14	0.0000	96000.00
99	M	+	1*O2	=	2*O			1.80000E+18	-1.0000	118020.00
100	1*CH	+	1*N2	=	1*HCN	+	1*N	1.00000E+11	0.0000	19000.00
101	1*CN	+	1*H2	=	1*HCN	+	1*H	6.00000E+13	0.0000	5300.00
102	1*O	+	1*HCN	=	1*OH	+	1*CN	1.40000E+11	0.6800	16900.00
103	1*OH	+	1*HCN	=	1*HNCO	+	1*H	4.00000E+11	0.0000	2800.00
104	1*CN	+	1*O	=	1*CO	+	1*N	1.20000E+13	0.0000	0.00
105	1*CN	+	1*OH	=	1*NCO	+	1*H	2.50000E+14	0.0000	6000.00
106	1*H2	+	1*NCO	=	1*HNCO	+	1*H	1.00000E+14	0.0000	9000.00
107	1*HNCO	+	1*H	=	1*NH2	+	1*CO	1.00000E+14	0.0000	8500.00
108	1*CN	+	1*O2	=	1*NCO	+	1*O	3.20000E+13	0.0000	1000.00
109	1*CN	+	1*CO2	=	1*NCO	+	1*CO	3.70000E+12	0.0000	0.00
110	1*O	+	1*NCO	=	1*NO	+	1*CO	2.00000E+13	0.0000	0.00
111	1*N	+	1*NCO	=	1*N2	+	1*CO	1.00000E+13	0.0000	0.00
112	1*H	+	1*NCO	=	1*NH	+	1*CO	2.00000E+13	0.0000	0.00
113	1*CH	+	1*NO	=	1*N	+	1*HCO	1.60000E+13	0.0000	9940.00
114	1*CH	+	1*NO	=	1*O	+	1*HCN	2.00000E+12	0.0000	0.00
115	1*NH	+	1*OH	=	1*N	+	1*H2O	5.00000E+11	0.5000	2000.00
116	1*HO2	+	1*NO	=	1*NO2	+	1*OH	2.09000E+12	0.0000	-477.00
117	1*O	+	1*NO2	=	1*NO	+	1*O2	1.00000E+13	0.0000	596.00
118	1*NO	+	1*O	=	1*NO2	+	M	5.62000E+15	0.0000	-1160.00
119	1*NO2	+	1*H	=	1*NO	+	1*OH	3.47000E+14	0.0000	1470.00
120	1*NO	+	1*H	=	1*N	+	1*OH	2.63000E+14	0.0000	50410.00
121	1*NO	+	1*O	=	1*N	+	1*O2	3.80000E+09	1.0000	41370.00
122	1*O	+	1*N2	=	1*NO	+	1*N	1.80000E+14	0.0000	76250.00
123	1*N	+	1*NO2	=	2*NO			4.00000E+12	0.0000	0.00
124	M	+	1*N2O	=	1*N2	+	1*O	6.92000E+23	-2.5000	65000.00
125	1*O	+	1*N2O	=	1*N2	+	1*O2	1.00000E+14	0.0000	28020.00
126	1*O	+	1*N2O	=	2*NO			6.92000E+13	0.0000	26630.00
127	1*N2O	+	1*H	=	1*N2	+	1*OH	7.59000E+13	0.0000	15100.00
128	1*NO2	+	1*H2	=	1*HNO2	+	1*H	2.40000E+13	0.0000	29000.00
129	1*OH	+	1*NO2	=	1*HNO3	+	M	3.00000E+15	0.0000	-3800.00
130	1*OH	+	1*NO	=	1*HNO2	+	M	5.60000E+15	0.0000	-1700.00
131	1*HNO	+	1*H	=	1*H2	+	1*NO	5.00000E+12	0.0000	0.00
132	1*H	+	1*NO	=	1*HNO	+	M	5.40000E+15	0.0000	-600.00
133	1*HNO	+	1*OH	=	1*H2O	+	1*NO	3.60000E+13	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2 , 93) =	2.30000	M(O2 , 93) =	0.78000	M(H2O , 93) =	6.00000	M(H2O2 , 93) =	6.60000
M(O2 , 95) =	1.30000	M(N2 , 95) =	1.30000	M(H2O , 95) =	21.30000	M(CO2 , 95) =	7.00000
M(H2 , 96) =	4.00000	M(O2 , 96) =	1.50000	M(H2O , 96) =	20.00000	M(N2 , 96) =	1.50000
M(CO2 , 96) =	4.00000	M(H2 , 98) =	4.10000	M(O2 , 98) =	2.00000	M(H2O , 98) =	15.00000
M(N2 , 98) =	2.00000	M(O2 ,129) =	0.70000	M(H2 ,129) =	1.40000		

TIME 1.87696E-04 SEC AREA 1.02322E+03 SQ CM AXIAL POSITION 3.00000E+01 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.73000
VELOCITY (CM/SEC)	159827.59
DENSITY (G/CM**3)	3.41933E-04
TEMPERATURE (DEG K)	1738.22
MASS FLOW RATE (G/SEC)	5.59193E+04
ENTROPY (CAL/G/DEG K)	2.1560
MACH NUMBER	1.9774
GAMMA	1.2743
ENTHALPY (CAL/G)	3.79343E+02
SP. HEAT (CP) (CAL/G/DEG K)	3.27469E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	80
AVERAGE STEP SIZE	0.38091E+00
METHOD ORDER	5
TOTAL NUMBER OF STEPS	80
FUNCT EVALUATIONS	103
JACOBIAN EVALUATIONS	17

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
CH4	4.91663E-07	4.05355E-02	-2.04428E-03	1	1.7243E+06	4.22765E+06	0.45858
CH3	1.87424E-08	1.54523E-03	2.41396E-04	2	4.0194E+12	8.95979E+05	0.85780
H	1.00305E-10	8.26970E-06	2.62788E-06	3	7.2249E+06	-4.50456E+06	0.54351
H2	8.70599E-09	7.17771E-04	1.82136E-04	4	6.3852E+12	1.07993E+07	0.99612
O2	2.33987E-06	1.92912E-01	-1.51872E-03	5	5.8617E+12	-1.74675E+08	0.98245
HO2	2.14976E-09	1.77238E-04	1.86213E-05	6	5.9459E+09	6.31448E+07	0.98890
O	1.62638E-10	1.34088E-05	3.58719E-06	7	6.3000E+12	-1.90904E+07	0.76078
OH	5.01110E-10	4.13143E-05	1.17881E-05	8	1.1445E+11	4.90885E+07	1.00000
H2O	9.19391E-08	7.57998E-03	2.06236E-03	9	1.2139E+13	-3.56356E+08	0.10895
CH3O	2.01636E-10	1.66240E-05	3.28997E-06	10	7.9611E+12	-6.25094E+05	0.99997

TABLE D.2.—Continued.

(h) Continued.

CH2O	3.40861E-08	2.81025E-03	3.90598E-04
C2H6	1.48603E-08	1.22517E-03	1.90737E-04
C2H5	1.84233E-12	1.51892E-07	-1.11263E-08
C2H4	6.93688E-09	5.71916E-04	2.45640E-04
CH2	1.02897E-12	8.48343E-08	5.54917E-08
C2H3	1.26767E-12	1.04514E-07	6.77191E-08
C2H2	1.13146E-10	9.32836E-06	6.13771E-06
HCO	4.78502E-12	3.94504E-07	1.77276E-07
C2H2O	6.17333E-13	5.08965E-08	3.52495E-08
C2H	6.19563E-16	5.10803E-11	-2.48645E-11
CO	1.45973E-08	1.20348E-03	5.18771E-04
C2HO	2.20257E-13	1.81592E-08	1.64241E-08
CH	1.45162E-16	1.19680E-11	5.61504E-12
CO2	9.07745E-11	7.48396E-06	4.75308E-06
H2O2	2.85151E-12	2.35095E-07	3.47544E-08
N2	9.10447E-06	7.50624E-01	-8.48242E-10
HCN	4.05268E-16	3.34126E-11	1.22506E-11
N	5.18291E-17	4.27309E-12	1.22165E-12
CN	1.64557E-17	1.35670E-12	8.77729E-15
HNCO	1.01663E-12	8.38170E-08	2.70655E-09
NCO	5.76588E-14	4.75372E-09	-3.88585E-09
NH2	2.62917E-14	2.16764E-09	8.64340E-10
NO	7.73732E-14	6.37908E-09	4.33469E-10
NH	2.87343E-14	2.36902E-09	-5.25303E-11
NO2	1.04519E-14	8.61711E-10	5.99231E-11
N2O	4.01764E-14	3.31237E-09	7.78525E-10
HNO2	4.10931E-19	3.38795E-14	9.28872E-15
HNO3	7.84827E-21	6.47056E-16	1.84475E-16
HNO	1.53856E-18	1.26848E-13	3.57553E-14

11	1.1643E+13	-1.03316E+06	1.00000
12	3.1401E+13	-4.23370E+07	1.00000
13	1.2656E+13	9.00755E+07	0.96218
14	4.7029E+11	-1.89483E+05	0.84696
15	4.8000E+13	-4.92020E+03	0.99007
16	2.0000E+13	-2.06356E+05	0.99973
17	7.8275E+12	-1.14722E+05	0.99970
18	2.7825E+07	8.34820E+05	1.00000
19	3.3619E+12	-1.74650E+06	0.99996
20	1.5147E+12	2.44946E+04	0.03569
21	2.3792E+12	-6.16035E+05	1.00000
22	5.8787E+12	-4.19932E+05	0.99990
23	2.8425E+11	1.64693E+06	0.99779
24	4.2787E+12	-8.62319E+06	1.00000
25	6.0000E+12	-3.91618E+02	0.99942
26	3.3000E+13	-4.71286E+03	1.00000
27	5.0000E+12	-2.03896E+03	0.99993
28	3.0000E+13	-1.82981E+01	0.83495
29	3.0000E+13	-1.63287E-02	0.97593
30	1.4789E+03	2.00478E+00	0.90810
31	9.1334E+12	-6.87260E+04	1.00000
32	1.8271E+13	-6.65457E+04	1.00000
33	8.3027E+11	3.19646E+03	0.99702
34	3.0200E+11	-3.33966E+03	0.99997
35	3.2387E+13	-1.25336E+04	0.99999
36	2.0000E+13	-2.53939E+00	0.99655
37	7.0798E+11	-2.55945E+05	1.00000
38	1.2020E+12	-3.63790E+01	1.00000
39	1.0000E+13	-2.55052E+02	0.99999
40	5.0000E+13	-2.27145E+02	0.97460
41	3.0000E+13	-5.53197E+00	1.00000
42	5.6045E+12	-2.92364E-01	0.91892
43	1.0000E+13	-3.13858E-01	1.00000
44	2.8000E+13	1.58583E+03	0.58445
45	3.1468E+12	-9.65093E+01	0.67340
46	4.1886E+12	1.29688E+03	0.94764
47	7.3996E+12	1.42157E+01	0.62214
48	4.9330E+12	-1.32298E+00	0.92770
49	2.0000E+13	-1.75647E+03	1.00000
50	5.7163E+08	2.10655E+03	0.74408
51	5.0000E+13	-3.15580E+00	1.00000
52	1.2546E+12	-1.57440E+08	1.00000
53	2.0000E+13	-2.89578E+05	1.00000
54	3.2710E+06	1.04331E+06	0.99995
55	2.1195E+13	-8.98342E+07	1.00000
56	7.8753E+12	-3.22448E+06	0.99999
57	1.2669E+13	-7.28970E+06	1.00000
58	7.3394E+10	-5.86167E+06	0.99991
59	1.2508E+13	-8.58946E+05	0.99995
60	2.0000E+13	-1.52351E+08	0.99998
61	5.9291E+04	1.24694E+04	0.98660
62	2.3492E+10	2.04299E+03	0.99648
63	1.7812E+10	3.38694E+03	0.99990
64	2.3492E+10	-1.80751E+04	0.99957
65	3.7000E+12	-2.65679E-02	0.99599
66	1.0000E+13	-2.09304E+03	1.00000
67	2.7793E+12	-3.46240E+06	1.00000
68	2.1146E+10	-1.77309E-02	0.99991
69	3.7775E+12	-2.90787E+02	0.99957
70	1.4071E+13	-3.03568E+01	0.99654
71	5.0000E+12	-3.19027E+00	0.99998
72	4.0000E+13	-4.72748E+01	1.00000
73	3.0000E+13	-1.04318E+08	0.99988
74	3.0000E+13	-1.73829E+04	1.00000
75	3.0000E+13	-6.39424E+04	1.00000
76	2.0000E+13	-7.30031E+03	0.99999
77	3.1971E+12	2.42608E+07	0.99997
78	7.3234E+14	-2.29399E+04	1.00000
79	2.5222E+06	-5.95223E+03	1.00000
80	3.1218E+11	-4.85167E+05	0.99974
81	7.5272E+10	-1.18821E+06	1.00000
82	3.3377E+11	5.60904E+05	0.77862
83	1.6385E+12	5.50100E+07	0.99735
84	7.8421E+12	1.72419E+05	0.97268
85	3.9339E+13	-3.56870E+06	0.93509
86	3.7432E+13	-5.66904E+06	0.99823
87	8.0000E+12	-4.94382E+06	0.99199
88	9.8304E+13	-6.15819E+06	1.00000
89	5.6869E+10	1.71386E+05	0.98969
90	4.0321E+12	1.84062E+04	0.91649
91	1.8000E+12	-2.38757E+06	0.99933
92	7.8000E+11	-1.29745E+02	0.99994
93	2.7309E+11	4.11537E+06	0.99826
94	8.1108E+12	-3.98209E+06	0.87659
95	1.9502E+15	1.07256E+07	0.75285
96	7.8431E+01	-4.30735E+03	0.96759
97	4.0846E+15	-7.02361E+02	0.99282
98	1.8714E+02	-1.01453E+02	0.73735
99	1.5007E+00	2.73343E+01	0.63000
100	4.0841E+08	1.51216E-02	1.00000
101	1.2935E+13	-3.09113E-01	0.99521
102	1.6770E+11	-9.53688E-03	0.82456
103	1.7783E+11	1.15967E+00	0.99633
104	1.2000E+13	-2.11495E-02	1.00000
105	4.4010E+13	2.66821E+00	0.97381
106	7.3861E+12	-3.15352E+02	0.96577
107	8.5365E+12	-6.51284E+01	0.99293
108	2.3956E+13	-4.49856E+01	0.89861
109	3.7000E+12	-1.21137E+01	0.99999
110	2.0000E+13	-1.64033E+02	1.00000
111	1.0000E+13	-4.53663E-05	1.00000
112	2.0000E+13	-3.52399E+01	0.99986
113	9.0021E+11	-3.49269E-06	0.99876
114	2.0000E+12	-1.38230E-05	0.99984
115	1.1683E+13	-5.05361E+01	0.99975
116	2.3995E+12	-1.58091E+01	0.96025
117	8.4152E+12	-5.36672E+00	0.95539
118	7.8629E+15	4.47638E+01	0.98349
119	2.2673E+14	-5.92424E+01	0.99988
120	1.2073E+08	-4.63221E-01	0.99916
121	4.1530E+07	-6.36365E+01	1.00000
122	4.6581E+04	4.43828E+01	1.00000
123	4.0000E+12	-1.43670E-06	1.00000

TABLE D.2.—Continued.

(h) Continued.

124	3.6920E+07	-2.59910E+02	0.97684
125	2.9991E+10	1.53282E+01	0.99143
126	3.1036E+10	-6.14560E-02	1.00000
127	9.5871E+11	-1.42067E+00	0.69023
128	5.4198E+09	1.06158E-01	0.99950
129	9.0137E+15	-7.80955E-05	0.00034
130	9.1608E+15	2.06336E-01	0.10093
131	5.0000E+12	-2.55037E-04	0.70678
132	6.4244E+15	-2.67106E-02	0.10426
133	3.6000E+13	-1.59443E-02	0.96381

DERIVATIVES (CGS UNITS): T 5.52418E+00 RHO -1.17628E-06 V 3.11322E+00

MIXTURE MOLECULAR WEIGHT 28.19088 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) -8.47574E+08 MASS FRACTION SUM 1.00000000

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 4.559998E+00 S UP TO THIS TIME - 4.559998E+00 S

TIME 2.94056E-04 SEC AREA 1.43983E+03 SQ CM AXIAL POSITION 4.70000E+01 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.73099
VELOCITY (CM/SEC)	159772.69
DENSITY (G/CM**3)	2.43059E-04
TEMPERATURE (DEG K)	2389.90
MASS FLOW RATE (G/SEC)	5.59145E+04
ENTROPY (CAL/G/DEG K)	2.3067
MACH NUMBER	1.6664
GAMMA	1.2739
ENTHALPY (CAL/G)	3.80606E+02
SP. HEAT (CP) (CAL/G/DEG K)	3.35629E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	88
AVERAGE STEP SIZE	0.80410E-01
METHOD ORDER	3
TOTAL NUMBER OF STEPS	201
FUNCT EVALUATIONS	329
JACOBIAN EVALUATIONS	42

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	6.02064E-11	6.82084E-06	-5.87364E-06
CH3	1.19228E-09	1.35075E-04	-1.20699E-04
H	4.30898E-08	4.88168E-03	-5.41198E-04
H2	3.85719E-08	4.36984E-03	-2.36473E-04
O2	8.63190E-07	9.77915E-02	-1.07343E-03
HO2	1.74059E-10	1.97193E-05	-5.79197E-07
O	1.10579E-07	1.25275E-02	-8.86814E-04
OH	1.49823E-07	1.69736E-02	-1.37747E-04
H2O	7.20497E-07	8.16257E-02	7.73146E-04
CH3O	6.46103E-12	7.31976E-07	-5.46729E-07
CH2O	1.83927E-11	2.08373E-06	-1.59315E-06
C2H6	8.02425E-14	9.09074E-09	-4.07503E-08
C2H5	6.65571E-16	7.54031E-11	-7.03961E-10
C2H4	3.70903E-13	4.20199E-08	-7.96112E-08
CH2	1.08162E-11	1.22538E-06	-1.05343E-06
C2H3	1.23486E-14	1.39899E-09	-3.10263E-09
C2H2	6.54397E-14	7.41372E-09	-1.35717E-08
HCO	1.13443E-12	1.28520E-07	-9.92805E-08
C2H2O	1.85990E-14	2.10709E-09	-2.84900E-09
C2H	3.82673E-16	4.33534E-11	-7.74788E-11
CO	1.33005E-07	1.50683E-02	-2.11330E-03
C2HO	8.24620E-14	9.34220E-09	-1.63594E-08
CH	2.29895E-12	2.60450E-07	-2.33637E-07
CO2	2.94490E-07	3.33630E-02	2.24375E-03
H2O2	1.00854E-11	1.14258E-06	-1.66092E-07
N2	6.47146E-06	7.33158E-01	-1.39162E-05
HCN	3.70069E-13	4.19255E-08	-2.92180E-08
N	1.07008E-12	1.21230E-07	1.50882E-08
CN	2.42331E-15	2.74539E-10	-1.86181E-10
HNCO	5.24095E-14	5.93752E-09	-1.41584E-09
NCO	1.58350E-14	1.79396E-09	-1.00964E-09
NH2	2.39470E-12	2.71298E-07	1.01137E-08
NO	6.36990E-10	7.21651E-05	2.77805E-05
NH	6.78360E-14	7.68520E-09	1.22212E-09
NO2	4.20865E-13	4.76801E-08	1.94602E-08
N2O	6.50891E-12	7.37401E-07	1.75638E-08
HNO2	2.70052E-14	3.05944E-09	7.63746E-10
HNO3	3.13644E-18	3.55330E-13	9.72204E-14
HNO	9.25358E-14	1.04835E-08	1.98449E-09

REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	1.7934E+09	-5.63144E+07	0.97085
2	1.0284E+13	4.87310E+04	0.17515
3	6.0086E+08	-8.10281E+04	0.74230
4	1.6106E+13	8.02175E+05	0.17803
5	8.7054E+12	-3.40203E+06	0.17782
6	5.7214E+10	1.20753E+06	0.04232
7	6.3000E+12	9.19504E+06	0.04069
8	6.0059E+11	1.18884E+07	1.00000
9	1.0687E+13	-1.07608E+06	0.04666
10	1.7121E+13	-6.17155E+03	0.99996
11	2.1638E+13	-1.39501E+04	0.99996
12	4.1460E+13	-1.78596E+05	0.99996
13	1.4626E+14	4.90362E+05	0.87112
14	6.9790E+11	-8.62886E+01	0.98542
15	4.8000E+13	-1.52163E+03	0.99690
16	2.0000E+13	-2.72888E+05	0.99900
17	1.7512E+13	-1.16610E+04	0.99919
18	1.4561E+10	3.36432E+04	1.00000
19	3.7048E+12	-6.08421E+04	0.99919
20	1.6340E+12	-2.24112E+04	0.99211
21	2.6012E+12	-4.84566E+04	1.00000
22	8.7238E+12	-4.48370E+04	0.99997
23	3.5548E+12	2.89131E+05	0.99840
24	4.1951E+12	-6.01287E+04	1.00000
25	6.0000E+12	-3.24505E+03	0.99996
26	3.3000E+13	-6.17739E+04	1.00000
27	5.0000E+12	-1.17527E+04	0.99996
28	3.0000E+13	-4.40179E+00	0.99115
29	3.0000E+13	-1.99072E-04	0.99923
30	6.8928E+06	-9.27869E+00	0.51982
31	1.9939E+13	-1.16664E+05	0.99914
32	4.2387E+13	-1.19334E+05	0.99324
33	1.4428E+12	1.81146E+03	0.95008
34	3.0680E+11	-1.14685E+03	0.98770
35	3.6459E+13	-5.50197E+03	0.86475
36	2.0000E+13	-8.05112E+02	0.86453
37	8.6245E+11	-8.52231E+04	1.00000
38	1.2020E+12	-1.83268E+04	1.00000
39	1.0000E+13	-5.65020E+04	1.00000
40	5.0000E+13	-6.47548E+04	0.87289
41	3.0000E+13	-4.30850E+01	0.99998
42	6.5630E+12	-2.90165E+00	0.99994
43	1.0000E+13	-8.70650E-02	1.00000
44	2.8000E+13	-2.00975E+04	0.99986
45	3.9877E+12	-1.45773E+03	0.45025
46	5.4903E+12	3.62811E+04	0.93782
47	1.3915E+13	-1.86508E+02	0.44847
48	9.2767E+12	-4.89658E+01	0.45039
49	2.0000E+13	-7.12066E+04	1.00000
50	6.5192E+10	-2.68353E+04	0.65700
51	5.0000E+13	-2.61963E+03	0.99880
52	2.2096E+12	-6.48701E+06	1.00000
53	2.0000E+13	-7.88882E+06	1.00000
54	1.9577E+09	4.81299E+05	0.99179
55	2.3302E+13	-3.15263E+07	0.99980

TABLE D.2.—Continued.

(h) Concluded.

56	1.0791E+13	-2.02655E+06	0.99980
57	1.6714E+13	-6.98141E+06	0.99980
58	1.3820E+11	-7.49698E+02	0.99976
59	1.4666E+13	-2.99182E+04	0.99518
60	2.0000E+13	-1.23798E+06	0.79714
61	8.1934E+07	1.31009E+06	0.81871
62	2.2115E+11	1.03927E+06	0.99564
63	1.6821E+11	2.72626E+06	0.99566
64	2.2115E+11	-6.37970E+06	0.99565
65	3.7000E+12	-2.71234E+06	1.00000
66	1.0000E+13	-2.42006E+07	1.00000
67	5.6453E+12	-5.39733E+07	0.99999
68	2.0256E+11	-2.23498E+03	0.93021
69	7.0570E+12	-3.14433E+06	0.93020
70	2.6033E+13	-4.68386E+05	0.92997
71	5.0000E+12	-6.97522E+02	0.99981
72	4.0000E+13	-1.03379E+04	1.00000
73	3.0000E+13	-1.77206E+07	0.98129
74	3.0000E+13	-5.52331E+06	0.99604
75	3.0000E+13	-8.93434E+06	0.99604
76	2.0000E+13	-1.46561E+06	0.99602
77	1.0929E+13	2.36345E+07	0.83462
78	1.0122E+15	-2.78245E+08	0.98353
79	1.0885E+08	-5.36054E+05	0.31370
80	3.3782E+11	-8.84910E+08	0.31254
81	4.6003E+11	-9.06117E+06	0.85463
82	1.4226E+12	8.23685E+06	0.00025
83	5.9804E+12	1.06713E+08	0.00169
84	2.3219E+13	1.09010E+07	0.00348
85	4.6528E+13	-2.44673E+08	0.78744
86	4.0506E+13	-5.27725E+08	0.78818
87	8.0000E+12	-1.88176E+08	0.78813
88	1.0697E+14	-3.63733E+08	0.78854
89	4.0926E+11	-6.72749E+06	0.88377
90	4.5140E+12	-3.47400E+06	0.88415
91	1.8000E+12	2.56925E+04	0.45321
92	7.8000E+11	-3.80603E+05	0.97550
93	9.9220E+12	-2.35229E+07	0.02159
94	1.3126E+13	-6.22577E+07	0.00323
95	1.8022E+15	-1.42386E+09	0.88687
96	3.1563E+05	-5.07962E+08	0.97603
97	2.9708E+15	-2.11259E+08	0.97604
98	3.6600E+05	-2.66489E+07	0.97595
99	1.2142E+04	-7.58392E+06	0.97600
100	1.8302E+09	1.50970E+03	1.00000
101	1.9655E+13	6.07974E+03	0.90889
102	7.9062E+11	1.06870E+04	0.90921
103	2.2182E+11	-2.71972E+03	0.94565
104	1.2000E+13	-4.18981E+03	0.99975
105	7.0673E+13	-5.50064E+03	0.54791
106	1.5031E+13	5.11157E+02	0.24211
107	1.6699E+13	-1.50819E+03	0.26818
108	2.5924E+13	-3.19571E+03	0.54868
109	3.7000E+12	2.65170E+01	0.34238
110	2.0000E+13	-6.06163E+04	0.99999
111	1.0000E+13	-5.05770E-01	0.99349
112	2.0000E+13	-8.22439E+03	0.99941
113	1.9730E+12	-1.97772E+03	1.00000
114	2.0000E+12	-3.56666E+03	0.99980
115	1.6042E+13	-7.38369E+03	0.07615
116	2.3108E+12	-2.49651E+02	0.01194
117	8.8206E+12	-2.50632E+05	0.78562
118	7.1749E+15	-4.90809E+06	0.88803
119	2.5463E+14	-1.79043E+06	0.78598
120	6.4580E+09	-7.04101E+06	0.97980
121	1.4962E+09	-2.73988E+06	0.97984
122	1.9161E+07	1.74320E+07	0.99831
123	4.0000E+12	-2.35361E+00	0.99568
124	2.8189E+09	-7.34631E+05	0.86997
125	2.7394E+11	-2.15135E+05	0.81540
126	2.5402E+11	-1.09650E+05	0.99999
127	3.1578E+12	-7.61702E+05	0.81571
128	5.3486E+10	-2.91988E+03	0.88751
129	6.6776E+15	-8.14530E-02	0.00003
130	8.0103E+15	-6.42917E+03	0.00113
131	5.0000E+12	-1.77807E+04	0.96366
132	6.1272E+15	-4.21056E+05	0.33831
133	3.6000E+13	-5.67397E+05	0.96378

```
DERIVATIVES (CGS UNITS): T          2.14301E+01    RHO        -1.83017E-06     V          1.99510E+00

MIXTURE MOLECULAR WEIGHT     27.53632     TOTAL ENERGY EXCHANGE RATE   -4.83687E+09      MASS FRACTION SUM    1.00000003
                                            (CAL-CM**3/G**2/SEC)

_____________________________________________________

   COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP -  5.949997E+00  S     UP TO THIS TIME -  1.321999E+01  S

(LSENS)     END OF THIS CASE

            SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

               TOTAL NO. OF STEPS -                    201
               TOTAL NO. OF DERIVATIVE EVALUATIONS -   329
               TOTAL NO. OF JACOBIAN EVALUATIONS -      42
               TOTAL CPU TIME -                 13.219994 S


                        TOTAL CPU TIME (INCLUDING I/O) REQUIRED =     15.500000 S


(LSENS)     READ DATA FOR NEXT CASE
```

TABLE D.2.—Continued.

(i) Case 9

```
                    **  DATA LINES  **
              1         2         3         4         5         6         7         8
CC  12345678901234567890123456789012345678901234567890123456789012345678901234567890

      LSENS   METHANE  AIR  MECHANISM   ASSIGNED (CONST.) TEMP. FLOW PROBLEM  CASE 9
     REPEAT
     DISTANCE  PRESSURE
      &prob  cx0=1.730, combus=.true., exchr=.false.,
        print=25.0,42.0,48.0,  &end
      &tmpdat  cx0=1700.0,  &end
      &start  area=1000.0, mach=2.0,  &end
     CH4        0.049768
     O2         0.199072
     N2         0.75116
     CN         0.0000001
     END
      &solver  emax=1.0E-4, atolsp=1.0E-13,  &end
     FINIS
```

```
                    **  EQUILIBRIUM CALCULATION  **

          THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED TEMPERATURE AND PRESSURE

                          INITIAL STATE              FINAL STATE              FINAL/INITIAL RATIO

PRESSURE                       1.7300                   1.7300                    1.0000
 (ATM)
VELOCITY                       0.00                     0.00                      1.0000
 (CM/SEC)
DENSITY                     3.49869E-04              3.49843E-04                  0.9999
 (G/CM**3)
TEMPERATURE                   1700.00                  1700.00                     1.0000
 (DEG K)
ENTHALPY                      379.22696                 41.16700                   0.10856
 (CAL/G)
INTERNAL ENERGY               259.48010                -78.58891                  -0.30287
 (CAL/G)
SP. HEAT (CP)                   0.32691                  0.33141                   1.01374
 (CAL/G/DEG K)
ENTROPY                         2.1420                   2.1511                    1.0042
 (CAL/G/DEG K)
MACH NUMBER                     0.0000                   0.0000                    1.0000

GAMMA                           1.2746                   1.2699                    0.9963

SONIC VELOCITY                79913.95                 79789.35                    0.9984
 (CM/SEC)

                                                  SPECIES     MOLE FRACTION
                                                   CH4         2.82089E-10
                                                   CH3         2.82089E-10
                                                   H           2.43981E-07
                                                   H2          4.80198E-06
                                                   O2          9.84867E-02
                                                   HO2         9.40550E-07
                                                   O           1.05975E-05
                                                   OH          2.67611E-04
                                                   H2O         9.93892E-02
                                                   CH3O        2.82089E-10
                                                   CH2O        2.82089E-10
                                                   C2H6        2.82089E-10
                                                   C2H5        2.82089E-10
                                                   C2H4        2.82089E-10
                                                   CH2         2.82089E-10
                                                   C2H3        2.82089E-10
                                                   C2H2        2.82089E-10
                                                   HCO         2.82089E-10
                                                   C2H2O       2.82089E-10
                                                   C2H         2.82089E-10
                                                   CO          8.17330E-06
                                                   C2HO        2.82089E-10
                                                   CH          2.82089E-10
                                                   CO2         4.97562E-02
                                                   H2O2        2.40530E-08
                                                   N2          7.50131E-01
                                                   HCN         2.82089E-10
                                                   N           2.82089E-10
                                                   CN          2.82089E-10
                                                   HNCO        2.82089E-10
                                                   NCO         2.82089E-10
                                                   NH2         2.82089E-10
                                                   NO          1.93922E-03
                                                   NH          2.82089E-10
                                                   NO2         5.54534E-06
                                                   N2O         1.46579E-07
                                                   HNO2        8.25410E-08
                                                   HNO3        2.82089E-10
                                                   HNO         2.82089E-10

MIXTURE MOLECULAR WEIGHT                                       28.20888

D(LOG VOLUME)/D(LOG T)                                          1.0010
    AT CONSTANT P

D(LOG VOLUME)/D(LOG P)                                         -1.0000
    AT CONSTANT T


                COMPUTATIONAL WORK REQUIRED FOR EQUILIBRIUM CALCULATION:
                NO. OF ITERATIONS =     23     CPU TIME =  8.000183E-02 S
```

TABLE D.2.—Continued.

(i) Continued.

** INITIAL CONDITIONS **

TIME 0.00000E+00 SEC AREA 1.00000E+03 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.73000
VELOCITY (CM/SEC)	159827.88
DENSITY (G/CM**3)	3.49869E-04
TEMPERATURE (DEG K)	1700.00
MASS FLOW RATE (G/SEC)	5.59188E+04
ENTROPY (CAL/G/DEG K)	2.1420
MACH NUMBER	2.0000
GAMMA	1.2746
ENTHALPY (CAL/G)	3.79227E+02
SP. HEAT (CP) (CAL/G/DEG K)	3.26913E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	6.17216E-07	4.97680E-02	-1.50903E-05
CH3	0.00000E+00	0.00000E+00	1.50903E-05
H	0.00000E+00	0.00000E+00	7.44369E-06
H2	0.00000E+00	0.00000E+00	0.00000E+00
O2	2.46886E-06	1.99072E-01	-8.05210E-05
HO2	0.00000E+00	0.00000E+00	7.64658E-06
O	0.00000E+00	0.00000E+00	7.28745E-05
OH	0.00000E+00	0.00000E+00	0.00000E+00
H2O	0.00000E+00	0.00000E+00	0.00000E+00
CH3O	0.00000E+00	0.00000E+00	0.00000E+00
CH2O	0.00000E+00	0.00000E+00	0.00000E+00
C2H6	0.00000E+00	0.00000E+00	0.00000E+00
C2H5	0.00000E+00	0.00000E+00	0.00000E+00
C2H4	0.00000E+00	0.00000E+00	0.00000E+00
CH2	0.00000E+00	0.00000E+00	0.00000E+00
C2H3	0.00000E+00	0.00000E+00	0.00000E+00
C2H2	0.00000E+00	0.00000E+00	0.00000E+00
HCO	0.00000E+00	0.00000E+00	0.00000E+00
C2H2O	0.00000E+00	0.00000E+00	0.00000E+00
C2H	0.00000E+00	0.00000E+00	0.00000E+00
CO	0.00000E+00	0.00000E+00	0.00000E+00
C2HO	0.00000E+00	0.00000E+00	0.00000E+00
CH	0.00000E+00	0.00000E+00	0.00000E+00
CO2	0.00000E+00	0.00000E+00	0.00000E+00
H2O2	0.00000E+00	0.00000E+00	0.00000E+00
N2	9.31578E-06	7.51160E-01	-1.20855E-11
HCN	0.00000E+00	0.00000E+00	0.00000E+00
N	0.00000E+00	0.00000E+00	0.00000E+00
CN	1.24019E-12	1.00000E-07	-7.28744E-05
HNCO	0.00000E+00	0.00000E+00	0.00000E+00
NCO	0.00000E+00	0.00000E+00	7.28744E-05
NH2	0.00000E+00	0.00000E+00	0.00000E+00
NO	0.00000E+00	0.00000E+00	0.00000E+00
NH	0.00000E+00	0.00000E+00	0.00000E+00
NO2	0.00000E+00	0.00000E+00	0.00000E+00
N2O	0.00000E+00	0.00000E+00	1.20855E-11
HNO2	0.00000E+00	0.00000E+00	0.00000E+00
HNO3	0.00000E+00	0.00000E+00	0.00000E+00
HNO	0.00000E+00	0.00000E+00	0.00000E+00

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	9.7244E+05	6.08103E+01	1.00000
2	3.7198E+12	0.00000E+00	0.00000
3	5.0180E+06	6.24678E+01	1.00000
4	5.9162E+12	0.00000E+00	0.00000
5	5.6736E+12	0.00000E+00	0.00000
6	4.9334E+09	0.00000E+00	0.00000
7	6.3000E+12	0.00000E+00	0.00000
8	9.9825E+10	0.00000E+00	0.00000
9	1.2247E+13	0.00000E+00	0.00000
10	7.4740E+12	0.00000E+00	0.00000
11	1.1064E+13	0.00000E+00	0.00000
12	3.0690E+13	0.00000E+00	0.00000
13	1.0344E+13	0.00000E+00	0.00000
14	4.5524E+11	0.00000E+00	0.00000
15	4.8000E+13	0.00000E+00	0.00000
16	2.0000E+13	0.00000E+00	0.00000
17	7.3247E+12	0.00000E+00	0.00000
18	1.6606E+07	0.00000E+00	0.00000
19	3.3351E+12	0.00000E+00	0.00000
20	1.5053E+12	0.00000E+00	0.00000
21	2.3618E+12	0.00000E+00	0.00000
22	5.6904E+12	0.00000E+00	0.00000
23	2.3080E+11	0.00000E+00	0.00000
24	4.2857E+12	0.00000E+00	0.00000
25	6.0000E+12	0.00000E+00	0.00000
26	3.3000E+13	0.00000E+00	0.00000
27	5.0000E+12	0.00000E+00	0.00000
28	3.0000E+13	0.00000E+00	0.00000
29	3.0000E+13	0.00000E+00	0.00000
30	7.3700E+02	0.00000E+00	0.00000
31	8.5640E+12	0.00000E+00	0.00000
32	1.7046E+13	0.00000E+00	0.00000
33	7.9329E+11	0.00000E+00	0.00000
34	3.0160E+11	0.00000E+00	0.00000
35	3.2072E+13	0.00000E+00	0.00000
36	2.0000E+13	0.00000E+00	0.00000
37	6.9656E+11	0.00000E+00	0.00000
38	1.2020E+12	0.00000E+00	0.00000
39	1.0000E+13	0.00000E+00	0.00000
40	5.0000E+13	0.00000E+00	0.00000
41	3.0000E+13	0.00000E+00	0.00000
42	5.5320E+12	0.00000E+00	0.00000
43	1.0000E+13	0.00000E+00	0.00000
44	2.8000E+13	0.00000E+00	0.00000
45	3.0859E+12	0.00000E+00	0.00000
46	4.0962E+12	0.00000E+00	0.00000
47	7.0241E+12	0.00000E+00	0.00000
48	4.6827E+12	0.00000E+00	0.00000
49	2.0000E+13	0.00000E+00	0.00000
50	3.8682E+08	0.00000E+00	0.00000
51	5.0000E+13	0.00000E+00	0.00000
52	1.1974E+12	0.00000E+00	0.00000
53	2.0000E+13	0.00000E+00	0.00000
54	1.9307E+06	0.00000E+00	0.00000
55	2.1031E+13	0.00000E+00	0.00000
56	7.6735E+12	0.00000E+00	0.00000
57	1.2383E+13	0.00000E+00	0.00000
58	6.9803E+10	0.00000E+00	0.00000
59	1.2369E+13	0.00000E+00	0.00000
60	2.0000E+13	0.00000E+00	0.00000
61	3.2663E+04	0.00000E+00	0.00000
62	1.9580E+10	0.00000E+00	0.00000
63	1.4842E+10	0.00000E+00	0.00000
64	1.9580E+10	0.00000E+00	0.00000
65	3.7000E+12	0.00000E+00	0.00000
66	1.0000E+13	0.00000E+00	0.00000
67	2.6268E+12	0.00000E+00	0.00000
68	1.7601E+10	0.00000E+00	0.00000
69	3.5950E+12	0.00000E+00	0.00000
70	1.3413E+13	0.00000E+00	0.00000
71	5.0000E+12	0.00000E+00	0.00000
72	4.0000E+13	0.00000E+00	0.00000
73	3.0000E+13	0.00000E+00	0.00000
74	3.0000E+13	0.00000E+00	0.00000
75	3.0000E+13	0.00000E+00	0.00000
76	2.0000E+13	0.00000E+00	0.00000
77	2.8889E+12	0.00000E+00	0.00000
78	7.1305E+14	0.00000E+00	0.00000

TABLE D.2.—Continued.

(i) Continued.

79	1.8492E+06	0.00000E+00	0.00000
80	3.1015E+11	0.00000E+00	0.00000
81	6.4836E+10	0.00000E+00	0.00000
82	2.9616E+11	0.00000E+00	0.00000
83	1.4726E+12	0.00000E+00	0.00000
84	7.1708E+12	0.00000E+00	0.00000
85	3.8799E+13	0.00000E+00	0.00000
86	3.7189E+13	0.00000E+00	0.00000
87	8.0000E+12	0.00000E+00	0.00000
88	9.7622E+13	0.00000E+00	0.00000
89	4.8329E+10	0.00000E+00	0.00000
90	3.9948E+12	0.00000E+00	0.00000
91	1.8000E+12	0.00000E+00	0.00000
92	7.8000E+11	0.00000E+00	0.00000
93	2.0307E+11	0.00000E+00	0.00000
94	7.7952E+12	0.00000E+00	0.00000
95	1.9630E+15	0.00000E+00	0.00000
96	3.9562E+01	0.00000E+00	0.00000
97	4.1765E+15	0.00000E+00	0.00000
98	1.0018E+02	0.00000E+00	0.00000
99	7.1175E-01	1.78032E-04	1.00000
100	3.6090E+08	0.00000E+00	0.00000
101	1.2497E+13	0.00000E+00	0.00000
102	1.4798E+11	0.00000E+00	0.00000
103	1.7462E+11	0.00000E+00	0.00000
104	1.2800E+13	0.00000E+00	0.00000
105	4.2324E+13	0.00000E+00	0.00000
106	6.9658E+12	0.00000E+00	0.00000
107	8.0770E+12	0.00000E+00	0.00000
108	2.3801E+13	5.95338E+02	1.00000
109	3.7000E+12	0.00000E+00	0.00000
110	2.0000E+13	0.00000E+00	0.00000
111	1.0000E+13	0.00000E+00	0.00000
112	2.0000E+13	0.00000E+00	0.00000
113	8.4381E+11	0.00000E+00	0.00000
114	2.0000E+12	0.00000E+00	0.00000
115	1.1405E+13	0.00000E+00	0.00000
116	2.4070E+12	0.00000E+00	0.00000
117	8.3826E+12	0.00000E+00	0.00000
118	7.9225E+15	0.00000E+00	0.00000
119	2.2457E+14	0.00000E+00	0.00000
120	8.6958E+07	0.00000E+00	0.00000
121	3.1028E+07	0.00000E+00	0.00000
122	2.8358E+04	0.00000E+00	0.00000
123	4.0000E+12	0.00000E+00	0.00000
124	2.5566E+07	0.00000E+00	0.00000
125	2.4991E+10	-9.87306E-05	1.00000
126	2.6097E+10	0.00000E+00	0.00000
127	8.6897E+11	0.00000E+00	0.00000
128	4.4875E+09	0.00000E+00	0.00000
129	9.2394E+15	0.00000E+00	0.00000
130	9.2627E+15	0.00000E+00	0.00000
131	5.0000E+12	0.00000E+00	0.00000
132	6.4495E+15	0.00000E+00	0.00000
133	3.6000E+13	0.00000E+00	0.00000

DERIVATIVES (CGS UNITS): T 0.00000E+00 RHO -1.31388E-09 V 0.00000E+00

MIXTURE MOLECULAR WEIGHT 28.21102 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 5.92105E+06 MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 1.190010 S

TIME 3.00323E-04 SEC AREA 1.00533E+03 SQ CM AXIAL POSITION 4.80000E+01 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.73000
VELOCITY (CM/SEC)	159827.88
DENSITY (G/CM**3)	3.48013E-04
TEMPERATURE (DEG K)	1700.00
MASS FLOW RATE (G/SEC)	5.59188E+04
ENTROPY (CAL/G/DEG K)	2.1620
MACH NUMBER	1.9915
GAMMA	1.2787
ENTHALPY (CAL/G)	3.22341E+02
SP. HEAT (CP) (CAL/G/DEG K)	3.24936E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	6
AVERAGE STEP SIZE	0.10519E+01
METHOD ORDER	4
TOTAL NUMBER OF STEPS	137
FUNCT EVALUATIONS	184
JACOBIAN EVALUATIONS	25

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
CH4	2.88178E-07	2.32367E-02	-2.67162E-03	1	9.7244E+05	-1.35854E+02	0.82561
CH3	1.91140E-08	1.54122E-03	6.04892E-06	2	3.7198E+12	1.98822E+03	0.72567
H	3.09554E-10	2.49603E-05	4.69517E-06	3	5.0180E+06	-2.16252E+02	0.89255
H2	2.98194E-08	2.40443E-03	2.39713E-04	4	5.9162E+12	5.33818E+03	0.99295
O2	2.18046E-06	1.75817E-01	-3.02746E-03	5	5.6736E+12	1.55999E+04	0.95284
HO2	3.45739E-09	2.78780E-04	1.33554E-05	6	4.9336E+09	1.63935E+03	0.96563
O	3.81901E-10	3.07938E-05	5.71794E-06	7	6.3000E+12	-5.92180E+03	0.83083
OH	1.21275E-09	9.77881E-05	1.69045E-05	8	9.9825E+10	2.13057E+03	1.00000
H2O	3.78990E-07	3.05592E-02	4.30922E-03	9	1.2247E+13	8.16156E+03	0.22092
CH3O	2.08432E-10	1.68065E-05	-5.14536E-07	10	7.4740E+12	4.52179E+02	0.99990
CH2O	4.37161E-08	3.52496E-03	-1.69220E-04	11	1.1064E+13	8.25857E+02	1.00000
C2H6	2.36730E-08	1.90883E-03	-4.73879E-05	12	3.0690E+13	7.27479E+03	0.99998

TABLE D.2.—Continued.

(i) Continued.

C2H5	9.88112E-12	7.96745E-07	1.38219E-07
C2H4	4.70382E-08	3.79284E-03	5.12019E-04
CH2	1.79722E-11	1.44916E-06	5.07118E-07
C2H3	2.42732E-11	1.95723E-06	6.49998E-07
C2H2	2.30923E-09	1.86200E-04	5.30853E-05
HCO	1.72899E-11	1.39414E-06	2.03886E-07
C2H2O	1.96327E-11	1.58304E-06	5.91704E-07
C2H	3.13259E-14	2.52590E-09	1.47195E-09
CO	1.13925E-07	9.18610E-03	1.72638E-03
C2HO	1.07987E-11	8.70729E-07	4.19384E-07
CH	6.98679E-15	5.63366E-10	3.47858E-10
CO2	2.59512E-09	2.09253E-04	6.91888E-05
H2O2	9.50117E-12	7.66109E-07	6.55731E-08
N2	9.26636E-06	7.47175E-01	-1.72464E-09
HCN	2.55361E-15	2.05905E-10	4.97298E-11
N	7.78540E-17	6.27760E-12	7.50689E-13
CN	3.20665E-18	2.58562E-13	6.29686E-13
HNCO	9.54948E-13	7.70004E-08	-2.18034E-09
NCO	1.44339E-15	1.16385E-10	4.35551E-12
NH2	1.62101E-13	1.30707E-08	2.12906E-09
NO	1.05015E-13	8.46765E-09	4.81276E-10
NH	1.33005E-14	1.07246E-09	-1.74864E-10
NO2	1.16014E-14	9.35452E-10	-6.06635E-11
N2O	1.33766E-13	1.07860E-08	1.59959E-09
HNO2	1.80283E-18	1.45368E-13	3.08435E-14
HNO3	2.81432E-20	2.26928E-15	2.14810E-16
HNO	7.99676E-18	6.44803E-13	1.36210E-13

13	1.0344E+13	8.49427E+03	0.81160
14	4.5524E+11	5.62227E+01	0.69424
15	4.8000E+13	1.20132E+00	0.99099
16	2.0000E+13	5.67153E+01	0.99979
17	7.3247E+12	8.79821E+02	0.99909
18	1.6606E+07	7.99856E+01	0.99999
19	3.3351E+12	1.57065E+03	0.99984
20	1.5053E+12	6.56109E+02	0.92540
21	2.3618E+12	3.50311E+02	1.00000
22	5.6904E+12	8.43917E+02	0.99987
23	2.3080E+11	5.68072E+02	0.99023
24	4.2857E+12	1.87287E+03	1.00000
25	6.0000E+12	3.72067E-01	0.99953
26	3.3000E+13	2.52581E+00	1.00000
27	5.0000E+12	1.21519E+00	0.99992
28	3.0000E+13	1.07325E-01	0.99321
29	3.0000E+13	1.87195E-04	0.99388
30	7.3700E+02	-1.03774E-04	0.37322
31	8.5640E+12	6.23591E+01	1.00000
32	1.7046E+13	1.24122E+02	0.99999
33	7.9329E+11	1.81026E+01	0.98688
34	3.0160E+11	6.97369E+00	0.99995
35	3.2072E+13	1.80878E+01	0.99998
36	2.0000E+13	6.25400E-03	0.99688
37	6.9656E+11	1.35420E+02	1.00000
38	1.2020E+12	4.09293E-02	1.00000
39	1.0000E+13	1.08131E+00	1.00000
40	5.0000E+13	1.35345E+00	0.98075
41	3.0000E+13	4.80731E-02	1.00000
42	5.5320E+12	8.81928E-03	0.99488
43	1.0000E+13	9.62829E-03	1.00000
44	2.8000E+13	4.79306E+00	0.87075
45	3.0859E+12	1.50609E-01	0.24826
46	4.0962E+12	-4.57247E-02	0.18198
47	7.0241E+12	-1.18874E+00	0.77131
48	4.6827E+12	2.57325E-01	0.88765
49	2.0000E+13	1.23814E+00	1.00000
50	3.8682E+08	-5.90714E-01	0.43169
51	5.0000E+13	4.93893E-03	1.00000
52	1.1974E+12	4.49318E+03	0.99999
53	2.0000E+13	1.06547E+01	1.00000
54	1.9307E+06	8.63618E+00	0.99924
55	2.1031E+13	9.20600E+03	0.99999
56	7.6735E+12	8.57356E+02	0.99996
57	1.2383E+13	1.70697E+03	1.00000
58	6.9803E+10	4.81523E+02	0.99987
59	1.2369E+13	3.37507E+01	0.99996
60	2.0000E+13	1.09126E+04	0.99997
61	3.2663E+04	-2.80915E-02	0.30527
62	1.9580E+10	8.90671E-01	0.93114
63	1.4842E+10	8.92983E-01	0.99823
64	1.9580E+10	3.70312E+00	0.98816
65	3.7000E+12	5.53889E-04	0.99995
66	1.0000E+13	1.25787E+00	1.00000
67	2.6268E+12	8.49934E+02	1.00000
68	1.7601E+10	9.97184E-04	0.99973
69	3.5950E+12	6.45812E-01	0.99822
70	1.3413E+13	6.09738E-01	0.98962
71	5.0000E+12	1.33347E-02	1.00000
72	4.0000E+13	1.06678E-01	1.00000
73	3.0000E+13	9.33507E+03	0.99965
74	3.0000E+13	1.63558E+00	1.00000
75	3.0000E+13	5.19391E+00	1.00000
76	2.0000E+13	8.83818E-01	0.99999
77	2.8889E+12	5.11367E+03	0.99978
78	7.1305E+14	3.17676E+00	1.00000
79	1.8492E+06	3.79270E+00	0.99999
80	3.1015E+11	3.53445E+02	0.99895
81	6.4836E+10	2.10859E+02	1.00000
82	2.9616E+11	3.01034E+02	0.85055
83	1.4726E+12	8.15945E+03	0.99419
84	7.1708E+12	6.56932E+02	0.97431
85	3.8799E+13	3.32748E+02	0.97052
86	3.7189E+13	4.05126E+02	0.99924
87	8.0000E+12	2.75559E+02	0.99493

TABLE D.2.—Continued.
(i) Concluded.

88	9.7622E+13	8.62659E+02	1.00000
89	4.8329E+10	4.02368E+01	0.97804
90	3.9948E+12	-2.59592E+00	0.87229
91	1.8000E+12	1.77541E+02	0.99935
92	7.8000E+11	1.89410E-02	0.99997
93	2.0307E+11	2.19813E+02	0.99581
94	7.7952E+12	1.92744E+03	0.82808
95	1.9630E+15	-1.60454E+02	0.38383
96	3.9562E+01	-3.79522E-01	0.99178
97	4.1765E+15	5.04961E-02	0.99877
98	1.0018E+02	-1.43576E-02	0.95216
99	7.1175E-01	-5.92713E-04	0.78857
100	3.6090E+08	1.92921E-04	1.00000
101	1.2497E+13	8.63664E-06	0.87538
102	1.4798E+11	9.45868E-07	0.79383
103	1.7462E+11	-2.09982E-04	0.97918
104	1.2000E+13	1.21336E-07	1.00000
105	4.2324E+13	-6.12937E-06	0.81852
106	6.9658E+12	-2.13415E-04	0.07937
107	8.0770E+12	1.75791E-02	0.89171
108	2.3801E+13	1.33002E-03	0.96796
109	3.7000E+12	-1.33691E-03	0.99981
110	2.0000E+13	9.10278E-05	1.00000
111	1.0000E+13	9.27635E-12	0.99978
112	2.0000E+13	7.34138E-05	0.99499
113	8.4381E+11	5.11150E-09	0.99992
114	2.0000E+12	1.21159E-08	0.99998
115	1.1405E+13	1.51722E-03	0.99890
116	2.4070E+12	6.87200E-03	0.95237
117	8.3826E+12	3.01776E-04	0.98410
118	7.9225E+15	-4.00037E-04	0.92479
119	2.2457E+14	6.65828E-03	0.99991
120	8.6958E+07	-3.29896E-05	0.99929
121	3.1028E+07	-2.49967E-03	1.00000
122	2.8358E+04	8.28589E-04	1.00000
123	4.0000E+12	2.98303E-11	1.00000
124	2.5566E+07	-1.34240E-02	0.97458
125	2.4991E+10	-7.71212E-05	0.87975
126	2.6097E+10	1.10076E-05	1.00000
127	8.6897E+11	2.82732E-04	0.95165
128	4.4875E+09	1.27908E-05	0.99787
129	9.2394E+15	1.77363E-09	0.00014
130	9.2627E+15	-1.25361E-05	0.09402
131	5.0000E+12	9.61607E-08	0.94095
132	6.4495E+15	4.07424E-06	0.18977
133	3.6000E+13	2.85343E-06	0.98985

```
DERIVATIVES (CGS UNITS): T          0.00000E+00    RHO        -1.83068E-07    V          0.00000E+00

MIXTURE MOLECULAR WEIGHT     28.06136     TOTAL ENERGY EXCHANGE RATE   -1.95990E+09      MASS FRACTION SUM    1.00000001
                                               (CAL-CM**3/G**2/SEC)


COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP -  3.499985E-01  S     UP TO THIS TIME -  6.219994E+00  S


(LSENS)     END OF THIS CASE


            SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

               TOTAL NO. OF STEPS -                        137
               TOTAL NO. OF DERIVATIVE EVALUATIONS -       184
               TOTAL NO. OF JACOBIAN EVALUATIONS -          25
               TOTAL CPU TIME -                     6.219994 S


                          TOTAL CPU TIME (INCLUDING I/O) REQUIRED =      8.700005 S


(LSENS)     READ DATA FOR NEXT CASE
```

TABLE D.2.—Continued.

(j) Case 10

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

LSENS METHANOL - AIR COMBUSTION CASE 10

REACTION NUMBER	REACTION							REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	M	+	1*CH3OH	=	1*CH3	+	1*OH	3.20000E+18	0.0000	80000.00
2	1*O2	+	1*CH3OH	=	1*CH2OH	+	1*HO2	4.00000E+13	0.0000	50900.00
3	1*OH	+	1*CH3OH	=	1*CH2OH	+	1*H2O	4.00000E+12	0.0000	2000.00
4	1*O	+	1*CH3OH	=	1*CH2OH	+	1*OH	1.60000E+12	0.0000	2300.00
5	1*H	+	1*CH3OH	=	1*CH2OH	+	1*H2	3.20000E+13	0.0000	7000.00
6	1*H	+	1*CH3OH	=	1*CH3	+	1*H2O	5.00000E+12	0.0000	5300.00
7	1*CH3	+	1*CH3OH	=	1*CH2OH	+	1*CH4	2.00000E+11	0.0000	9800.00
8	1*HO2	+	1*CH3OH	=	1*CH2OH	+	1*H2O2	6.30000E+12	0.0000	19400.00
9	M	+	1*CH2OH	=	1*CH2O	+	1*H	2.50000E+13	0.0000	29000.00
10	1*O2	+	1*CH2OH	=	1*CH2O	+	1*HO2	1.00000E+12	0.0000	6000.00
11	M	+	1*CH4	=	1*CH3	+	1*H	2.00000E+17	0.0000	88000.00
12	1*H	+	1*CH4	=	1*CH3	+	1*H2	1.26000E+14	0.0000	11900.00
13	1*CH4	+	1*O2	=	1*CH3	+	1*HO2	7.94000E+13	0.0000	56000.00
14	1*O	+	1*CH4	=	1*CH3	+	1*OH	1.90000E+14	0.0000	11720.00
15	1*OH	+	1*CH4	=	1*CH3	+	1*H2O	2.50000E+13	0.0000	5010.00
16	1*CH3	+	1*O2	=	1*CH3O	+	1*O	2.40000E+13	0.0000	28680.00
17	1*CH3	+	1*OH	=	1*CH3O	+	1*H	6.30000E+12	0.0000	0.00
18	M	+	1*CH3O	=	1*CH2O	+	1*H	5.00000E+13	0.0000	21000.00
19			2*CH3	=	1*C2H6			2.40000E+14	-0.4000	0.00
20	1*H	+	1*C2H6	=	1*C2H5	+	1*H2	1.32000E+14	0.0000	9700.00
21	1*O	+	1*C2H6	=	1*C2H5	+	1*OH	1.13000E+14	0.0000	7850.00
22	1*OH	+	1*C2H6	=	1*C2H5	+	1*H2O	8.70000E+13	0.0000	3520.00
23	M	+	1*C2H5	=	1*C2H4	+	1*H	1.00000E+17	0.0000	31000.00
24	1*C2H5	+	1*O2	=	1*C2H4	+	1*HO2	2.00000E+12	0.0000	5000.00
25	1*H	+	1*C2H5	=	1*C2H4	+	1*H2	4.80000E+13	0.0000	0.00
26	1*CH3	+	1*CH2	=	1*C2H4	+	1*H	2.00000E+13	0.0000	0.00
27	1*H	+	1*C2H4	=	1*H2	+	1*C2H3	1.50000E+14	0.0000	10200.00
28	M	+	1*C2H4	=	1*C2H2	+	1*H2	2.60000E+17	0.0000	79300.00
29	1*C2H4	+	1*OH	=	1*C2H3	+	1*H2O	4.80000E+12	0.0000	1230.00
30	1*C2H4	+	1*OH	=	1*CH3	+	1*CH2O	2.00000E+12	0.0000	960.00
31	1*C2H4	+	1*O	=	1*CH3	+	1*HCO	3.30000E+12	0.0000	1130.00
32	1*C2H4	+	1*O	=	1*CH2O	+	1*CH2	2.50000E+13	0.0000	5000.00
33	M	+	1*C2H3	=	1*C2H2	+	1*H	3.00000E+15	0.0000	32000.00
34	1*C2H3	+	1*O2	=	1*CH2O	+	1*HCO	3.98000E+12	0.0000	-250.00
35	1*C2H3	+	1*H	=	1*C2H2	+	1*H2	6.00000E+12	0.0000	0.00
36	1*C2H3	+	1*O	=	1*C2H2O	+	1*H	3.30000E+13	0.0000	0.00
37	1*C2H3	+	1*OH	=	1*C2H2	+	1*H2O	5.00000E+12	0.0000	0.00
38	1*C2H3	+	1*CH2	=	1*C2H2	+	1*CH3	3.00000E+13	0.0000	0.00
39	1*C2H3	+	1*C2H	=	2*C2H2			3.00000E+13	0.0000	0.00
40	M	+	1*C2H2	=	1*C2H	+	1*H	4.20000E+16	0.0000	107000.00
41	1*C2H2	+	1*O	=	1*CH2	+	1*CO	1.60000E+14	0.0000	9890.00
42	1*C2H2	+	1*O	=	1*C2HO	+	1*H	4.00000E+14	0.0000	10660.00
43	1*C2H2	+	1*OH	=	1*C2H	+	1*H2O	6.30000E+12	0.0000	7000.00
44	1*C2H2	+	1*OH	=	1*C2H2O	+	1*H	3.20000E+11	0.0000	200.00
45	1*C2H	+	1*O2	=	1*C2HO	+	1*O	5.00000E+13	0.0000	1500.00
46	1*C2H	+	1*OH	=	1*C2HO	+	1*H	2.00000E+13	0.0000	0.00
47	1*C2HO	+	1*O2	=	2*CO	+	1*OH	1.46000E+12	0.0000	2500.00
48	1*C2HO	+	1*O	=	2*CO	+	1*H	1.20200E+12	0.0000	0.00
49	1*C2HO	+	1*OH	=	2*HCO			1.00000E+13	0.0000	0.00
50	1*C2HO	+	1*H	=	1*CH2	+	1*CO	5.00000E+13	0.0000	0.00
51	1*C2HO	+	1*CH2	=	1*C2H3	+	1*CO	3.00000E+13	0.0000	0.00
52	1*C2HO	+	1*CH2	=	1*CH2O	+	1*C2H	1.00000E+13	0.0000	2000.00
53			2*C2HO	=	1*C2H2	+	2*CO	1.00000E+13	0.0000	0.00
54	1*C2H2O	+	1*OH	=	1*CH2O	+	1*HCO	2.80000E+13	0.0000	0.00
55	1*C2H2O	+	1*OH	=	1*C2HO	+	1*H2O	7.50000E+12	0.0000	3000.00
56	1*C2H2O	+	1*H	=	1*CH3	+	1*CO	1.13000E+13	0.0000	3428.00
57	1*C2H2O	+	1*H	=	1*C2HO	+	1*H2	7.50000E+13	0.0000	8000.00
58	1*C2H2O	+	1*O	=	1*C2HO	+	1*OH	5.00000E+13	0.0000	8000.00
59	1*C2H2O	+	1*O	=	1*CH2O	+	1*CO	2.00000E+13	0.0000	0.00
60	M	+	1*C2H2O	=	1*CH2	+	1*CO	2.00000E+16	0.0000	60000.00
61	1*C2H	+	1*O	=	1*CO	+	1*CH	5.00000E+13	0.0000	0.00
62	1*CH3O	+	1*O2	=	1*CH2O	+	1*HO2	1.00000E+13	0.0000	7170.00
63	1*CH3O	+	1*H	=	1*CH2O	+	1*H2	2.00000E+13	0.0000	0.00
64	M	+	1*CH2O	=	1*HCO	+	1*H	5.00000E+16	0.0000	81000.00
65	1*CH2O	+	1*OH	=	1*HCO	+	1*H2O	3.00000E+13	0.0000	1200.00
66	1*CH2O	+	1*H	=	1*HCO	+	1*H2	2.50000E+13	0.0000	3990.00
67	1*CH2O	+	1*O	=	1*HCO	+	1*OH	3.50000E+13	0.0000	3510.00
68	1*CH3	+	1*CH2O	=	1*CH4	+	1*HCO	1.00000E+10	0.5000	6000.00
69	1*CH3	+	1*HCO	=	1*CH4	+	1*CO	3.00000E+11	0.5000	0.00
70	1*CH3	+	1*HO2	=	1*CH3O	+	1*OH	2.00000E+13	0.0000	0.00
71	M	+	1*CH3	=	1*CH2	+	1*H	1.95000E+16	0.0000	91600.00
72	1*H	+	1*CH3	=	1*H2	+	1*CH2	2.70000E+11	0.6700	25700.00
73	1*O	+	1*CH3	=	1*OH	+	1*CH2	1.90000E+11	0.6800	25700.00
74	1*OH	+	1*CH3	=	1*H2O	+	1*CH2	2.70000E+11	0.6700	25700.00
75	1*CH	+	1*CO2	=	1*HCO	+	1*CO	3.70000E+12	0.0000	0.00
76	1*CH	+	1*O2	=	1*HCO	+	1*O	1.00000E+13	0.0000	0.00
77	1*CH2	+	1*O2	=	1*CH2O	+	1*O	5.00000E+11	0.5000	6960.00
78	1*CH2	+	1*O	=	1*CH	+	1*OH	2.00000E+11	0.7000	25800.00
79	1*CH2	+	1*OH	=	1*CH	+	1*H2O	5.00000E+11	0.5000	5900.00
80	1*CH2	+	1*H	=	1*CH	+	1*H2	3.20000E+11	0.7000	4970.00
81			2*CH2	=	1*C2H3	+	1*H	5.00000E+12	0.0000	0.00
82			2*CH2	=	1*C2H2	+	1*H2	4.00000E+13	0.0000	0.00
83	1*HCO	+	1*O2	=	1*CO	+	1*HO2	3.00000E+13	0.0000	0.00
84	1*HCO	+	1*O	=	1*CO	+	1*OH	3.00000E+13	0.0000	0.00
85	1*HCO	+	1*OH	=	1*CO	+	1*H2O	3.00000E+13	0.0000	0.00
86	1*HCO	+	1*H	=	1*CO	+	1*H2	2.00000E+13	0.0000	0.00
87	M	+	1*HCO	=	1*H	+	1*CO	2.90000E+14	0.0000	15570.00
88	1*CO	+	1*O	=	1*CO2	+	M	2.40000E+15	0.0000	4100.00
89	1*CO	+	1*O2	=	1*CO2	+	1*O	2.50000E+12	0.0000	47690.00
90	1*CO	+	1*OH	=	1*CO2	+	1*H	4.17000E+11	0.0000	1000.00
91	1*CO	+	1*HO2	=	1*CO2	+	1*OH	5.75000E+13	0.0000	22930.00
92	1*O	+	1*H2O	=	2*OH			6.80000E+13	0.0000	18365.00
93	1*H	+	1*O2	=	1*OH	+	1*O	1.89000E+14	0.0000	16400.00
94	1*O	+	1*H2	=	1*OH	+	1*H	4.20000E+14	0.0000	13750.00
95	1*H	+	1*HO2	=	1*H2	+	1*O2	7.28000E+13	0.0000	2126.00
96	1*O	+	1*HO2	=	1*OH	+	1*O2	5.00000E+13	0.0000	1000.00
97	1*HO2	+	1*OH	=	1*H2O	+	1*O2	8.00000E+12	0.0000	0.00
98	1*H	+	1*HO2	=	2*OH			1.34000E+14	0.0000	1070.00
99	1*H2	+	1*HO2	=	1*H2O2	+	1*H	7.91000E+13	0.0000	25000.00
100	1*OH	+	1*H2O2	=	1*H2O	+	1*HO2	6.10000E+12	0.0000	1430.00
101			2*HO2	=	1*H2O2	+	1*O2	1.80000E+12	0.0000	0.00
102	1*H	+	1*H2O2	=	1*OH	+	1*H2O	7.80000E+11	0.0000	0.00
103	M	+	1*H2O2	=	2*OH			1.44000E+17	0.0000	45510.00
104	1*H2	+	1*OH	=	1*H2O	+	1*H	4.74000E+13	0.0000	6098.00

TABLE D.2.—Continued.

(j) Continued.

105	1*H	+	1*O2	=	1*HO2	+	M	1.46000E+15	0.0000	-1000.00
106	M	+	1*H2O	=	1*H	+	1*OH	1.30000E+15	0.0000	105140.00
107	1*H	+	1*O	=	1*OH	+	M	7.10000E+18	-1.0000	0.00
108	M	+	1*H2	=	2*H			2.20000E+14	0.0000	96000.00
109	M	+	1*O2	=	2*O			1.80000E+18	-1.0000	118020.00
110	1*CH	+	1*N2	=	1*HCN	+	1*N	1.00000E+11	0.0000	19000.00
111	1*CN	+	1*H2	=	1*HCN	+	1*H	6.00000E+13	0.0000	5300.00
112	1*O	+	1*HCN	=	1*OH	+	1*CN	1.40000E+11	0.6800	16900.00
113	1*OH	+	1*HCN	=	1*HNCO	+	1*H	4.00000E+11	0.0000	2800.00
114	1*CN	+	1*O	=	1*CO	+	1*N	1.20000E+13	0.0000	0.00
115	1*CN	+	1*OH	=	1*HCO	+	1*H	2.50000E+14	0.0000	6000.00
116	1*H2	+	1*HCO	=	1*HNCO	+	1*H	1.00000E+14	0.0000	9000.00
117	1*HNCO	+	1*H	=	1*NH2	+	1*CO	1.00000E+14	0.0000	8500.00
118	1*CN	+	1*O2	=	1*NCO	+	1*O	3.20000E+13	0.0000	1000.00
119	1*CN	+	1*CO2	=	1*NCO	+	1*CO	3.70000E+12	0.0000	0.00
120	1*O	+	1*HCO	=	1*HO	+	1*CO	2.00000E+13	0.0000	0.00
121	1*N	+	1*HCO	=	1*H2	+	1*CO	1.00000E+13	0.0000	0.00
122	1*H	+	1*HCO	=	1*NH	+	1*CO	2.00000E+13	0.0000	0.00
123	1*CH	+	1*HO	=	1*H	+	1*HCO	1.60000E+13	0.0000	9940.00
124	1*CH	+	1*HO	=	1*O	+	1*HCN	2.00000E+12	0.0000	0.00
125	1*NH	+	1*OH	=	1*N	+	1*H2O	5.00000E+11	0.5000	2000.00
126	1*HO2	+	1*HO	=	1*HO2	+	1*OH	2.09000E+12	0.0000	-477.00
127	1*O	+	1*HO2	=	1*HO	+	1*O2	1.00000E+13	0.0000	596.00
128	1*NO	+	1*O	=	1*NO2	+	M	5.62000E+15	0.0000	-1160.00
129	1*NO2	+	1*H	=	1*NO	+	1*OH	3.47000E+14	0.0000	1470.00
130	1*NO	+	1*H	=	1*N	+	1*OH	2.63000E+14	0.0000	50410.00
131	1*NO	+	1*O	=	1*N	+	1*O2	3.80000E+09	1.0000	41370.00
132	1*O	+	1*N2	=	1*NO	+	1*N	1.80000E+14	0.0000	76250.00
133	1*N	+	1*NO2	=	2*NO			4.00000E+12	0.0000	0.00
134	M	+	1*N2O	=	1*N2	+	1*O	6.92000E+23	-2.5000	65000.00
135	1*O	+	1*N2O	=	1*N2	+	1*O2	1.00000E+14	0.0000	28020.00
136	1*O	+	1*N2O	=	2*NO			6.92000E+13	0.0000	26630.00
137	1*N2O	+	1*H	=	1*N2	+	1*OH	7.59000E+13	0.0000	15100.00
138	1*NO2	+	1*H2	=	1*HNO2	+	1*H	2.40000E+13	0.0000	29000.00
139	1*OH	+	1*NO2	=	1*HNO3	+	M	3.00000E+15	0.0000	-3800.00
140	1*OH	+	1*NO	=	1*HNO2	+	M	5.60000E+15	0.0000	-1700.00
141	1*HNO	+	1*H	=	1*H2	+	1*NO	5.00000E+12	0.0000	0.00
142	1*H	+	1*NO	=	1*HNO	+	M	5.40000E+15	0.0000	-600.00
143	1*HNO	+	1*OH	=	1*H2O	+	1*NO	3.60000E+13	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2	,103) =	2.30000	M(O2	,103) =	0.78000	M(H2O	,103) =	6.00000	M(H2O2	,103) =	6.60000
M(O2	,105) =	1.30000	M(N2	,105) =	1.30000	M(H2O	,105) =	21.30000	M(CO2	,105) =	7.00000
M(H2	,106) =	4.00000	M(O2	,106) =	1.50000	M(H2O	,106) =	20.00000	M(N2	,106) =	1.50000
M(CO2	,106) =	4.00000	M(H2	,108) =	4.10000	M(O2	,108) =	2.00000	M(H2O	,108) =	15.00000
M(H2	,108) =	2.00000	M(O2	,139) =	0.70000	M(H2	,139) =	1.40000			

** INITIAL CONDITIONS **

TIME 0.00000E+00 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.00000
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	2.77826E-04
TEMPERATURE (DEG K)	1300.00
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	2.1788
MACH NUMBER	0.0000
GAMMA	1.2066
ENTHALPY (CAL/G)	-1.90008E+01
SP. HEAT (CP) (CAL/G/DEG K)	3.91666E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
CH3OH	2.04685E-06	2.18343E-01	-2.53107E-06	1	1.1375E+05	2.82759E+01	1.00000
CH3	0.00000E+00	0.00000E+00	2.18255E-06	2	1.1092E+05	4.51524E+00	1.00000
OH	0.00000E+00	0.00000E+00	2.18255E-06	3	1.8443E+12	0.00000E+00	0.00000
O2	1.53514E-06	1.63757E-01	-1.76032E-03	4	6.5683E+11	0.00000E+00	0.00000
CH2OH	0.00000E+00	0.00000E+00	3.48520E-07	5	2.1298E+12	0.00000E+00	0.00000
HO2	0.00000E+00	0.00000E+00	3.48520E-07	6	6.4263E+11	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	0.00000E+00	7	4.5030E+09	0.00000E+00	0.00000
O*	0.00000E+00	0.00000E+00	1.75997E-03	8	3.4507E+09	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	0.00000E+00	9	3.3312E+08	0.00000E+00	0.00000
H2	0.00000E+00	0.00000E+00	0.00000E+00	10	9.8019E+10	0.00000E+00	0.00000
CH4	0.00000E+00	0.00000E+00	0.00000E+00	11	3.2129E+02	0.00000E+00	0.00000
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	12	1.2583E+12	0.00000E+00	0.00000
CH2O	0.00000E+00	0.00000E+00	0.00000E+00	13	3.0575E+04	0.00000E+00	0.00000
CH3O	0.00000E+00	0.00000E+00	0.00000E+00	14	2.0344E+12	0.00000E+00	0.00000
C2H6	0.00000E+00	0.00000E+00	0.00000E+00	15	3.5949E+12	0.00000E+00	0.00000
C2H5	0.00000E+00	0.00000E+00	0.00000E+00	16	3.6197E+08	0.00000E+00	0.00000
C2H4	0.00000E+00	0.00000E+00	0.00000E+00	17	6.3000E+12	0.00000E+00	0.00000
CH2	0.00000E+00	0.00000E+00	0.00000E+00	18	1.4742E+10	0.00000E+00	0.00000
C2H3	0.00000E+00	0.00000E+00	0.00000E+00	19	1.3634E+13	0.00000E+00	0.00000
C2H2	0.00000E+00	0.00000E+00	0.00000E+00	20	3.0893E+12	0.00000E+00	0.00000
HCO	0.00000E+00	0.00000E+00	1.43987E-03	21	5.4122E+12	0.00000E+00	0.00000
C2H2O	0.00000E+00	0.00000E+00	0.00000E+00	22	2.2272E+13	0.00000E+00	0.00000
C2H	0.00000E+00	0.00000E+00	0.00000E+00	23	6.1437E+11	0.00000E+00	0.00000
CO	0.00000E+00	0.00000E+00	8.38746E-07	24	2.8870E+11	0.00000E+00	0.00000
C2HO	0.00000E+00	0.00000E+00	0.00000E+00	25	4.8000E+13	0.00000E+00	0.00000

TABLE D.2.—Continued.

(j) Continued.

CH	9.37446E-11	1.00000E-05	-1.43990E-03
CO2	2.19831E-09	2.34500E-04	-8.38746E-07
N2	5.72199E-06	6.10380E-01	-3.43008E-08
HCN	0.00000E+00	0.00000E+00	3.43008E-08
N	9.37446E-12	1.00000E-06	-8.12589E-06
CN	9.37446E-12	1.00000E-06	-3.12776E-04
HNCO	0.00000E+00	0.00000E+00	0.00000E+00
NCO	0.00000E+00	0.00000E+00	3.12776E-04
NH2	0.00000E+00	0.00000E+00	0.00000E+00
NO	0.00000E+00	0.00000E+00	8.16019E-06
NH	0.00000E+00	0.00000E+00	0.00000E+00
NO2	0.00000E+00	0.00000E+00	0.00000E+00
N2O	0.00000E+00	0.00000E+00	2.20236E-16
HNO2	0.00000E+00	0.00000E+00	0.00000E+00
HNO3	0.00000E+00	0.00000E+00	0.00000E+00
HNO	0.00000E+00	0.00000E+00	0.00000E+00
AR	6.82936E-08	7.28507E-03	0.00000E+00

26	2.0000E+13	0.00000E+00	0.00000
27	2.8928E+12	0.00000E+00	0.00000
28	1.2118E+04	0.00000E+00	0.00000
29	2.9817E+12	0.00000E+00	0.00000
30	1.3792E+12	0.00000E+00	0.00000
31	2.1308E+12	0.00000E+00	0.00000
32	3.6088E+12	0.00000E+00	0.00000
33	1.2515E+10	0.00000E+00	0.00000
34	4.3844E+12	0.00000E+00	0.00000
35	6.0000E+12	0.00000E+00	0.00000
36	3.3000E+13	0.00000E+00	0.00000
37	5.0000E+12	0.00000E+00	0.00000
38	3.0000E+13	0.00000E+00	0.00000
39	3.0000E+13	0.00000E+00	0.00000
40	4.3144E-02	0.00000E+00	0.00000
41	3.4790E+12	0.00000E+00	0.00000
42	6.4558E+12	0.00000E+00	0.00000
43	4.1931E+11	0.00000E+00	0.00000
44	2.9616E+11	0.00000E+00	0.00000
45	2.7977E+13	0.00000E+00	0.00000
46	2.0000E+13	0.00000E+00	0.00000
47	5.5471E+11	0.00000E+00	0.00000
48	1.2020E+12	0.00000E+00	0.00000
49	1.0000E+13	0.00000E+00	0.00000
50	5.0000E+13	0.00000E+00	0.00000
51	3.0000E+13	0.00000E+00	0.00000
52	4.6107E+12	0.00000E+00	0.00000
53	1.0000E+13	0.00000E+00	0.00000
54	2.8000E+13	0.00000E+00	0.00000
55	2.3481E+12	0.00000E+00	0.00000
56	2.9976E+12	0.00000E+00	0.00000
57	3.3895E+12	0.00000E+00	0.00000
58	2.2597E+12	0.00000E+00	0.00000
59	2.0000E+13	0.00000E+00	0.00000
60	1.6373E+06	0.00000E+00	0.00000
61	5.0000E+13	0.00000E+00	0.00000
62	6.2318E+11	0.00000E+00	0.00000
63	2.0000E+13	0.00000E+00	0.00000
64	1.2068E+03	0.00000E+00	0.00000
65	1.8853E+13	0.00000E+00	0.00000
66	5.3353E+12	0.00000E+00	0.00000
67	8.9946E+12	0.00000E+00	0.00000
68	3.5341E+10	0.00000E+00	0.00000
69	1.0817E+13	0.00000E+00	0.00000
70	2.0000E+13	0.00000E+00	0.00000
71	7.7746E+00	0.00000E+00	0.00000
72	1.5745E+09	0.00000E+00	0.00000
73	1.1903E+09	0.00000E+00	0.00000
74	1.5745E+09	0.00000E+00	0.00000
75	3.7000E+12	9.87849E+00	1.00000
76	1.0000E+13	1.86443E+04	1.00000
77	1.2186E+12	0.00000E+00	0.00000
78	1.3913E+09	0.00000E+00	0.00000
79	1.8368E+12	0.00000E+00	0.00000
80	7.0693E+12	0.00000E+00	0.00000
81	5.0000E+12	0.00000E+00	0.00000
82	4.0000E+13	0.00000E+00	0.00000
83	3.0000E+13	0.00000E+00	0.00000
84	3.0000E+13	0.00000E+00	0.00000
85	3.0000E+13	0.00000E+00	0.00000
86	2.0000E+13	0.00000E+00	0.00000
87	6.9959E+11	0.00000E+00	0.00000
88	4.9084E+14	-3.26201E-11	1.00000
89	2.4017E+04	0.00000E+00	0.00000
90	2.8315E+11	0.00000E+00	0.00000
91	8.0313E+09	0.00000E+00	0.00000
92	5.5600E+10	0.00000E+00	0.00000
93	3.3065E+11	0.00000E+00	0.00000
94	2.0496E+12	0.00000E+00	0.00000
95	3.1968E+13	0.00000E+00	0.00000
96	3.3951E+13	0.00000E+00	0.00000
97	8.0000E+12	0.00000E+00	0.00000
98	8.8557E+13	0.00000E+00	0.00000
99	4.9579E+09	0.00000E+00	0.00000
100	3.5069E+12	0.00000E+00	0.00000
101	1.8000E+12	0.00000E+00	0.00000
102	7.8000E+11	0.00000E+00	0.00000
103	3.2169E+09	0.00000E+00	0.00000
104	4.4731E+12	0.00000E+00	0.00000
105	2.1501E+15	0.00000E+00	0.00000
106	2.7435E-03	0.00000E+00	0.00000
107	5.4615E+15	0.00000E+00	0.00000
108	1.5972E-02	0.00000E+00	0.00000
109	1.9970E-05	3.72320E-09	1.00000
110	6.3946E+07	4.44383E-01	1.00000
111	7.7115E+12	0.00000E+00	0.00000
112	2.6452E+10	0.00000E+00	0.00000
113	1.3531E+11	0.00000E+00	0.00000
114	1.2000E+13	0.00000E+00	0.00000
115	2.4505E+13	0.00000E+00	0.00000
116	3.0688E+12	0.00000E+00	0.00000
117	3.7241E+12	0.00000E+00	0.00000
118	2.1729E+13	4.05117E+03	1.00000
119	3.7000E+12	9.87849E-01	1.00000
120	2.0000E+13	0.00000E+00	0.00000
121	1.0000E+13	0.00000E+00	0.00000
122	2.0000E+13	0.00000E+00	0.00000
123	3.4124E+11	0.00000E+00	0.00000
124	2.0000E+12	0.00000E+00	0.00000
125	8.3121E+12	0.00000E+00	0.00000
126	2.5138E+12	0.00000E+00	0.00000
127	7.9397E+12	0.00000E+00	0.00000
128	8.8054E+15	0.00000E+00	0.00000
129	1.9643E+14	0.00000E+00	0.00000
130	8.8159E+05	0.00000E+00	0.00000
131	5.4802E+05	-1.05719E+02	1.00000
132	2.7320E+01	0.00000E+00	0.00000
133	4.0000E+12	0.00000E+00	0.00000
134	1.3420E+05	0.00000E+00	0.00000
135	1.9472E+09	-2.85326E-09	1.00000
136	2.3078E+09	0.00000E+00	0.00000
137	2.1964E+11	0.00000E+00	0.00000
138	3.1979E+08	0.00000E+00	0.00000

TABLE D.2.—Continued.

(j) Continued.

139	1.3060E+16	0.00000E+00	0.00000
140	1.0814E+16	0.00000E+00	0.00000
141	5.0000E+12	0.00000E+00	0.00000
142	6.8118E+15	0.00000E+00	0.00000
143	3.6000E+13	0.00000E+00	0.00000

DERIVATIVES (CGS UNITS): T 1.16420E+06 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 29.63652 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) -1.37013E+09 MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 2.320000 S

TIME 6.50000E-04 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.23771
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	2.77826E-04
TEMPERATURE (DEG K)	1558.04
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	2.2970
MACH NUMBER	0.0000
GAMMA	1.2057
ENTHALPY (CAL/G)	1.71763E+00
SP. HEAT (CP) (CAL/G/DEG K)	4.05863E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	22
AVERAGE STEP SIZE	0.66459E-05
METHOD ORDER	3
TOTAL NUMBER OF STEPS	169
FUNCT EVALUATIONS	233
JACOBIAN EVALUATIONS	31

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH3OH	1.63313E-06	1.68690E-01	-6.53904E-03
CH3	1.33680E-09	1.38082E-04	7.70793E-05
OH	1.32068E-09	1.36417E-04	3.77190E-05
O2	1.21777E-06	1.25787E-01	-5.26103E-03
CH2OH	2.74785E-08	2.83833E-03	6.17805E-04
HO2	3.63008E-08	3.74961E-03	2.38526E-04
H2O	5.47129E-07	5.65144E-02	1.01648E-02
O	4.03882E-11	4.17181E-06	1.94849E-06
H	1.60786E-10	1.66080E-05	6.73690E-06
H2	3.49320E-08	3.60823E-03	9.63257E-04
CH4	1.40417E-09	1.45041E-04	5.52713E-05
H2O2	4.42219E-09	4.56781E-04	-1.59208E-04
CH2O	1.74995E-07	1.80757E-02	7.45257E-04
CH3O	2.00942E-10	2.07559E-05	8.70415E-06
C2H6	1.73379E-10	1.79088E-05	1.34871E-05
C2H5	1.56951E-13	1.62119E-08	1.21006E-08
C2H4	1.00184E-10	1.03483E-05	7.00562E-06
CH2	1.87284E-14	1.93451E-09	2.00003E-09
C2H3	8.18959E-14	8.45925E-09	8.04100E-09
C2H2	7.69929E-13	7.95280E-08	7.80406E-08
HCO	9.08209E-11	9.38114E-06	2.94632E-06
C2H2O	1.46431E-11	1.51253E-06	4.90586E-07
C2H	1.71430E-17	1.77075E-12	1.54283E-12
CO	1.99746E-07	2.06323E-02	4.65676E-03
C2HO	7.94533E-14	8.20695E-09	5.48424E-09
CH	8.49693E-18	8.77672E-13	1.11920E-12
CO2	1.01831E-08	1.05184E-03	3.33056E-04
N2	5.72199E-06	5.91040E-01	-5.05261E-11
HCN	2.01536E-14	2.08172E-09	9.90791E-11
N	5.89751E-16	6.09170E-11	5.62587E-12
CN	4.90811E-17	5.06972E-12	-2.58885E-12
HNCO	8.91339E-12	9.20688E-07	-8.54386E-09
NCO	6.72064E-15	6.94193E-10	-3.75436E-10
NH2	2.54211E-13	2.62582E-08	8.79590E-09
NO	2.43236E-12	2.51245E-07	6.19354E-08
NH	6.89483E-14	7.12186E-09	-9.19723E-10
NO2	7.05138E-12	7.28356E-07	-6.09991E-08
N2O	1.12947E-15	1.16666E-10	4.97219E-11
HNO2	3.80009E-16	3.92522E-11	1.62051E-12
HNO3	6.23374E-17	6.43900E-12	-1.52202E-12
HNO	1.77972E-16	1.83832E-11	6.24962E-12
AR	6.82936E-08	7.05423E-03	0.00000E+00

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	1.9203E+07	3.85401E+03	0.97983
2	2.8986E+06	-1.76478E+03	0.95940
3	2.0966E+12	5.85032E+04	0.99861
4	7.6119E+11	6.48800E+02	0.99745
5	3.3361E+12	1.11148E+04	0.97935
6	9.0266E+11	3.07071E+03	0.99998
7	8.4404E+09	2.38172E+02	0.99768
8	1.1969E+10	9.05141E+03	0.98463
9	2.1382E+09	7.36906E+03	0.99999
10	1.4400E+11	6.24186E+04	0.99986
11	9.0586E+04	-1.14317E+01	0.99861
12	2.6985E+12	-6.23307E+01	0.88760
13	1.1081E+06	-2.60446E+02	0.99991
14	4.3128E+12	-3.15654E-01	0.09059
15	4.9565E+12	4.75206E+01	0.39906
16	2.2761E+09	3.84768E+01	0.80152
17	6.3000E+12	-7.93508E+03	0.98216
18	5.6657E+10	1.42790E+03	0.99999
19	1.2682E+13	2.60414E+02	0.88695
20	5.7535E+12	2.07708E+00	0.99959
21	8.9524E+12	8.12125E-01	0.99995
22	2.7910E+13	8.27936E+01	0.99997
23	4.4829E+12	8.50527E+01	0.96380
24	3.9780E+11	4.57667E-01	0.46462
25	4.8000E+13	1.56860E-02	0.99955
26	2.0000E+13	6.48297E-03	0.99936
27	5.5630E+12	1.15756E+00	0.99708
28	1.9560E+06	2.45783E-02	1.00000
29	3.2263E+12	5.52929E+00	0.99980
30	1.4668E+12	-1.23202E+01	0.83051
31	2.2909E+12	1.20085E-01	0.99995
32	4.9725E+12	2.60168E-01	0.99809
33	9.7365E+10	9.98414E-01	0.99830
34	4.3147E+12	5.57482E+00	1.00000
35	6.0000E+12	1.02354E-03	0.99998
36	3.3000E+13	1.41411E-03	1.00000
37	5.0000E+12	7.00620E-03	1.00000
38	3.0000E+13	5.91324E-07	0.99194
39	3.0000E+13	5.45639E-10	0.99996
40	4.1125E+01	-1.58106E-07	0.97550
41	6.5588E+12	2.64231E-03	1.00000
42	1.2787E+13	5.14950E-03	0.99966
43	6.5680E+11	8.35664E-03	0.96582
44	2.9998E+11	3.82266E-03	0.96732
45	3.0801E+13	8.33024E-03	0.99998
46	2.0000E+13	5.83425E-06	0.99453
47	6.5114E+11	8.16209E-01	1.00000
48	1.2020E+12	4.99717E-05	1.00000
49	1.0000E+13	1.35703E-02	0.99822
50	5.0000E+13	8.23793E-03	0.99549
51	3.0000E+13	5.78345E-07	1.00000
52	5.2415E+12	3.15611E-08	0.31234
53	1.0000E+13	8.17857E-07	1.00000
54	2.8000E+13	-7.63317E+00	0.52109
55	2.8461E+12	7.08983E-01	0.99428
56	3.7344E+12	9.72713E-02	0.85394
57	5.6609E+12	1.58040E-01	0.91527
58	3.7739E+12	2.86127E-02	0.98953
59	2.0000E+13	1.53239E-01	1.00000
60	7.6681E+07	1.36488E-01	0.96915
61	5.0000E+13	4.48502E-07	1.00000
62	9.8684E+11	3.12784E+03	0.99979
63	2.0000E+13	8.37147E+00	1.00000

TABLE D.2.—Continued.
(j) Concluded.

64	2.1722E+05	4.73997E+00	0.99417
65	2.0361E+13	6.09633E+04	1.00000
66	6.8905E+12	2.51158E+03	0.99993
67	1.1265E+13	1.03143E+03	0.99999
68	5.6840E+10	1.72264E+02	0.99999
69	1.1842E+13	1.86258E+01	1.00000
70	2.0000E+13	1.25735E+04	0.99998
71	2.7611E+03	3.65183E-04	0.78882
72	9.2340E+09	2.56459E-02	0.99738
73	6.9937E+09	4.89034E-03	0.99968
74	9.2340E+09	2.11169E-01	0.99982
75	3.7000E+12	4.07506E-06	0.98251
76	1.0000E+13	1.34054E-03	1.00000
77	2.0843E+12	6.15853E-01	0.99999
78	8.2567E+09	8.06615E-08	0.99690
79	2.9353E+12	9.39004E-04	0.99830
80	1.1036E+13	4.19718E-04	0.97489
81	5.0000E+12	2.27048E-08	0.99929
82	4.0000E+13	1.81768E-07	1.00000
83	3.0000E+13	4.29504E+04	0.99918
84	3.0000E+13	1.42566E+00	1.00000
85	3.0000E+13	4.66185E+01	1.00000
86	2.0000E+13	3.78370E+00	1.00000
87	1.8983E+12	2.16223E+04	0.99994
88	6.3840E+14	6.45965E-01	1.00000
89	5.1092E+05	1.61006E+00	1.00000
90	3.0190E+11	1.03115E+03	0.99938
91	3.4932E+10	3.28146E+03	1.00000
92	1.8047E+11	-4.28732E+01	0.45350
93	9.4623E+11	2.39177E+03	0.99646
94	4.9488E+12	7.92756E+01	0.87640
95	3.6636E+13	2.76799E+03	0.99916
96	3.6199E+13	6.87505E+02	0.99990
97	8.0000E+12	4.96858E+03	0.99994
98	9.4845E+13	7.17182E+03	1.00000
99	2.4624E+10	1.03391E+02	0.25558
100	3.8436E+12	2.64435E+02	0.90926
101	1.8000E+12	3.07104E+04	0.99938
102	7.8000E+11	7.18510E+00	1.00000
103	5.9507E+10	4.16562E+04	0.99996
104	6.6130E+12	3.68553E+03	0.93245
105	2.0166E+15	-1.61735E+03	0.93238
106	2.3212E+00	-4.64858E-01	0.99916
107	4.5570E+15	3.70595E-03	0.99847
108	7.5210E+00	-6.61221E-03	0.98760
109	3.2192E-02	-6.44117E-06	0.56710
110	2.1618E+08	1.36171E-07	0.99999
111	1.0832E+13	2.36344E-04	0.98230
112	8.8405E+10	-5.57884E-06	0.85682
113	1.6192E+11	-1.04156E-03	0.94912
114	1.2000E+13	3.08177E-07	1.00000
115	3.6000E+13	1.60391E-05	0.53053
116	5.4645E+12	4.30678E-03	0.25913
117	6.4222E+12	1.13955E-01	0.95566
118	2.3167E+13	1.79096E-02	0.99834
119	3.7000E+12	-1.81344E-02	0.99868
120	2.0000E+13	7.03312E-05	1.00000
121	1.0000E+13	5.13490E-10	1.00000
122	2.0000E+13	2.78145E-04	0.99341
123	6.4538E+11	1.66249E-10	0.96206
124	2.0000E+12	5.35464E-10	0.99990
125	1.0345E+13	1.21936E-02	0.99918
126	2.4381E+12	2.46566E+00	0.88406
127	8.2489E+12	3.04082E-02	0.99911
128	8.1743E+15	-4.86823E-02	0.99794
129	2.1584E+14	3.17031E+00	1.00000
130	2.2327E+07	-3.96171E-04	0.99971
131	9.3174E+06	-1.17350E-02	1.00000
132	3.6266E+03	1.02750E-05	0.94629
133	4.0000E+12	2.15504E-07	1.00000
134	5.5075E+06	-6.41358E-04	0.99878
135	1.1737E+10	-2.46452E-06	0.99719
136	1.2725E+10	7.52015E-09	0.99998
137	5.7827E+11	-3.55436E-07	0.20714
138	2.0526E+09	6.54586E-03	0.99932
139	1.0237E+16	-1.97185E-05	0.00171
140	9.6973E+15	-6.52487E-03	0.62547
141	5.0000E+12	1.79650E-06	0.96918
142	6.5548E+15	1.92159E-04	0.59765
143	3.6000E+13	1.09396E-04	0.99792

```
DERIVATIVES (CGS UNITS): T            4.95379E+06     RHO          0.00000E+00

MIXTURE MOLECULAR WEIGHT     28.69745     TOTAL ENERGY EXCHANGE RATE   -5.73830E+09       MASS FRACTION SUM    1.00000001

                                          (CAL-CM**3/G**2/SEC)

 ------------------------------------------------------------

    COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP -  1.650002E+00  S     UP TO THIS TIME -  1.115000E+01  S

(LSENS)     END OF THIS CASE


              SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

                 TOTAL NO. OF STEPS -                    169
                 TOTAL NO. OF DERIVATIVE EVALUATIONS -   233
                 TOTAL NO. OF JACOBIAN EVALUATIONS -      31
                 TOTAL CPU TIME -                  11.150002 S

                          TOTAL CPU TIME (INCLUDING I/O) REQUIRED =     14.839996 S


(LSENS)     READ DATA FOR NEXT CASE
```

TABLE D.2.—Continued.

(k) Case 11

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

LSENS PROPANE-AIR WELL-STIRRED REACTOR + ROCKET EXP; EMAX=10-4 CASE 11

REACTION NUMBER	REACTION							REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1			1*C3H8	=	1*C2H5	+	1*CH3	5.00000E+15	0.0000	83500.00
2	1*CH3	+	1*C3H8	=	1*CH4	+	1*C3H7	3.55000E+12	0.0000	10300.00
3			1*C3H7	=	1*C2H4	+	1*CH3	3.00000E+14	0.0000	33200.00
4	M	+	1*CH4	=	1*CH3	+	1*H	2.00000E+17	0.0000	88000.00
5	1*H	+	1*CH4	=	1*CH3	+	1*H2	1.26000E+14	0.0000	11900.00
6	1*CH4	+	1*O2	=	1*CH3	+	1*HO2	7.94000E+13	0.0000	56000.00
7	1*O	+	1*CH4	=	1*CH3	+	1*OH	1.90000E+14	0.0000	11720.00
8	1*OH	+	1*CH4	=	1*CH3	+	1*H2O	2.50000E+13	0.0000	5010.00
9	1*CH3	+	1*O2	=	1*CH3O	+	1*O	2.40000E+13	0.0000	28680.00
10	1*CH3	+	1*OH	=	1*CH3O	+	1*H	6.30000E+12	0.0000	0.00
11	M	+	1*CH3O	=	1*CH2O	+	1*H	5.00000E+13	0.0000	21000.00
12			2*CH3	=	1*C2H6			2.40000E+14	-0.4000	0.00
13	1*H	+	1*C2H6	=	1*C2H5	+	1*H2	1.32000E+14	0.0000	9700.00
14	1*O	+	1*C2H6	=	1*C2H5	+	1*OH	1.13000E+14	0.0000	7850.00
15	1*OH	+	1*C2H6	=	1*C2H5	+	1*H2O	8.70000E+13	0.0000	3520.00
16	M	+	1*C2H5	=	1*C2H4	+	1*H	1.00000E+17	0.0000	31000.00
17	1*C2H5	+	1*O2	=	1*C2H4	+	1*HO2	2.00000E+12	0.0000	5000.00
18	1*H	+	1*C2H5	=	1*C2H4	+	1*H2	4.80000E+13	0.0000	0.00
19	1*CH3	+	1*CH2	=	1*C2H4	+	1*H	2.00000E+13	0.0000	0.00
20	1*H	+	1*C2H4	=	1*H2	+	1*C2H3	1.50000E+14	0.0000	10200.00
21	M	+	1*C2H4	=	1*C2H2	+	1*H2	2.60000E+17	0.0000	79300.00
22	1*C2H4	+	1*OH	=	1*C2H3	+	1*H2O	4.80000E+12	0.0000	1230.00
23	1*C2H4	+	1*OH	=	1*CH3	+	1*CH2O	2.00000E+12	0.0000	960.00
24	1*C2H4	+	1*O	=	1*CH3	+	1*HCO	3.30000E+12	0.0000	1130.00
25	1*C2H4	+	1*O	=	1*CH2O	+	1*CH2	2.50000E+13	0.0000	5000.00
26	M	+	1*C2H3	=	1*C2H2	+	1*H	3.00000E+15	0.0000	32000.00
27	1*C2H3	+	1*O2	=	1*CH2O	+	1*HCO	3.98000E+12	0.0000	-250.00
28	1*C2H3	+	1*H	=	1*C2H2	+	1*H2	6.00000E+12	0.0000	0.00
29	1*C2H3	+	1*O	=	1*C2H2O	+	1*H	3.30000E+13	0.0000	0.00
30	1*C2H3	+	1*OH	=	1*C2H2	+	1*H2O	5.00000E+12	0.0000	0.00
31	1*C2H3	+	1*CH2	=	1*C2H2	+	1*CH3	3.00000E+13	0.0000	0.00
32	1*C2H3	+	1*C2H	=	2*C2H2			3.00000E+13	0.0000	0.00
33	M	+	1*C2H2	=	1*C2H	+	1*H	4.20000E+16	0.0000	107000.00
34	1*C2H2	+	1*O	=	1*CH2	+	1*CO	1.60000E+14	0.0000	9890.00
35	1*C2H2	+	1*O	=	1*C2HO	+	1*H	4.00000E+14	0.0000	10660.00
36	1*C2H2	+	1*OH	=	1*C2H	+	1*H2O	6.30000E+12	0.0000	7000.00
37	1*C2H2	+	1*OH	=	1*C2H2O	+	1*H	3.20000E+11	0.0000	200.00
38	1*C2H	+	1*O2	=	1*C2HO	+	1*O	5.00000E+13	0.0000	1500.00
39	1*C2H	+	1*OH	=	1*C2HO	+	1*H	2.00000E+13	0.0000	0.00
40	1*C2HO	+	1*O2	=	2*CO	+	1*OH	1.46000E+12	0.0000	2500.00
41	1*C2HO	+	1*O	=	2*CO	+	1*H	1.20200E+12	0.0000	0.00
42	1*C2HO	+	1*OH	=	2*HCO			1.00000E+13	0.0000	0.00
43	1*C2HO	+	1*H	=	1*CH2	+	1*CO	5.00000E+13	0.0000	0.00
44	1*C2HO	+	1*CH2	=	1*C2H3	+	1*CO	3.00000E+13	0.0000	0.00
45	1*C2HO	+	1*CH2	=	1*CH2O	+	1*C2H	1.00000E+13	0.0000	2000.00
46			2*C2HO	=	1*C2H2	+	2*CO	1.00000E+13	0.0000	0.00
47	1*C2H2O	+	1*OH	=	1*CH2O	+	1*HCO	2.80000E+13	0.0000	0.00
48	1*C2H2O	+	1*OH	=	1*C2HO	+	1*H2O	7.50000E+12	0.0000	3000.00
49	1*C2H2O	+	1*H	=	1*CH3	+	1*CO	1.13000E+13	0.0000	3428.00
50	1*C2H2O	+	1*H	=	1*C2HO	+	1*H2	7.50000E+13	0.0000	8000.00
51	1*C2H2O	+	1*O	=	1*C2HO	+	1*OH	5.00000E+13	0.0000	8000.00
52	1*C2H2O	+	1*O	=	1*CH2O	+	1*CO	2.00000E+13	0.0000	0.00
53	M	+	1*C2H2O	=	1*CH2	+	1*CO	2.00000E+16	0.0000	60000.00
54	1*C2H	+	1*O	=	1*CO	+	1*CH	5.00000E+13	0.0000	0.00
55	1*CH3O	+	1*O2	=	1*CH2O	+	1*HO2	1.00000E+13	0.0000	7170.00
56	1*CH3O	+	1*H	=	1*CH2O	+	1*H2	2.00000E+13	0.0000	0.00
57	M	+	1*CH2O	=	1*HCO	+	1*H	5.00000E+16	0.0000	81000.00
58	1*CH2O	+	1*OH	=	1*HCO	+	1*H2O	3.00000E+13	0.0000	1200.00
59	1*CH2O	+	1*H	=	1*HCO	+	1*H2	2.50000E+13	0.0000	3990.00
60	1*CH2O	+	1*O	=	1*HCO	+	1*OH	3.50000E+13	0.0000	3510.00
61	1*CH3	+	1*CH2O	=	1*CH4	+	1*HCO	1.00000E+10	0.5000	6000.00
62	1*CH3	+	1*HCO	=	1*CH4	+	1*CO	3.00000E+11	0.5000	0.00
63	1*CH3	+	1*HO2	=	1*CH3O	+	1*OH	2.00000E+13	0.0000	0.00
64	M	+	1*CH3	=	1*CH2	+	1*H	1.95000E+16	0.0000	91600.00
65	1*H	+	1*CH3	=	1*H2	+	1*CH2	2.70000E+11	0.6700	25700.00
66	1*O	+	1*CH3	=	1*OH	+	1*CH2	1.90000E+11	0.6800	25700.00
67	1*OH	+	1*CH3	=	1*H2O	+	1*CH2	2.70000E+11	0.6700	25700.00
68	1*CH	+	1*CO2	=	1*HCO	+	1*CO	3.70000E+12	0.0000	0.00
69	1*CH	+	1*O2	=	1*HCO	+	1*O	1.00000E+13	0.0000	0.00
70	1*CH2	+	1*O2	=	1*CH2O	+	1*O	5.00000E+11	0.5000	6960.00
71	1*CH2	+	1*O	=	1*CH	+	1*OH	2.00000E+11	0.7000	25800.00
72	1*CH2	+	1*OH	=	1*CH	+	1*H2O	5.00000E+11	0.5000	5900.00
73	1*CH2	+	1*H	=	1*CH	+	1*H2	3.20000E+11	0.7000	4970.00
74			2*CH2	=	1*C2H3	+	1*H	5.00000E+12	0.0000	0.00
75			2*CH2	=	1*C2H2	+	1*H2	4.00000E+13	0.0000	0.00
76	1*HCO	+	1*O2	=	1*CO	+	1*HO2	3.00000E+13	0.0000	0.00
77	1*HCO	+	1*O	=	1*CO	+	1*OH	3.00000E+13	0.0000	0.00
78	1*HCO	+	1*OH	=	1*CO	+	1*H2O	3.00000E+13	0.0000	0.00
79	1*HCO	+	1*H	=	1*CO	+	1*H2	2.00000E+13	0.0000	0.00
80	M	+	1*HCO	=	1*H	+	1*CO	2.90000E+14	0.0000	15570.00
81	1*CO	+	1*O	=	1*CO2	+	M	2.40000E+15	0.0000	4100.00
82	1*CO	+	1*O2	=	1*CO2	+	1*O	2.50000E+12	0.0000	47690.00
83	1*CO	+	1*OH	=	1*CO2	+	1*H	4.17000E+11	0.0000	1000.00
84	1*CO	+	1*HO2	=	1*CO2	+	1*OH	5.75000E+13	0.0000	22930.00
85	1*O	+	1*H2O	=	2*OH			6.80000E+13	0.0000	18365.00
86	1*H	+	1*O2	=	1*OH	+	1*O	1.89000E+14	0.0000	16400.00
87	1*O	+	1*H2	=	1*OH	+	1*H	4.20000E+14	0.0000	13750.00
88	1*H	+	1*HO2	=	1*H2	+	1*O2	7.28000E+13	0.0000	2126.00
89	1*O	+	1*HO2	=	1*OH	+	1*O2	5.00000E+13	0.0000	1000.00
90	1*HO2	+	1*OH	=	1*H2O	+	1*O2	8.00000E+12	0.0000	0.00
91	1*H	+	1*HO2	=	2*OH			1.34000E+14	0.0000	1070.00
92	1*H2	+	1*HO2	=	1*H2O2	+	1*H	7.91000E+13	0.0000	25000.00
93	1*OH	+	1*H2O2	=	1*H2O	+	1*HO2	6.10000E+12	0.0000	1430.00
94			2*HO2	=	1*H2O2	+	1*O2	1.80000E+12	0.0000	0.00
95	1*H	+	1*H2O2	=	1*OH	+	1*H2O	7.80000E+11	0.0000	0.00
96	M	+	1*H2O2	=	2*OH			1.44000E+17	0.0000	45510.00
97	1*H2	+	1*OH	=	1*H2O	+	1*H	4.74000E+13	0.0000	6098.00
98	1*H	+	1*O2	=	1*HO2	+	M	1.46000E+15	0.0000	-1000.00
99	M	+	1*H2O	=	1*H	+	1*OH	1.30000E+15	0.0000	105140.00
100	1*H	+	1*O	=	1*OH	+	M	7.10000E+18	-1.0000	0.00
101	M	+	1*H2	=	2*H			2.20000E+14	0.0000	96000.00
102	M	+	1*O2	=	2*O			1.80000E+18	-1.0000	118020.00
103	1*CH	+	1*N2	=	1*HCN	+	1*N	1.00000E+11	0.0000	19000.00
104	1*CN	+	1*H2	=	1*HCN	+	1*H	6.00000E+13	0.0000	5300.00

TABLE D.2.—Continued.

(k) Continued.

105	1*O	+	1*HCN	=	1*OH	+	1*CN	1.40000E+11	0.6800	16900.00
106	1*OH	+	1*HCN	=	1*HNCO	+	1*H	4.00000E+11	0.0000	2800.00
107	1*CN	+	1*O	=	1*CO	+	1*N	1.20000E+13	0.0000	0.00
108	1*CN	+	1*OH	=	1*NCO	+	1*H	2.50000E+14	0.0000	6000.00
109	1*H2	+	1*NCO	=	1*HNCO	+	1*H	1.00000E+14	0.0000	9000.00
110	1*HNCO	+	1*H	=	1*NH2	+	1*CO	1.00000E+14	0.0000	8500.00
111	1*CN	+	1*O2	=	1*NCO	+	1*O	3.20000E+13	0.0000	1000.00
112	1*CN	+	1*CO2	=	1*NCO	+	1*CO	3.70000E+12	0.0000	0.00
113	1*O	+	1*NCO	=	1*NO	+	1*CO	2.00000E+13	0.0000	0.00
114	1*N	+	1*NCO	=	1*N2	+	1*CO	1.00000E+13	0.0000	0.00
115	1*H	+	1*NCO	=	1*NH	+	1*CO	2.00000E+13	0.0000	0.00
116	1*CH	+	1*NO	=	1*N	+	1*HCO	1.60000E+13	0.0000	9940.00
117	1*CH	+	1*NO	=	1*O	+	1*HCN	2.00000E+12	0.0000	0.00
118	1*NH	+	1*OH	=	1*N	+	1*H2O	5.00000E+11	0.5000	2000.00
119	1*HO2	+	1*NO	=	1*NO2	+	1*OH	2.09000E+12	0.0000	-477.00
120	1*O	+	1*NO2	=	1*NO	+	1*O2	1.00000E+13	0.0000	596.00
121	1*NO	+	1*O	=	1*NO2	+	M	5.62000E+15	0.0000	-1160.00
122	1*NO2	+	1*H	=	1*NO	+	1*OH	3.47000E+14	0.0000	1470.00
123	1*NO	+	1*H	=	1*N	+	1*OH	2.63000E+14	0.0000	50410.00
124	1*NO	+	1*O	=	1*N	+	1*O2	3.80000E+09	1.0000	41370.00
125	1*O	+	1*N2	=	1*NO	+	1*N	1.80000E+14	0.0000	76250.00
126	1*N	+	1*NO2	=	2*NO			4.00000E+12	0.0000	0.00
127	M	+	1*H2O	=	1*N2	+	1*O	6.92000E+23	-2.5000	65000.00
128	1*O	+	1*H2O	=	1*N2	+	1*O2	1.00000E+14	0.0000	28020.00
129	1*O	+	1*H2O	=	2*NO			6.92000E+13	0.0000	26630.00
130	1*N2O	+	1*H	=	1*N2	+	1*OH	7.59000E+13	0.0000	15100.00
131	1*NO2	+	1*H2	=	1*HNO2	+	1*H	2.40000E+13	0.0000	29000.00
132	1*OH	+	1*NO2	=	1*HNO3	+	M	3.00000E+15	0.0000	-3800.00
133	1*OH	+	1*NO	=	1*HNO2	+	M	5.60000E+15	0.0000	-1700.00
134	1*HNO	+	1*H	=	1*H2	+	1*NO	5.00000E+12	0.0000	0.00
135	1*H	+	1*NO	=	1*HNO	+	M	5.40000E+15	0.0000	-600.00
136	1*HNO	+	1*OH	=	1*H2O	+	1*NO	3.60000E+13	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2 , 96) = 2.30000	M(O2 , 96) = 0.78000	M(H2O , 96) = 6.00000	M(H2O2 , 96) = 6.60000
M(O2 , 98) = 1.30000	M(N2 , 98) = 1.30000	M(H2O , 98) = 21.30000	M(CO2 , 98) = 7.00000
M(H2 , 99) = 4.00000	M(O2 , 99) = 1.50000	M(H2O , 99) = 20.00000	M(N2 , 99) = 1.50000
M(CO2 , 99) = 4.00000	M(H2 ,101) = 4.10000	M(O2 ,101) = 2.00000	M(H2O ,101) = 15.00000
M(N2 ,101) = 2.00000	M(O2 ,132) = 0.70000	M(H2 ,132) = 1.40000	

** INITIAL CONDITIONS **

TIME 0.00000E+00 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 2.00000E-01 CM

FLOW PROPERTIES

PRESSURE (ATM)	5.00000
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	2.96325E-03
TEMPERATURE (DEG K)	614.00
MASS FLOW RATE (G/SEC)	1.00000E+01
ENTROPY (CAL/G/DEG K)	1.7275
MACH NUMBER	0.0000
GAMMA	1.2954
ENTHALPY (CAL/G)	3.60515E+01
SP. HEAT (CP) (CAL/G/DEG K)	2.91858E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

HEAT LOSS(QDOT/MDOT) = -1.2180E+00 CAL/G

CHEMICAL PROPERTIES

SPECIES	MASS FRACTION	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE*CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
C3H8	8.73262E-02	5.91318E-02	-5.57359E-20	1	9.4978E-15	6.34742E-15	1.00000
C2H5	0.00000E+00	0.00000E+00	5.57359E-20	2	7.6560E+08	0.00000E+00	0.00000
CH3	0.00000E+00	0.00000E+00	5.57359E-20	3	4.5685E+02	0.00000E+00	0.00000
CH4	0.00000E+00	0.00000E+00	0.00000E+00	4	9.5046E-15	0.00000E+00	0.00000
C3H7	0.00000E+00	0.00000E+00	0.00000E+00	5	7.3221E+09	0.00000E+00	0.00000
C2H4	0.00000E+00	0.00000E+00	0.00000E+00	6	9.2670E-07	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	0.00000E+00	7	1.2796E+10	0.00000E+00	0.00000
H2	0.00000E+00	0.00000E+00	0.00000E+00	8	4.1177E+11	0.00000E+00	0.00000
O2	2.11232E-01	1.97108E-01	-1.91172E-34	9	1.4850E+03	0.00000E+00	0.00000
HO2	0.00000E+00	0.00000E+00	0.00000E+00	10	6.3000E+12	0.00000E+00	0.00000
O	0.00000E+00	0.00000E+00	1.96753E-34	11	1.6755E+06	0.00000E+00	0.00000
OH	0.00000E+00	0.00000E+00	0.00000E+00	12	1.8405E+13	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	0.00000E+00	13	4.6549E+10	0.00000E+00	0.00000
CH3O	0.00000E+00	0.00000E+00	0.00000E+00	14	1.8152E+11	0.00000E+00	0.00000
CH2O	0.00000E+00	0.00000E+00	0.00000E+00	15	4.8595E+12	0.00000E+00	0.00000
C2H6	0.00000E+00	0.00000E+00	0.00000E+00	16	9.2412E+05	0.00000E+00	0.00000
CH2	0.00000E+00	0.00000E+00	0.00000E+00	17	3.3213E+10	0.00000E+00	0.00000
C2H5	0.00000E+00	0.00000E+00	0.00000E+00	18	4.8000E+13	0.00000E+00	0.00000
C2H2	0.00000E+00	0.00000E+00	0.00000E+00	19	2.0000E+13	0.00000E+00	0.00000
HCO	0.00000E+00	0.00000E+00	0.00000E+00	20	3.5112E+10	0.00000E+00	0.00000
C2H2O	0.00000E+00	0.00000E+00	0.00000E+00	21	1.5438E-11	0.00000E+00	0.00000
C2H	0.00000E+00	0.00000E+00	0.00000E+00	22	1.7516E+12	0.00000E+00	0.00000

TABLE D.2.—Continued.

(k) Continued.

CO	0.00000E+00	0.00000E+00	1.16036E-40
C2HO	0.00000E+00	0.00000E+00	0.00000E+00
CH	0.00000E+00	0.00000E+00	0.00000E+00
CO2	4.16200E-04	2.82378E-04	-1.16036E-40
H2O2	0.00000E+00	0.00000E+00	0.00000E+00
N2	6.89289E-01	7.34705E-01	-1.85592E-34
HCN	0.00000E+00	0.00000E+00	0.00000E+00
N	0.00000E+00	0.00000E+00	0.00000E+00
CN	0.00000E+00	0.00000E+00	0.00000E+00
HNCO	0.00000E+00	0.00000E+00	0.00000E+00
NCO	0.00000E+00	0.00000E+00	0.00000E+00
NH2	0.00000E+00	0.00000E+00	0.00000E+00
NO	0.00000E+00	0.00000E+00	0.00000E+00
NH	0.00000E+00	0.00000E+00	0.00000E+00
NO2	0.00000E+00	0.00000E+00	0.00000E+00
N2O	0.00000E+00	0.00000E+00	1.85592E-34
HNO2	0.00000E+00	0.00000E+00	0.00000E+00
HNO3	0.00000E+00	0.00000E+00	0.00000E+00
HNO	0.00000E+00	0.00000E+00	0.00000E+00
AR	1.17370E-02	8.77283E-03	0.00000E+00

23	9.1059E+11	0.00000E+00	0.00000
24	1.3071E+12	0.00000E+00	0.00000
25	4.1516E+11	0.00000E+00	0.00000
26	1.2215E+04	0.00000E+00	0.00000
27	4.8851E+12	0.00000E+00	0.00000
28	6.0000E+12	0.00000E+00	0.00000
29	3.3000E+13	0.00000E+00	0.00000
30	5.0000E+12	0.00000E+00	0.00000
31	3.0000E+13	0.00000E+00	0.00000
32	3.0000E+13	0.00000E+00	0.00000
33	3.4452E-22	0.00000E+00	0.00000
34	4.8287E+10	0.00000E+00	0.00000
35	6.4224E+10	0.00000E+00	0.00000
36	2.0311E+10	0.00000E+00	0.00000
37	2.7162E+11	0.00000E+00	0.00000
38	1.4624E+13	0.00000E+00	0.00000
39	2.0000E+13	0.00000E+00	0.00000
40	1.8814E+11	0.00000E+00	0.00000
41	1.2020E+12	0.00000E+00	0.00000
42	1.0000E+13	0.00000E+00	0.00000
43	5.0000E+13	0.00000E+00	0.00000
44	3.0000E+13	0.00000E+00	0.00000
45	1.9414E+12	0.00000E+00	0.00000
46	1.0000E+13	0.00000E+00	0.00000
47	2.8000E+13	0.00000E+00	0.00000
48	6.4155E+11	0.00000E+00	0.00000
49	6.8061E+11	0.00000E+00	0.00000
50	1.0654E+11	0.00000E+00	0.00000
51	7.1026E+10	0.00000E+00	0.00000
52	2.0000E+13	0.00000E+00	0.00000
53	8.7978E-06	0.00000E+00	0.00000
54	5.0000E+13	0.00000E+00	0.00000
55	2.8047E+10	0.00000E+00	0.00000
56	2.0000E+13	0.00000E+00	0.00000
57	7.3703E-13	0.00000E+00	0.00000
58	1.1220E+13	0.00000E+00	0.00000
59	9.5000E+11	0.00000E+00	0.00000
60	1.9711E+12	0.00000E+00	0.00000
61	1.8131E+09	0.00000E+00	0.00000
62	7.4337E+12	0.00000E+00	0.00000
63	2.0000E+13	0.00000E+00	0.00000
64	4.8477E-17	0.00000E+00	0.00000
65	1.4180E+04	0.00000E+00	0.00000
66	1.0640E+04	0.00000E+00	0.00000
67	1.4180E+04	0.00000E+00	0.00000
68	3.7000E+12	0.00000E+00	0.00000
69	1.0000E+13	0.00000E+00	0.00000
70	4.1275E+10	0.00000E+00	0.00000
71	1.1732E+04	0.00000E+00	0.00000
72	9.8397E+10	0.00000E+00	0.00000
73	4.8733E+11	0.00000E+00	0.00000
74	5.0000E+12	0.00000E+00	0.00000
75	4.0000E+13	0.00000E+00	0.00000
76	3.0000E+13	0.00000E+00	0.00000
77	3.0000E+13	0.00000E+00	0.00000
78	3.0000E+13	0.00000E+00	0.00000
79	2.0000E+13	0.00000E+00	0.00000
80	8.3243E+08	0.00000E+00	0.00000
81	8.3337E+13	-1.32146E-35	1.00000
82	2.6482E-05	0.00000E+00	0.00000
83	1.8373E+11	0.00000E+00	0.00000
84	3.9616E+05	0.00000E+00	0.00000
85	1.9751E+07	0.00000E+00	0.00000
86	2.7477E+08	0.00000E+00	0.00000
87	5.3582E+09	0.00000E+00	0.00000
88	1.2747E+13	0.00000E+00	0.00000
89	2.2031E+13	0.00000E+00	0.00000
90	8.0000E+12	0.00000E+00	0.00000
91	5.5750E+13	0.00000E+00	0.00000
92	9.9901E+04	0.00000E+00	0.00000
93	1.8894E+12	0.00000E+00	0.00000
94	1.8000E+12	0.00000E+00	0.00000
95	7.8000E+11	0.00000E+00	0.00000
96	9.1062E+00	0.00000E+00	0.00000
97	3.2006E+11	0.00000E+00	0.00000
98	3.3136E+15	0.00000E+00	0.00000
99	4.8974E-23	0.00000E+00	0.00000
100	1.1564E+16	0.00000E+00	0.00000
101	1.4852E-20	0.00000E+00	0.00000
102	2.8745E-27	6.35490E-31	1.00000
103	1.7261E+04	0.00000E+00	0.00000
104	7.7920E+11	0.00000E+00	0.00000
105	1.0632E+07	0.00000E+00	0.00000
106	4.0310E+10	0.00000E+00	0.00000
107	1.2000E+13	0.00000E+00	0.00000
108	1.8293E+12	0.00000E+00	0.00000
109	6.2590E+10	0.00000E+00	0.00000
110	9.4292E+10	0.00000E+00	0.00000
111	1.4100E+13	0.00000E+00	0.00000
112	3.7000E+12	0.00000E+00	0.00000
113	2.0000E+13	0.00000E+00	0.00000
114	1.0000E+13	0.00000E+00	0.00000
115	2.0000E+13	0.00000E+00	0.00000
116	4.6348E+09	0.00000E+00	0.00000
117	2.0000E+12	0.00000E+00	0.00000
118	2.4053E+12	0.00000E+00	0.00000
119	3.0898E+12	0.00000E+00	0.00000
120	6.1356E+12	0.00000E+00	0.00000
121	1.4542E+16	0.00000E+00	0.00000
122	1.0401E+14	0.00000E+00	0.00000
123	2.9978E-04	0.00000E+00	0.00000
124	4.3907E-03	0.00000E+00	0.00000
125	1.3017E-13	0.00000E+00	0.00000
126	4.0000E+12	0.00000E+00	0.00000
127	5.4114E-07	0.00000E+00	0.00000
128	1.0628E+04	-2.11359E-29	1.00000
129	2.2978E+04	0.00000E+00	0.00000
130	3.2025E+08	0.00000E+00	0.00000
131	1.1424E+03	0.00000E+00	0.00000
132	6.7563E+16	0.00000E+00	0.00000

TABLE D.2.—Continued.

(k) Continued.

133	2.2558E+16	0.00000E+00	0.00000
134	5.0000E+12	0.00000E+00	0.00000
135	8.8300E+15	0.00000E+00	0.00000
136	3.6000E+13	0.00000E+00	0.00000

MIXTURE MOLECULAR WEIGHT 29.85917 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 5.42968E-10 MASS FRACTION SUM 1.00000008

CPU TIME FOR INITIALIZATION OF LSENS = 2.010002 S

**EQUILIBRIUM CONDITIONS **

TIME 0.00000E+00 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 2.00000E-01 CM

FLOW PROPERTIES

PRESSURE (ATM)	5.00000
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	7.12405E-04
TEMPERATURE (DEG K)	2205.10
MASS FLOW RATE (G/SEC)	1.00000E+01
ENTROPY (CAL/G/DEG K)	2.3430
MACH NUMBER	0.0000
GAMMA	1.2663
ENTHALPY (CAL/G)	3.60518E+01
SP. HEAT (CP) (CAL/G/DEG K)	3.66532E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

HEAT LOSS(QDOT/MDOT) = 6.7375E+00 CAL/G

CHEMICAL PROPERTIES

SPECIES	MASS FRACTION	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
C3H8	4.40962E-09	2.57807E-09	-1.88763E-06
C2H5	2.90615E-09	2.57807E-09	-1.64737E-04
CH3	1.50347E-09	2.57807E-09	1.09630E-02
CH4	1.60426E-09	2.57807E-09	4.94927E-08
C3H7	4.30883E-09	2.57807E-09	-1.09486E-02
C2H4	2.80536E-09	2.57807E-09	1.11153E-02
H	2.52153E-05	6.44928E-04	1.67780E-04
H2	4.89789E-03	6.26407E-02	-4.66564E-06
O2	1.73353E-06	1.39666E-06	6.34629E-09
HO2	3.30067E-09	2.57807E-09	2.22312E-08
O	9.10483E-07	1.46711E-06	7.32341E-08
OH	1.37839E-04	2.08944E-04	1.86705E-04
H2O	9.86353E-02	1.41152E-01	-8.80070E-07
CH3O	3.10341E-09	2.57807E-09	-7.27513E-06
CH2O	2.42160E-08	2.07920E-08	8.53875E-07
C2H6	3.00694E-09	2.57807E-09	-3.06632E-06
CH2	1.40268E-09	2.57807E-09	1.09127E-06
C2H3	2.70457E-09	2.57807E-09	-4.01556E-06
C2H2	2.60378E-09	2.57807E-09	4.70061E-06
HCO	8.92784E-08	7.93176E-08	3.54979E-07
C2H2O	4.20373E-09	2.57807E-09	1.40355E-07
C2H	2.50299E-09	2.57807E-09	-7.14720E-07
CO	1.16640E-01	1.07355E-01	6.14452E-07
C2HO	4.10293E-09	2.57807E-09	-2.43131E-07
CH	1.30189E-09	2.57807E-09	-1.35362E-06
CO2	7.86172E-02	4.60536E-02	-4.93828E-07
H2O2	3.40146E-09	2.57807E-09	-7.97699E-06
N2	6.89273E-01	6.34337E-01	-4.74891E-09
HCN	8.56052E-08	8.16619E-08	2.17771E-06
N	1.40067E-09	2.57807E-09	4.27903E-08
CN	2.60177E-09	2.57807E-09	-2.34320E-06
HNCO	4.02371E-08	2.41102E-08	1.53519E-06
NCO	4.20171E-09	2.57807E-09	-1.39270E-06
NH2	2.19562E-08	3.53282E-08	-9.96718E-14
NO	3.44264E-05	2.95785E-05	2.43727E-05
NH	1.20716E-08	2.07275E-08	2.57321E-09
NO2	4.60055E-09	2.57807E-09	1.37363E-04
N2O	4.40128E-09	2.57807E-09	1.52331E-09
HNO2	4.70134E-09	2.57807E-09	-2.55091E-05
HNO3	6.30128E-09	2.57807E-09	-1.37720E-04
HNO	3.10140E-09	2.57807E-09	1.47813E-06
AR	1.17370E-02	7.57455E-03	0.00000E+00

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE*CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	2.6497E+07	3.71932E+00	1.00000
2	3.3836E+11	-4.57303E-10	0.11906
3	1.5369E+11	2.15727E+04	1.00000
4	3.7953E+08	-4.97462E-03	0.77164
5	8.3358E+12	-7.04647E-02	0.77165
6	2.2366E+08	-4.25136E-09	0.77820
7	1.3097E+13	-2.51853E-04	0.77165
8	7.9688E+12	-2.18241E-02	0.77165
9	3.4491E+10	-4.63861E-04	0.99960
10	6.3000E+12	-1.26755E+01	0.99960
11	4.1461E+11	1.60820E+00	1.00000
12	1.1037E+13	-6.00128E+00	1.00000
13	1.4428E+13	2.15546E-02	0.59721
14	1.8839E+13	6.40254E-05	0.59721
15	3.8963E+13	1.88587E-02	0.59721
16	8.4636E+13	3.28232E+02	0.99982
17	6.3896E+11	3.46091E-06	0.99981
18	4.8000E+13	1.20054E-01	0.99982
19	2.0000E+13	-1.41827E-05	0.98609
20	1.4627E+13	-5.16927E-02	0.58553
21	3.5930E+09	1.39276E-02	0.99933
22	3.6252E+12	-4.15075E-03	0.58553
23	1.6065E+12	1.30202E-03	1.00000
24	2.5499E+12	1.45106E-05	1.00000
25	7.9870E+12	4.54482E-05	0.99992
26	2.0210E+12	7.83700E+00	0.99972
27	4.2137E+12	2.28275E-05	1.00000
28	6.0000E+12	1.50054E-02	0.99972
29	3.3000E+13	1.87777E-04	0.99991
30	5.0000E+12	4.05122E-03	0.99972
31	3.0000E+13	2.99999E-07	1.00000
32	3.0000E+13	3.00000E-07	1.00000
33	1.0432E+06	-5.42732E-03	0.99926
34	1.6746E+13	8.34364E-05	0.87554
35	3.5118E+13	-5.71053E-04	0.74076
36	1.2752E+12	-1.38619E+00	0.99926
37	3.0572E+11	1.67923E-04	0.67772
38	3.5506E+13	1.91801E-04	0.99713
39	2.0000E+13	1.61628E-02	0.99713
40	8.2523E+11	4.47065E-06	1.00000
41	1.2020E+12	6.84023E-06	1.00000
42	1.0000E+13	8.10465E-03	1.00000
43	5.0000E+13	1.21044E-01	0.96774
44	3.0000E+13	2.69818E-07	0.89939
45	6.3355E+12	6.09884E-08	0.96265
46	1.0000E+13	9.99999E-08	1.00000
47	2.8000E+13	2.26922E-02	0.99996
48	3.7821E+12	-3.36226E-02	0.91645
49	5.1680E+12	1.28386E-02	0.99306
50	1.2083E+13	-3.31554E-01	0.91645
51	8.0553E+12	-5.02823E-04	0.91645
52	2.0000E+13	1.13810E-04	0.99996
53	2.2613E+10	5.38408E-02	0.61382
54	5.0000E+13	2.83649E-04	0.99688
55	1.9470E+12	1.05480E-05	1.00000
56	2.0000E+13	5.00317E-02	1.00000
57	4.6878E+08	6.12826E-08	0.00000

TABLE D.2.—Continued.

(k) Continued.

58	2.2813E+13	-2.00079E-07	0.00000
59	1.0057E+13	-1.41921E-07	0.00000
60	1.5710E+13	-4.40742E-10	0.00000
61	1.1941E+11	7.43132E-09	0.77165
62	1.4088E+13	3.34447E-06	0.77164
63	2.0000E+13	-4.82236E-04	0.99959
64	1.6273E+07	-3.44902E-03	0.98203
65	1.3314E+11	-1.81995E-02	0.98203
66	1.0119E+11	-3.14655E-05	0.98203
67	1.3314E+11	-5.89629E-03	0.98203
68	3.7000E+12	6.60950E-01	1.00000
69	1.0000E+13	5.41746E-05	1.00000
70	4.7959E+12	2.59789E-05	0.99989
71	1.2144E+11	-2.25645E-05	0.97028
72	6.1084E+12	-1.61644E-01	0.97028
73	2.2541E+13	-1.84111E+00	0.97028
74	5.0000E+12	-1.05910E-07	0.67930
75	4.0000E+13	3.99655E-07	0.99914
76	3.0000E+13	-1.47829E-04	0.02872
77	3.0000E+13	-2.06588E-08	0.00000
78	3.0000E+13	-3.48865E-06	0.00000
79	2.0000E+13	-6.18997E-06	0.00000
80	8.3030E+12	8.49213E-04	0.00000
81	9.4158E+14	-3.51168E-05	0.00001
82	4.6917E+07	-2.36450E-09	0.00000
83	3.3191E+11	-1.01411E-02	0.00000
84	3.0694E+11	3.66970E-03	0.02871
85	1.0288E+12	2.34161E-04	0.00000
86	4.4775E+12	4.13785E-06	0.00000
87	1.8217E+13	2.22077E-04	0.00000
88	4.4815E+13	3.21879E-03	0.02871
89	3.9798E+13	6.50254E-06	0.02871
90	8.0000E+12	1.86154E-04	0.02871
91	1.0497E+14	7.53943E-03	0.02871
92	2.6327E+11	-6.23228E-02	0.49349
93	4.4015E+12	1.76041E-03	0.49349
94	1.8000E+12	-1.65168E-08	0.47852
95	7.8000E+11	9.91290E-04	0.50803
96	4.4444E+12	1.56525E+01	0.50803
97	1.1787E+13	-1.49093E-01	0.00000
98	1.8343E+15	-8.79791E-03	0.02872
99	4.9363E+04	2.50316E-04	0.00001
100	3.2198E+15	-6.06735E-07	0.00000
101	6.7260E+04	1.17654E-04	0.00000
102	1.6396E+03	1.88539E-11	0.00001
103	1.3088E+09	3.22042E-03	1.00000
104	1.7900E+13	4.28116E+00	0.98432
105	5.5550E+11	-6.28647E-03	0.98432
106	2.1113E+11	-2.67956E-09	0.00000
107	1.2000E+13	6.76986E-05	0.99136
108	6.3573E+13	2.38200E-02	0.46231
109	1.2823E+13	3.02489E+00	0.97084
110	1.4373E+13	-1.96390E-07	0.00000
111	2.5471E+13	6.37923E-05	0.46231
112	3.7000E+12	3.05564E-01	0.46231
113	2.0000E+13	1.10496E-04	0.97084
114	1.0000E+13	9.47097E-08	0.94710
115	2.0000E+13	4.85729E-02	0.97084
116	1.6556E+12	1.89949E-04	1.00000
117	2.0000E+12	2.29462E-04	1.00000
118	1.4875E+13	4.35028E-02	0.44882
119	2.3304E+12	-2.79051E-03	0.91257
120	8.7283E+12	4.54522E-05	0.91508
121	7.3233E+15	-1.42368E-01	0.91508
122	2.4811E+14	5.67949E-01	0.91508
123	2.6532E+09	3.41768E-02	0.44882
124	6.6525E+08	1.94941E-05	0.44882
125	4.9894E+06	3.13554E-03	0.44882
126	4.0000E+12	3.38369E-08	0.84592
127	1.0947E+09	-1.23741E-03	0.22565
128	1.6707E+11	-2.77063E-07	0.22565
129	1.5877E+11	-2.63297E-07	0.22565
130	2.4192E+12	-1.76353E-03	0.22565
131	3.2062E+10	-8.54691E-03	0.52316
132	7.1407E+15	-2.71359E+02	1.00000
133	8.2542E+15	-5.02538E+01	0.95950
134	5.0000E+12	-1.73611E-02	0.58124
135	6.1924E+15	2.85459E+00	0.58124
136	3.6000E+13	-4.04976E-02	0.58124

MIXTURE MOLECULAR WEIGHT 25.78071 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 5.63445E+08 MASS FRACTION SUM 1.00000027

COMPUTATIONAL WORK REQUIRED FOR EQUILIBRIUM CALCULATION:
NO. OF ITERATIONS = 14 CPU TIME = 9.000397E-02 S

INITIAL ESTIMATES (SIGMAS) AT TEMPERATURE = 2205.10 K:

C3H8	1.00000E-10
C2H5	1.00000E-10
CH3	1.00000E-10
CH4	1.00000E-10
C3H7	1.00000E-10
C2H4	1.00000E-10
H	2.50159E-05
H2	2.42975E-03
O2	5.41748E-08
HO2	1.00000E-10
O	5.69073E-08
OH	8.10468E-06
H2O	5.47511E-03
CH3O	1.00000E-10
CH2O	8.06494E-10
C2H6	1.00000E-10
CH2	1.00000E-10
C2H3	1.00000E-10

TABLE D.2.—Continued.

(k) Continued.

C2H2	1.00000E-10
HCO	3.07663E-09
C2H2O	1.00000E-10
C2H	1.00000E-10
CO	4.16416E-03
C2HO	1.00000E-10
CH	1.00000E-10
CO2	1.78636E-03
H2O2	1.00000E-10
N2	2.46051E-02
HCN	3.16756E-09
N	1.00000E-10
CN	1.00000E-10
HNCO	9.35203E-10
NCO	1.00000E-10
NH2	1.37034E-09
NO	1.14731E-06
NH	8.03991E-10
NO2	1.00000E-10
N2O	1.00000E-10
HNO2	1.00000E-10
HNO3	1.00000E-10
HNO	1.00000E-10
AR	2.93807E-04

WELLSTIRRED REACTOR CALCULATION.... LSENS PROPANE-AIR WELL-STIRRED REACTOR + ROCKET EXP; EMAX=10-4 CASE 11

		INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE	ATM	5.00000	5.00000	1.00000
TEMP.	DEG K	614.000	2190.94	3.56831
ENTROPY	CAL/GM/K	1.72748	2.33746	1.35310
DENSITY	GM/CM**3	2.96325E-03	7.19404E-04	0.24278
ENTHALPY	CAL/GM	36.0515	29.3850	0.815084
SP. HEAT (CP)	CAL/GM/K	2.91858E-01	3.66534E-01	1.25586
MOL. WT. OF MIXT		29.8592	25.8669	
GAMMA		1.2954	1.2652	

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
C3H8	5.91318E-02	8.73262E-02	1.01303E-07	1.72695E-07
C2H5	0.00000E+00	0.00000E+00	2.58669E-09	2.90615E-09
CH3	0.00000E+00	0.00000E+00	2.73015E-04	1.58685E-04
CH4	0.00000E+00	0.00000E+00	9.45262E-04	5.86249E-04
C3H7	0.00000E+00	0.00000E+00	2.58669E-09	4.30883E-09
C2H4	0.00000E+00	0.00000E+00	8.88892E-06	9.64034E-06
H	0.00000E+00	0.00000E+00	7.91521E-04	3.08436E-05
H2	0.00000E+00	0.00000E+00	5.90258E-02	4.59986E-03
O2	1.97108E-01	2.11232E-01	8.04592E-05	9.95324E-05
HO2	0.00000E+00	0.00000E+00	7.60364E-08	9.70239E-08
O	0.00000E+00	0.00000E+00	2.62396E-06	1.62299E-06
OH	0.00000E+00	0.00000E+00	2.68915E-04	1.76810E-04
H2O	0.00000E+00	0.00000E+00	1.42406E-01	9.91795E-02
CH3O	0.00000E+00	0.00000E+00	1.02584E-07	1.23076E-07
CH2O	0.00000E+00	0.00000E+00	5.73864E-06	6.66138E-06
C2H6	0.00000E+00	0.00000E+00	7.57872E-07	8.81000E-07
CH2	0.00000E+00	0.00000E+00	6.74832E-06	3.65940E-06
C2H3	0.00000E+00	0.00000E+00	2.69585E-07	2.81870E-07
C2H2	0.00000E+00	0.00000E+00	5.91869E-04	5.95779E-04
HCO	0.00000E+00	0.00000E+00	1.15555E-07	1.29633E-07
C2H2O	0.00000E+00	0.00000E+00	4.41671E-06	7.17776E-06
C2H	0.00000E+00	0.00000E+00	5.43488E-07	5.25902E-07
CO	0.00000E+00	0.00000E+00	1.03864E-01	1.12470E-01
C2HO	0.00000E+00	0.00000E+00	8.02887E-07	1.27352E-06
CH	0.00000E+00	0.00000E+00	1.93182E-07	9.72290E-08
CO2	2.82378E-04	4.16200E-04	4.76000E-02	8.09863E-02
H2O2	0.00000E+00	0.00000E+00	2.58669E-09	3.40146E-09
N2	7.34705E-01	6.89289E-01	6.36424E-01	6.89235E-01
HCN	0.00000E+00	0.00000E+00	9.35685E-06	9.77598E-06
N	0.00000E+00	0.00000E+00	2.99478E-08	1.62165E-08
CN	0.00000E+00	0.00000E+00	2.58669E-09	2.60177E-09
HNCO	0.00000E+00	0.00000E+00	2.61621E-06	4.35160E-06
NCO	0.00000E+00	0.00000E+00	1.04164E-08	1.69200E-08
NH2	0.00000E+00	0.00000E+00	4.95708E-06	3.07051E-06
NO	0.00000E+00	0.00000E+00	8.14463E-05	9.44791E-05
NH	0.00000E+00	0.00000E+00	1.38717E-07	8.05189E-08
NO2	0.00000E+00	0.00000E+00	2.58669E-09	4.60055E-09
N2O	0.00000E+00	0.00000E+00	2.58669E-09	4.40128E-09
HNO2	0.00000E+00	0.00000E+00	2.58669E-09	4.70134E-09
HNO3	0.00000E+00	0.00000E+00	2.58669E-09	6.30128E-09
HNO	0.00000E+00	0.00000E+00	2.21709E-08	2.65825E-08
AR	8.77283E-03	1.17370E-02	7.59988E-03	1.17370E-02

HEAT LOSS(QDOT/MDOT) = 6.6668E+00 CAL/GM

VOLUME 300.000 CM**3 MASS FLO 10.0000 GM/SEC

MDOT/VOLUME = 0.03333 RESIDENCE TIME = 21.5821 MSEC ITERATIONS = 12

TABLE D.2.—Continued.

(k) Continued.

```
WELLSTIRRED REACTOR CALCULATION....  LSENS   PROPANE-AIR WELL-STIRRED REACTOR + ROCKET EXP; EMAX=10-4    CASE 11
```

		INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE	ATM	5.00000	5.00000	1.00000
TEMP.	DEG K	614.000	2148.67	3.49947
ENTROPY	CAL/GM/K	1.72748	2.33082	1.34926
DENSITY	GM/CM**3	2.96325E-03	7.36115E-04	0.24841
ENTHALPY	CAL/GM	36.0515	36.0111	0.998881
SP. HEAT (CP)	CAL/GM/K	2.91858E-01	3.66061E-01	1.25424
MOL. WT. OF MIXT		29.8592	25.9571	
GAMMA		1.2954	1.2644	

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
C3H8	5.91318E-02	8.73262E-02	2.31540E-05	3.93342E-05
C2H5	0.00000E+00	0.00000E+00	7.64447E-07	8.55872E-07
CH3	0.00000E+00	0.00000E+00	1.73760E-03	1.00644E-03
CH4	0.00000E+00	0.00000E+00	1.21288E-03	7.49611E-04
C3H7	0.00000E+00	0.00000E+00	2.59571E-09	4.30883E-09
C2H4	0.00000E+00	0.00000E+00	3.05887E-04	3.30592E-04
H	0.00000E+00	0.00000E+00	4.66244E-03	1.81053E-04
H2	0.00000E+00	0.00000E+00	4.73052E-02	3.67367E-03
O2	1.97108E-01	2.11232E-01	2.19454E-03	2.70533E-03
HO2	0.00000E+00	0.00000E+00	3.15334E-06	4.00975E-06
O	0.00000E+00	0.00000E+00	1.52471E-04	9.39801E-05
OH	0.00000E+00	0.00000E+00	1.93598E-03	1.26847E-03
H2O	0.00000E+00	0.00000E+00	1.46084E-01	1.01388E-01
CH3O	0.00000E+00	0.00000E+00	8.13630E-07	9.72770E-07
CH2O	0.00000E+00	0.00000E+00	6.71907E-05	7.77237E-05
C2H6	0.00000E+00	0.00000E+00	3.17376E-05	3.67656E-05
CH2	0.00000E+00	0.00000E+00	1.73602E-04	9.38117E-05
C2H3	0.00000E+00	0.00000E+00	1.95693E-05	2.03900E-05
C2H2	0.00000E+00	0.00000E+00	2.66249E-03	2.67077E-03
HCO	0.00000E+00	0.00000E+00	2.80311E-06	3.13369E-06
C2H2O	0.00000E+00	0.00000E+00	4.49156E-05	7.27403E-05
C2H	0.00000E+00	0.00000E+00	1.26075E-05	1.21572E-05
CO	0.00000E+00	0.00000E+00	9.93922E-02	1.07254E-01
C2HO	0.00000E+00	0.00000E+00	5.26326E-05	8.31942E-05
CH	0.00000E+00	0.00000E+00	3.38357E-05	1.69704E-05
CO2	2.82378E-04	4.16200E-04	4.54745E-02	7.71012E-02
H2O2	0.00000E+00	0.00000E+00	1.48198E-07	1.94201E-07
N2	7.34705E-01	6.89289E-01	6.38598E-01	6.89187E-01
HCN	0.00000E+00	0.00000E+00	2.82088E-05	2.93700E-05
N	0.00000E+00	0.00000E+00	3.93803E-07	2.12500E-07
CN	0.00000E+00	0.00000E+00	9.97618E-08	9.99946E-08
HNCO	0.00000E+00	0.00000E+00	4.02982E-06	6.67960E-06
NCO	0.00000E+00	0.00000E+00	1.23855E-07	2.00486E-07
NH2	0.00000E+00	0.00000E+00	4.75288E-05	2.93380E-05
NO	0.00000E+00	0.00000E+00	1.07732E-04	1.24536E-04
NH	0.00000E+00	0.00000E+00	5.63310E-07	3.25840E-07
NO2	0.00000E+00	0.00000E+00	2.59571E-09	4.60055E-09
N2O	0.00000E+00	0.00000E+00	3.33234E-08	5.65030E-08
HNO2	0.00000E+00	0.00000E+00	2.59571E-09	4.70134E-09
HNO3	0.00000E+00	0.00000E+00	2.59571E-09	6.30128E-09
HNO	0.00000E+00	0.00000E+00	1.79560E-07	2.14542E-07
AR	8.77283E-03	1.17370E-02	7.62638E-03	1.17370E-02

```
HEAT LOSS(QDOT/MDOT) =   4.0346E-02  CAL/GM
VOLUME     300.000      CM**3          MASS FLO   1600.00      GM/SEC
MDOT/VOLUME =      5.33333   RESIDENCE TIME =          0.1380  MSEC   ITERATIONS =   4

                    COMPUTATIONAL WORK REQUIRED FOR PSR CALCULATION:
                NO. OF ITERATIONS =    22      CPU TIME =  4.480003E+00 S

                          **  INITIAL CONDITIONS  **

TIME   0.00000E+00  SEC            AREA   1.90000E+01  SQ CM            AXIAL POSITION   2.00000E-01  CM

   FLOW PROPERTIES                                          INTEGRATION INDICATORS

     PRESSURE                 5.00000                        STEPS FROM LAST PRINT              0
      (ATM)
     VELOCITY            114398.68                           AVERAGE STEP SIZE            0.00000E+00
      (CM/SEC)
     DENSITY             7.36114E-04                         METHOD ORDER                       0
      (G/CM**3)
     TEMPERATURE             2148.67
      (DEG K)
     MASS FLOW RATE      1.60000E+03                         TOTAL NUMBER OF STEPS              0
      (G/SEC)
     ENTROPY                 2.3308                          FUNCT EVALUATIONS                  0
      (CAL/G/DEG K)
     MACH NUMBER             1.2263                          JACOBIAN EVALUATIONS               0

     GAMMA                   1.2644

     ENTHALPY            3.60111E+01
      (CAL/G)
     SP. HEAT (CP)       3.66061E-01
      (CAL/G/DEG K)
```

TABLE D.2.—Continued.

(k) Continued.

CHAMBER PRESS = 73.5 PSIA THROAT AREA = 2.32500E+00 SQ IN

ISP = 1144.0 METERS/SEC = 116.7 LB-SEC/LB IVAC = 1745.6 METERS/SEC = 178.0 LB-SEC/LB

CSTAR = 1558.7 FT/SEC THRUST COEFF = 2.4079 AREA RATIO = 1.267

HEAT LOSS(QDOT/MDOT) = 4.0346E-02 CAL/(G-CM)

CHEMICAL PROPERTIES

SPECIES	MASS FRACTION	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
C3H8	3.93342E-05	2.31540E-05	-1.05572E-02
C2H5	8.55872E-07	7.64447E-07	1.57005E-07
CH3	1.00644E-03	1.73760E-03	9.49976E-03
CH4	7.49611E-04	1.21288E-03	2.49208E-04
C3H7	4.30883E-09	2.59571E-09	-9.14273E-03
C2H4	3.30592E-04	3.05887E-04	9.20558E-03
H	1.81053E-04	4.66244E-03	9.59796E-04
H2	3.67367E-03	4.73052E-02	9.71962E-03
O2	2.70533E-03	2.19454E-03	-3.47558E-02
HO2	4.00975E-06	3.15334E-06	6.36669E-07
O	9.39801E-05	1.52471E-04	3.12865E-05
OH	1.26847E-03	1.93598E-03	4.93335E-04
H2O	1.01388E-01	1.46084E-01	3.00154E-02
CH3O	9.72770E-07	8.13630E-07	1.66997E-07
CH2O	7.77237E-05	6.71907E-05	1.38072E-05
C2H6	3.67656E-05	3.17376E-05	6.51821E-06
CH2	9.38117E-05	1.73602E-04	3.56721E-05
C2H3	2.03900E-05	1.95693E-05	4.02397E-06
C2H2	2.67077E-03	2.66249E-03	5.47053E-04
HCO	3.13369E-06	2.80311E-06	5.80057E-07
C2H2O	7.27403E-05	4.49156E-05	9.22834E-06
C2H	1.21572E-05	1.26075E-05	2.58966E-06
CO	1.07254E-01	9.93922E-02	2.04218E-02
C2HO	8.31942E-05	5.26326E-05	1.08105E-05
CH	1.69704E-05	3.38357E-05	6.95098E-06
CO2	7.71012E-02	4.54745E-02	9.29308E-03
H2O2	1.94201E-07	1.48198E-07	3.04412E-08
N2	6.89187E-01	6.38598E-01	-1.94100E-05
HCN	2.93700E-05	2.82088E-05	5.79600E-06
N	2.12500E-07	3.93803E-07	8.09213E-08
CN	9.99946E-08	9.97618E-08	2.04971E-08
HNCO	6.67960E-06	4.02982E-06	8.27995E-07
NCO	2.00486E-07	1.23855E-07	2.54486E-08
NH2	2.93380E-05	4.75288E-05	9.76560E-06
NO	1.24536E-04	1.07732E-04	2.62632E-06
NH	3.25840E-07	5.63310E-07	1.15742E-07
NO2	4.60055E-09	2.59571E-09	1.16773E-04
N2O	5.65030E-08	3.33234E-08	6.84688E-09
HNO2	4.70134E-09	2.59571E-09	1.77305E-05
HNO3	6.30128E-09	2.59571E-09	-1.14993E-04
HNO	2.14542E-07	1.79560E-07	3.68919E-08
AR	1.17370E-02	7.62638E-03	0.00000E+00

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE*CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	1.6065E+07	1.94640E+04	0.99986
2	3.1811E+11	1.89934E+01	0.99991
3	1.2596E+11	1.68917E+04	0.98718
4	2.2398E+08	-3.43897E+04	0.98841
5	7.7621E+12	2.28150E+04	0.35021
6	1.5990E+08	-3.71835E+00	0.85479
7	1.2209E+13	1.47023E+03	0.43876
8	7.7331E+12	9.78723E+03	0.36316
9	2.9044E+10	1.49213E+02	0.90775
10	6.3000E+12	2.48595E+02	0.00790
11	3.6558E+11	4.41374E+02	0.99980
12	1.1152E+13	6.60346E+03	0.13214
13	1.3613E+13	2.98679E+03	0.99903
14	1.7973E+13	1.28977E+02	0.99917
15	3.8149E+13	3.47566E+03	0.99905
16	7.0287E+13	2.58011E+04	0.32354
17	6.2010E+11	1.46062E+00	0.94602
18	4.8000E+13	2.52622E+02	0.99491
19	2.0000E+13	8.94556E+03	0.99905
20	1.3760E+13	2.86697E+04	0.98435
21	2.2339E+09	1.00839E+03	0.99428
22	3.5986E+12	3.11438E+03	0.98467
23	1.5973E+12	1.40013E+03	0.99732
24	2.5327E+12	1.75312E+02	1.00000
25	7.7512E+12	5.35807E+02	0.99862
26	1.6683E+12	3.07399E+04	0.63439
27	4.2200E+12	2.68978E+02	1.00000
28	6.0000E+12	8.10270E+02	0.99725
29	3.3000E+13	1.46137E+02	0.99999
30	5.0000E+12	2.80389E+02	0.99730
31	3.0000E+13	1.50564E+02	0.99537
32	3.0000E+13	1.09451E+01	0.99634
33	5.4938E+05	-2.14891E+02	0.99000
34	1.5782E+13	9.50850E+03	0.99995
35	3.2945E+13	1.97593E+04	0.99544
36	1.2228E+12	2.45186E+03	0.26210
37	3.0536E+11	2.32732E+03	0.99626
38	3.5188E+13	1.44403E+03	0.99935
39	2.0000E+13	7.19438E+02	0.99299
40	8.1296E+11	1.39365E+02	1.00000
41	1.2020E+12	1.43164E+01	1.00000
42	1.0000E+13	1.51232E+03	1.00000
43	5.0000E+13	1.79997E+04	0.98842
44	3.0000E+13	4.06834E+02	1.00000
45	6.2600E+12	8.48614E+01	0.99963
46	1.0000E+13	4.11146E+01	1.00000
47	2.8000E+13	3.61354E+03	0.99997
48	3.7147E+12	-1.82554E+02	0.27578
49	5.0629E+12	1.53042E+03	0.97254
50	1.1517E+13	-1.46366E+03	0.29021
51	7.6782E+12	-1.69263E+01	0.17823
52	2.0000E+13	2.03284E+02	1.00000
53	1.5783E+10	-1.22768E+03	0.53849
54	5.0000E+13	1.42644E+02	0.99995
55	1.8651E+12	4.94269E+00	0.99998
56	2.0000E+13	1.12605E+02	1.00000
57	2.8851E+08	2.47993E+01	0.86196
58	2.2650E+13	4.36838E+03	0.99898
59	9.8198E+12	4.56100E+03	0.99896
60	1.5383E+13	2.33694E+02	0.99910
61	1.1371E+11	1.96723E+01	0.99840
62	1.3906E+13	1.00282E+02	0.99756
63	2.0000E+13	1.61422E+02	0.99248
64	9.3984E+06	-1.88849E+03	0.98733
65	1.1217E+11	5.47249E+02	0.40575
66	8.5229E+10	1.63117E+01	0.48673
67	1.1217E+11	2.33868E+02	0.41760
68	3.7000E+12	8.44952E+03	1.00000
69	1.0000E+13	1.10206E+03	1.00000
70	4.5407E+12	2.56751E+03	1.00000
71	1.0217E+11	1.68649E+00	0.42016
72	5.8203E+12	9.93108E+02	0.34207
73	2.1486E+13	8.48369E+03	0.32868
74	5.0000E+12	2.23643E+02	0.99997
75	4.0000E+13	1.78919E+03	1.00000
76	3.0000E+13	2.69292E+02	0.98317
77	3.0000E+13	1.90039E+01	0.99863
78	3.0000E+13	2.41254E+02	0.99844
79	2.0000E+13	3.87330E+02	0.99841
80	7.5634E+12	2.48318E+04	0.78916
81	9.1872E+14	5.83201E+02	0.99521
82	3.5254E+07	1.06319E+01	0.93158
83	3.2993E+11	2.48913E+04	0.26417
84	2.6753E+11	1.23752E+02	0.99442
85	9.2158E+11	3.61643E+03	0.11870
86	4.0584E+12	5.59004E+04	0.90702
87	1.6776E+13	2.44723E+04	0.13627
88	4.4247E+13	8.74413E+02	0.90564
89	3.9560E+13	2.59288E+01	0.91850
90	8.0000E+12	6.57821E+01	0.90752
91	1.0430E+14	2.25860E+03	0.99242
92	2.2664E+11	-2.76187E-01	0.00547
93	4.3639E+12	4.70124E-02	0.02530
94	1.8000E+12	2.40442E-02	0.90512
95	7.8000E+11	7.93997E-01	0.99261

TABLE D.2.—Continued.

(k) Continued.

96	3.3835E+12	-1.14933E+00	0.00086
97	1.1564E+13	3.07904E+04	0.01993
98	1.8453E+15	3.23997E+03	0.92020
99	2.6288E+04	-3.35336E+03	0.99262
100	3.3044E+15	9.82273E+01	0.99350
101	3.7836E+04	-1.34185E+03	0.99247
102	8.2955E+02	-3.59256E-02	0.93005
103	1.1680E+09	3.74563E+01	0.99999
104	1.7341E+13	-2.57872E+01	0.17513
105	4.9322E+11	9.05306E-01	0.28754
106	2.0762E+11	1.08876E+01	0.64699
107	1.2000E+13	2.70856E-01	0.99981
108	6.1328E+13	9.38431E+00	0.53382
109	1.2150E+13	8.66268E+00	0.08199
110	1.3659E+13	1.80222E+01	0.04731
111	2.5318E+13	7.87019E+00	0.95665
112	3.7000E+12	9.12932E+00	0.36645
113	2.0000E+13	5.60551E-01	0.99999
114	1.0000E+13	7.23902E-04	1.00000
115	2.0000E+13	1.71129E+01	0.99834
116	1.5599E+12	8.43899E+00	1.00000
117	2.0000E+12	1.08202E+01	1.00000
118	1.4509E+13	1.68993E+01	0.71962
119	2.3370E+12	1.15078E+00	0.97662
120	8.6972E+12	-1.26993E-02	0.71312
121	7.3744E+15	4.99607E+00	0.97993
122	2.4593E+14	2.98561E+00	0.67588
123	1.9614E+09	-5.60612E+01	0.97458
124	5.0589E+08	-5.20566E+00	0.99764
125	3.1593E+06	-1.64848E+00	0.78311
126	4.0000E+12	6.01853E-06	0.99176
127	7.9120E+08	-4.79388E-01	0.92453
128	1.4125E+11	7.78928E-05	0.07313
129	1.3535E+11	1.01038E-03	0.98990
130	2.2099E+12	4.65664E-01	0.91382
131	2.6947E+10	-1.11662E-01	0.95787
132	7.3052E+15	-2.12217E+02	0.99999
133	8.3388E+15	3.28330E+01	0.44853
134	5.0000E+12	6.15514E+00	0.99073
135	6.2147E+15	2.46284E+01	0.18745
136	3.6000E+13	1.84052E+01	0.99092

DERIVATIVES (CGS UNITS): T -1.61242E+03 RHO -2.23801E-03 V 2.27387E+05

MIXTURE MOLECULAR WEIGHT 25.95711 TOTAL ENERGY EXCHANGE RATE -4.71633E+09 (CAL-CM**3/G**2/SEC) MASS FRACTION SUM 1.00000018

CPU TIME FOR INITIALIZATION OF LSENS = 0.599998 S

TIME 2.10833E-05 SEC AREA 9.50000E+01 SQ CM AXIAL POSITION 4.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	0.31213
VELOCITY (CM/SEC)	205745.31
DENSITY (G/CM**3)	8.18530E-05
TEMPERATURE (DEG K)	1207.44
MASS FLOW RATE (G/SEC)	1.59988E+03
ENTROPY (CAL/G/DEG K)	2.3367
MACH NUMBER	2.9058
GAMMA	1.2975
ENTHALPY (CAL/G)	-3.13534E+02
SP. HEAT (CP) (CAL/G/DEG K)	3.33538E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	16
AVERAGE STEP SIZE	0.13189E+00
METHOD ORDER	4
TOTAL NUMBER OF STEPS	158
FUNCT EVALUATIONS	203
JACOBIAN EVALUATIONS	30

CHAMBER PRESS = 73.5 PSIA THROAT AREA = 2.32500E+00 SQ IN

ISP = 2057.5 METERS/SEC = 209.8 LB-SEC/LB IVAC = 2245.2 METERS/SEC = 229.0 LB-SEC/LB

CSTAR = 1558.8 FT/SEC THRUST COEFF = 4.3304 AREA RATIO = 6.333

HEAT LOSS(QDOT/MDOT) = 1.0933E-02 CAL/(G-CM)

CHEMICAL PROPERTIES

SPECIES	MASS FRACTION	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE*CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
C3H8	3.56854E-07	2.10267E-07	3.30566E-08	1	3.8480E+00	-4.93770E+00	0.99992
C2H5	1.56557E-05	1.39970E-05	3.50952E-06	2	4.8518E+10	3.80296E-03	0.99990
CH3	1.45636E-04	2.51684E-04	-3.70288E-05	3	2.9365E+08	-7.65783E-02	0.04339
CH4	6.30941E-04	1.02187E-03	2.24521E-05	4	2.3593E+01	-6.25179E+03	1.00000
C3H7	2.02770E-11	1.22271E-11	5.38548E-10	5	8.8397E+11	2.64015E+03	0.77877
C2H4	2.07228E-04	1.91929E-04	-2.31085E-06	6	5.8032E+03	-3.87778E-02	0.99987
H	9.82910E-05	2.53365E-03	-1.85952E-04	7	1.4368E+12	1.34998E+01	0.89058
H2	3.87762E-03	4.99803E-02	8.23327E-05	8	3.0982E+12	2.57790E+02	0.79349
O2	7.11964E-04	5.78104E-04	-9.71503E-06	9	1.5454E+08	3.26544E-02	0.98037
HO2	3.94974E-07	3.10919E-07	1.56193E-08	10	6.3000E+12	-2.37944E+00	0.01441
O	4.29184E-06	6.96981E-06	-1.55144E-06	11	7.9052E+09	6.13064E-03	0.77605
OH	4.53450E-05	6.92747E-05	-2.30869E-05	12	1.4043E+13	1.31744E+03	0.99981
H2O	1.02841E-01	1.48323E-01	1.39377E-05	13	2.3166E+12	1.01474E+03	0.99734
CH3O	8.05791E-10	6.74628E-10	-5.73168E-10	14	4.2875E+12	5.17334E+00	0.99869

TABLE D.2.—Continued.

(k) Continued.

CH2O	3.36934E-05	2.91559E-05	2.76605E-06
C2H6	1.35432E-04	1.17025E-04	3.83272E-07
CH2	7.14120E-06	1.32280E-05	-3.22903E-06
C2H3	2.44702E-04	2.35083E-04	2.96100E-05
C2H2	2.54527E-03	2.53987E-03	-3.01363E-05
HCO	2.99220E-06	2.67917E-06	4.73737E-07
C2H2O	2.86666E-05	1.77184E-05	-2.00549E-07
C2H	1.62951E-07	1.69152E-07	-7.94274E-08
CO	1.08064E-01	1.00241E-01	8.02278E-07
C2HO	2.94028E-06	1.86198E-06	-4.13144E-07
CH	4.95284E-07	9.88464E-07	-3.69731E-07
CO2	7.92424E-02	4.67832E-02	1.33748E-05
H2O2	1.47428E-08	1.12615E-08	-3.47037E-09
N2	6.89186E-01	6.39222E-01	5.36243E-09
HCN	2.97705E-05	2.86215E-05	1.36261E-09
N	9.46478E-08	1.75572E-07	-6.57106E-09
CN	2.73080E-09	2.72711E-09	-9.76126E-10
HNCO	2.93575E-06	1.77288E-06	-6.56809E-08
NCO	6.21521E-09	3.84336E-09	-1.28310E-09
NH2	3.11674E-05	5.05420E-05	6.69983E-08
NO	1.25553E-04	1.08717E-04	9.90332E-09
NH	2.85269E-07	4.93653E-07	-6.13020E-10
NO2	1.23908E-09	6.99794E-10	1.50145E-12
N2O	3.77522E-08	2.22867E-08	-7.81921E-11
HNO2	3.55661E-08	1.96560E-08	-1.79580E-10
HNO3	1.17750E-13	4.85525E-14	7.88724E-15
HNO	5.78710E-07	4.84825E-07	-1.35304E-08
AR	1.17370E-02	7.63385E-03	0.00000E+00

15	2.0063E+13	2.40326E+02	0.99752
16	2.4486E+11	-1.79301E+03	0.26100
17	2.4890E+11	2.98311E+00	0.99994
18	4.8000E+13	2.52151E+03	1.00000
19	2.0000E+13	9.86315E+01	1.00000
20	2.1373E+12	1.09689E+03	0.71248
21	1.1520E+03	-3.14093E-04	0.48954
22	2.8748E+12	4.14227E+01	0.73161
23	1.3405E+12	2.63897E+01	0.99957
24	2.0605E+12	4.08301E+00	1.00000
25	3.1112E+12	6.16304E+00	0.99970
26	4.8421E+09	-9.80229E+03	0.85323
27	4.4171E+12	8.89198E+02	1.00000
28	6.0000E+12	5.29367E+03	1.00000
29	3.3000E+13	8.00928E+01	1.00000
30	5.0000E+12	1.20616E+02	1.00000
31	3.0000E+13	1.38189E+02	1.00000
32	3.0000E+13	1.76709E+00	1.00000
33	1.8028E-03	-5.76105E+00	1.00000
34	2.5942E+12	6.80256E+01	1.00000
35	4.7051E+12	1.23376E+02	0.99998
36	3.4066E+11	-1.74895E-01	0.00197
37	2.9441E+11	7.66952E+01	0.99953
38	2.6759E+13	3.87603E+00	1.00000
39	2.0000E+13	3.47137E-01	0.99996
40	5.1505E+11	8.21231E-01	1.00000
41	1.2020E+12	2.31067E-02	1.00000
42	1.0000E+13	1.91068E+00	1.00000
43	5.0000E+13	3.49275E+02	0.99962
44	3.0000E+13	1.09453E+00	1.00000
45	4.3450E+12	1.58526E-01	1.00000
46	1.0000E+13	5.13558E-02	1.00000
47	2.8000E+13	5.09073E+01	0.99997
48	2.1481E+12	3.54671E+00	0.90811
49	2.7077E+12	1.80052E+02	0.99997
50	2.6732E+12	1.60266E+02	0.90156
51	1.7822E+12	3.10136E-01	0.95131
52	2.0000E+13	3.65857E+00	1.00000
53	2.7597E+05	-2.12019E+02	0.99997
54	5.0000E+13	8.73185E-02	1.00000
55	5.0374E+11	2.91014E-04	0.99999
56	2.0000E+13	5.06383E-02	1.00000
57	1.0908E+02	-1.12592E+00	1.00000
58	1.8194E+13	5.44169E+01	0.99972
59	4.7396E+12	5.18464E+02	0.99970
60	8.1049E+12	2.43931E+00	0.99985
61	2.8505E+10	3.09415E-01	0.99863
62	1.0424E+13	1.04123E+01	1.00000
63	2.0000E+13	2.31830E+00	1.00000
64	5.1308E-01	-2.13862E+02	1.00000
65	6.9894E+08	-2.72597E-01	0.29223
66	5.2802E+08	4.13225E-04	0.30118
67	6.9894E+08	-5.75676E-03	0.24180
68	3.7000E+12	2.53449E+02	1.00000
69	1.0000E+13	8.46456E+00	1.00000
70	9.5526E+11	1.08208E+01	1.00000
71	6.1442E+08	7.20734E-05	0.85893
72	1.4859E+12	1.47994E+00	0.73376
73	5.7926E+12	2.05554E+02	0.71479
74	5.0000E+12	1.29597E+00	1.00000
75	4.0000E+13	1.03678E+01	1.00000
76	3.0000E+13	6.88273E+01	0.99999
77	3.0000E+13	8.29810E-01	1.00000
78	5.0000E+13	8.24770E+00	1.00000
79	2.0000E+13	2.01101E+02	1.00000
80	4.4074E+11	1.42434E+03	0.81431
81	4.3461E+14	1.41695E+00	1.00000
82	5.8334E+03	4.98748E-04	0.99604
83	2.7487E+11	2.24808E+03	0.79510
84	4.0670E+09	1.87760E-01	1.00000
85	3.2240E+10	2.32112E+01	0.47015
86	2.0324E+11	4.32438E+02	0.98066
87	1.3629E+12	3.55427E+02	0.50540
88	3.0014E+13	3.50218E+01	0.99997
89	3.2958E+13	1.05795E-01	0.99999
90	8.0000E+12	2.55234E-01	0.99997
91	8.5789E+13	1.00107E+02	1.00000
92	2.3611E+09	-8.04912E-01	0.93675
93	3.3612E+12	3.65489E-03	0.94096
94	1.8000E+12	2.57635E-04	0.99954
95	7.8000E+11	3.29667E-02	1.00000
96	8.3354E+08	-3.23303E-01	0.92791
97	3.7327E+12	1.27344E+03	0.06652
98	2.2149E+15	6.78746E+01	0.99996
99	1.2115E-04	-9.99179E+01	1.00000
100	5.8802E+15	4.84565E-01	1.00000
101	9.2503E-04	-2.09796E+02	1.00000
102	6.4783E-07	-1.71688E-05	1.00000
103	3.6387E+07	3.40474E-02	0.99974
104	6.5893E+12	1.23214E-01	0.09262
105	1.5235E+10	2.04800E-03	0.45491
106	1.2452E+11	2.70201E-01	0.73881
107	1.2000E+13	3.37864E-04	1.00000
108	2.0508E+13	4.51371E-03	0.78649
109	2.3495E+12	-7.35703E-02	0.09914
110	2.8939E+12	9.99988E+00	0.51934
111	2.1093E+13	4.90565E-02	0.99587
112	3.7000E+12	-2.93813E-02	0.04032
113	2.0000E+13	7.93595E-04	1.00000
114	1.0000E+13	9.99550E-06	1.00000
115	2.0000E+13	2.88466E-01	0.99993
116	2.5407E+11	4.04434E-02	1.00000
117	2.0000E+12	3.18365E-01	1.00000
118	7.5491E+12	3.79962E-01	0.99359
119	2.5497E+12	1.27528E-01	0.99894
120	7.8005E+12	5.55963E-05	0.98650
121	9.1138E+15	3.22260E-02	1.00000
122	1.8804E+14	4.93738E-01	0.99974
123	1.9752E+05	-5.53383E-01	0.99985
124	1.4913E+05	-5.94259E-02	1.00000

TABLE D.2.—Continued.
(k) Concluded.

125	2.8432E+00	-8.22740E-01	1.00000
126	4.0000E+12	7.27987E-07	1.00000
127	2.3457E+04	-6.60741E-05	0.98842
128	8.4782E+08	1.95076E-07	1.00000
129	1.0471E+09	2.40855E-07	0.99966
130	1.4031E+11	1.17363E-02	1.00000
131	1.3525E+08	-3.34266E-01	0.99998
132	1.4619E+16	1.17722E-06	0.34903
133	1.1373E+16	3.07462E-01	0.76920
134	5.0000E+12	9.09786E+00	1.00000
135	6.9342E+15	8.86939E+00	0.99509
136	3.6000E+13	1.79102E+00	1.00000

DERIVATIVES (CGS UNITS): T -8.25079E+01 RHO -1.95264E-05 V 5.76675E+03

MIXTURE MOLECULAR WEIGHT 25.98253 TOTAL ENERGY EXCHANGE RATE -2.08273E+09 MASS FRACTION SUM 1.00000017
(CAL-CM**3/G**2/SEC)

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 8.799896E-01 S UP TO THIS TIME - 1.016998E+01 S

(LSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

TOTAL NO. OF STEPS - 158
TOTAL NO. OF DERIVATIVE EVALUATIONS - 203
TOTAL NO. OF JACOBIAN EVALUATIONS - 30
TOTAL CPU TIME - 10.169983 S

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 12.259995 S

(LSENS) READ DATA FOR NEXT CASE

TABLE D.2.—Continued.
(l) Case 12

DISTANCE-AREA VERSION LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

LSENS HIGH TEMPERATURE AIR IONIZATION CASE 12

REACTION NUMBER	REACTION								REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1*N	+	1*O2	=	1*NO	+	1*O		6.40000E+09	1.0000	6250.00
2	1*O	+	1*N2	=	1*NO	+	1*N		1.80000E+14	0.0000	76250.00
3	1*N	+	1*O	=	1*NO	+	M		6.40000E+16	-0.5000	0.00
4			2*O	=	1*O2	+	M		5.70000E+13	0.0000	-1790.00
5	M	+	1*N2	=	2*N				3.72000E+21	-1.6000	225000.00
6	1*NO	+	1*O	=	1*NO2	+	M		5.62000E+15	0.0000	-1160.00
7	M	+	1*N2O	=	1*N2	+	1*O		6.92000E+23	-2.5000	65000.00
8	1*O	+	1*N2O	=	1*N2	+	1*O2		1.00000E+14	0.0000	28020.00
9	1*NO+	+	1*E	=	1*N	+	1*O		1.45000E+21	-1.5000	0.00
10	1*O+	+	1*E	=	1*O	+	M		2.00000E+26	-2.5000	0.00
11	1*O2	+	1*E	=	1*O2-	+	M		1.52000E+21	-1.0000	1190.00
12	1*O2	+	1*O-	=	1*O2-	+	1*O		6.00000E+12	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(N2O , 3) = 2.25000 M(N2 , 6) = 1.55000 M(O2 , 10) = 4.50000 M(N , 10) = 0.03000
M(NO , 10) = 50.00000 M(O , 10) = 0.03000 M(N2 , 11) = 0.00002

** INITIAL CONDITIONS **

TIME 0.00000E+00 SEC AREA 1.00000E+03 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.68030
VELOCITY (CM/SEC)	47002.00
DENSITY (G/CM**3)	1.22560E-04
TEMPERATURE (DEG K)	4820.00
MASS FLOW RATE (G/SEC)	5.76058E+03
ENTROPY (CAL/G/DEG K)	2.3905
MACH NUMBER	0.3535
GAMMA	1.2726
ENTHALPY (CAL/G)	1.35458E+03
SP. HEAT (CP) (CAL/G/DEG K)	3.21566E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
N	0.00000E+00	0.00000E+00	8.53190E-06	1	1.6063E+13	0.00000E+00	0.00000
O2	8.90048E-07	2.09500E-01	-2.31733E-02	2	6.2795E+10	0.00000E+00	0.00000
NO	0.00000E+00	0.00000E+00	0.00000E+00	3	9.2184E+14	0.00000E+00	0.00000
O	0.00000E+00	0.00000E+00	4.33027E-02	4	6.8713E+13	-1.34005E+06	1.00000
N2	3.35839E-06	7.90500E-01	-3.04911E-03	5	2.9899E+05	2.83998E+02	1.00000
NO2	0.00000E+00	0.00000E+00	0.00000E+00	6	6.3436E+15	0.00000E+00	0.00000
N2O	0.00000E+00	0.00000E+00	3.04484E-03	7	4.8444E+11	0.00000E+00	0.00000
NO+	0.00000E+00	0.00000E+00	0.00000E+00	8	5.3643E+12	-2.02705E+05	1.00000
E	0.00000E+00	0.00000E+00	4.38522E-07	9	4.3331E+15	0.00000E+00	0.00000
O+	0.00000E+00	0.00000E+00	0.00000E+00	10	1.2400E+17	0.00000E+00	0.00000
O2-	4.24844E-15	1.00000E-09	-4.38522E-07	11	2.7851E+17	-2.91938E+01	1.00000
O-	0.00000E+00	0.00000E+00	0.00000E+00	12	6.0000E+12	0.00000E+00	0.00000

DERIVATIVES (CGS UNITS): T -1.44460E+03 RHO 2.89845E-05 V -1.11156E+04

MIXTURE MOLECULAR WEIGHT 28.84834 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 1.75700E+11 MASS FRACTION SUM 1.00000000

SPECIES MOLE NUMBERS (MOLE SPECIES I/G MIXTURE) AND DERIVATIVES (CGS UNITS: MOLE SPECIES I/G MIXTURE/S OR CM)

SPECIES	SIGMA(I)	DSIGMA(I)/DIVAR	SPECIES	SIGMA(I)	DSIGMA(I)/DIVAR	SPECIES	SIGMA(I)	DSIGMA(I)/DIVAR
N	0.00000E+00	0.14811E-05	O2	0.72621E-02	-0.40227E-02	NO	0.00000E+00	0.00000E+00
O	0.00000E+00	0.75171E-02	N2	0.27402E-01	-0.52931E-03	NO2	0.00000E+00	0.00000E+00
N2O	0.00000E+00	0.52856E-03	NO+	0.00000E+00	0.00000E+00	E	0.00000E+00	0.76125E-07
O+	0.00000E+00	0.00000E+00	O2-	0.34664E-10	-0.76125E-07	O-	0.00000E+00	0.00000E+00

TABLE D.2.—Continued.

(l) Continued.

OMEGA(I,J) RATE OF PRODUCTION OF SPECIES I BY REACTION J (MOLE SPECIES I/CC/S)

SPECIES	REACTION 1	2	3	4	5	6	7	8
	9	10	11	12				
N	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.85319E-05	0.00000E+00	0.00000E+00	0.00000E+00
	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00				
O2	0.00000E+00	0.00000E+00	0.00000E+00	-0.20129E-01	0.00000E+00	0.00000E+00	0.00000E+00	-0.30448E-02
	0.00000E+00	0.00000E+00	0.43852E-06	0.00000E+00				
NO	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00				
O	0.00000E+00	0.00000E+00	0.00000E+00	0.40258E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.30448E-02
	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00				
N2	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-0.42659E-05	0.00000E+00	0.00000E+00	-0.30448E-02
	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00				
NO2	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00				
N2O	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.30448E-02
	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00				
NO+	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00				
E	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
	0.00000E+00	0.00000E+00	0.43852E-06	0.00000E+00				
O+	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00				
O2-	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
	0.00000E+00	0.00000E+00	-0.43852E-06	0.00000E+00				
O-	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00				

CPU TIME FOR INITIALIZATION OF LSENS = 0.949997 S

TIME 1.59489E-05 SEC AREA 1.00000E+03 SQ CM AXIAL POSITION 7.00000E-01 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.70904
VELOCITY (CM/SEC)	41946.49
DENSITY (G/CM**3)	1.37332E-04
TEMPERATURE (DEG K)	4238.68
MASS FLOW RATE (G/SEC)	5.76058E+03
ENTROPY (CAL/G/DEG K)	2.4163
MACH NUMBER	0.3292
GAMMA	1.2873
ENTHALPY (CAL/G)	1.35995E+03
SP. HEAT (CP) (CAL/G/DEG K)	3.18551E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	4
AVERAGE STEP SIZE	0.50398E-01
METHOD ORDER	4
TOTAL NUMBER OF STEPS	57
FUNCT EVALUATIONS	73
JACOBIAN EVALUATIONS	14

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
N	1.44539E-09	2.94154E-04	-2.40893E-05	1	1.2917E+13	2.93986E+05	0.44160
O2	6.72505E-07	1.36862E-01	-9.27740E-03	2	2.1075E+10	2.85929E+05	0.23345
NO	3.44095E-07	7.00273E-02	1.08092E-02	3	9.8302E+14	-6.75873E+03	0.98355
O	3.05299E-07	6.21318E-02	7.75744E-03	4	7.0497E+13	-1.84687E+05	0.99082
N2	3.59017E-06	7.30639E-01	-5.37990E-03	5	1.4649E+04	1.35292E+01	0.98739
NO2	1.13223E-11	2.30421E-06	5.15564E-07	6	6.4498E+15	2.73364E+01	0.00011
N2O	2.06908E-10	4.21081E-05	-1.29661E-05	7	2.6338E+11	1.39241E+04	0.98071
NO+	1.54269E-12	3.13954E-07	1.06516E-07	8	3.5914E+12	-1.32366E+04	0.52390
E	1.53645E-12	3.12686E-07	1.05370E-07	9	5.2544E+15	-5.64771E+00	0.89532
O+	2.74119E-18	5.57863E-13	8.04637E-14	10	1.7098E+17	-4.26638E-06	0.99979
O2-	3.47934E-15	7.08084E-10	2.43515E-10	11	3.1135E+17	6.07560E-02	0.00269
O-	7.51715E-15	1.52983E-09	9.02342E-10	12	6.0000E+12	-4.78443E-02	0.02889

DERIVATIVES (CGS UNITS): T -3.73835E+02 RHO 1.10772E-05 V -3.38343E+03

MIXTURE MOLECULAR WEIGHT 27.94853 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 3.68408E+10 MASS FRACTION SUM 1.00000002

SPECIES MOLE NUMBERS (MOLE SPECIES I/G MIXTURE) AND DERIVATIVES (CGS UNITS: MOLE SPECIES I/G MIXTURE/S OR CM)

SPECIES	SIGMA(I)	DSIGMA(I)/DIVAR	SPECIES	SIGMA(I)	DSIGMA(I)/DIVAR	SPECIES	SIGMA(I)	DSIGMA(I)/DIVAR
N	0.10525E-04	-0.41818E-05	O2	0.48969E-02	-0.16105E-02	NO	0.25056E-02	0.18764E-02
O	0.22231E-02	0.13466E-02	N2	0.26142E-01	-0.93392E-03	NO2	0.82445E-07	0.89499E-07
N2O	0.15066E-05	-0.22508E-05	NO+	0.11233E-07	0.18490E-07	E	0.11188E-07	0.18292E-07
O+	0.19960E-13	0.13968E-13	O2-	0.25335E-10	0.42273E-10	O-	0.54737E-10	0.15664E-09

TABLE D.2.—Continued.

(l) Continued.

OMEGA(I,J) RATE OF PRODUCTION OF SPECIES I BY REACTION J (MOLE SPECIES I/CC/S)

SPECIES	REACTION 1	2	3	4	5	6	7	8
	9	10	11	12				
N	-0.55446E-02	0.53926E-02	0.12747E-03	0.00000E+00	0.51032E-06	0.00000E+00	0.00000E+00	0.00000E+00
	-0.10652E-06	0.00000E+00	0.00000E+00	0.00000E+00				
O2	-0.55446E-02	0.00000E+00	0.00000E+00	-0.34832E-02	0.00000E+00	0.00000E+00	0.00000E+00	-0.24964E-03
	0.00000E+00	0.00000E+00	-0.11459E-08	0.90234E-09				
NO	0.55446E-02	0.53926E-02	-0.12747E-03	0.00000E+00	0.00000E+00	-0.51556E-06	0.00000E+00	0.00000E+00
	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00				
O	0.55446E-02	-0.53926E-02	0.12747E-03	0.69664E-02	0.00000E+00	-0.51556E-06	0.26261E-03	0.24964E-03
	-0.10652E-06	-0.80464E-13	0.00000E+00	-0.90234E-09				
N2	0.00000E+00	-0.53926E-02	0.00000E+00	0.00000E+00	-0.25516E-06	0.00000E+00	0.26261E-03	-0.24964E-03
	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00				
NO2	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.51556E-06	0.00000E+00	0.00000E+00
	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00				
N2O	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-0.26261E-03	0.24964E-03
	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00				
NO+	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
	0.10652E-06	0.00000E+00	0.00000E+00	0.00000E+00				
E	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
	0.10652E-06	0.80464E-13	-0.11459E-08	0.00000E+00				
O+	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
	0.00000E+00	0.80464E-13	0.00000E+00	0.00000E+00				
O2-	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
	0.00000E+00	0.00000E+00	0.11459E-08	-0.90234E-09				
O-	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
	0.00000E+00	0.00000E+00	0.00000E+00	0.90234E-09				

COMPUTER TIME (CPU) REQUIRED, FOR THIS STEP - 3.999329E-02 S UP TO THIS TIME - 3.999939E-01 S

TIME 1.59489E-05 SEC AXIAL POSITION 7.00000E-01 CM

REACTION IMPORTANCE FOR SPECIES FORMATION AND RATES

REACTION NUMBER (J)

SPECIES (I)

OMEGA(I,J) RATE OF PRODUCTION OF SPECIES I BY REACTION J (MOLE/CM**3/S)

SPECIES										
N	1	2	3	5	9					
	-5.545E-03	5.393E-03	1.275E-04	5.103E-07	-1.065E-07					
O2	1	4	8	11	12					
	-5.545E-03	-3.483E-03	-2.496E-04	-1.146E-09	9.023E-10					
NO	1	2	3	6						
	5.545E-03	5.393E-03	-1.275E-04	-5.156E-07						
O	4	1	2	7	8	3	6	9	12	10
	6.966E-03	5.545E-03	-5.393E-03	2.626E-04	2.496E-04	1.275E-04	-5.156E-07	-1.065E-07	-9.023E-10	-8.046E-14
N2	2	7	8	5						
	-5.393E-03	2.626E-04	-2.496E-04	-2.552E-07						
NO2	6									
	5.156E-07									

TABLE D.2.—Continued.
(l) Concluded.

```
                 7           8
N2O
          -2.626E-04   2.496E-04

                 9
NO+
           1.065E-07

                 9          11          10
E
           1.065E-07  -1.146E-09   8.046E-14

                10
O+
           8.046E-14

                11          12
O2-
           1.146E-09  -9.023E-10

                12
O-
           9.023E-10


(LSENS)     END OF THIS CASE

              SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:
                 TOTAL NO. OF STEPS -                        57
                 TOTAL NO. OF DERIVATIVE EVALUATIONS -       73
                 TOTAL NO. OF JACOBIAN EVALUATIONS -         14
                 TOTAL CPU TIME -                     0.399994 S


                                TOTAL CPU TIME (INCLUDING I/O) REQUIRED =      1.910004 S


(LSENS)     READ DATA FOR NEXT CASE
```

TABLE D.2.—Continued.

(m) Case 13

```
                              **  DATA LINES  **

                 1         2         3         4         5         6         7         8
CC  12345678901234567890123456789012345678901234567890123456789012345678901234567890

     LSENS   HIGH PRESSURE HYDROGEN - CARBON MONOXIDE REACTION                CASE 13
    NEW
       CH3     +   OH       =   CH3O    +   H            6.3E+12   0.          0.
       M       +   CH3O     =   CH2O    +   H            5.0E+13   0.         21000.
       CH3O    +   H        =   CH2O    +   H2           2.0E+13    0.         0.
       CH3     +   HCO      =   CH4     +   CO           3.0E+11   .5          0.
       CH3     +   HO2      =   CH3O    +   OH           2.0E+13   0.          0.
       M           CH4      =   CH3     +   H            2.0E+17   0.         88000.
       H       +   CH4      =   CH3     +   H2          1.26E+14   0.         11900.
       OH      +   CH4      =   CH3     +   H2O          2.5E+13   0.         5010.
       CH2O    +   H        =   HCO     +   H2           2.5E+13   0.          3990.
       CH2O    +   OH       =   HCO     +   H2O          3.0E+13   0.          1200.
       M       +   CH2O     =   H       +   HCO          5.0E+16  0.         81000.
       HCO     +   H        =   CO      +   H2           2.0E+13    0.         0.
       HCO     +   OH       =   CO      +   H2O          3.0E+13   0.         0.
       M       +   HCO      =   H       +   CO           2.9E+14   0.         15570.
       CO      +   OH       =   CO2     +   H           4.17E+11   0.0        1000.
       CO      +   HO2      =   CO2     +   OH          5.75E+13   0.         22930.
       H       +   HO2      =2.00H                      1.34E+14   0.         1070.
       H2      +   HO2      =   H2O2    +   H           7.91E+13   0.         25000.
       OH      +   H2O2     =   H2O     +   HO2          6.1E+12   0.         1430.
       M       +   H2O2     =2.00H                      1.44E+17   0.         45510.
       THIRDBODY
    H2          2.30    H2O2         6.6     H2O          6.0    END
       H2      +   OH       =   H2O     +   H           4.74E+13   0.         6098.
       M       +   H2O      =   H       +   OH          1.30E+15   0.         105140.
       THIRDBODY
    H2          4.00    CO2          4.0     H2O          20.0   END
       M       +   H2       =   H       +   H            2.2E+14   0.          96000.
       THIRDBODY
    H2          4.10    H2O         15.0     END
                                     -  BLANK LINE  -
    END
    TIME
     &prob  print=1.0,1.E+6,1.E+8,1.E+9, combus=.true.,
       rhocon=.true., tcon=.true.,  &end
     &start  t=1000.0, p=100.0,  &end
    H2        0.99
    CO        0.01
    END
     &solver  emax=1.0E-3, atolsp=1.0E-12,  &end
    FINIS
```

```
                              **  EQUILIBRIUM CALCULATION  **

                THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED TEMPERATURE AND DENSITY

                                INITIAL STATE                FINAL STATE                FINAL/INITIAL RATIO

PRESSURE                          100.0000                     98.0001                          0.9800
 (ATM)
VELOCITY                            0.00                        0.00                            1.0000
 (CM/SEC)
DENSITY                         2.77341E-03                 2.77341E-03                         1.0000
 (G/CM**3)
TEMPERATURE                       1000.00                     1000.00                           1.0000
 (DEG K)
ENTHALPY                         2057.01343                  1820.27039                         0.88491
 (CAL/G)
INTERNAL ENERGY                  1183.82056                   964.54108                         0.81477
 (CAL/G)
SP. HEAT (CP)                      3.17527                      3.16527                         0.99685
 (CAL/G/DEG K)
ENTROPY                            13.5443                      13.4256                          0.9912
 (CAL/G/DEG K)
MACH NUMBER                         0.0000                       0.0000                          1.0000

GAMMA                               1.3793                       1.3705                          0.9936

SONIC VELOCITY                   224481.86                   221517.92                           0.9868
 (CM/SEC)

                                                        SPECIES     MOLE FRACTION
                                                         CH3         2.32219E-11
                                                         OH          2.32219E-11
                                                         CH3O        2.32219E-11
                                                         H           2.32219E-11
                                                         CH2O        2.32219E-11
                                                         H2          9.79592E-01
                                                         HCO         2.32219E-11
                                                         CH4         1.02038E-02
                                                         CO          2.86966E-07
                                                         HO2         2.32219E-11
                                                         H2O         1.02038E-02
                                                         CO2         2.32219E-11
                                                         H2O2        2.32219E-11

MIXTURE MOLECULAR WEIGHT                                          2.32219

D(LOG VOLUME)/D(LOG T)                                            1.0000
    AT CONSTANT P

D(LOG VOLUME)/D(LOG P)                                           -1.0000
    AT CONSTANT T


                COMPUTATIONAL WORK REQUIRED FOR EQUILIBRIUM CALCULATION:
                NO. OF ITERATIONS =     11      CPU TIME =  2.000427E-02 S
```

TABLE D.2.—Continued.
(m) Continued.

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

LSENS HIGH PRESSURE HYDROGEN - CARBON MONOXIDE REACTION CASE 13

REACTION NUMBER	REACTION							REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1*CH3	+	1*OH	=	1*CH3O	+	1*H	6.30000E+12	0.0000	0.00
2	M	+	1*CH3O	=	1*CH2O	+	1*H	5.00000E+13	0.0000	21000.00
3	1*CH3O	+	1*H	=	1*CH2O	+	1*H2	2.00000E+13	0.0000	0.00
4	1*CH3	+	1*HCO	=	1*CH4	+	1*CO	3.00000E+11	0.5000	0.00
5	1*CH3	+	1*HO2	=	1*CH3O	+	1*OH	2.00000E+13	0.0000	0.00
6	M	+	1*CH4	=	1*CH3	+	1*H	2.00000E+17	0.0000	88000.00
7	1*H	+	1*CH4	=	1*CH3	+	1*H2	1.26000E+14	0.0000	11900.00
8	1*OH	+	1*CH4	=	1*CH3	+	1*H2O	2.50000E+13	0.0000	5010.00
9	1*CH2O	+	1*H	=	1*HCO	+	1*H2	2.50000E+13	0.0000	3990.00
10	1*CH2O	+	1*OH	=	1*HCO	+	1*H2O	3.00000E+13	0.0000	1200.00
11	M	+	1*CH2O	=	1*H	+	1*HCO	5.00000E+16	0.0000	81000.00
12	1*HCO	+	1*H	=	1*CO	+	1*H2	2.00000E+13	0.0000	0.00
13	1*HCO	+	1*OH	=	1*CO	+	1*H2O	3.00000E+13	0.0000	0.00
14	M	+	1*HCO	=	1*H	+	1*CO	2.90000E+14	0.0000	15570.00
15	1*CO	+	1*OH	=	1*CO2	+	1*H	4.17000E+11	0.0000	1000.00
16	1*CO	+	1*HO2	=	1*CO2	+	1*OH	5.75000E+13	0.0000	22930.00
17	1*H	+	1*HO2	=	2*OH			1.34000E+14	0.0000	1070.00
18	1*H2	+	1*HO2	=	1*H2O2	+	1*H	7.91000E+13	0.0000	25000.00
19	1*OH	+	1*H2O2	=	1*H2O	+	1*HO2	6.10000E+12	0.0000	1430.00
20	M	+	1*H2O2	=	2*OH			1.44000E+17	0.0000	45510.00
21	1*H2	+	1*OH	=	1*H2O	+	1*H	4.74000E+13	0.0000	6098.00
22	M	+	1*H2O	=	1*H	+	1*OH	1.30000E+15	0.0000	105140.00
23	M	+	1*H2	=	2*H			2.20000E+14	0.0000	96000.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2 , 20) = 2.30000	M(H2O2 , 20) = 6.60000	M(H2O , 20) = 6.00000	M(H2 , 22) = 4.00000
M(CO2 , 22) = 4.00000	M(H2O , 22) = 20.00000	M(H2 , 23) = 4.10000	M(H2O , 23) = 15.00000

** INITIAL CONDITIONS **

TIME 0.00000E+00 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	100.00000
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	2.77341E-03
TEMPERATURE (DEG K)	1000.00
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	13.5443
MACH NUMBER	0.0000
GAMMA	1.3793
ENTHALPY (CAL/G)	2.05701E+03
SP. HEAT (CP) (CAL/G/DEG K)	3.17527E+00

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH3	0.00000E+00	0.00000E+00	0.00000E+00
OH	0.00000E+00	0.00000E+00	0.00000E+00
CH3O	0.00000E+00	0.00000E+00	0.00000E+00
H	0.00000E+00	0.00000E+00	2.79263E-12
CH2O	0.00000E+00	0.00000E+00	0.00000E+00
H2	1.20649E-03	9.90000E-01	-1.41686E-12
HCO	0.00000E+00	0.00000E+00	4.10895E-14
CH4	0.00000E+00	0.00000E+00	0.00000E+00
CO	1.21868E-05	1.00000E-02	-4.10895E-14
HO2	0.00000E+00	0.00000E+00	0.00000E+00
H2O	0.00000E+00	0.00000E+00	0.00000E+00
CO2	0.00000E+00	0.00000E+00	0.00000E+00
H2O2	0.00000E+00	0.00000E+00	0.00000E+00

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	6.3000E+12	0.00000E+00	0.00000
2	1.2865E+09	0.00000E+00	0.00000
3	2.0000E+13	0.00000E+00	0.00000
4	9.4868E+12	0.00000E+00	0.00000
5	2.0000E+13	0.00000E+00	0.00000
6	1.1712E-02	0.00000E+00	0.00000
7	3.1596E+11	0.00000E+00	0.00000
8	2.0091E+12	0.00000E+00	0.00000
9	3.3568E+12	0.00000E+00	0.00000
10	1.6401E+13	0.00000E+00	0.00000
11	9.9183E-02	0.00000E+00	0.00000
12	2.0000E+13	-5.34200E-09	1.00000
13	3.0000E+13	0.00000E+00	0.00000
14	1.1470E+11	0.00000E+00	0.00000
15	2.5211E+11	0.00000E+00	0.00000
16	5.6017E+08	0.00000E+00	0.00000
17	7.8209E+13	0.00000E+00	0.00000
18	2.7191E+08	0.00000E+00	0.00000
19	2.9703E+12	0.00000E+00	0.00000
20	1.6299E+07	0.00000E+00	0.00000
21	2.2032E+12	0.00000E+00	0.00000
22	1.3665E-08	0.00000E+00	0.00000
23	2.2996E-07	1.78862E-07	1.00000

DERIVATIVES (CGS UNITS): T 0.00000E+00 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 2.27575 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 1.91134E-02 MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 1.049988 S

TABLE D.2.—Continued.
(m) Concluded.

TIME 1.00000E+09 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	98.00324
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	2.77341E-03
TEMPERATURE (DEG K)	1000.00
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	13.4259
MACH NUMBER	0.0000
GAMMA	1.3706
ENTHALPY (CAL/G)	1.82065E+03
SP. HEAT (CP) (CAL/G/DEG K)	3.16510E+00

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	32
AVERAGE STEP SIZE	0.28531E+08
METHOD ORDER	4
TOTAL NUMBER OF STEPS	122
FUNCT EVALUATIONS	161
JACOBIAN EVALUATIONS	30

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH3	5.61735E-14	4.70329E-11	-2.46945E-13
OH	6.45768E-18	5.40687E-15	-4.00448E-15
CH3O	2.45959E-21	2.05936E-18	6.16723E-19
H	2.69224E-13	2.25416E-10	-1.18634E-14
CH2O	2.54826E-12	2.13360E-09	-3.30179E-16
H2	1.16999E-03	9.79609E-01	-2.51061E-13
HCO	1.17880E-17	9.86985E-15	2.62903E-13
CH4	1.21671E-05	1.01872E-02	2.47068E-13
CO	1.94159E-08	1.62565E-05	-2.62672E-13
HO2	3.51516E-31	2.94317E-28	-6.64869E-32
H2O	1.21668E-05	1.01870E-02	4.15303E-15
CO2	2.91174E-10	2.43794E-07	-2.50644E-17
H2O2	3.25150E-26	2.72241E-23	1.43246E-27

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	6.3000E+12	-1.60552E-11	0.98183
2	1.2865E+09	-1.61333E-11	0.03179
3	2.0000E+13	-5.65353E-17	0.03179
4	9.4868E+12	-1.33068E-16	0.00016
5	2.0000E+13	-2.77355E-24	0.98182
6	1.1712E-02	5.80922E-12	0.00000
7	3.1596E+11	-3.21271E-08	0.00000
8	2.0091E+12	2.17912E-13	0.00000
9	3.3568E+12	2.67861E-11	0.00009
10	1.6401E+13	3.14786E-15	0.00009
11	9.9183E-02	3.53072E-15	0.00009
12	2.0000E+13	-1.34648E-15	0.00016
13	3.0000E+13	-4.83715E-20	0.00016
14	1.1470E+11	-3.41529E-08	0.00016
15	2.5211E+11	-3.25859E-12	0.00079
16	5.6017E+08	-2.99657E-28	0.00060
17	7.8209E+13	1.82740E-28	0.00019
18	2.7191E+08	2.78229E-24	0.00019
19	2.9703E+12	-1.54997E-29	0.00019
20	1.6299E+07	-1.83450E-22	0.00000
21	2.2032E+12	5.39709E-10	0.00000
22	1.3665E-08	2.68750E-17	0.00000
23	2.2996E-07	8.75260E-14	0.00000

DERIVATIVES (CGS UNITS): T 0.00000E+00 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 2.32211 TOTAL ENERGY EXCHANGE RATE -5.50202E-04 MASS FRACTION SUM 1.00000000

(CAL-CM**3/G**2/SEC)

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 1.499939E-01 S UP TO THIS TIME - 6.199951E-01 S

(LSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

TOTAL NO. OF STEPS - 122
TOTAL NO. OF DERIVATIVE EVALUATIONS - 161
TOTAL NO. OF JACOBIAN EVALUATIONS - 30
TOTAL CPU TIME - 0.619995 S

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 2.089996 S

(LSENS) READ DATA FOR NEXT CASE

TABLE D.2.—Continued.

(n) Case 14

```
                    ** DATA LINES **

          1         2         3         4         5         6         7         8
CC  12345678901234567890123456789012345678901234567890123456789012345678901234567890

   LSENS   HYDROGEN - OXYGEN LOW TEMPERATURE PHOTOLYTIC IGNITION          CASE 14
  NEW
     O       +   H2O      =   OH      +   OH          6.8E+13    0.       18365.
     H       +   O2       =   OH      +   O          1.89E+14   0.       16400.
     O       +   H2       =   OH      +   H          4.20E+14   0.       13750.
     H       +   HO2      =   H2      +   O2         7.28E+13   0.       2126.
     O       +   HO2      =   OH      +   O2          5.0E+13   0.       1000.
     HO2     +   OH       =   H2O     +   O2          8.0E+12            0.
     H       +   HO2      =2.00H                     1.34E+14   0.       1070.
     H2      +   HO2      =   H2O2    +   H          7.91E+13   0.       25000.
     OH      +   H2O2     =   H2O     +   HO2         6.1E+12   0.       1430.
     HO2     +   HO2      =   H2O2    +   O2          1.8E+12   0.        0.
     H       +   H2O2     =   OH      +   H2O         7.8E+11   0.        0.
     M       +   H2O2     =   OH      +   OH         1.44E+17   0.       45510.
     THIRDBODY
  H2          2.30    O2          .78     H2O          6.0    H2O2        6.6
  END
     H2      +   OH       =   H2O     +   H          4.74E+13   0.       6098.
     H       +   O2       =   HO2     +   M          1.46E+15   0.       -1000.
     THIRDBODY
  O2          1.30    H2          3.0     H2O          21.3   END
     M       +   H2O      =   H       +   OH         1.30E+15   0.       105140.
     THIRDBODY
  H2          4.00    O2          1.5     H2O          20.0   END
     H       +   O        =   OH      +   M           7.1E+18   -1.        0.
     M       +   H2       =   H       +   H           2.2E+14   0.        96000.
     THIRDBODY
  H2          4.10    O2          2.0     H2O          15.0   END
     M       +   O2       =   O       +   O          1.80E+18   -1.       118020.
     HNU     +   H2       >2.0H                         .003   0.          0.
     HNU     +   O2       >2.00                         .005     0.        0.
                                  -  BLANK LINE  -
  END
  TIME
   &prob  rhocon=.true., iprint=100, combus=.true., end=1.0173,  &end
   &start  t=700.0, p=2.0,  &end
  H2        0.667
  O2        0.333
  END
   &solver  emax=1.0E-6, atolsp=1.0E-11,  &end
  FINIS
```

```
                    ** EQUILIBRIUM CALCULATION **

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED INTERNAL ENERGY AND DENSITY

                          INITIAL STATE              FINAL STATE              FINAL/INITIAL RATIO

PRESSURE                       2.0000                   8.4135                    4.2068
 (ATM)
VELOCITY                        0.00                     0.00                     1.0000
 (CM/SEC)
DENSITY                    4.17838E-04              4.17838E-04                  1.0000
 (G/CM**3)
TEMPERATURE                   700.00                  3526.93                     5.0385
 (DEG K)
ENTHALPY                     238.98650                610.70337                  2.55539
 (CAL/G)
INTERNAL ENERGY              123.06985                123.07077                  1.00001
 (CAL/G)
SP. HEAT (CP)                  0.60975                  4.34787                   7.13058
 (CAL/G/DEG K)
ENTROPY                         3.5907                  4.2549                    1.1850
 (CAL/G/DEG K)
MACH NUMBER                     0.0000                  0.0000                    1.0000

GAMMA                           1.3728                  1.0328                    0.7523

SONIC VELOCITY                81597.60                151475.22                    1.8564
 (CM/SEC)

                                                 SPECIES     MOLE FRACTION
                                                  O           4.05365E-02
                                                  H2O         5.23165E-01
                                                  OH          1.33129E-01
                                                  H           8.74128E-02
                                                  O2          5.02276E-02
                                                  H2          1.65334E-01
                                                  HO2         1.83876E-04
                                                  H2O2        1.08549E-05

MIXTURE MOLECULAR WEIGHT                                 14.37269

D(LOG VOLUME)/D(LOG T)                                    2.4893
    AT CONSTANT P

D(LOG VOLUME)/D(LOG P)                                   -1.0863
    AT CONSTANT T

                COMPUTATIONAL WORK REQUIRED FOR EQUILIBRIUM CALCULATION:
                NO. OF ITERATIONS =      7     CPU TIME =  9.994507E-03 S
```

TABLE D.2.—Continued.

(n) Continued.

** INITIAL CONDITIONS **

TIME 0.00000E+00 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	2.00000
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	4.17838E-04
TEMPERATURE (DEG K)	700.00
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	3.5907
MACH NUMBER	0.0000
GAMMA	1.3728
ENTHALPY (CAL/G)	2.38986E+02
SP. HEAT (CP) (CAL/G/DEG K)	6.09751E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
O	0.00000E+00	0.00000E+00	1.15949E-07	1	1.2552E+08	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	0.00000E+00	2	1.4327E+09	0.00000E+00	0.00000
OH	0.00000E+00	0.00000E+00	0.00000E+00	3	2.1395E+10	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	1.39348E-07	4	1.5789E+13	-2.31827E-06	1.00000
O2	1.15949E-05	3.33000E-01	-5.79748E-08	5	2.4364E+13	0.00000E+00	0.00000
H2	2.32246E-05	6.67000E-01	-6.96741E-08	6	8.0000E+12	0.00000E+00	0.00000
HO2	0.00000E+00	0.00000E+00	4.04743E-13	7	6.2092E+13	0.00000E+00	0.00000
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	8	1.2383E+06	0.00000E+00	0.00000
				9	2.1820E+12	0.00000E+00	0.00000
				10	1.8000E+12	0.00000E+00	0.00000
				11	7.8000E+11	0.00000E+00	0.00000
				12	8.9023E+02	0.00000E+00	0.00000
				13	5.9142E+11	0.00000E+00	0.00000
				14	2.9962E+15	0.00000E+00	0.00000
				15	1.9398E-18	0.00000E+00	0.00000
				16	1.0143E+16	0.00000E+00	0.00000
				17	2.3436E-16	3.69149E-18	1.00000
				18	3.6533E-22	8.44797E-25	1.00000
				19	3.0000E-03	3.99074E-01	1.00000
				20	5.0000E-03	3.32063E-01	1.00000

DERIVATIVES (CGS UNITS): T -7.61641E+01 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 12.00014 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 8.11371E+04 MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 0.949997 S

TIME 1.01636E+00 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	2.69601
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	4.17838E-04
TEMPERATURE (DEG K)	956.82
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	3.7233
MACH NUMBER	0.0000
GAMMA	1.3529
ENTHALPY (CAL/G)	2.79326E+02
SP. HEAT (CP) (CAL/G/DEG K)	6.26068E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	100
AVERAGE STEP SIZE	0.51403E-02
METHOD ORDER	4
TOTAL NUMBER OF STEPS	200
FUNCT EVALUATIONS	295
JACOBIAN EVALUATIONS	36

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
O	1.62898E-12	4.74388E-08	1.42767E-09	1	4.3420E+09	3.19301E-02	0.99639
H2O	7.91009E-07	2.30355E-02	1.10181E-04	2	3.3922E+10	6.40247E+01	1.00000
OH	2.51101E-12	7.31248E-08	1.70843E-09	3	3.0378E+11	6.33436E+01	1.00000
H	2.96556E-11	8.63623E-07	2.47190E-08	4	2.3797E+13	1.86430E+01	0.99555
O2	1.11117E-05	3.23593E-01	-4.94514E-05	5	2.9550E+13	1.27731E+00	1.00000
H2	2.23482E-05	6.50819E-01	-1.03666E-04	6	8.0000E+12	5.33040E-01	1.00000
HO2	4.63275E-09	1.34914E-04	1.77515E-06	7	7.6331E+13	6.00665E+01	1.00000
H2O2	8.29927E-08	2.41689E-03	-7.41585E-06	8	1.5411E+08	-6.74639E+01	0.42469
				9	2.8754E+12	3.43084E+00	0.99961
				10	1.8000E+12	2.19563E+02	0.99226
				11	7.8000E+11	1.09958E+01	1.00000
				12	5.7976E+06	1.80149E+02	1.00000
				13	1.9183E+12	6.16155E+02	0.99932
				14	2.4704E+15	4.58919E+02	0.99997
				15	1.2546E-09	-6.89258E-03	1.00000
				16	7.4205E+15	7.05052E-05	1.00000
				17	2.5984E-08	-2.83597E-03	1.00000
				18	2.0751E-12	-5.41356E-08	1.00000
				19	3.0000E-03	3.84015E-01	1.00000
				20	5.0000E-03	3.18227E-01	1.00000

DERIVATIVES (CGS UNITS): T 3.19339E+04 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 12.16816 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) -3.50769E+07 MASS FRACTION SUM 1.00000001

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 6.699982E-01 S UP TO THIS TIME - 1.240005E+00 S

TABLE D.2.—Continued.
(n) Concluded.

TIME 1.01730E+00 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	2.88438
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	4.17838E-04
TEMPERATURE (DEG K)	1026.93
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	3.7533
MACH NUMBER	0.0000
GAMMA	1.3477
ENTHALPY (CAL/G)	2.90243E+02
SP. HEAT (CP) (CAL/G/DEG K)	6.30997E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	32
AVERAGE STEP SIZE	0.29456E-04
METHOD ORDER	4
TOTAL NUMBER OF STEPS	232
FUNCT EVALUATIONS	349
JACOBIAN EVALUATIONS	41

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
O	1.18540E-11	3.46311E-07	9.14943E-08	1	8.3967E+09	5.83952E-01	0.99108
H2O	1.03350E-06	3.01934E-02	8.87724E-04	2	6.1129E+10	7.69581E+02	0.99998
OH	1.65441E-11	4.83332E-07	1.45325E-07	3	4.9774E+11	7.47452E+02	0.99999
H	1.99828E-10	5.83791E-06	1.47962E-06	4	2.5685E+13	3.05426E+02	0.99808
O2	1.09995E-05	3.21347E-01	-4.19885E-04	5	3.0630E+13	2.16481E+01	1.00000
H2	2.21176E-05	6.46157E-01	-8.49624E-04	6	8.0000E+12	7.89108E+00	1.00000
HO2	1.04092E-08	3.04102E-04	2.96330E-05	7	7.9321E+13	9.45039E+02	1.00000
H2O2	6.81766E-08	1.99175E-03	-5.37281E-05	8	3.7821E+08	-5.72629E+02	0.53449
				9	3.0269E+12	1.95408E+01	0.99926
				10	1.8000E+12	1.11250E+03	0.99588
				11	7.8000E+11	6.08654E+01	1.00000
				12	2.9718E+07	7.67210E+02	1.00000
				13	2.3879E+12	4.99676E+03	0.99841
				14	2.3833E+15	3.08257E+03	0.99993
				15	5.4735E-08	-1.88330E-01	1.00000
				16	6.9138E+15	3.21086E-03	1.00000
				17	8.1639E-07	-9.76464E-02	1.00000
				18	1.3395E-10	-2.58887E-06	1.00000
				19	3.0000E-03	3.80052E-01	1.00000
				20	5.0000E-03	3.15013E-01	1.00000

DERIVATIVES (CGS UNITS): T 2.55051E+05 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 12.20699 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) -2.83276E+08 MASS FRACTION SUM 1.00000001

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 2.200012E-01 S UP TO THIS TIME - 1.460007E+00 S

(LSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

TOTAL NO. OF STEPS - 232
TOTAL NO. OF DERIVATIVE EVALUATIONS - 349
TOTAL NO. OF JACOBIAN EVALUATIONS - 41
TOTAL CPU TIME - 1.460007 S

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 2.680008 S

(LSENS) READ DATA FOR NEXT CASE

TABLE D.2.—Continued.

(o) Case 15

DISTANCE-AREA VERSION LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

LSENS METHANE AIR MECHAN.; MON. DECR. TABULAR AREA WITH APRINT CASE 15

REACTION NUMBER	REACTION							REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	M	+	1*CH4	=	1*CH3	+	1*H	2.00000E+17	0.0000	88000.00
2	1*H	+	1*CH4	=	1*CH3	+	1*H2	1.26000E+14	0.0000	11900.00
3	1*CH4	+	1*O2	=	1*CH3	+	1*HO2	7.94000E+13	0.0000	56000.00
4	1*O	+	1*CH4	=	1*CH3	+	1*OH	1.90000E+14	0.0000	11720.00
5	1*OH	+	1*CH4	=	1*CH3	+	1*H2O	2.50000E+13	0.0000	5010.00
6	1*CH3	+	1*O2	=	1*CH3O	+	1*O	2.40000E+13	0.0000	28680.00
7	1*CH3	+	1*OH	=	1*CH3O	+	1*H	6.30000E+12	0.0000	0.00
8	M	+	1*CH3O	=	1*CH2O	+	1*H	5.00000E+13	0.0000	21000.00
9			2*CH3	=	1*C2H6			2.40000E+14	-0.4000	0.00
10	1*H	+	1*C2H6	=	1*C2H5	+	1*H2	1.32000E+14	0.0000	9700.00
11	1*O	+	1*C2H6	=	1*C2H5	+	1*OH	1.13000E+14	0.0000	7850.00
12	1*OH	+	1*C2H6	=	1*C2H5	+	1*H2O	8.70000E+13	0.0000	3520.00
13	M	+	1*C2H5	=	1*C2H4	+	1*H	1.00000E+17	0.0000	31000.00
14	1*C2H5	+	1*O2	=	1*C2H4	+	1*HO2	2.00000E+12	0.0000	5000.00
15	1*H	+	1*C2H5	=	1*C2H4	+	1*H2	4.80000E+13	0.0000	0.00
16	1*CH3	+	1*CH2	=	1*C2H4	+	1*H	2.00000E+13	0.0000	0.00
17	1*H	+	1*C2H4	=	1*H2	+	1*C2H3	1.50000E+14	0.0000	10200.00
18	M	+	1*C2H4	=	1*C2H2	+	1*H2	2.60000E+17	0.0000	79300.00
19	1*C2H4	+	1*OH	=	1*C2H3	+	1*H2O	4.80000E+12	0.0000	1230.00
20	1*C2H4	+	1*OH	=	1*CH3	+	1*CH2O	2.00000E+12	0.0000	960.00
21	1*C2H4	+	1*O	=	1*CH3	+	1*HCO	3.30000E+12	0.0000	1130.00
22	1*C2H4	+	1*O	=	1*CH2O	+	1*CH2	2.50000E+13	0.0000	5000.00
23	M	+	1*C2H3	=	1*C2H2	+	1*H	3.00000E+15	0.0000	32000.00
24	1*C2H3	+	1*O2	=	1*CH2O	+	1*HCO	3.98000E+12	0.0000	-250.00
25	1*C2H3	+	1*H	=	1*C2H2	+	1*H2	6.00000E+12	0.0000	0.00
26	1*C2H3	+	1*O	=	1*C2H2O	+	1*H	3.30000E+13	0.0000	0.00
27	1*C2H3	+	1*OH	=	1*C2H2	+	1*H2O	5.00000E+12	0.0000	0.00
28	1*C2H3	+	1*CH2	=	1*C2H2	+	1*CH3	3.00000E+13	0.0000	0.00
29	1*C2H3	+	1*C2H	=	2*C2H2			3.00000E+13	0.0000	0.00
30	M	+	1*C2H2	=	1*C2H	+	1*H	4.20000E+16	0.0000	107000.00
31	1*C2H2	+	1*O	=	1*CH2	+	1*CO	1.60000E+14	0.0000	9890.00
32	1*C2H2	+	1*O	=	1*C2HO	+	1*H	4.00000E+14	0.0000	10660.00
33	1*C2H2	+	1*OH	=	1*C2H	+	1*H2O	6.30000E+12	0.0000	7000.00
34	1*C2H2	+	1*OH	=	1*C2H2O	+	1*H	3.20000E+11	0.0000	200.00
35	1*C2H	+	1*O2	=	1*C2HO	+	1*O	5.00000E+13	0.0000	1500.00
36	1*C2H	+	1*OH	=	1*C2HO	+	1*H	2.00000E+13	0.0000	0.00
37	1*C2HO	+	1*O2	=	2*CO	+	1*OH	1.46000E+12	0.0000	2500.00
38	1*C2HO	+	1*O	=	2*CO	+	1*H	1.20200E+12	0.0000	0.00
39	1*C2HO	+	1*OH	=	2*HCO			1.00000E+13	0.0000	0.00
40	1*C2HO	+	1*H	=	1*CH2	+	1*CO	5.00000E+13	0.0000	0.00
41	1*C2HO	+	1*CH2	=	1*C2H3	+	1*CO	3.00000E+13	0.0000	0.00
42	1*C2HO	+	1*CH2	=	1*CH2O	+	1*C2H	1.00000E+13	0.0000	2000.00
43			2*C2HO	=	1*C2H2	+	2*CO	1.00000E+13	0.0000	0.00
44	1*C2H2O	+	1*OH	=	1*CH2O	+	1*HCO	2.80000E+13	0.0000	0.00
45	1*C2H2O	+	1*OH	=	1*C2HO	+	1*H2O	7.50000E+12	0.0000	3000.00
46	1*C2H2O	+	1*H	=	1*CH3	+	1*CO	1.13000E+13	0.0000	3428.00
47	1*C2H2O	+	1*H	=	1*C2HO	+	1*H2	7.50000E+13	0.0000	8000.00
48	1*C2H2O	+	1*O	=	1*C2HO	+	1*OH	5.00000E+13	0.0000	8000.00
49	1*C2H2O	+	1*O	=	1*CH2O	+	1*CO	2.00000E+13	0.0000	0.00
50	M	+	1*C2H2O	=	1*CH2	+	1*CO	2.00000E+16	0.0000	60000.00
51	1*C2H	+	1*O	=	1*CO	+	1*CH	5.00000E+13	0.0000	0.00
52	1*CH3O	+	1*O2	=	1*CH2O	+	1*HO2	1.00000E+13	0.0000	7170.00
53	1*CH3O	+	1*H	=	1*CH2O	+	1*H2	2.00000E+13	0.0000	0.00
54	M	+	1*CH2O	=	1*HCO	+	1*H	5.00000E+16	0.0000	81000.00
55	1*CH2O	+	1*OH	=	1*HCO	+	1*H2O	3.00000E+13	0.0000	1200.00
56	1*CH2O	+	1*H	=	1*HCO	+	1*H2	2.50000E+13	0.0000	3990.00
57	1*CH2O	+	1*O	=	1*HCO	+	1*OH	3.50000E+13	0.0000	3510.00
58	1*CH3	+	1*CH2O	=	1*CH4	+	1*HCO	1.00000E+10	0.5000	6000.00
59	1*CH3	+	1*HCO	=	1*CH4	+	1*CO	3.00000E+11	0.5000	0.00
60	1*CH3	+	1*HO2	=	1*CH3O	+	1*OH	2.00000E+13	0.0000	0.00
61	M	+	1*CH3	=	1*CH2	+	1*H	1.95000E+16	0.0000	91600.00
62	1*H	+	1*CH3	=	1*H2	+	1*CH2	2.70000E+11	0.6700	25700.00
63	1*O	+	1*CH3	=	1*OH	+	1*CH2	1.90000E+11	0.6800	25700.00
64	1*OH	+	1*CH3	=	1*H2O	+	1*CH2	2.70000E+11	0.6700	25700.00
65	1*CH	+	1*CO2	=	1*HCO	+	1*CO	3.70000E+12	0.0000	0.00
66	1*CH	+	1*O2	=	1*HCO	+	1*O	1.00000E+13	0.0000	0.00
67	1*CH2	+	1*O2	=	1*CH2O	+	1*O	5.00000E+11	0.5000	6960.00
68	1*CH2	+	1*O	=	1*CH	+	1*OH	2.00000E+11	0.7000	25800.00
69	1*CH2	+	1*OH	=	1*CH	+	1*H2O	5.00000E+11	0.5000	5900.00
70	1*CH2	+	1*H	=	1*CH	+	1*H2	3.20000E+11	0.7000	4970.00
71			2*CH2	=	1*C2H3	+	1*H	5.00000E+12	0.0000	0.00
72			2*CH2	=	1*C2H2	+	1*H2	4.00000E+13	0.0000	0.00
73	1*HCO	+	1*O2	=	1*CO	+	1*HO2	3.00000E+13	0.0000	0.00
74	1*HCO	+	1*O	=	1*CO	+	1*OH	3.00000E+13	0.0000	0.00
75	1*HCO	+	1*OH	=	1*CO	+	1*H2O	3.00000E+13	0.0000	0.00
76	1*HCO	+	1*H	=	1*CO	+	1*H2	2.00000E+13	0.0000	0.00
77	M	+	1*HCO	=	1*H	+	1*CO	2.90000E+14	0.0000	15570.00
78	1*CO	+	1*O	=	1*CO2	+	M	2.40000E+15	0.0000	4100.00
79	1*CO	+	1*O2	=	1*CO2	+	1*O	2.50000E+12	0.0000	47690.00
80	1*CO	+	1*OH	=	1*CO2	+	1*H	4.17000E+11	0.0000	1000.00
81	1*CO	+	1*HO2	=	1*CO2	+	1*OH	5.75000E+13	0.0000	22930.00
82	1*O	+	1*H2O	=	2*OH			6.80000E+13	0.0000	18365.00
83	1*H	+	1*O2	=	1*OH	+	1*O	1.89000E+14	0.0000	16400.00
84	1*O	+	1*H2	=	1*OH	+	1*H	4.20000E+14	0.0000	13750.00
85	1*H	+	1*HO2	=	1*H2	+	1*O2	7.28000E+13	0.0000	2126.00
86	1*O	+	1*HO2	=	1*OH	+	1*O2	5.00000E+13	0.0000	1000.00
87	1*HO2	+	1*OH	=	1*H2O	+	1*O2	8.00000E+12	0.0000	0.00
88	1*H	+	1*HO2	=	2*OH			1.34000E+14	0.0000	1070.00
89	1*H2	+	1*HO2	=	1*H2O2	+	1*H	7.91000E+13	0.0000	25000.00
90	1*OH	+	1*H2O2	=	1*H2O	+	1*HO2	6.10000E+12	0.0000	1430.00
91			2*HO2	=	1*H2O2	+	1*O2	1.80000E+12	0.0000	0.00
92	1*H	+	1*H2O2	=	1*OH	+	1*H2O	7.80000E+11	0.0000	0.00
93	M	+	1*H2O2	=	2*OH			1.44000E+17	0.0000	45510.00
94	1*H2	+	1*OH	=	1*H2O	+	1*H	4.74000E+13	0.0000	6098.00
95	1*H	+	1*O2	=	1*HO2	+	M	1.46000E+15	0.0000	-1000.00
96	M	+	1*H2O	=	1*H	+	1*OH	1.30000E+15	0.0000	105140.00
97	1*H	+	1*O	=	1*OH	+	M	7.10000E+18	-1.0000	0.00
98	M	+	1*H2	=	2*H			2.20000E+14	0.0000	96000.00
99	M	+	1*O2	=	2*O			1.80000E+18	-1.0000	118020.00
100	1*CH	+	1*N2	=	1*HCN	+	1*N	1.00000E+11	0.0000	19000.00
101	1*CN	+	1*H2	=	1*HCN	+	1*H	6.00000E+13	0.0000	5300.00
102	1*O	+	1*HCN	=	1*OH	+	1*CN	1.40000E+11	0.6800	16900.00
103	1*OH	+	1*HCN	=	1*HNCO	+	1*H	4.00000E+11	0.0000	2800.00
104	1*CN	+	1*O	=	1*CO	+	1*N	1.20000E+13	0.0000	0.00

TABLE D.2.—Continued.

(o) Continued.

105	1*CN	+	1*OH	=	1*NCO	+	1*H	2.50000E+14	0.0000	6000.00
106	1*H2	+	1*NCO	=	1*HNCO	+	1*H	1.00000E+14	0.0000	9000.00
107	1*HNCO	+	1*H	=	1*NH2	+	1*CO	1.00000E+14	0.0000	8500.00
108	1*CN	+	1*O2	=	1*NCO	+	1*O	3.20000E+13	0.0000	1000.00
109	1*CN	+	1*CO2	=	1*NCO	+	1*CO	3.70000E+12	0.0000	0.00
110	1*O	+	1*NCO	=	1*NO	+	1*CO	2.00000E+13	0.0000	0.00
111	1*N	+	1*NCO	=	1*N2	+	1*CO	1.00000E+13	0.0000	0.00
112	1*H	+	1*NCO	=	1*NH	+	1*CO	2.00000E+13	0.0000	0.00
113	1*CH	+	1*NO	=	1*N	+	1*HCO	1.60000E+13	0.0000	9940.00
114	1*CH	+	1*NO	=	1*O	+	1*HCN	2.00000E+12	0.0000	0.00
115	1*NH	+	1*OH	=	1*N	+	1*H2O	5.00000E+11	0.5000	2000.00
116	1*HO2	+	1*NO	=	1*NO2	+	1*OH	2.09000E+12	0.0000	-477.00
117	1*O	+	1*NO2	=	1*NO	+	1*O2	1.00000E+13	0.0000	596.00
118	1*NO	+	1*O	=	1*NO2	+	M	5.62000E+15	0.0000	-1160.00
119	1*HO2	+	1*H	=	1*NO	+	1*OH	3.47000E+14	0.0000	1470.00
120	1*NO	+	1*H	=	1*N	+	1*OH	2.63000E+14	0.0000	50410.00
121	1*NO	+	1*O	=	1*N	+	1*O2	3.80000E+09	1.0000	41370.00
122	1*O	+	1*N2	=	1*NO	+	1*N	1.80000E+14	0.0000	76250.00
123	1*N	+	1*NO2	=	2*NO			4.00000E+12	0.0000	0.00
124	M	+	1*N2O	=	1*N2	+	1*O	6.92000E+23	-2.5000	65000.00
125	1*O	+	1*N2O	=	1*N2	+	1*O2	1.00000E+14	0.0000	28020.00
126	1*O	+	1*N2O	=	2*NO			6.92000E+13	0.0000	26630.00
127	1*N2O	+	1*H	=	1*N2	+	1*OH	7.59000E+13	0.0000	15100.00
128	1*HO2	+	1*H2	=	1*HNO2	+	1*H	2.40000E+13	0.0000	29000.00
129	1*OH	+	1*NO2	=	1*HNO3	+	M	3.00000E+15	0.0000	-3800.00
130	1*OH	+	1*NO	=	1*HNO2	+	M	5.60000E+15	0.0000	-1700.00
131	1*HNO	+	1*H	=	1*H2	+	1*NO	5.00000E+12	0.0000	0.00
132	1*H	+	1*NO	=	1*HNO	+	M	5.40000E+15	0.0000	-600.00
133	1*HNO	+	1*OH	=	1*H2O	+	1*NO	3.60000E+13	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2 , 93) =	2.30000	M(O2 , 93) =	0.78000	M(H2O , 93) =	6.00000	M(H2O2 , 93) =	6.60000
M(O2 , 95) =	1.30000	M(N2 , 95) =	1.30000	M(H2O , 95) =	21.30000	M(CO2 , 95) =	7.00000
M(H2 , 96) =	4.00000	M(O2 , 96) =	1.50000	M(H2O , 96) =	20.00000	M(N2 , 96) =	1.50000
M(CO2 , 96) =	4.00000	M(H2 , 98) =	4.10000	M(O2 , 98) =	2.00000	M(H2O , 98) =	15.00000
M(N2 , 98) =	2.00000	M(O2 ,129) =	0.70000	M(H2 ,129) =	1.40000		

** NEW INPUT DATA GIVEN IN CGS UNITS ** ** OUTPUT REQUIRED IN CGS UNITS **

** ASSIGNED VARIABLE PROFILE **

THE AREA IS CALCULATED BY INTERPOLATION FROM THE FOLLOWING TABLE

STATION	AXIAL DISTANCE (CM)	AREA (CM**2)
1	0.00000E+00	1.20000E+03
2	5.00000E+00	1.18000E+03
3	1.00000E+01	1.16000E+03
4	1.50000E+01	1.14000E+03
5	2.00000E+01	1.12000E+03
6	2.50000E+01	1.10000E+03
7	3.00000E+01	1.08000E+03
8	3.20000E+01	1.06000E+03
9	3.40000E+01	1.04000E+03
10	3.60000E+01	1.02000E+03
11	3.80000E+01	1.00000E+03
12	4.00000E+01	9.80000E+02
13	4.20000E+01	9.60000E+02
14	4.40000E+01	9.40000E+02

NUMBER OF REACTING SPECIES: 39

NUMBER OF INERT SPECIES: 0

NUMBER OF SPECIES ODE'S REQUIRED FOR THIS CASE: 39

TOTAL NUMBER OF ODE'S REQUIRED FOR THIS CASE: 42

INTEGRATION CONTROLS

INTEGRATION METHOD (MF): 21 MAXIMUM RELATIVE ERROR: 1.00000E-05 SPECIES ABSOLUTE ERROR: 1.00000E-14

MAXIMUM NUMBER OF STEPS ALLOWED FOR THE COMPLETE PROBLEM: 2000

** OUTPUT REQUIRED AT 4 ASSIGNED-VARIABLE VALUES WHICH CORRESPOND TO THE FOLLOWING PRINT STATIONS **

STATION	AXIAL DISTANCE (CM)
1	5.00000E+00
2	1.24954E+01
3	2.24363E+01
4	4.30002E+01

TABLE D.2.—Continued.

(o) Continued.

** INITIAL CONDITIONS **

TIME 0.00000E+00 SEC AREA 1.20000E+03 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.73000
VELOCITY (CM/SEC)	155259.65
DENSITY (G/CM**3)	3.71736E-04
TEMPERATURE (DEG K)	1600.00
MASS FLOW RATE (G/SEC)	6.92587E+04
ENTROPY (CAL/G/DEG K)	2.1223
MACH NUMBER	2.0000
GAMMA	1.2780
ENTHALPY (CAL/G)	3.46688E+02
SP. HEAT (CP) (CAL/G/DEG K)	3.23820E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	6.55792E-07	4.97680E-02	-4.71274E-06
CH3	0.00000E+00	0.00000E+00	4.71274E-06
H	0.00000E+00	0.00000E+00	1.64958E-06
H2	0.00000E+00	0.00000E+00	0.00000E+00
O2	2.62317E-06	1.99072E-01	-8.38235E-05
HO2	0.00000E+00	0.00000E+00	3.06316E-06
O	0.00000E+00	0.00000E+00	8.07603E-05
OH	0.00000E+00	0.00000E+00	0.00000E+00
H2O	0.00000E+00	0.00000E+00	0.00000E+00
CH3O	0.00000E+00	0.00000E+00	0.00000E+00
CH2O	0.00000E+00	0.00000E+00	0.00000E+00
C2H6	0.00000E+00	0.00000E+00	0.00000E+00
C2H5	0.00000E+00	0.00000E+00	0.00000E+00
C2H4	0.00000E+00	0.00000E+00	0.00000E+00
CH2	0.00000E+00	0.00000E+00	0.00000E+00
C2H3	0.00000E+00	0.00000E+00	0.00000E+00
C2H2	0.00000E+00	0.00000E+00	0.00000E+00
HCO	0.00000E+00	0.00000E+00	0.00000E+00
C2H2O	0.00000E+00	0.00000E+00	0.00000E+00
C2H	0.00000E+00	0.00000E+00	0.00000E+00
CO	0.00000E+00	0.00000E+00	0.00000E+00
C2HO	0.00000E+00	0.00000E+00	0.00000E+00
CH	0.00000E+00	0.00000E+00	0.00000E+00
CO2	0.00000E+00	0.00000E+00	0.00000E+00
H2O2	0.00000E+00	0.00000E+00	0.00000E+00
N2	9.89802E-06	7.51160E-01	-1.79633E-12
HCN	0.00000E+00	0.00000E+00	0.00000E+00
N	0.00000E+00	0.00000E+00	0.00000E+00
CN	1.31770E-12	1.00000E-07	-8.07603E-05
HNCO	0.00000E+00	0.00000E+00	0.00000E+00
NCO	0.00000E+00	0.00000E+00	8.07603E-05
NH2	0.00000E+00	0.00000E+00	0.00000E+00
NO	0.00000E+00	0.00000E+00	0.00000E+00
NH	0.00000E+00	0.00000E+00	0.00000E+00
NO2	0.00000E+00	0.00000E+00	0.00000E+00
N2O	0.00000E+00	0.00000E+00	1.79633E-12
HNO2	0.00000E+00	0.00000E+00	0.00000E+00
HNO3	0.00000E+00	0.00000E+00	0.00000E+00
HNO	0.00000E+00	0.00000E+00	0.00000E+00

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	1.9089E+05	1.19373E+01	1.00000
2	2.9847E+12	0.00000E+00	0.00000
3	1.7806E+06	2.21667E+01	1.00000
4	4.7630E+12	0.00000E+00	0.00000
5	5.1714E+12	0.00000E+00	0.00000
6	2.9021E+09	0.00000E+00	0.00000
7	6.3000E+12	0.00000E+00	0.00000
8	6.7687E+10	0.00000E+00	0.00000
9	1.2548E+13	0.00000E+00	0.00000
10	6.2462E+12	0.00000E+00	0.00000
11	9.5679E+12	0.00000E+00	0.00000
12	2.8755E+13	0.00000E+00	0.00000
13	5.8291E+12	0.00000E+00	0.00000
14	4.1501E+11	0.00000E+00	0.00000
15	4.8000E+13	0.00000E+00	0.00000
16	2.0000E+13	0.00000E+00	0.00000
17	6.0651E+12	0.00000E+00	0.00000
18	3.8291E+06	0.00000E+00	0.00000
19	3.2601E+12	0.00000E+00	0.00000
20	1.4788E+12	0.00000E+00	0.00000
21	2.3129E+12	0.00000E+00	0.00000
22	5.1877E+12	0.00000E+00	0.00000
23	1.2768E+11	0.00000E+00	0.00000
24	4.3056E+12	0.00000E+00	0.00000
25	6.0000E+12	0.00000E+00	0.00000
26	3.3000E+13	0.00000E+00	0.00000
27	5.0000E+12	0.00000E+00	0.00000
28	3.0000E+13	0.00000E+00	0.00000
29	3.0000E+13	0.00000E+00	0.00000
30	1.0180E+02	0.00000E+00	0.00000
31	7.1320E+12	0.00000E+00	0.00000
32	1.3995E+13	0.00000E+00	0.00000
33	6.9692E+11	0.00000E+00	0.00000
34	3.0049E+11	0.00000E+00	0.00000
35	3.1195E+13	0.00000E+00	0.00000
36	2.0000E+13	0.00000E+00	0.00000
37	6.6507E+11	0.00000E+00	0.00000
38	1.2020E+12	0.00000E+00	0.00000
39	1.0000E+13	0.00000E+00	0.00000
40	5.0000E+13	0.00000E+00	0.00000
41	3.0000E+13	0.00000E+00	0.00000
42	5.3311E+12	0.00000E+00	0.00000
43	1.0000E+13	0.00000E+00	0.00000
44	2.8000E+13	0.00000E+00	0.00000
45	2.9193E+12	0.00000E+00	0.00000
46	3.8445E+12	0.00000E+00	0.00000
47	6.0578E+12	0.00000E+00	0.00000
48	4.0385E+12	0.00000E+00	0.00000
49	2.0000E+13	0.00000E+00	0.00000
50	1.2747E+08	0.00000E+00	0.00000
51	5.0000E+13	0.00000E+00	0.00000
52	1.0486E+12	0.00000E+00	0.00000
53	2.0000E+13	0.00000E+00	0.00000
54	4.3141E+05	0.00000E+00	0.00000
55	2.0569E+13	0.00000E+00	0.00000
56	7.1274E+12	0.00000E+00	0.00000
57	1.1604E+13	0.00000E+00	0.00000
58	6.0604E+10	0.00000E+00	0.00000
59	1.2000E+13	0.00000E+00	0.00000
60	2.0000E+13	0.00000E+00	0.00000
61	5.9987E+03	0.00000E+00	0.00000
62	1.1686E+10	0.00000E+00	0.00000
63	8.8532E+09	0.00000E+00	0.00000
64	1.1686E+10	0.00000E+00	0.00000
65	3.7000E+12	0.00000E+00	0.00000
66	1.0000E+13	0.00000E+00	0.00000
67	2.2405E+12	0.00000E+00	0.00000
68	1.0466E+10	0.00000E+00	0.00000
69	3.1270E+12	0.00000E+00	0.00000
70	1.1726E+13	0.00000E+00	0.00000
71	5.0000E+12	0.00000E+00	0.00000
72	4.0000E+13	0.00000E+00	0.00000
73	3.0000E+13	0.00000E+00	0.00000
74	3.0000E+13	0.00000E+00	0.00000
75	3.0000E+13	0.00000E+00	0.00000
76	2.0000E+13	0.00000E+00	0.00000
77	2.1659E+12	0.00000E+00	0.00000
78	6.6096E+14	0.00000E+00	0.00000
79	7.6523E+05	0.00000E+00	0.00000
80	3.0447E+11	0.00000E+00	0.00000
81	4.2421E+10	0.00000E+00	0.00000
82	2.1085E+11	0.00000E+00	0.00000
83	1.0872E+12	0.00000E+00	0.00000
84	5.5602E+12	0.00000E+00	0.00000
85	3.7302E+13	0.00000E+00	0.00000

TABLE D.2.—Continued.

(o) Continued.

86	3.6507E+13	0.00000E+00	0.00000
87	8.0000E+12	0.00000E+00	0.00000
88	9.5708E+13	0.00000E+00	0.00000
89	3.0432E+10	0.00000E+00	0.00000
90	3.8905E+12	0.00000E+00	0.00000
91	1.8000E+12	0.00000E+00	0.00000
92	7.8000E+11	0.00000E+00	0.00000
93	8.7496E+10	0.00000E+00	0.00000
94	6.9635E+12	0.00000E+00	0.00000
95	1.9996E+15	0.00000E+00	0.00000
96	5.6558E+00	0.00000E+00	0.00000
97	4.4375E+15	0.00000E+00	0.00000
98	1.6960E+01	0.00000E+00	0.00000
99	8.5187E-02	2.13082E-05	1.00000
100	2.5393E+08	0.00000E+00	0.00000
101	1.1329E+13	0.00000E+00	0.00000
102	1.0387E+11	0.00000E+00	0.00000
103	1.6581E+11	0.00000E+00	0.00000
104	1.2000E+13	0.00000E+00	0.00000
105	3.7877E+13	0.00000E+00	0.00000
106	5.8974E+12	0.00000E+00	0.00000
107	6.9017E+12	0.00000E+00	0.00000
108	2.3364E+13	5.84425E+02	1.00000
109	3.7000E+12	0.00000E+00	0.00000
110	2.0000E+13	0.00000E+00	0.00000
111	1.0000E+15	0.00000E+00	0.00000
112	2.0000E+13	0.00000E+00	0.00000
113	7.0207E+11	0.00000E+00	0.00000
114	2.0000E+12	0.00000E+00	0.00000
115	1.0662E+13	0.00000E+00	0.00000
116	2.4283E+12	0.00000E+00	0.00000
117	8.2907E+12	0.00000E+00	0.00000
118	8.0944E+15	0.00000E+00	0.00000
119	2.1854E+14	0.00000E+00	0.00000
120	3.4219E+07	0.00000E+00	0.00000
121	1.3584E+07	0.00000E+00	0.00000
122	6.9185E+03	0.00000E+00	0.00000
123	4.0000E+12	0.00000E+00	0.00000
124	8.9376E+06	0.00000E+00	0.00000
125	1.4882E+10	-1.29992E-05	1.00000
126	1.5945E+10	0.00000E+00	0.00000
127	6.5717E+11	0.00000E+00	0.00000
128	2.6242E+09	0.00000E+00	0.00000
129	9.9124E+15	0.00000E+00	0.00000
130	9.5587E+15	0.00000E+00	0.00000
131	5.0000E+12	0.00000E+00	0.00000
132	6.5215E+15	0.00000E+00	0.00000
133	3.6000E+13	0.00000E+00	0.00000

DERIVATIVES (CGS UNITS): T 1.97928E+00 RHO 1.65526E-06 V -1.72834E+02

MIXTURE MOLECULAR WEIGHT 28.21102 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) -1.27744E+06 MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 2.220001 S

TIME 1.46451E-04 SEC AREA 1.10936E+03 SQ CM AXIAL POSITION 2.24363E+01 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.98504
VELOCITY (CM/SEC)	150959.76
DENSITY (G/CM**3)	4.13563E-04
TEMPERATURE (DEG K)	1650.17
MASS FLOW RATE (G/SEC)	6.92587E+04
ENTROPY (CAL/G/DEG K)	2.1234
MACH NUMBER	1.9161
GAMMA	1.2763
ENTHALPY (CAL/G)	3.62423E+02
SP. HEAT (CP) (CAL/G/DEG K)	3.25371E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	29
AVERAGE STEP SIZE	0.35712E+00
METHOD ORDER	4
TOTAL NUMBER OF STEPS	161
FUNCT EVALUATIONS	199
JACOBIAN EVALUATIONS	25

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
CH4	7.17624E-07	4.89515E-02	-2.51430E-04	1	4.4284E+05	2.65382E+01	0.97428
CH3	3.70822E-09	2.52950E-04	5.03006E-05	2	3.3445E+12	9.58538E+01	0.97496
H	7.00621E-12	4.77918E-07	1.25105E-07	3	3.0419E+06	2.82779E+01	0.76098
H2	7.91112E-10	5.39645E-05	1.66017E-05	4	5.3278E+12	3.79712E+02	0.99957
O2	2.91153E-06	1.98605E-01	-1.46771E-04	5	5.4252E+12	9.45846E+02	0.99824
HO2	9.44564E-10	6.44319E-05	7.30120E-06	6	3.8178E+09	2.40782E+02	0.99910
O	1.69934E-11	1.15917E-06	2.71685E-07	7	6.3000E+12	-9.40210E+00	0.62316
OH	4.16255E-11	2.83942E-06	7.69567E-07	8	8.2740E+10	1.72728E+02	1.00000
H2O	7.12085E-09	4.85737E-04	1.68311E-04	9	1.2394E+13	2.67191E+02	0.26815
CH3O	2.43557E-11	1.66139E-06	4.42876E-07	10	6.8533E+12	5.08339E-01	1.00000
CH2O	4.35616E-09	2.97148E-04	1.03105E-04	11	1.0314E+13	1.85554E+00	1.00000
C2H6	1.81074E-09	1.23516E-04	4.30530E-05	12	2.9739E+13	1.31057E+01	1.00000
C2H5	2.28401E-14	1.55800E-09	7.69219E-10	13	7.8404E+12	1.53007E+01	0.99685
C2H4	5.74154E-11	3.91650E-06	2.72323E-06	14	4.3534E+11	1.64308E-01	0.97073
CH2	1.33148E-15	9.08247E-11	6.47922E-11	15	4.8000E+13	4.47719E-05	0.99693
C2H3	6.99639E-16	4.77248E-11	4.59942E-11	16	2.0000E+13	5.77222E-04	0.99976
C2H2	1.40319E-13	9.57162E-09	8.59543E-09	17	6.6865E+12	1.57259E-02	0.99998
HCO	4.83642E-14	3.29909E-09	1.94312E-09	18	8.1738E+06	4.02252E-02	1.00000
C2H2O	3.63527E-16	2.47974E-11	2.56029E-11	19	3.2987E+12	4.60939E-02	1.00000
C2H	4.71926E-20	3.21916E-15	3.95994E-15	20	1.4924E+12	-6.02946E-01	0.96657

TABLE D.2.—Continued.

(o) Continued.

CO	1.30390E-10	8.89436E-06	6.00063E-06
C2HO	2.00636E-17	1.36860E-12	1.57301E-12
CH	1.04070E-20	7.09898E-16	7.22928E-16
CO2	1.42213E-13	9.70085E-09	8.80828E-09
H2O2	8.54763E-13	5.83063E-08	1.03216E-08
N2	1.10117E-05	7.51146E-01	-9.52715E-11
HCN	4.10903E-18	2.80291E-13	1.90069E-13
N	1.46099E-18	9.96594E-14	4.38093E-14
CN	5.12271E-18	3.49437E-13	1.22003E-13
HNCO	2.59465E-13	1.76990E-08	5.95718E-09
NCO	1.17461E-12	8.01242E-08	-6.53491E-09
NH2	2.97443E-16	2.02896E-11	1.36082E-11
NO	2.14401E-14	1.46250E-09	3.66046E-10
NH	8.96606E-15	6.11605E-10	1.60472E-10
NO2	1.38841E-15	9.47083E-11	4.26103E-11
N2O	4.48392E-15	3.05864E-10	9.25858E-11
HNO2	1.76860E-20	1.20643E-15	5.84728E-16
HNO3	1.71978E-22	1.17312E-17	7.01640E-18
HNO	6.02737E-20	4.11148E-15	1.98166E-15

21	2.3381E+12	1.33377E-02	1.00000
22	5.4417E+12	3.10423E-02	0.99998
23	1.7339E+11	1.03905E-02	0.99930
24	4.2953E+12	5.11571E-02	1.00000
25	6.0000E+12	1.71843E-07	0.99932
26	3.3000E+13	2.29396E-06	1.00000
27	5.0000E+12	8.51335E-07	0.99995
28	3.0000E+13	-3.29911E-09	0.95281
29	3.0000E+13	4.32687E-15	0.74712
30	2.8320E+02	3.39666E-09	0.99724
31	7.8394E+12	1.09293E-04	1.00000
32	1.5497E+13	2.16050E-04	1.00000
33	7.4517E+11	2.54429E-05	0.99981
34	3.0107E+11	1.02814E-05	0.99999
35	3.1645E+13	2.54226E-05	1.00000
36	2.0000E+13	2.29331E-10	0.99835
37	6.8116E+11	2.32647E-04	1.00000
38	1.2020E+12	2.39612E-09	1.00000
39	1.0000E+13	4.88248E-08	0.99990
40	5.0000E+13	3.98351E-08	0.96936
41	3.0000E+13	4.68574E-12	0.99999
42	5.4340E+12	-2.84658E-12	0.77032
43	1.0000E+13	2.35361E-14	1.00000
44	2.8000E+13	-1.17593E-04	0.97937
45	3.0043E+12	2.56633E-07	0.96552
46	3.9726E+12	-2.76520E-05	0.99787
47	6.5394E+12	4.95944E-08	0.50928
48	4.3596E+12	1.56133E-07	0.99156
49	2.0000E+13	7.22375E-07	1.00000
50	2.2625E+08	6.94081E-06	0.98456
51	5.0000E+13	2.34445E-10	1.00000
52	1.1231E+12	4.65627E+02	1.00000
53	2.0000E+13	1.99541E-02	1.00000
54	9.3599E+05	3.49479E-01	1.00000
55	2.0806E+13	2.20583E+01	1.00000
56	7.4046E+12	1.32131E+00	1.00000
57	1.2001E+13	5.19399E+00	1.00000
58	6.5181E+10	6.15586E+00	0.99996
59	1.2187E+13	1.27777E-02	0.99991
60	2.0000E+13	4.09585E+02	1.00000
61	1.4403E+04	4.57785E-03	0.99997
62	1.5254E+10	2.31704E-03	0.99997
63	1.1560E+10	4.25900E-03	1.00000
64	1.5254E+10	1.37665E-02	1.00000
65	3.7000E+12	-5.25069E-15	0.14089
66	1.0000E+13	1.77160E-06	1.00000
67	2.4319E+12	5.51211E-02	1.00000
68	1.3688E+10	1.81075E-09	1.00000
69	3.3600E+12	1.08877E-06	0.99998
70	1.2566E+13	6.85206E-07	0.99976
71	5.0000E+12	5.18176E-11	0.99982
72	4.0000E+13	4.14616E-10	1.00000
73	3.0000E+13	2.46987E+01	0.99998
74	3.0000E+13	1.44159E-04	1.00000
75	3.0000E+13	3.53120E-04	1.00000
76	2.0000E+13	3.96236E-05	1.00000
77	2.5136E+12	1.04200E+01	1.00000
78	6.8739E+14	1.30550E-04	1.00000
79	1.2074E+06	2.67993E-03	1.00000
80	3.0739E+11	9.75451E-03	0.99997
81	5.2820E+10	3.80361E-02	1.00000
82	2.5132E+11	1.34282E-01	0.75519
83	1.2718E+12	1.51638E+02	0.99966
84	6.3415E+12	4.89877E-01	0.98280
85	3.8068E+13	1.31865E+00	0.89523
86	3.6858E+13	3.45282E+00	0.99820
87	8.0000E+12	1.82553E+00	0.99264
88	9.6693E+13	3.74132E+00	1.00000
89	3.8651E+10	1.67619E-01	0.99261
90	3.9440E+12	-6.97878E-03	0.89480
91	1.8000E+12	9.38245E+00	0.99923
92	7.8000E+11	2.73111E-05	0.99999
93	1.3520E+11	9.49668E+00	0.99992
94	7.3817E+12	1.32137E+00	0.92973
95	1.9806E+15	-3.71788E+01	0.89238
96	1.5457E+01	-1.90679E-04	0.93159
97	4.3026E+15	4.31723E-05	0.98325
98	4.2473E+01	-1.53311E-07	0.02648
99	2.5532E-01	6.24295E-05	0.97979
100	3.0453E+08	2.04044E-10	1.00000
101	1.1918E+13	2.82378E-07	0.99991
102	1.2468E+11	-9.51698E-09	0.99468
103	1.7030E+11	-8.19194E-07	0.99979
104	1.2000E+13	6.10770E-09	1.00000
105	4.0114E+13	-7.76301E-05	0.99936
106	6.4274E+12	3.49108E-02	0.99972
107	7.4861E+12	7.95644E-05	0.99997
108	2.3589E+13	9.75761E-04	0.47435
109	3.7000E+12	-8.99142E-04	1.00000
110	2.0000E+13	2.33411E-03	1.00000
111	1.0000E+13	1.00337E-10	1.00000
112	2.0000E+13	9.62332E-04	1.00000
113	7.7207E+11	9.97601E-16	0.99044
114	2.0000E+12	2.60178E-15	0.99717
115	1.1037E+13	2.40839E-05	0.99999
116	2.4172E+12	2.85250E-04	0.99662
117	8.3381E+12	5.36939E-07	0.46681
118	8.0051E+15	-2.29534E-05	0.98923
119	2.2164E+14	1.26032E-05	0.99982
120	5.5414E+07	-1.46332E-08	0.99669
121	2.0808E+07	-3.95127E-05	1.00000
122	1.4344E+04	1.56934E-05	1.00000
123	4.0000E+12	4.74400E-14	1.00000
124	1.5404E+07	-5.04319E-04	0.98840
125	1.9454E+10	-3.69577E-05	0.99977
126	2.0569E+10	9.16355E-09	1.00000
127	7.5925E+11	-6.18438E-08	0.30722
128	3.4628E+09	2.22342E-08	0.99981
129	9.5586E+15	4.10234E-11	0.00092

TABLE D.2.—Continued.

(o) Continued.

130	9.4045E+15	-1.88154E-08	0.02549
131	5.0000E+12	-1.70434E-12	0.12131
132	6.4842E+15	1.20705E-08	0.14458
133	3.6000E+13	4.85855E-10	0.92002

DERIVATIVES (CGS UNITS): T 2.88791E+00 RHO 2.20037E-06 V -2.27804E+02

MIXTURE MOLECULAR WEIGHT 28.21051 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) -4.25939E+07 MASS FRACTION SUM 1.00000000

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 1.649994E+00 S UP TO THIS TIME - 9.000000E+00 S

TIME 2.83463E-04 SEC AREA 9.54999E+02 SQ CM AXIAL POSITION 4.25001E+01 CM

FLOW PROPERTIES

PRESSURE (ATM)	3.17523
VELOCITY (CM/SEC)	133515.05
DENSITY (G/CM**3)	5.43172E-04
TEMPERATURE (DEG K)	1993.74
MASS FLOW RATE (G/SEC)	6.92581E+04
ENTROPY (CAL/G/DEG K)	2.1774
MACH NUMBER	1.5379
GAMMA	1.2725
ENTHALPY (CAL/G)	4.21727E+02
SP. HEAT (CP) (CAL/G/DEG K)	3.31576E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	118
AVERAGE STEP SIZE	0.16567E+00
METHOD ORDER	4
TOTAL NUMBER OF STEPS	279
FUNCT EVALUATIONS	359
JACOBIAN EVALUATIONS	38

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	3.40604E-07	1.75491E-02	-6.38759E-02
CH3	1.27900E-07	6.58980E-03	1.67191E-02
H	3.51845E-09	1.81282E-04	1.43170E-03
H2	4.92214E-08	2.53605E-03	3.55775E-03
O2	3.34688E-06	1.72442E-01	-6.64194E-02
HO2	5.69348E-09	2.93347E-04	2.42905E-04
O	6.36081E-09	3.27730E-04	2.81115E-03
OH	1.75676E-08	9.05141E-04	7.32808E-03
H2O	6.74531E-07	3.47541E-02	8.94642E-02
CH3O	9.89933E-10	5.10046E-05	6.96576E-05
CH2O	5.29882E-08	2.73013E-03	-5.09769E-03
C2H6	2.91571E-08	1.50227E-03	-2.83783E-03
C2H5	3.55738E-11	1.83288E-06	8.32677E-06
C2H4	7.70981E-08	3.97235E-03	7.73786E-03
CH2	2.79446E-10	1.43980E-05	1.57683E-04
C2H3	2.38724E-10	1.22998E-05	1.10005E-04
C2H2	8.96820E-09	4.62071E-04	2.59896E-03
HCO	1.53395E-10	7.90341E-06	4.93156E-05
C2H2O	1.07069E-10	5.51652E-06	5.17763E-05
C2H	1.44852E-12	7.46325E-08	1.08700E-06
CO	1.98863E-07	1.02461E-02	3.46349E-02
C2HO	4.59648E-10	2.36826E-05	3.20739E-04
CH	1.24851E-12	6.43273E-08	1.27908E-06
CO2	4.31797E-09	2.22476E-04	1.35990E-03
H2O2	4.15768E-12	2.14218E-07	4.19770E-07
N2	1.44628E-05	7.45169E-01	-2.43752E-07
HCN	2.20298E-14	1.13505E-09	1.56265E-08
N	7.46803E-15	3.84777E-10	5.38870E-09
CN	4.41513E-17	2.27482E-12	2.28840E-11
HNCO	1.42240E-12	7.32866E-08	-6.26817E-08
NCO	1.34495E-14	6.92964E-10	2.97262E-09
NH2	3.21244E-13	1.65516E-08	5.63250E-08
NO	4.62605E-13	2.38349E-08	1.60872E-07
NH	1.58641E-14	8.17373E-10	-2.61956E-09
NO2	6.34113E-15	3.26716E-10	-3.17438E-10
N2O	6.29665E-13	3.24424E-08	1.55942E-07
HNO2	1.44678E-17	7.45429E-13	8.41252E-12
HNO3	3.28768E-20	1.69392E-15	6.30472E-15
HNO	4.46481E-17	2.30041E-12	2.28086E-11

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	4.5147E+07	-2.98324E+03	0.74678
2	6.2505E+12	1.95450E+04	0.76983
3	5.7703E+07	-1.02029E+03	0.82067
4	9.8634E+12	7.00746E+04	0.96748
5	7.0592E+12	1.34032E+05	0.93620
6	1.7233E+10	2.31976E+04	0.92778
7	6.3000E+12	-3.74404E+04	0.43831
8	2.4945E+11	1.62448E+04	1.00000
9	1.1491E+13	6.62632E+04	0.10401
10	1.1410E+13	3.96710E+03	0.99994
11	1.5580E+13	9.79384E+03	0.99999
12	3.5782E+13	6.21209E+04	0.99998
13	3.9979E+13	7.56667E+04	0.80876
14	5.6616E+11	1.66776E+02	0.72996
15	4.8000E+13	2.01363E+01	0.98885
16	2.0000E+13	2.42156E+03	0.99948
17	1.1428E+13	1.04976E+04	0.99904
18	5.2753E+08	2.67555E+03	0.99999
19	3.5189E+12	1.61502E+04	0.99973
20	1.5696E+12	6.83922E+03	0.94914
21	2.4811E+12	4.12407E+03	1.00000
22	7.0770E+12	1.17617E+04	0.99986
23	9.3184E+11	1.45445E+04	0.99390
24	4.2392E+12	1.14802E+04	1.00000
25	6.0000E+12	1.70753E+01	0.99964
26	3.3000E+13	1.69843E+02	1.00000
27	5.0000E+12	7.10657E+01	0.99990
28	3.0000E+13	6.65805E+00	0.98154
29	3.0000E+13	3.49208E-02	0.99316
30	7.8362E+04	4.99331E-03	0.10801
31	1.3182E+13	2.54882E+03	1.00000
32	2.7135E+13	5.24583E+03	0.99986
33	1.0765E+12	5.66568E+02	0.98559
34	3.0425E+11	1.62444E+02	0.99985
35	3.4241E+13	5.62223E+02	0.99925
36	2.0000E+13	1.69326E+00	0.98159
37	7.7680E+11	4.05041E+03	1.00000
38	1.2020E+12	1.19115E+01	1.00000
39	1.0000E+13	2.73693E+02	1.00000
40	5.0000E+13	2.73128E+02	0.99654
41	3.0000E+13	1.30608E+01	1.00000
42	6.0362E+12	2.62413E+00	0.99856
43	1.0000E+13	7.16104E+00	1.00000
44	2.8000E+13	1.71727E+02	0.96201
45	3.5173E+12	-1.70451E+01	0.43186
46	4.7567E+12	-8.54544E-01	0.12334
47	9.9567E+12	-6.80129E+01	0.84251
48	6.6378E+12	1.57825E+00	0.10300
49	2.0000E+13	4.61667E+01	1.00000
50	5.2959E+09	2.32358E+01	0.62293
51	5.0000E+13	1.56146E+00	1.00000
52	1.6370E+12	1.83826E+04	0.99999
53	2.0000E+13	2.36109E+02	1.00000
54	6.6054E+07	2.29953E+02	0.99871
55	2.2160E+13	6.99178E+04	0.99998
56	9.1319E+12	5.77015E+03	0.99993
57	1.4431E+13	1.64862E+04	0.99999
58	9.8203E+10	2.25505E+03	0.99967
59	1.3395E+13	8.90699E+02	0.99993
60	2.0000E+13	4.93423E+04	0.99958
61	1.7742E+06	9.99327E+00	0.66944
62	6.6827E+10	9.99656E+01	0.98073
63	5.0739E+10	1.39529E+02	0.99728

TABLE D.2.—Continued.
(o) Concluded.

64	6.6827E+10	5.06215E+02	0.99466
65	3.7000E+12	6.76047E-02	0.99995
66	1.0000E+13	1.41631E+02	1.00000
67	3.8536E+12	1.22159E+04	1.00000
68	6.0625E+10	3.64215E-01	0.99718
69	5.0357E+12	8.33265E+01	0.99447
70	1.8626E+13	6.08322E+01	0.98004
71	5.0000E+12	1.32337E+00	0.99997
72	4.0000E+13	1.05872E+01	1.00000
73	3.0000E+13	5.21839E+04	0.99963
74	3.0000E+13	9.92130E+01	1.00000
75	3.0000E+13	2.74011E+02	1.00000
76	2.0000E+13	3.65857E+01	0.99998
77	5.6970E+12	5.74726E+04	0.99974
78	8.5266E+14	7.09507E+01	0.99998
79	1.4800E+07	3.33836E+01	0.99992
80	3.2398E+11	3.82864E+03	0.99801
81	1.7625E+11	6.76362E+02	1.00000
82	6.5974E+11	4.70486E+03	0.49038
83	3.0111E+12	1.15308E+05	0.95944
84	1.3062E+13	1.19028E+04	0.85874
85	4.2568E+13	2.77096E+03	0.95872
86	3.8846E+13	4.74054E+03	0.99417
87	8.0000E+12	2.68107E+03	0.98856
88	1.0229E+14	6.94330E+03	0.99976
89	1.4379E+11	1.34325E+02	0.98351
90	4.2518E+12	-1.66421E+01	0.94051
91	1.8000E+12	1.97632E+02	0.99932
92	7.8000E+11	3.85206E-02	0.99602
93	1.4779E+12	3.47138E+02	0.75391
94	1.0170E+13	2.15446E+04	0.72280
95	1.8792E+15	-1.18888E+03	0.29180
96	3.8787E+03	-2.22968E+01	0.98384
97	3.5612E+15	5.19979E+00	0.99177
98	6.5929E+03	-8.31950E-01	0.94171
99	1.0434E+02	-9.02043E-02	0.79701
100	8.2652E+08	5.05851E-02	1.00000
101	1.5746E+13	-1.64104E-05	0.12395
102	3.4463E+11	1.43426E-04	0.87625
103	1.9730E+11	-2.53547E-03	0.90738
104	1.2000E+13	1.14214E-05	0.99990
105	5.4983E+13	-8.33520E-04	0.85221
106	1.0314E+13	-1.90100E-02	0.45097
107	1.1702E+13	1.90909E-01	0.96180
108	2.4862E+13	9.03448E-03	0.72554
109	3.7000E+12	-8.13011E-03	0.99971
110	2.0000E+13	5.79929E-03	1.00000
111	1.0000E+13	3.39816E-09	0.99817
112	2.0000E+13	3.20608E-03	0.99945
113	1.3017E+12	2.54700E-06	0.99951
114	2.0000E+12	3.91488E-06	0.99991
115	1.3476E+13	1.20849E-02	0.94934
116	2.3574E+12	1.97377E-02	0.93788
117	8.6033E+12	1.06576E-03	0.90613
118	7.5317E+15	-1.69459E-03	0.53754
119	2.3944E+14	1.80375E-02	0.99619
120	7.8362E+08	-2.13842E-02	0.99980
121	2.2108E+08	-2.68944E-01	0.99999
122	7.8865E+05	2.45908E-01	1.00000
123	4.0000E+12	6.42033E-10	1.00000
124	2.9225E+08	-5.28373E-01	0.97760
125	8.4820E+10	-9.28385E-03	0.88966
126	8.3363E+10	1.13167E-03	1.00000
127	1.6788E+12	7.97228E-03	0.63240
128	1.5896E+10	1.57207E-05	0.93485
129	7.8284E+15	2.13693E-08	0.00039
130	8.6008E+15	1.27928E-05	0.00278
131	5.0000E+12	2.45321E-06	0.92148
132	6.2830E+15	1.73385E-04	0.25773
133	3.6000E+13	9.36237E-05	0.97823

```
DERIVATIVES (CGS UNITS): T          2.54030E+02    RHO          4.61298E-05     V          -9.94097E+03

MIXTURE MOLECULAR WEIGHT     27.98600     TOTAL ENERGY EXCHANGE RATE   -1.25658E+10      MASS FRACTION SUM    1.00000001
                                             (CAL-CM**3/G**2/SEC)


COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP -  5.866669E+00  S     UP TO THIS TIME -  1.396667E+01  S


          (LSENS)     END OF THIS CASE


                SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

                   TOTAL NO. OF STEPS -                    279
                   TOTAL NO. OF DERIVATIVE EVALUATIONS -   359
                   TOTAL NO. OF JACOBIAN EVALUATIONS -      38
                   TOTAL CPU TIME -                 13.966667 S


                                TOTAL CPU TIME (INCLUDING I/O) REQUIRED =     16.533325 S


          (LSENS)     READ DATA FOR NEXT CASE
```

TABLE D.2.—Continued.

(p) Case 16

```
                                   ** DATA LINES **
                   1         2         3         4         5         6         7         8
CC  12345678901234567890123456789012345678901234567890123456789012345678901234567890123456789


    LSENS METHANE - AIR WITH TAB. AREA PROFILE OF CASE 15, BUT PRINT ASSIG; CASE 16
    REPEAT
    DISTANCE  AREA
     &prob xtb= 0.0,5.0,10.0,15.0,20.0,25.0,30.0,32.0,34.0,36.0,38.0,40.0,42.0,44.0,
       atb= 1200.0,1180.0,1160.0,1140.0,1120.0,1100.0,1080.0,1060.0,1040.0,1020.0,
       1000.0, 980.0, 960.0, 940.0,
      print = 5.0, 12.4954, 22.4363, 43.0002,   &end
     &start  t=1600.0, mach=2.0, p=1.730,  &end
    CH4         0.049768
    O2          0.199072
    N2          0.75116
    CN          0.0000001
    END
     &solver  emax=1.0E-5, atolsp=1.0E-14,  &end
    FINIS
```

```
                                   ** INITIAL CONDITIONS **

TIME   0.00000E+00  SEC            AREA   1.20000E+03  SQ CM            AXIAL POSITION   0.00000E+00  CM

    FLOW PROPERTIES                                          INTEGRATION INDICATORS

      PRESSURE                 1.73000                         STEPS FROM LAST PRINT              0
       (ATM)
      VELOCITY            155259.65                            AVERAGE STEP SIZE            0.00000E+00
       (CM/SEC)
      DENSITY             3.71736E-04                          METHOD ORDER                       0
       (G/CM**3)
      TEMPERATURE             1600.00
       (DEG K)
      MASS FLOW RATE      6.92587E+04                          TOTAL NUMBER OF STEPS              0
       (G/SEC)
      ENTROPY                  2.1223                          FUNCT EVALUATIONS                  0
       (CAL/G/DEG K)
      MACH NUMBER              2.0000                          JACOBIAN EVALUATIONS               0

      GAMMA                    1.2780

      ENTHALPY            3.46688E+02
       (CAL/G)
      SP. HEAT (CP)       3.23820E-01
       (CAL/G/DEG K)
```

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSI-TIVE DIR RATE
CH4	6.55792E-07	4.97680E-02	-4.71274E-06	1	1.9089E+05	1.19373E+01	1.00000
CH3	0.00000E+00	0.00000E+00	4.71274E-06	2	2.9847E+12	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	1.64958E-06	3	1.7806E+06	2.21667E+01	1.00000
H2	0.00000E+00	0.00000E+00	0.00000E+00	4	4.7630E+12	0.00000E+00	0.00000
O2	2.62317E-06	1.99072E-01	-8.38235E-05	5	5.1714E+12	0.00000E+00	0.00000
HO2	0.00000E+00	0.00000E+00	3.06316E-06	6	2.9021E+09	0.00000E+00	0.00000
O	0.00000E+00	0.00000E+00	8.07603E-05	7	6.3000E+12	0.00000E+00	0.00000
OH	0.00000E+00	0.00000E+00	0.00000E+00	8	6.7687E+10	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	0.00000E+00	9	1.2548E+13	0.00000E+00	0.00000
CH3O	0.00000E+00	0.00000E+00	0.00000E+00	10	6.2462E+12	0.00000E+00	0.00000
CH2O	0.00000E+00	0.00000E+00	0.00000E+00	11	9.5679E+12	0.00000E+00	0.00000
C2H6	0.00000E+00	0.00000E+00	0.00000E+00	12	2.8755E+13	0.00000E+00	0.00000
C2H5	0.00000E+00	0.00000E+00	0.00000E+00	13	5.8291E+12	0.00000E+00	0.00000
C2H4	0.00000E+00	0.00000E+00	0.00000E+00	14	4.1501E+11	0.00000E+00	0.00000
CH2	0.00000E+00	0.00000E+00	0.00000E+00	15	4.8000E+13	0.00000E+00	0.00000
C2H3	0.00000E+00	0.00000E+00	0.00000E+00	16	2.0000E+13	0.00000E+00	0.00000
C2H2	0.00000E+00	0.00000E+00	0.00000E+00	17	6.0651E+12	0.00000E+00	0.00000
HCO	0.00000E+00	0.00000E+00	0.00000E+00	18	3.8291E+06	0.00000E+00	0.00000
C2H2O	0.00000E+00	0.00000E+00	0.00000E+00	19	3.2601E+12	0.00000E+00	0.00000
C2H	0.00000E+00	0.00000E+00	0.00000E+00	20	1.4788E+12	0.00000E+00	0.00000
CO	0.00000E+00	0.00000E+00	0.00000E+00	21	2.3129E+12	0.00000E+00	0.00000
C2HO	0.00000E+00	0.00000E+00	0.00000E+00	22	5.1877E+12	0.00000E+00	0.00000
CH	0.00000E+00	0.00000E+00	0.00000E+00	23	1.2768E+11	0.00000E+00	0.00000
CO2	0.00000E+00	0.00000E+00	0.00000E+00	24	4.3056E+12	0.00000E+00	0.00000
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	25	6.0000E+12	0.00000E+00	0.00000
N2	9.89802E-06	7.51160E-01	-1.79633E-12	26	3.3000E+13	0.00000E+00	0.00000
HCN	0.00000E+00	0.00000E+00	0.00000E+00	27	5.0000E+12	0.00000E+00	0.00000
N	0.00000E+00	0.00000E+00	0.00000E+00	28	3.0000E+13	0.00000E+00	0.00000
CN	1.31770E-12	1.00000E-07	-8.07603E-05	29	3.0000E+13	0.00000E+00	0.00000
HNCO	0.00000E+00	0.00000E+00	0.00000E+00	30	1.0180E+02	0.00000E+00	0.00000
NCO	0.00000E+00	0.00000E+00	8.07603E-05	31	7.1320E+12	0.00000E+00	0.00000
NH2	0.00000E+00	0.00000E+00	0.00000E+00	32	1.3995E+13	0.00000E+00	0.00000
NO	0.00000E+00	0.00000E+00	0.00000E+00	33	6.9692E+11	0.00000E+00	0.00000
NH	0.00000E+00	0.00000E+00	0.00000E+00	34	3.0049E+11	0.00000E+00	0.00000
NO2	0.00000E+00	0.00000E+00	0.00000E+00	35	3.1195E+13	0.00000E+00	0.00000
N2O	0.00000E+00	0.00000E+00	1.79633E-12	36	2.0000E+13	0.00000E+00	0.00000
HNO2	0.00000E+00	0.00000E+00	0.00000E+00	37	6.6507E+11	0.00000E+00	0.00000
HNO3	0.00000E+00	0.00000E+00	0.00000E+00	38	1.2020E+12	0.00000E+00	0.00000
HNO	0.00000E+00	0.00000E+00	0.00000E+00	39	1.0000E+13	0.00000E+00	0.00000
				40	5.0000E+13	0.00000E+00	0.00000
				41	3.0000E+13	0.00000E+00	0.00000
				42	5.3311E+12	0.00000E+00	0.00000
				43	1.0000E+13	0.00000E+00	0.00000
				44	2.8000E+13	0.00000E+00	0.00000
				45	2.9193E+12	0.00000E+00	0.00000
				46	3.8445E+12	0.00000E+00	0.00000
				47	6.0578E+12	0.00000E+00	0.00000
				48	4.0385E+12	0.00000E+00	0.00000
				49	2.0000E+13	0.00000E+00	0.00000
				50	1.2747E+08	0.00000E+00	0.00000

TABLE D.2.—Continued.

(p) Continued.

51	5.0000E+13	0.00000E+00	0.00000
52	1.0486E+12	0.00000E+00	0.00000
53	2.0000E+13	0.00000E+00	0.00000
54	4.3141E+05	0.00000E+00	0.00000
55	2.0569E+13	0.00000E+00	0.00000
56	7.1274E+12	0.00000E+00	0.00000
57	1.1604E+13	0.00000E+00	0.00000
58	6.0604E+10	0.00000E+00	0.00000
59	1.2000E+13	0.00000E+00	0.00000
60	2.0000E+13	0.00000E+00	0.00000
61	5.9987E+03	0.00000E+00	0.00000
62	1.1686E+10	0.00000E+00	0.00000
63	8.8532E+09	0.00000E+00	0.00000
64	1.1686E+10	0.00000E+00	0.00000
65	3.7000E+12	0.00000E+00	0.00000
66	1.0000E+13	0.00000E+00	0.00000
67	2.2405E+12	0.00000E+00	0.00000
68	1.0466E+10	0.00000E+00	0.00000
69	3.1270E+12	0.00000E+00	0.00000
70	1.1726E+13	0.00000E+00	0.00000
71	5.0000E+12	0.00000E+00	0.00000
72	4.0000E+13	0.00000E+00	0.00000
73	3.0000E+13	0.00000E+00	0.00000
74	3.0000E+13	0.00000E+00	0.00000
75	3.0000E+13	0.00000E+00	0.00000
76	2.0000E+13	0.00000E+00	0.00000
77	2.1659E+12	0.00000E+00	0.00000
78	6.6096E+14	0.00000E+00	0.00000
79	7.6523E+05	0.00000E+00	0.00000
80	3.0447E+11	0.00000E+00	0.00000
81	4.2421E+10	0.00000E+00	0.00000
82	2.1085E+11	0.00000E+00	0.00000
83	1.0872E+12	0.00000E+00	0.00000
84	5.5602E+12	0.00000E+00	0.00000
85	3.7302E+13	0.00000E+00	0.00000
86	3.6507E+13	0.00000E+00	0.00000
87	8.0000E+12	0.00000E+00	0.00000
88	9.5708E+13	0.00000E+00	0.00000
89	3.0432E+10	0.00000E+00	0.00000
90	3.8905E+12	0.00000E+00	0.00000
91	1.8000E+12	0.00000E+00	0.00000
92	7.8000E+11	0.00000E+00	0.00000
93	8.7496E+10	0.00000E+00	0.00000
94	6.9635E+12	0.00000E+00	0.00000
95	1.9996E+15	0.00000E+00	0.00000
96	5.6558E+00	0.00000E+00	0.00000
97	4.4375E+15	0.00000E+00	0.00000
98	1.6960E+01	0.00000E+00	0.00000
99	8.5187E-02	2.13082E-05	1.00000
100	2.5393E+08	0.00000E+00	0.00000
101	1.1329E+13	0.00000E+00	0.00000
102	1.0387E+11	0.00000E+00	0.00000
103	1.6581E+11	0.00000E+00	0.00000
104	1.2000E+13	0.00000E+00	0.00000
105	3.7877E+13	0.00000E+00	0.00000
106	5.8974E+12	0.00000E+00	0.00000
107	6.9017E+12	0.00000E+00	0.00000
108	2.3364E+13	5.84425E+02	1.00000
109	3.7000E+12	0.00000E+00	0.00000
110	2.0000E+13	0.00000E+00	0.00000
111	1.0000E+13	0.00000E+00	0.00000
112	2.0000E+13	0.00000E+00	0.00000
113	7.0207E+11	0.00000E+00	0.00000
114	2.0000E+12	0.00000E+00	0.00000
115	1.0662E+13	0.00000E+00	0.00000
116	2.4283E+12	0.00000E+00	0.00000
117	8.2907E+12	0.00000E+00	0.00000
118	8.0944E+15	0.00000E+00	0.00000
119	2.1854E+14	0.00000E+00	0.00000
120	3.4219E+07	0.00000E+00	0.00000
121	1.3584E+07	0.00000E+00	0.00000
122	6.9185E+03	0.00000E+00	0.00000
123	4.0000E+12	0.00000E+00	0.00000
124	8.9376E+06	0.00000E+00	0.00000
125	1.4882E+10	-1.29992E-05	1.00000
126	1.5945E+10	0.00000E+00	0.00000
127	6.5717E+11	0.00000E+00	0.00000
128	2.6242E+09	0.00000E+00	0.00000
129	9.9124E+15	0.00000E+00	0.00000
130	9.5587E+15	0.00000E+00	0.00000
131	5.0000E+12	0.00000E+00	0.00000
132	6.5215E+15	0.00000E+00	0.00000
133	3.6000E+13	0.00000E+00	0.00000

DERIVATIVES (CGS UNITS): T 1.97928E+00 RHO 1.65526E-06 V -1.72834E+02

MIXTURE MOLECULAR WEIGHT 28.21102 TOTAL ENERGY EXCHANGE RATE -1.27744E+06 (CAL-CM**3/G**2/SEC) MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 1.069992 S

TABLE D.2.—Continued.

(p) Continued.

TIME 1.46451E-04 SEC AREA 1.10936E+03 SQ CM AXIAL POSITION 2.24363E+01 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.98504
VELOCITY (CM/SEC)	150959.76
DENSITY (G/CM**3)	4.13563E-04
TEMPERATURE (DEG K)	1650.17
MASS FLOW RATE (G/SEC)	6.92587E+04
ENTROPY (CAL/G/DEG K)	2.1234
MACH NUMBER	1.9161
GAMMA	1.2763
ENTHALPY (CAL/G)	3.62423E+02
SP. HEAT (CP) (CAL/G/DEG K)	3.25371E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	29
AVERAGE STEP SIZE	0.35712E+00
METHOD ORDER	4
TOTAL NUMBER OF STEPS	161
FUNCT EVALUATIONS	199
JACOBIAN EVALUATIONS	25

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	7.17624E-07	4.89515E-02	-2.51430E-04
CH3	3.70822E-09	2.52950E-04	5.03006E-05
H	7.00622E-12	4.77918E-07	1.25105E-07
H2	7.91113E-10	5.39645E-05	1.66017E-05
O2	2.91153E-06	1.98605E-01	-1.46771E-04
HO2	9.44564E-10	6.44319E-05	7.30120E-06
O	1.69934E-11	1.15918E-06	2.71685E-07
OH	4.16255E-11	2.83942E-06	7.69568E-07
H2O	7.12085E-09	4.85737E-04	1.68311E-04
CH3O	2.43557E-11	1.66139E-06	4.42876E-07
CH2O	4.35616E-09	2.97149E-04	1.03105E-04
C2H6	1.81074E-09	1.23516E-04	4.30530E-05
C2H5	2.28401E-14	1.55800E-09	7.69218E-10
C2H4	5.74155E-11	3.91650E-06	2.72323E-06
CH2	1.33148E-15	9.08248E-11	6.47923E-11
C2H3	6.99640E-16	4.77249E-11	4.59943E-11
C2H2	1.40319E-13	9.57163E-09	8.59544E-09
HCO	4.83643E-14	3.29909E-09	1.94312E-09
C2H2O	3.63528E-16	2.47974E-11	2.56030E-11
C2H	4.71927E-20	3.21917E-15	3.95995E-15
CO	1.30390E-10	8.89437E-06	6.00064E-06
C2HO	2.00636E-17	1.36861E-12	1.57302E-12
CH	1.04070E-20	7.09899E-16	7.22929E-16
CO2	1.42213E-13	9.70086E-09	8.80830E-09
H2O2	8.54763E-13	5.83063E-08	1.03216E-08
N2	1.10117E-05	7.51146E-01	-9.52715E-11
HCN	4.10904E-18	2.80291E-13	1.90069E-13
N	1.46100E-18	9.96595E-14	4.38094E-14
CN	5.12271E-18	3.49438E-13	1.22003E-13
HNCO	2.59465E-13	1.76990E-08	5.95719E-09
NCO	1.17461E-12	8.01242E-08	-6.53491E-09
NH2	2.97443E-16	2.02896E-11	1.36082E-11
NO	2.14401E-14	1.46250E-09	3.66047E-10
NH	8.96606E-15	6.11606E-10	1.60472E-10
NO2	1.38841E-15	9.47084E-11	4.26104E-11
N2O	4.48392E-15	3.05864E-10	9.25858E-11
HNO2	1.76861E-20	1.20643E-15	- 5.84729E-16
HNO3	1.71978E-22	1.17312E-17	7.01639E-18
HNO	6.02738E-20	4.11148E-15	1.98167E-15

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	4.4284E+05	2.65382E+01	0.97428
2	3.3445E+12	9.58538E+01	0.97496
3	3.0419E+06	2.82779E+01	0.76098
4	5.3278E+12	3.79712E+02	0.99957
5	5.4252E+12	9.45847E+02	0.99824
6	3.8178E+09	2.40782E+02	0.99910
7	6.3000E+12	-9.40211E+00	0.62316
8	8.2740E+10	1.72728E+02	1.00000
9	1.2394E+13	2.67192E+02	0.26815
10	6.8533E+12	5.08339E-01	1.00000
11	1.0314E+13	1.85554E+00	1.00000
12	2.9739E+13	1.31057E+01	1.00000
13	7.8404E+12	1.53007E+01	0.99685
14	4.3534E+11	1.64308E-01	0.97073
15	4.8000E+13	4.47720E-05	0.99493
16	2.0000E+13	5.77223E-04	0.99976
17	6.6865E+12	1.57259E-02	0.99998
18	8.1738E+06	4.02253E-02	1.00000
19	3.2987E+12	4.60940E-02	1.00000
20	1.4924E+12	-6.02946E-01	0.96657
21	2.3381E+12	1.33377E-02	1.00000
22	5.4417E+12	3.10424E-02	0.99998
23	1.7339E+11	1.03905E-02	0.99930
24	4.2953E+12	5.11572E-02	1.00000
25	6.0000E+12	1.71843E-07	0.99932
26	3.3000E+13	2.29396E-06	1.00000
27	5.0000E+12	8.51337E-07	0.99995
28	3.0000E+13	-3.29912E-09	0.95281
29	3.0000E+13	4.32689E-15	0.74712
30	2.8320E+02	3.39666E-09	0.99724
31	7.8394E+12	1.09293E-04	1.00000
32	1.5497E+13	2.16050E-04	1.00000
33	7.4517E+11	2.54429E-05	0.99981
34	3.0107E+11	1.02814E-05	0.99999
35	3.1645E+13	2.54227E-05	1.00000
36	2.0000E+13	2.29332E-10	0.99835
37	6.8116E+11	2.32647E-04	1.00000
38	1.2020E+12	2.39613E-09	1.00000
39	1.0000E+13	4.88249E-08	0.99990
40	5.0000E+13	3.98352E-08	0.96936
41	3.0000E+13	4.68576E-12	0.99999
42	5.4340E+12	-2.84658E-12	0.77032
43	1.0000E+13	2.35361E-14	1.00000
44	2.8000E+13	-1.17593E-04	0.97937
45	3.0043E+12	2.56633E-07	0.96552
46	3.9726E+12	-2.76520E-05	0.99787
47	6.5394E+12	4.95945E-08	0.50928
48	4.3596E+12	1.56134E-07	0.99156
49	2.0000E+13	7.22376E-07	1.00000
50	2.2625E+08	6.94083E-06	0.98456
51	5.0000E+13	2.34445E-10	1.00000
52	1.1231E+12	4.65628E+02	1.00000
53	2.0000E+13	1.99541E-02	1.00000
54	9.3599E+05	3.49479E-01	1.00000
55	2.0806E+13	2.20584E+01	1.00000
56	7.4046E+12	1.32131E+00	1.00000
57	1.2001E+13	5.19400E+00	1.00000
58	6.5181E+10	6.15586E+00	0.99996
59	1.2187E+13	1.27778E-02	0.99991
60	2.0000E+13	4.09585E+02	1.00000
61	1.4403E+04	4.57785E-03	0.99997
62	1.5254E+10	2.31704E-03	0.99997
63	1.1560E+10	4.25901E-03	1.00000
64	1.5254E+10	1.37665E-02	1.00000
65	3.7000E+12	-5.25067E-15	0.14089
66	1.0000E+13	1.77160E-06	1.00000
67	2.4319E+12	5.51212E-02	1.00000
68	1.3688E+10	1.81075E-09	1.00000
69	3.3600E+12	1.08878E-06	0.99998
70	1.2566E+13	6.85208E-07	0.99976
71	5.0000E+12	5.18177E-11	0.99982
72	4.0000E+13	4.14617E-10	1.00000
73	3.0000E+13	2.46987E+01	0.99998
74	3.0000E+13	1.44159E-04	1.00000
75	3.0000E+13	3.53120E-04	1.00000
76	2.0000E+13	3.96237E-05	1.00000
77	2.5136E+12	1.04200E+01	1.00000
78	6.8739E+14	1.30550E-04	1.00000
79	1.2074E+06	2.67994E-03	1.00000
80	3.0739E+11	9.75453E-03	0.99997
81	5.2820E+10	3.80361E-02	1.00000

TABLE D.2.—Continued.

(p) Continued.

82	2.5132E+11	1.34282E-01	0.75519
83	1.2718E+12	1.51638E+02	0.99966
84	6.3415E+12	4.89878E-01	0.98280
85	3.8068E+13	1.31865E+00	0.89523
86	3.6858E+13	3.45282E+00	0.99820
87	8.0000E+12	1.82553E+00	0.99264
88	9.6693E+13	3.74133E+00	1.00000
89	3.8651E+10	1.67619E-01	0.99261
90	3.9440E+12	-6.97879E-03	0.89480
91	1.8000E+12	9.38246E+00	0.99923
92	7.8000E+11	2.73111E-05	0.99999
93	1.3520E+11	9.49668E+00	0.99992
94	7.3817E+12	1.32137E+00	0.92973
95	1.9806E+15	-3.71788E+01	0.89238
96	1.5457E+01	-1.90679E-04	0.93159
97	4.3026E+15	4.31723E-05	0.98325
98	4.2473E+01	-1.53312E-07	0.02648
99	2.5532E-01	6.24295E-05	0.97979
100	3.0453E+08	2.04045E-10	1.00000
101	1.1918E+13	2.82378E-07	0.99991
102	1.2468E+11	-9.51699E-09	0.99468
103	1.7030E+11	-8.19194E-07	0.99979
104	1.2000E+13	6.10771E-09	1.00000
105	4.0114E+13	-7.76301E-05	0.99936
106	6.4274E+12	3.49108E-02	0.99972
107	7.4861E+12	7.95645E-05	0.99997
108	2.3589E+13	9.75762E-04	0.47435
109	3.7000E+12	-8.99143E-04	1.00000
110	2.0000E+13	2.33411E-03	1.00000
111	1.0000E+13	1.00337E-10	1.00000
112	2.0000E+13	9.62332E-04	1.00000
113	7.7207E+11	9.97604E-16	0.99044
114	2.0000E+12	2.60178E-15	0.99717
115	1.1037E+13	2.40839E-05	0.99999
116	2.4172E+12	2.85250E-04	0.99662
117	8.3381E+12	5.36940E-07	0.46681
118	8.0051E+15	-2.29534E-05	0.98923
119	2.2164E+14	1.26033E-05	0.99982
120	5.5414E+07	-1.46332E-08	0.99669
121	2.0808E+07	-3.95127E-05	1.00000
122	1.4344E+04	1.56934E-05	1.00000
123	4.0000E+12	4.74400E-14	1.00000
124	1.5404E+07	-5.04320E-04	0.98840
125	1.9454E+10	-3.69577E-05	0.99977
126	2.0569E+10	9.16356E-09	1.00000
127	7.5925E+11	-6.18438E-08	0.30722
128	3.4628E+09	2.22342E-08	0.99981
129	9.5586E+15	4.10234E-11	0.00092
130	9.4045E+15	-1.88154E-08	0.02549
131	5.0000E+12	-1.70434E-12	0.12131
132	6.4842E+15	1.20705E-08	0.14458
133	3.6000E+13	4.85856E-10	0.92002

DERIVATIVES (CGS UNITS): T 2.88791E+00 RHO 2.20037E-06 V -2.27804E+02

MIXTURE MOLECULAR WEIGHT 28.21051 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) -4.25939E+07 MASS FRACTION SUM 1.00000000

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 1.660004E+00 S UP TO THIS TIME - 9.010025E+00 S

TIME 2.83463E-04 SEC AREA 9.54999E+02 SQ CM AXIAL POSITION 4.25001E+01 CM

FLOW PROPERTIES

PRESSURE (ATM)	3.17520
VELOCITY (CM/SEC)	133515.39
DENSITY (G/CM**3)	5.43171E-04
TEMPERATURE (DEG K)	1993.73
MASS FLOW RATE (G/SEC)	6.92581E+04
ENTROPY (CAL/G/DEG K)	2.1774
MACH NUMBER	1.5379
GAMMA	1.2725
ENTHALPY (CAL/G)	4.21726E+02
SP. HEAT (CP) (CAL/G/DEG K)	3.31576E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	118
AVERAGE STEP SIZE	0.16567E+00
METHOD ORDER	4
TOTAL NUMBER OF STEPS	279
FUNCT EVALUATIONS	359
JACOBIAN EVALUATIONS	38

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
CH4	3.40620E-07	1.75499E-02	-6.38713E-02	1	4.5143E+07	-2.98280E+03	0.74676
CH3	1.27895E-07	6.58958E-03	1.67178E-02	2	6.2504E+12	1.95436E+04	0.76983
H	3.51808E-09	1.81263E-04	1.43144E-03	3	5.7700E+07	-1.02023E+03	0.82066
H2	4.92203E-08	2.53600E-03	3.55768E-03	4	9.8633E+12	7.00692E+04	0.96749
O2	3.34689E-06	1.72443E-01	-6.64127E-02	5	7.0591E+12	1.34024E+05	0.93620
HO2	5.69341E-09	2.93344E-04	2.42879E-04	6	1.7232E+10	2.31964E+04	0.92779
O	6.36007E-09	3.27693E-04	2.81061E-03	7	6.3000E+12	-3.74380E+04	0.43833
OH	1.75657E-08	9.05044E-04	7.32672E-03	8	2.4945E+11	1.62441E+04	1.00000
H2O	6.74506E-07	3.47529E-02	8.94564E-02	9	1.1491E+13	6.62581E+04	0.10401
CH3O	9.89912E-10	5.10037E-05	6.96517E-05	10	1.1410E+13	3.96674E+03	0.99994
CH2O	5.29894E-08	2.73019E-03	-5.09736E-03	11	1.5580E+13	9.79289E+03	0.99999
C2H6	2.91577E-08	1.50231E-03	-2.83738E-03	12	3.5782E+13	6.21155E+04	0.99998
C2H5	3.55715E-11	1.83277E-06	8.32578E-06	13	3.9978E+13	7.56601E+04	0.80876
C2H4	7.70959E-08	3.97224E-03	7.73785E-03	14	5.6616E+11	1.66765E+02	0.72996
CH2	2.79405E-10	1.43959E-05	1.57649E-04	15	4.8000E+13	2.01330E+01	0.98885
C2H3	2.38695E-10	1.22984E-05	1.09986E-04	16	2.0000E+13	2.42113E+03	0.99948
C2H2	8.96751E-09	4.62037E-04	2.59869E-03	17	1.1428E+13	1.04961E+04	0.99904

TABLE D.2.—Continued.

(p) Continued.

HCO	1.53382E-10	7.90275E-06	4.93072E-05
C2H2O	1.07055E-10	5.51584E-06	5.17669E-05
C2H	1.44824E-12	7.46182E-08	1.08673E-06
CO	1.98853E-07	1.02456E-02	3.46313E-02
C2HO	4.59564E-10	2.36783E-05	3.20663E-04
CH	1.24818E-12	6.43104E-08	1.27865E-06
CO2	4.31761E-09	2.22458E-04	1.35970E-03
H2O2	4.15756E-12	2.14212E-07	4.19630E-07
N2	1.44627E-05	7.45169E-01	-2.43711E-07
HCN	2.20257E-14	1.13484E-09	1.56221E-08
N	7.46662E-15	3.84706E-10	5.38724E-09
CN	4.41453E-17	2.27452E-12	2.28789E-11
HNCO	1.42241E-12	7.32875E-08	-6.26747E-08
NCO	1.34487E-14	6.92925E-10	2.97220E-09
NH2	3.21229E-13	1.65508E-08	5.63190E-08
NO	4.62562E-13	2.38328E-08	1.60839E-07
NH	1.58648E-14	8.17408E-10	-2.61949E-09
NO2	6.34119E-15	3.26720E-10	-3.17522E-10
N2O	6.29623E-13	3.24404E-08	1.55920E-07
HNO2	1.44656E-17	7.45318E-13	8.41042E-12
HNO3	3.28750E-20	1.69383E-15	6.30338E-15
HNO	4.46421E-17	2.30011E-12	2.28034E-11

18	5.2749E+08	2.67525E+03	0.99999
19	3.5189E+12	1.61480E+04	0.99973
20	1.5696E+12	6.83826E+03	0.94913
21	2.4811E+12	4.12349E+03	1.00000
22	7.0770E+12	1.17600E+04	0.99986
23	9.3180E+11	1.45422E+04	0.99390
24	4.2392E+12	1.14789E+04	1.00000
25	6.0000E+12	1.70715E+01	0.99964
26	3.3000E+13	1.69803E+02	1.00000
27	5.0000E+12	7.10497E+01	0.99990
28	3.0000E+13	6.65628E+00	0.98154
29	3.0000E+13	3.49100E-02	0.99316
30	7.8352E+04	4.99591E-03	0.10809
31	1.3182E+13	2.54831E+03	1.00000
32	2.7135E+13	5.24478E+03	0.99986
33	1.0765E+12	5.66461E+02	0.98559
34	3.0425E+11	1.62415E+02	0.99985
35	3.4241E+13	5.62117E+02	0.99925
36	2.0000E+13	1.69276E+00	0.98159
37	7.7679E+11	4.04969E+03	1.00000
38	1.2020E+12	1.19080E+01	1.00000
39	1.0000E+13	2.73614E+02	1.00000
40	5.0000E+13	2.73051E+02	0.99654
41	3.0000E+13	1.30566E+01	1.00000
42	6.0362E+12	2.62327E+00	0.99856
43	1.0000E+13	7.15847E+00	1.00000
44	2.8000E+13	1.71686E+02	0.96201
45	3.5173E+12	-1.70409E+01	0.43186
46	4.7567E+12	-8.55105E-01	0.12344
47	9.9566E+12	-6.79987E+01	0.84252
48	6.6377E+12	1.57859E+00	0.10305
49	2.0000E+13	4.61558E+01	1.00000
50	5.2955E+09	2.32313E+01	0.62292
51	5.0000E+13	1.56099E+00	1.00000
52	1.6369E+12	1.83822E+04	0.99999
53	2.0000E+13	2.36080E+02	1.00000
54	6.6048E+07	2.29938E+02	0.99871
55	2.2160E+13	6.99119E+04	0.99998
56	9.1319E+12	5.76966E+03	0.99993
57	1.4431E+13	1.64847E+04	0.99999
58	9.8202E+10	2.25501E+03	0.99967
59	1.3395E+13	8.90594E+02	0.99993
60	2.0000E+13	4.93401E+04	0.99958
61	1.7740E+06	9.99241E+00	0.66947
62	6.6825E+10	9.99487E+01	0.98073
63	5.0737E+10	1.39504E+02	0.99728
64	6.6825E+10	5.06128E+02	0.99466
65	3.7000E+12	6.75815E-02	0.99995
66	1.0000E+13	1.41594E+02	1.00000
67	3.8535E+12	1.22140E+04	1.00000
68	6.0623E+10	3.64109E-01	0.99718
69	5.0356E+12	8.33047E+01	0.99447
70	1.8626E+13	6.08166E+01	0.98004
71	5.0000E+12	1.32298E+00	0.99997
72	4.0000E+13	1.05841E+01	1.00000
73	3.0000E+13	5.21798E+04	0.99963
74	3.0000E+13	9.91935E+01	1.00000
75	3.0000E+13	2.73959E+02	1.00000
76	2.0000E+13	3.65788E+01	0.99998
77	5.6969E+12	5.74668E+04	0.99974
78	8.5266E+14	7.09389E+01	0.99998
79	1.4799E+07	3.33805E+01	0.99992
80	3.2398E+11	3.82805E+03	0.99801
81	1.7624E+11	6.76307E+02	1.00000
82	6.5972E+11	4.70431E+03	0.49041
83	3.0110E+12	1.15295E+05	0.95944
84	1.3061E+13	1.19012E+04	0.85875
85	4.2568E+13	2.77063E+03	0.95872
86	3.8846E+13	4.73994E+03	0.99417
87	8.0000E+12	2.68075E+03	0.98856
88	1.0229E+14	6.94249E+03	0.99976
89	1.4378E+11	1.34318E+02	0.98351
90	4.2518E+12	-1.66407E+01	0.94052
91	1.8000E+12	1.97628E+02	0.99932
92	7.8000E+11	3.85156E-02	0.99602
93	1.4778E+12	3.47126E+02	0.75394
94	1.0170E+13	2.15420E+04	0.72281
95	1.8792E+15	-1.18888E+03	0.29182
96	3.8783E+03	-2.22921E+01	0.98384
97	3.5612E+15	5.19866E+00	0.99177
98	6.5922E+03	-8.31771E-01	0.94171
99	1.0433E+02	-9.01815E-02	0.79699
100	8.2650E+08	5.05707E-02	1.00000
101	1.5746E+13	-1.63874E-05	0.12382
102	3.4462E+11	1.43379E-04	0.87624
103	1.9730E+11	-2.53524E-03	0.90740
104	1.2000E+13	1.14186E-05	0.99990
105	5.4983E+13	-8.33371E-04	0.85222
106	1.0314E+13	-1.90072E-02	0.45096
107	1.1701E+13	1.90890E-01	0.96180
108	2.4862E+13	9.03348E-03	0.72555
109	3.7000E+12	-8.12931E-03	0.99971
110	2.0000E+13	5.79830E-03	1.00000

TABLE D.2.—Concluded.
(p) Concluded.

111	1.0000E+13	3.39733E-09	0.99817
112	2.0000E+13	3.20557E-03	0.99945
113	1.3017E+12	2.54607E-06	0.99951
114	2.0000E+12	3.91350E-06	0.99991
115	1.3476E+13	1.20841E-02	0.94934
116	2.3574E+12	1.97357E-02	0.93788
117	8.6033E+12	1.06566E-03	0.90613
118	7.5317E+15	-1.69469E-03	0.53760
119	2.3944E+14	1.80359E-02	0.99619
120	7.8357E+08	-2.13779E-02	0.99980
121	2.2107E+08	-2.68891E-01	0.99999
122	7.8859E+05	2.45860E-01	1.00000
123	4.0000E+12	6.41922E-10	1.00000
124	2.9223E+08	-5.28300E-01	0.97760
125	8.4817E+10	-9.28288E-03	0.88967
126	8.3361E+10	1.13144E-03	1.00000
127	1.6788E+12	7.97087E-03	0.63240
128	1.5895E+10	1.57204E-05	0.93487
129	7.8284E+15	2.13649E-08	0.00039
130	8.6008E+15	1.27862E-05	0.00278
131	5.0000E+12	2.45262E-06	0.92147
132	6.2830E+15	1.73344E-04	0.25772
133	3.6000E+13	9.36013E-05	0.97823

DERIVATIVES (CGS UNITS): T 2.54007E+02 RHO 4.61257E-05 V -9.94004E+03

MIXTURE MOLECULAR WEIGHT 27.98601 TOTAL ENERGY EXCHANGE RATE -1.25648E+10 MASS FRACTION SUM 1.00000001
(CAL-CM**3/G**2/SEC)

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 5.866669E+00 S UP TO THIS TIME - 1.390001E+01 S

(LSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

TOTAL NO. OF STEPS - 279
TOTAL NO. OF DERIVATIVE EVALUATIONS - 359
TOTAL NO. OF JACOBIAN EVALUATIONS - 38
TOTAL CPU TIME - 13.900009 S

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 15.649994 S

(LSENS) READ DATA FOR NEXT CASE

Appendix E
Sensitivity Test Cases

In addition to the kinetics-only test cases described in appendix D we have prepared a set of nine kinetics-plus-sensitivity-analysis test cases. These example problems are also supplied with LSENS. The first six cases are constant-temperature problems whose results have been published in the literature. Results for cases 1 and 2 were also computed analytically. Excellent agreement between the LSENS and literature results was obtained for all cases. The last three cases are non-isothermal problems that illustrate the application of sensitivity analysis to combustion problems. As for the kinetics-only test cases, all sensitivity cases are set up in one file for execution in a single computer run. Cases 1, 2, 5, and 7 involve dummy species used in simple reactions. The thermodynamic data for these species are not read from the standard thermodynamic data file. Their coefficients are placed at the beginning of the problem data file. In this appendix we describe these cases. We then list the complete input file in table E.1. Cases 8 and 9 will be especially useful to users as models for their own sensitivity analysis computations.

Description of Test Cases

Case 1

Case 1 is the constant-volume isothermal reaction

$$A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} B$$

where k_1 and k_{-1}, the forward and reverse rate coefficients, are given separately by writing the two separate irreversible reactions $A \rightarrow B$ and $B \rightarrow A$. This case was first studied by Hwang (ref. 12) and was later used by Radhakrishnan (ref. 13) to compare sensitivity analysis methods. Note that in namelist PROB both the variables SENSTD and SENCAL are set equal to TRUE. This action tells LSENS to compute sensitivity coefficients for the time derivatives of the dependent variables as well as for the variables themselves. The variable ALLSP is used after the keyword INIT to obtain initial value sensitivities with respect to all species and after the keyword SENSVAR to obtain sensitivities for all species concentrations at each print station. In namelist SENRXN we have set ALLRXN equal to TRUE to obtain sensitivities with respect to all reactions. For this and all other isothermal reactions only the variable SENSAJ is set equal to TRUE for sensitivities with respect to the preexponential factors. Coefficients with respect to the temperature exponent and activation energy of any reaction will be the same as those for the preexponential factor.

Case 2

Case 2 is the constant-volume isothermal reaction $A \rightleftharpoons B \rightleftharpoons C$. Each forward and reverse reaction is written separately, so that the case has four reactions, $A \rightarrow B$, $B \rightarrow A$, $B \rightarrow C$, and $C \rightarrow B$. This test case was used by Hwang et al. (ref. 14). The keyword INIT does not appear in the sensitivity analysis data, and therefore no sensitivities with respect to initial conditions are computed.

Case 3

Case 3 is the constant-volume isothermal pyrolysis of ethane using the mechanism of Kramer et al. (ref. 15). This same case was also used by Dunker (ref. 16) and Radhakrishnan (refs. 13 and 17) to compare sensitivity analysis methods. The data require sensitivities for all species with respect to the initial ethane concentration and temperature and for all species with respect to the rate coefficients of reactions 1 and 2.

Case 4

Case 4 is the isothermal constant-volume ignition of a methane-oxygen-argon mixture containing trace concentra-

tions of carbon dioxide and hydrogen. The mechanism is that of Boni and Penner (ref. 18). Sensitivity coefficients for all species with respect to all reaction preexponential coefficients are required. Separate forward and reverse rate coefficients are given for the reversible reactions.

Case 5

Case 5 is the isothermal, constant-volume oxidation of formaldehyde using the mechanism of Dougherty et al. (ref. 19). In this case the variable TINY is set equal to 0.1 in namelist PROB to set equal to zero any sensitivity coefficients whose magnitudes are less than 0.1. Also, in namelist SENRXN the variable ORDER is set equal to TRUE in order to have a second type of table printed out for the sensitivity coefficients. The second table is organized by dependent variable, and for each one the coefficients are listed in order of decreasing magnitude. The rate-controlling reactions can then be seen at a glance. Note that the chemical mechanism has two reactions that simulate the destruction of species at the wall of the reaction chamber. These are $H_2O_2 \rightarrow H_2O_2W$ and $HO_2 \rightarrow HO_2W$, where the species on the right side of each reaction has the same thermodynamic properties as the species on the left side.

Case 6

Problem 6 is the isothermal, constant-volume oxidation of wet carbon monoxide. We use the mechanism of Yetter et al. (ref. 20). Sensitivity coefficients with respect to all rate parameters for concentrations of the two variables hydrogen and carbon monoxide are to be computed, as are sensitivities with respect to six initial concentrations. In namelist SENRXN we have set ORDER equal to TRUE and have also set the variable OUTPUT equal to FALSE. This suppresses the printing of the standard type of sensitivity-coefficient table. Only the table organized by dependent variable is printed.

Case 7

Case 7 is the first nonisothermal case, the constant-pressure, irreversible conversion of one reactant to one product with the rate coefficient expression

$$k = 1.0T$$

This test problem, first used by Radhakrishnan (refs. 13 and 17), can be solved analytically and so permits an objective evaluation of the accuracy of the code. Sensitivity coefficients of all dependent variables and their derivatives are required. This is done very simply by placing the one word ALL on the line after the keyword SENSVAR and setting the variable SENSTD equal to TRUE in namelist PROB. The word ALL is also placed after the keyword INIT to obtain sensitivity coefficients with respect to the initial values of all dependent variables. In namelist SENRXN we have set the variables SENSNJ and SENSEJ as well as SENSAJ equal to TRUE in order to obtain sensitivity coefficients with respect to all three rate coefficient parameters in this nonisothermal reaction.

Case 8

Case 8 is the constant-pressure static ignition of a stoichiometric hydrogen-air mixture seeded with 0.45 mol % nitric oxide to catalyze the low-initial-temperature (950.66 K) reaction. The mechanism is the same as that used for kinetics test case 2 and described in appendix D. Four reactions of carbon monoxide and carbon dioxide have also been added because the air contains a small amount of carbon dioxide. The latter reactions and rate coefficients are also taken from the kinetics test cases. The variable TINY is set to 1.0×10^{-7} in namelist PROB. Sensitivity coefficients are required for seven dependent variables, six species concentrations and temperature. Initial value sensitivities are required for eight variables. Note that this list is ended by inserting a blank line because there are exactly eight names written on the line following the keyword INIT. Rate coefficient sensitivities are to be computed for the six reactions whose numbers are listed in the array RXNUM in namelist SENRXN.

Case 9

Problem 9 is the constant-volume static ignition of a stoichiometric benzene-oxygen mixture that has been shock heated to an initial temperature of 1405 K. The chemical mechanism was developed by Bittker (ref. 21) to match a wide range of experimental ignition delay times and composition profile data reported for this fuel. Sensitivity coefficients for 10 dependent variables are required, including temperature, density, and pressure. Sensitivities with respect to the initial values of five variables, including temperature and density, will be computed as well as sensitivities to the rate parameters A_j and E_j for 24 reactions listed in the array RXNUM.

Listing of Results

The test case file in table E.1 was also executed on the Sun SPARCstation 1 that was used to execute the kinetics-only cases. Total execution time for the nine cases was approximately 139 s. Sample results are given in table E.2. Of course, these cases too will execute more rapidly on the newer workstations and mainframe computers.

TABLE E.1.—PROBLEM DATA FILE FOR SENSITIVITY ANALYSIS TEST CASES

```
CARD
   300.000  1000.000  5000.000
DUMA                L 5/66A  1.00 0.00 0.00 0.G   300.000  5000.000  1.0          1
 0.25161474E 01       0.00000000      0.00000000      0.00000000      0.00000000    2
     0.00000000       0.00000000 0.25161474E 01       0.00000000      0.00000000    3
     0.00000000       0.00000000      0.00000000      0.00000000      0.00000000    4
DUMB                L 5/66A  1.00 0.00 0.00 0.G   300.000  5000.000  1.0          1
 0.25161474E 01       0.00000000      0.00000000      0.00000000      0.00000000    2
     0.00000000       0.00000000 0.25161474E 01       0.00000000      0.00000000    3
     0.00000000       0.00000000      0.00000000      0.00000000      0.00000000    4
DUMC                L 5/66A  1.00 0.00 0.00 0.G   300.000  5000.000   1.0          1
 0.25161474E 01       0.00000000      0.00000000      0.00000000      0.00000000    2
     0.00000000       0.00000000 0.25161474E 01       0.00000000      0.00000000    3
     0.00000000       0.00000000      0.00000000 .    0.00000000      0.00000000    4
DUMP                L 5/66A  1.00 0.00 0.00 0.G   300.000  5000.000          1.0  1
 0.25161474E 01       0.00000000      0.00000000      0.00000000      0.00000000    2
-0.25161474E 04       0.00000000 0.25161474E 01       0.00000000      0.00000000    3
     0.00000000       0.00000000-0.25161474E 04       0.00000000      0.00000000    4
DUMR                L 5/66A  1.00 0.00 0.00 0.G   300.000  5000.000   1.0          1
 0.25161474E 01       0.00000000      0.00000000      0.00000000      0.00000000    2
     0.00000000       0.00000000 0.25161474E 01       0.00000000      0.00000000    3
     0.00000000       0.00000000      0.00000000      0.00000000      0.00000000    4
HO2W                J 9/78H  1.O  2.   0.   0.G   300.000  5000.000     33.00669 1
 0.40173060E 01 0.22175883E-02-0.57710171E-06 0.71372882E-10-0.36458591E-14    2
-0.11412445E 04 0.37846051E 01 0.35964102E 01 0.52500748E-03 0.75118344E-05    3
-0.95674952E-08 0.36597628E-11-0.89333502E 03 0.66372671E 01      0.00000000    4
H2O2W               L 3/85H  2.O  2.   0.   0.G   300.000  5000.000     34.01460 1
 0.47928858E 01 0.36300865E-02-0.11136435E-05 0.14868513E-09-0.68958511E-14    2
-0.18132195E 05-0.51306415E 00 0.34546633E 01 0.55575930E-02 0.92103738E-06    3
-0.46279780E-08 0.21458200E-11-0.17672328E 05 0.68402452E 01-0.16394994E 05    4
SPECA               L 5/66A  1.00 0.00 0.00 0.G   300.000  5000.000 0.999001E-03 1
 0.25161474E 01       0.00000000      0.00000000      0.00000000      0.00000000    2
     0.00000000       0.00000000 0.25161474E 01       0.00000000      0.00000000    3
     0.00000000       0.00000000      0.00000000      0.00000000      0.00000000    4
SPECB               L 5/66A  1.00 0.00 0.00 0.G   300.000  5000.000 0.999001E-03 1
 0.25161474E 01       0.00000000      0.00000000      0.00000000      0.00000000    2
     0.00000000       0.00000000 0.25161474E 01       0.00000000      0.00000000    3
     0.00000000       0.00000000      0.00000000      0.00000000      0.00000000    4
END
SIMPLE TEST CASE A=B: HWANG, JT, PROC. NSC TAIWAN, PART B, V6, P37, 1982. CASE 1
   SPECA                 >   SPECB                    1.00E+03
   SPECB                 >   SPECA                    1.00E+00


TIME
 &prob  rhocon=.true., tcon=.true., sencal=.true., senstd=.true.,
   print=1.5E-04,1.0E-03,2.0E-02,  &end
 &start p=1.0, t=300.0,   &end
SPECA      0.999001
SPECB      0.000999
END
 &solver  emax=1.0E-06, atolsp=0.0,   &end
INIT
ALLSP      END
SENSVAR
ALLSP      END
REAC
 &senrxn  sensaj=.true.,  allrxn=.true.,  &end
FINIS
SIMPLE TEST CASE A=B=C: HWANG ET AL, J. CHEM PHYS, V69, P5180, 1978.      CASE 2
NEW
                DUMA      >   DUMB                    1.0
                DUMB      >   DUMA                    100.0
                DUMB      >   DUMC                    100.0
                DUMC      >   DUMB                    1.0


TIME
 &prob   rhocon=.true., tcon=.true., sencal=.true.,
   print= 0.1, 2.5, 4.5,  &end
 &start t=300.0, p=1.0,   &end
DUMA       1.00
END
 &solver  emax=1.0E-6, atolsp=1.0E-8,  &end
SENSVAR
ALLSP      END
REAC
 &senrxn allrxn=.true., sensaj=.true.,    &end
FINIS
```

TABLE E.1.—Continued.

```
ETHANE PYROLYSIS: KRAMER ET AL, APPL MATH MODELLING, V5, P432, 1981.    CASE 3
NEW
                C2H6      >2.0CH3                        1.20E+12   0.0       59218.0
   C2H6     +   CH3       >   C2H5     +   CH4           8.01E+08   0.0       11943.0
                C2H5      >   C2H4     +   H             3.00E+11   0.0       34974.0
   H        +   C2H6      >   C2H5     +   H2            1.30E+11   0.0       8982.0
   H        +   H         >   H2                         6.99E+13   0.0       0.0


TIME
 &prob  rhocon=.true., tcon=.true., sencal=.true.,
   print=  1.0,  20.0,   &end
 &start   p=0.4507,  t=923.0,  &end
C2H6        1.0
END
 &solver  emax=1.0E-6, atolsp=1.0E-8,   &end
INIT
C2H6      TEMP      END
SENSVAR
ALLSP     END
REAC
 &senrxn  sensaj=.true., rxnum = 1.0, 2.0,   &end
FINIS
CH4-O2-AR SHOCK IGNITION: BONI & PENNER, COMB SCI & TECH, V15, P99, 1977. CASE 4
NEW
   M        +   CH4       >   CH3      +   H             4.337E+07   0.0       0.0
   H        +   CH3       >   CH4      +   M             1.106E+17   0.0       0.0
   OH       +   CH4       >   CH3      +   H2O           2.590E+13   0.0       0.0
   CH3      +   H2O       >   OH       +   CH4           1.048E+11   0.0       0.0
   H        +   CH4       >   CH3      +   H2            1.988E+13   0.0       0.0
   CH3      +   H2        >   H        +   CH4           8.071E+11   0.0       0.0
   O        +   CH4       >   CH3      +   OH            2.168E+12   0.0       0.0
   CH3      +   OH        >   O        +   CH4           6.625E+10   0.0       0.0
   CH3      +   O         >   CH2O     +   H               1.0E+14   0.0       0.0
   CH2O     +   H         >   CH3      +   O               5.3E+07   0.0       0.0
   CH3      +   O2        >   CH2O     +   OH              2.0E+10   0.0       0.0
   CH2O     +   OH        >   CH3      +   O2            4.337E+04   0.0       0.0
   CH2O     +   O         >   HCO      +   OH            1.584E+13   0.0       0.0
   HCO      +   OH        >   CH2O     +   O             9.035E+09   0.0       0.0
   CH2O     +   OH        >   HCO      +   H2O           1.108E+14   0.0       0.0
   HCO      +   H2O       >   CH2O     +   OH            8.553E+09   0.0       0.0
   CH2O     +   H         >   HCO      +   H2            5.240E+12   0.0       0.0
   HCO      +   H2        >   CH2O     +   H             4.216E+09   0.0       0.0
   M        +   CH2O      >   HCO      +   H             3.843E+08   0.0       0.0
   HCO      +   H         >   CH2O     +   M             1.959E+16   0.0       0.0
   HCO      +   O         >   CO       +   OH              1.0E+14   0.0       0.0
   CO       +   OH        >   HCO      +   O             1.144E+05   0.0       0.0
   HCO      +   OH        >   CO       +   H2O             1.0E+14   0.0       0.0
   CO       +   H2O       >   HCO      +   OH            1.265E+04   0.0       0.0
   HCO      +   H         >   CO       +   H2              2.0E+14   0.0       0.0
   CO       +   H2        >   HCO      +   H             2.771E+05   0.0       0.0
   M        +   HCO       >   H        +   CO            4.216E+10   0.0       0.0
   H        +   CO        >   HCO      +   M             3.628E+12   0.0       0.0
   CO       +   OH        >   CO2      +   H             5.360E+11   0.0       0.0
   CO2      +   H         >   CO       +   OH            2.289E+11   0.0       0.0
   H2       +   OH        >   H2O      +   H             1.807E+13   0.0       0.0
   H2O      +   H         >   H2       +   OH            1.807E+12   0.0       0.0
   O        +   H2        >   OH       +   H             7.228E+12   0.0       0.0
   OH       +   H         >   O        +   H2            6.625E+12   0.0       0.0
   H        +   O2        >   OH       +   O             3.216E+12   0.0       0.0
   OH       +   O         >   H        +   O2            1.385E+13   0.0       0.0
   H        +   OH        >   H2O      +   M             2.104E+15   0.0       0.0
   THIRDBODY
H2O       16.7      END
   M        +   H2O       >   H        +   OH            3.096E+03   0.0       0.0
   THIRDBODY
H2O       16.7      END
   H        +   HO2       >2.0OH                         1.554E+14   0.0       0.0
             2.0OH       >   H        +   HO2           6.023E+08   0.0       0.0
   H        +   O2        >   HO2      +   M             1.930E+15   0.0       0.0
   M        +   HO2       >   H        +   O2            2.168E+10   0.0       0.0
   OH       +   OH        >   O        +   H2O           9.456E+12   0.0       0.0
   O        +   H2O       >   OH       +   OH            1.205E+12   0.0       0.0

AR
TIME
 &prob    rhocon=.true., tcon=.true., sencal=.true., print= 2.5E-5,
     &end
 &start  t=2000.0, p=6.729, &end
CH4       0.09172
O2        0.18344
AR        0.72484
```

TABLE E.1.—Continued.

```
CO2             4.0494E-20
H2              4.0494E-20
END
 &solver  mf=21, emax=1.0E-3, atolsp=1.0E-12,   &end
SENSVAR
ALLSP     END
REAC
 &senrxn   sensaj=.true., allrxn=.true.,   &end
FINIS
FORMALDEHYDE OXID.: DOUGHERTY ET AL, J. CHEM PHYS, V71, P1794, 1979.      CASE 5
NEW
   HCO      +   O2       >   CO       +   HO2          6.02E+10   0.        0.
   HO2      +   CH2O     >   H2O2     +   HCO          3.43E+10   0.        0.
   M        +   H2O2     >2.0OH                       4.01E+06   0.        0.
   CH2O     +   OH       >   HCO      +   H2O          9.64E+13   0.        0.
   OH       +   H2O2     >   H2O      +   HO2          3.07E+12   0.        0.
                H2O2     >   H2O2W                      1.05E+2   0.        0.
                HO2      >   HO2W                       1.05E+1   0.        0.
   HO2      +   HO2      >   H2O2     +   O2           1.81E+12   0.        0.
   CO       +   OH       >   CO2      +   H            1.99E+11   0.        0.
   CO       +   HO2      >   CO2      +   OH           7.23E+08   0.        0.
   CH2O     +   H        >   HCO      +   H2           1.63E+12   0.        0.
   H        +   O2       >   OH       +   O            3.32E+10   0.        0.
   H        +   O2       >   HO2      +   M            3.63E+15   0.        0.
   M        +   HO2      >   H        +   O2           2.83E+05   0.        0.
   O        +   H2       >   OH       +   H            1.82E+11   0.        0.
   CH2O     +   O        >   HCO      +   OH           6.02E+13   0.        0.
   H        +   H2O2     >   HO2      +   H2           7.83E+11   0.        0.
   H        +   H2O2     >   H2O      +   OH           3.55E+12   0.        0.
   O        +   H2O2     >   OH       +   HO2          6.02E+10   0.        0.
                HCO      >   H        +   CO           4.60E-12   0.        0.
   H2       +   OH       >   H2O      +   H            6.02E+12   0.        0.
   CH2O     +   O2       >   HCO      +   HO2          1.75E+04   0.        0.
   H        +   HO2      >2.0OH                       3.01E+12   0.        0.
   HO2      +   H        >   H2O      +   O            3.01E+13   0.        0.
   H        +   HO2      >   H2       +   O2           2,71E+13   0.        0.

N2
TIME
 &prob  rhocon=.true., tcon=.true., sencal=.true., tiny=0.1,
   print= 1.0E-06,5.0E-03,  &end
 &start t=952.0, p=0.918066,   &end
CH2O       0.009564
CO         0.399833
O2         0.179453
N2         0.411150
END
 &solver  emax=1.0E-06, atolsp=1.0E-08,  &end
SENSVAR
ALLSP     END
REAC
 &senrxn  allrxn=.true., sensaj=.true., order=.true.,  &end
FINIS
 WET CO OXIDATION: YETTER ET AL, COMB & FLAME, V59, P107, 1985.          CASE 6
NEW
   HCO      +   H        >   CO       +   H2            2.0E+14   0.        0.
   CO       +   H2       >   HCO      +   H            1.716E-3   0.        0.
   HCO      +   OH       >   CO       +   H2O           1.0E+14   0.        0.
   CO       +   H2O      >   HCO      +   OH          3.656E-06   0.        0.
   HCO      +   O        >   CO       +   OH          3.012E+13   0.        0.
   CO       +   OH       >   O        +   HCO         2.867E-04   0.        0.
   HCO      +   O2       >   CO       +   HO2         3.015E+12   0.        0.
   CO       +   HO2      >   HCO      +   O2          2.590E+06   0.        0.
   CO       +   HO2      >   CO2      +   OH          3.084E+09   0.        0.
   CO2      +   OH       >   CO       +   HO2         1.777E-02   0.        0.0
   CO       +   OH       >   CO2      +   H           1.921E+11   0.        0.
   CO2      +   H        >   CO       +   OH          7.890E+08   0.0       0.0
   CO2      +   O        >   CO       +   O2          4.434E+02   0.        0.
   CO       +   O2       >   CO2      +   O           8.492E+02   0.        0.0
   H        +   O2       >   OH       +   O           1.126E+11   0.        0.
   OH       +   O        >   H        +   O2          1.385E+13   0.        0.0
   O        +   H2       >   OH       +   H           3.385E+11   0.        0.
   OH       +   H        >   O        +   H2          3.831E+11   0.0       0.0
   O        +   H2O      >   OH       +   OH          1.650E+10   0.        0.
   OH       +   OH       >   O        +   H2O         4.108E+12   0.        0.0
   H2O      +   H        >   OH       +   H2          7.709E+09   0.        0.
   OH       +   H2       >   H2O      +   H           1.837E+12   0.        0.0
   OH       +   H2O2     >   H2O      +   HO2         3.632E+12   0.        0.
   H2O      +   HO2      >   OH       +   H2O2        7.107E+06   0.        0.0
   O        +   HO2      >   OH       +   O2          2.168E+13   0.        0.
   OH       +   O2       >   O        +   HO2         2.475E+02   0.        0.0
   H        +   HO2      >2.0OH                       1.126E+14   0.        0.0
```

TABLE E.1.—Continued.

```
   OH      +   OH      >   H       +   HO2       1.385E+05   0.        0.0
   H       +   HO2     >   H2      +   O2        2.506E+13   0.        0.0
   H2      +   O2      >   H       +   HO2       2.487E+02   0.        0.0
   HO2     +   OH      >   H2O     +   O2        1.313E+13   0.        0.0
   H2O     +   O2      >   HO2     +   OH        5.529E-01   0.        0.0
   O2      +   H2O2    >2.0HO2                   1.349E+05   0.        0.0
   HO2     +   HO2     >   O2      +   H2O2      6.324E+12   0.        0.0
   HO2     +   H2      >   H2O2    +   H         1.403E+08   0.        0.
   H2O2    +   H       >   HO2     +   H2        3.054E+11   0.        0.0
   M       +   O2      >   O       +   O         2.030E-08   0.        0.
   O       +   O       >   O2      +   M         1.861E+14   0.        0.0
   M       +   H2      >   H       +   H         1.850E-05   0.        0.
   H       +   H       >   H2      +   M         3.000E+15   0.        0.0
   M       +   OH      >   O       +   H         1.807E-04   0.        0.
   O       +   H       >   OH      +   M         1.001E+16   0.        0.0
   M       +   H2O2    >2.0OH                    1.090E+08   0.        0.
   OH      +   OH      >   H2O2    +   M         9.251E+15   0.        0.0
   M       +   H2O     >   H       +   OH        3.012E-05   0.0       0.
   H       +   OH      >   H2O     +   M         1.157E+17   0.0       0.0
   M       +   HO2     >   H       +   O2        1.753E+06   0.        0.
   H       +   O2      >   HO2     +   M         2.605E+15   0.        0.0
   M       +   CO2     >   CO      +   O         3.234E-08   0.        0.
   CO      +   O       >   CO2     +   M         9.069E+14   0.0       0.0
   M       +   HCO     >   H       +   CO        2.777E+10    0.       0.
   H       +   CO      >   HCO     +   M         3.210E+14    0.       0.0

N2
TIME
 &prob  rhocon=.true., tcon=.true., sencal=.true.,
   print=1.0E-4,1.0E-1,1.0E2,  &end
 &start t=1100.0, p=1.0,  &end
CO        0.002
H2O       0.01
O2        0.028
N2        0.96
END
 &solver   emax=1.0E-3, atolsp=1.0E-12,  &end
SENSVAR
CO        H2
END
INIT
HCO       H         OH        O         HO2       H2O2      END
REAC
 &senrxn  sensaj=.true.,  allrxn=.true., output=.false., order=.true.,
  &end
FINIS
   SIMPLE NONISOTHERMAL TEST CASE  R>P                                  CASE 7
NEW
               DUMR     >   DUMP                        1.0   1.0       0.0


TIME      PRESSURE
 &prob   pcon=.true., sencal=.true., senstd=.true.,
   print=1.0E-06,1.0E-04,1.0E-02,   &end
 &start t=1000.0, p=1.0,   &end
DUMR      1.00
END
 &solver  emax=1.0E-3, atolsp=1.0E-12, &end
INIT
ALL       END
SENSVAR
ALL       END
REAC
 &senrxn  sensaj=.true., sensnj=.true., sensej=.true., allrxn=.true.,
  &end
FINIS
  HYDROGEN COMBUSTION IN STANDARD AIR AT 3.10 ATM.                      CASE 8
NEW
   CO      +   O       =   CO2     +   M         5.888E+15   0.        4100.
   CO      +   O2      =   CO2     +   O         2.512E+12   0.        47690.
   CO      +   OH      =   CO2     +   H         4.169E+11   0.         1000.
   CO      +   HO2     =   CO2     +   OH        5.754E+13   0.        22930.
   O       +   H2O     =   OH      +   OH          6.8E+13   0.0       18365.
   H       +   O2      =   OH      +   O          1.89E+14   0.        16400.
   O       +   H2      =   OH      +   H          4.20E+14   0.        13750.
   H       +   HO2     =   H2      +   O2         7.28E+13   0.        2126.
   O       +   HO2     =   OH      +   O2          5.0E+13   0.        1000.
   HO2     +   OH      =   H2O     +   O2          8.0E+12   0.           0.
   H       +   HO2     =2.0OH                    1.34E+14   0.        1070.
   H2      +   HO2     =   H2O2    +   H         7.91E+13   0.        25000.
   OH      +   H2O2    =   H2O     +   HO2         6.1E+12   0.        1430.
   HO2     +   HO2     =   H2O2    +   O2          1.8E+12   0.         0.
```

TABLE E.1.—Continued.

```
   H        +   H2O2      =   OH       +   H2O          7.8E+11   0.          0.
   M        +   H2O2      =2.0OH                       1.44E+17   0.         45510.
   THIRDBODY
H2          2.30    O2          .78      H2O          6.0    H2O2          6.6
END
   H2       +   OH        =   H2O      +   H           4.74E+13   0.         6098.
   H        +   O2        =   HO2      +   M           1.46E+15   0.         -1000.
   THIRDBODY
O2          1.30    N2          1.3      H2O          21.3   H2            5.0
END
   M        +   H2O       =   H        +   OH          1.30E+15   0.         105140.
   THIRDBODY
H2          4.00    O2          1.5      H2O          20.0   N2            1.5
END
   H        +   O         =   OH       +   M            7.1E+18   -1.         0.
   M        +   H2        =   H        +   H            2.2E+14   0.          96000.
   THIRDBODY
H2          4.10    O2          2.0      H2O          15.0   N2            2.0
END
   M        +   O2        =   O        +   O           1.80E+18   -1.         118020.
   HO2      +   NO        =   NO2      +   OH          2.09E+12   0.0         -477.
   O        +   NO2       =   NO       +   O2           1.0E+13   0.0         596.
   NO       +   O         =   NO2      +   M           5.62E+15   0.          -1160.
   NO2      +   H         =   NO       +   OH          3.47E+14   0.           1470.
   NO       +   O         =   N        +   O2            3.8E+9   1.0         41370.
   O        +   N2        =   NO       +   N            1.8E+14   0.          76250.
   NO       +   H         =   N        +   OH          2.63E+14   0.          50410.
   M        +   N2O       =   N2       +   O           6.92E+23   -2.5        65000.
   O        +   N2O       =   N2       +   O2           1.0E+14   0.          28020.
   O        +   N2O       =2.0NO                       6.92E+13   0.          26630.
   N        +   NO2       =2.0NO                        4.0E+12   0.          0.0
   N2O      +   H         =   N2       +   OH          7.59E+13   0.          15100.
   NO2      +   H2        =   HNO2     +   H            2.4E+13   0.          29000.
   OH       +   NO2       =   HNO3     +   M            3.0E+15   0.          -3800.
   THIRDBODY
O2          0.70    H2          1.4      END
   OH       +   NO        =   HNO2     +   M            5.6E+15   0.          -1700.
   HNO      +   H         =   H2       +   NO           5.0E+12   0.          0.
   H        +   NO        =   HNO      +   M            5.4E+15   0.          -600.
   HNO      +   OH        =   H2O      +   NO           3.6E+13   0.          0.

AR
TIME      PRESSURE
 &prob sencal=.true., tiny=1.0E-7,
   print= 1.0E-4, 1.8E-4, 2.0E-4, ct0=3.1,    &end
 &start   t= 950.66,    &end
H2          0.2952726
O2          0.1476404
CO2              2.1140E-4
N2          0.5458075
NO          0.0045
AR               6.5681E-3
END
 &solver  emax= 1.0E-4,  atolsp= 1.0E-13,    &end
INIT
CO        H2        O2        HO2       H2O2      NO        TEMP      DENSITY

REAC
 &senrxn  sensaj=.true.,  sensej=.true., output=.false., order=.true.,
  rxnum=5.0,6.0,8.0,11.0,17.0,18.0,  &end
SENSVAR
CO        CO2       OH        H2O       H2        NO        TEMP      END
FINIS
  BENZENE-OXYGEN-AR SHOCK IGNITION - WITH SENSITIVITY  MECHANISM K-70   CASE 9
NEW
   C6H6     +   O2        =   C6H5O    +   OH           4.0E+13   0.          34000.
   C6H6     +   C6H5      =   C12H10   +   H            4.0E+11   0.          4000.
                C6H6      =   C6H5     +   H            1.0E+16   0.          108000.
   C6H6     +   H         =   C6H5     +   H2           2.5E+14   0.          16000.
   C6H6     +   O         =   C6H5O    +   H          2.783E+13   0.          4910.
   C6H6     +   OH        =   C6H5     +   H2O        2.132E+13   0.          4580.
   M        +   C4H3      =   C4H2     +   H            1.0E+16   0.0         60000.
                C6H5O     =   C5H5     +   CO          2.51E+11   0.          43900.
   C6H5     +   O2        =   C6H5O    +   O            2.1E+12   0.           7470.
   C6H5     +   HO2       =   C6H5O    +   OH           2.0E+13   0.          1000.
                C6H5      =   C4H3     +   C2H2        4.50E+13   0.          72530.
                C6H5OH    =   C6H5O    +   H           2.00E+16   0.          88000.
   C6H5OH   +   H         =   C6H6     +   OH          2.20E+13   0.           7910.
   C6H5OH   +   H         =   C6H5O    +   H2          1.15E+14   0.          12405.
   C5H5     +   C6H5OH    =   C6H5O    +   C5H6        2.67E+14   0.          25227.
                C5H6      =   C5H5     +   H           8.13E+24   -2.981       78682.
   C5H6     +   O2        =   C5H5O    +   OH           1.0E+13   0.          20712.
```

TABLE E.1.—Continued.

C6H5OH	+	OH	=	C6H5O	+	H2O	3.0E+13	0.	0.
C6H5OH	+	HO2	=	C6H5O	+	H2O2	3.0E+13	0.	1500.
		C5H5O	=	C4H5	+	CO	3.0E+16	0.	15000.
C5H5	+	O	=	C5H5O			1.0E+13	0.	0.
C5H5	+	OH	=	C5H4OH	+	H	1.0E+13	0.	0.
		C5H4OH	=	C4H4	+	HCO	1.0E+15	0.	22000.
C5H5	+	HO2	=	C5H5O	+	OH	2.0E+13	0.	0.
		2.0C6H5	=	C12H10			3.1E+12	0.	0.
		C4H5	=	C2H3	+	C2H2	1.4E+13	0.	32900.
C4H2	+	O	=	C2HO	+	C2H	1.0E+13	0.	0.
C4H2	+	OH	=	HCO	+	C3H2	3.0E+13	0.	0.
C4H2	+	O	=	CO	+	C3H2	1.2E+12	0.	0.
M	+	C2H4	=	C2H2	+	H2	9.33E+16	0.	77200.
C2H4	+	OH	=	C2H3	+	H2O	4.786E+12	0.	1230.
C2H4	+	O	=	CH3	+	HCO	3.311E+12	0.	1130.
C2H4	+	O	=	CH2O	+	CH2	2.512E+13	0.	5000.
C2H4	+	OH	=	CH3	+	CH2O	1.995E+12	0.	960.
M	+	C2H3	=	C2H2	+	H	3.0E+15	0.	32000.
C2H3	+	O2	=	CH2O	+	HCO	3.98E+12	0.	-250.
C2H3	+	H	=	C2H2	+	H2	6.0E+12	0.	0.
C2H3	+	OH	=	C2H2	+	H2O	5.012E+12	0.	0.
C2H3	+	CH2	=	C2H2	+	CH3	3.020E+13	0.	0.
C2H3	+	C2H	=2.0C2H2				3.020E+13	0.	0.
C2H3	+	O	=	C2H2O	+	H	3.3E+13	0.	0.
CH2	+	CH2	=	C2H2	+	H2	4.0E+13	0.	0.
CH2	+	CH2	=	C2H3	+	H	5.012E+12	0.	0.
CH2	+	OH	=	CH	+	H2O	2.51E+11	.67	25700.
CH2	+	O	=	CH	+	OH	2.0E+11	.68	25000.
CH2	+	O2	=	CO2	+2.0H		1.59E+12	0.	1000.
M	+	C2H2	=	C2H	+	H	4.169E+16	0.	107000.
C2H2	+	C2H2	=	C4H3	+	H	2.0E+12	0.	45900.
C2H2	+	O	=	CH2	+	CO	1.6E+14	0.0	9890.
C2H2	+	O	=	C2HO	+	H	4.0E+14	0.0	10660.
C2H2	+	OH	=	C2H	+	H2O	6.310E+12	0.	7000.
C2H2	+	OH	=	C2H2O	+	H	3.2E+11	0.	200.
C2H2	+	C2H	=	C4H2	+	H	3.0E+13	0.	0.
C2H2	+	CH2	=	C3H3	+	H	1.2E+13	0.	6600.
M	+	C3H4	=	C3H3	+	H	2.0E+17	0.	65000.
C2H2O	+	OH	=	CH2O	+	HCO	2.8E+13	0.	0.
C2H2O	+	OH	=	C2HO	+	H2O	7.5E+12	0.	3000.
C2H2O	+	H	=	CH3	+	CO	1.13E+13	0.	3428.
C2H2O	+	H	=	C2HO	+	H2	7.5E+13	0.	8000.
C2H2O	+	O	=	C2HO	+	OH	5.0E+13	0.	8000.
C2H2O	+	O	=	CH2O	+	CO	2.0E+13	0.	0.
M	+	C2H2O	=	CH2	+	CO	2.0E+16	0.	60000.
C2HO	+	O2	=2.0CO		+	OH	1.46E+12	0.	2500.
C2HO	+	O	=2.0CO		+	H	1.202E+12	0.	0.
C2HO	+	OH	=2.0HCO				1.0E+13	0.	0.
C2HO	+	H	=	CH2	+	CO	5.0E+13	0.	0.
C2HO	+	CH2	=	C2H3	+	CO	3.0E+13	0.	0.
C2HO	+	CH2	=	CH2O	+	C2H	1.0E+13	0.	2000.
		2.0C2HO	=	C2H2	+2.0CO		1.0E+13	0.	0.
C2H	+	OH	=	C2HO	+	H	2.0E+13	0.	0.
C2H	+	O2	=	C2HO	+	O	5.00E+13	0.	1500.
C2H	+	O	=	CO	+	CH	5.012E+13	0.	0.
M	+	CH4	=	CH3	+	H	2.0E+17	0.	88000.
CH4	+	O2	=	CH3	+	HO2	7.943E+13	0.	56000.
CH4	+	H	=	CH3	+	H2	1.26E+14	0.	11900.
OH	+	CH4	=	CH3	+	H2O	2.5E+13	0.	5010.
O	+	CH4	=	CH3	+	OH	1.9E+14	0.	11720.
CH3	+	O2	=	CH3O	+	O	4.786E+13	0.	29000.
CH3	+	OH	=	CH3O	+	H	6.3E+12	0.	0.
M	+	CH3O	=	CH2O	+	H	5.0E+13	0.	21000.
CH3O	+	O2	=	CH2O	+	HO2	1.0E+12	0.	6000.
CH3O	+	H	=	CH2O	+	H2	2.0E+13	0.	0.
CH3	+	CH3	=	C2H4	+	H2	1.0E+16	0.	32000.
CH3	+	O	=	CH2O	+	H	1.288E+14	0.	2000.
CH3	+	CH2O	=	CH4	+	HCO	1.0E+10	0.5	6000.
CH3	+	HCO	=	CH4	+	CO	3.020E+11	.5	0.
CH3	+	HO2	=	CH3O	+	OH	2.00E+13	0.	0.
M	+	CH2O	=	HCO	+	H	5.0E+16	0.	81000.
CH2O	+	OH	=	HCO	+	H2O	3.0E+13	0.	1200.
CH2O	+	H	=	HCO	+	H2	2.5E+13	0.	3990.
CH2O	+	O	=	HCO	+	OH	3.5E+13	0.	3510.
HCO	+	HO2	=	CH2O	+	O2	1.0E+14	0.	3000.
M	+	HCO	=	H	+	CO	2.94E+14	0.	15569.
HCO	+	O2	=	CO	+	HO2	3.311E+12	0.	7000.
HCO	+	OH	=	CO	+	H2O	1.0E+14	0.	0.
HCO	+	H	=	CO	+	H2	1.995E+14	0.	0.
HCO	+	O	=	CO	+	OH	1.0E+14	0.	0.
CH	+	O2	=	HCO	+	O	1.0E+13	0.	0.
CO	+	O	=	CO2	+	M	5.9E+15	0.	4100.

TABLE E.1.—Concluded.

```
   CO       +   O2       =   CO2      +   O          2.5E+12   0.        47690.
   CO       +   OH       =   CO2      +   H         4.17E+11   0.         1000.
   CO       +   HO2      =   CO2      +   OH        5.75E+13   0.        22930.
   O        +   H2O      =   OH       +   OH         6.8E+13    0.       18365.
   H        +   O2       =   OH       +   O         1.89E+14   0.        16400.
   O        +   H2       =   OH       +   H         4.20E+14   0.        13750.
   H        +   HO2      =   H2       +   O2        7.28E+13   0.        2126.
   O        +   HO2      =   OH       +   O2         5.0E+13   0.        1000.
   HO2      +   OH       =   H2O      +   O2         8.0E+12               0.
   H        +   HO2      =2.0OH                     1.34E+14   0.        1070.
   H2       +   HO2      =   H2O2     +   H         7.91E+13   0.        25000.
   OH       +   H2O2     =   H2O      +   HO2        6.1E+12   0.        1430.
   HO2      +   HO2      =   H2O2     +   O2         1.8E+12   0.         0.
   H        +   H2O2     =   OH       +   H2O        7.8E+11   0.         0.
   M        +   H2O2     =   OH       +   OH        1.44E+17   0.        45510.
   THIRDBODY
H2          2.30    O2          .78     H2O         6.0    H2O2         6.6
END
   H2       +   OH       =   H2O      +   H         4.74E+13   0.        6098.
   H        +   O2       =   HO2      +   M         1.46E+15   0.        -1000.
   THIRDBODY
O2          1.30    CO2         7.0     H2O         21.3   H2           3.0
C6H6        20.0    CH4         5.0     END
   M        +   H2O      =   H        +   OH        1.30E+15   0.        105140.
   THIRDBODY
H2          4.00    O2          1.5     H2O         20.0   C6H6        20.0
CO2         4.00    END
   H        +   O        =   OH       +   M          7.1E+18   -1.        0.
   M        +   H2       =   H        +   H          2.2E+14   0.         96000.
   THIRDBODY
H2          4.10    O2          2.0     H2O         15.0   END
   M        +   O2       =   O        +   O         1.80E+18   -1.       118020.

AR
TIME
 &prob    iprint=50,  rhocon =.true., sencal=.true., tiny=1.0E-7,
   end=3.07E-4,  &end
 &start  t= 1405.0,  p=2.3868,       &end
C6H6       0.01690
O2         0.12582
AR         0.85728
END
 &solver  emax= 1.0E-4,  atolsp= 1.0E-13,   &end
SENSVAR
C6H6      C6H5      H2O       CO        C2H2      C6H5OH    C5H6      TEMP
DENSITY   PRESSURE  END
INIT
C6H6      OH        AR        TEMP      DENSITY   END
REAC
 &senrxn  sensaj=.true., sensej=.true.,
  rxnum=1.0,2.0,3.0,4.0,5.0,6.0,7.0,8.0,10.0,11.0,12.0,13.0,
   14.0,15.0,16.0,17.0,18.0,19.0,20.0,21.0,101.0,104.0,116.0,  &end
FINIS
```

TABLE E.2.—SELECTED SENSITIVITY TEST CASE RESULTS

(a) Case 1

```
                                    **  DATA LINES  **
                 1         2         3         4         5         6         7         8
CC  12345678901234567890123456789012345678901234567890123456789012345678901234567890

    SIMPLE TEST CASE A=B: HWANG, JT, PROC. NSC TAIWAN, PART B, V6, P37, 1982. CASE 1
       SPECA                  >   SPECB                    1.00E+03
       SPECB                  >   SPECA                    1.00E+00
                                    -  BLANK LINE  -
                                    -  BLANK LINE  -
    TIME
     &prob  rhocon=.true., tcon=.true., sencal=.true., senstd=.true.,
       print=1.5E-04,1.0E-03,2.0E-02,  &end
     &start p=1.0, t=300.0,   &end
    SPECA      0.999001
    SPECB      0.000999
    END
     &solver  emax=1.0E-06, atolsp=0.0,   &end
    INIT
    ALLSP      END
    SENSVAR
    ALLSP      END
    REAC
     &senrxn  sensaj=.true.,  allrxn=.true.,  &end
    FINIS
```

```
*** THE FOLLOWING  1 ELEMENTS CONSIDERED FOR THIS PROBLEM ***

     A


*** THE FOLLOWING  2 REACTING SPECIES CONSIDERED FOR THIS PROBLEM ***

     SPECA     SPECB

*** NO INERT SPECIES CONSIDERED FOR THIS PROBLEM ***



                *** THERMODYNAMIC DATA, MOLECULAR WEIGHT AND HEAT OF FORMATION AT 25 C ***


 SPECA              MWT =       0.00099900          H(25 C) =    1.4907E+03 CAL/MOLE
0.25161474E+01   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00
0.25161474E+01   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00

 SPECB              MWT =       0.00099900          H(25 C) =    1.4907E+03 CAL/MOLE
0.25161474E+01   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00
0.25161474E+01   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00



                         LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM        NASA LEWIS RESEARCH CENTER

              SIMPLE TEST CASE A=B: HWANG, JT, PROC. NSC TAIWAN, PART B, V6, P37, 1982. CASE 1

REACTION                                                                  REACTION RATE VARIABLES
 NUMBER                                                                     A                N          ACTIVATION
                                                                                                          ENERGY
   1                    1*SPECA     >    1*SPECB                          1.00000E+03        0.0000          0.00
   2                    1*SPECB     >    1*SPECA                          1.00000E+00        0.0000          0.00
```

TABLE E.2.—Continued.
(a) Continued.

```
** NEW INPUT DATA GIVEN IN CGS  UNITS  **                    **  OUTPUT REQUIRED IN CGS  UNITS  **

                    ** ASSIGNED VARIABLE PROFILE **

THIS IS A CONSTANT DENSITY PROBLEM - AN ASSIGNED VARIABLE IS NOT REQUIRED

THE TEMPERATURE WILL BE HELD CONSTANT FOR THIS CASE

NUMBER OF REACTING SPECIES:    2
   NUMBER OF INERT SPECIES:    0

NUMBER OF SPECIES ODE'S REQUIRED FOR THIS CASE:    2
  TOTAL NUMBER OF ODE'S REQUIRED FOR THIS CASE:    2

                    INTEGRATION CONTROLS
INTEGRATION METHOD (MF):  21        MAXIMUM RELATIVE ERROR:    1.00000E-06        SPECIES ABSOLUTE ERROR:    0.00000E+00

MAXIMUM NUMBER OF STEPS ALLOWED FOR THE COMPLETE PROBLEM:  2000

                    **** SENSITIVITY ANALYSIS REQUIRED ****

                    *** SENSITIVITY OF FOLLOWING   2 VARIABLES WILL BE CALCULATED ***
SPECA     SPECB

                    *** SENSITIVITY WRT INITIAL VALUES OF FOLLOWING   2 VARIABLES REQUIRED ***
SPECA     SPECB

*** CONSTANT TEMPERATURE CASE SO SENSITIVITY COEFFICIENTS WRT ONLY PREEXPONENTIAL FACTORS WILL BE CALCULATED ***
                    NORMALIZATION FACTOR FOR AJ = AJ

                    ** SENSITIVITY COEFFICIENTS WRT RATE CONSTANT PARAMETERS REQUIRED FOR FOLLOWING    2  REACTIONS **


 1    2

                    *** SENSITIVITY COEFFICIENTS OF FIRST-ORDER TIME DERIVATIVES ALSO REQUIRED ***

                    **  OUTPUT REQUIRED AT FOLLOWING   3  PRINT STATIONS  **

                    STATION          TIME (SEC)
                       1            1.50000E-04
                       2            1.00000E-03
                       3            2.00000E-02
```

TABLE E.2.—Continued.
(a) Continued.

```
                              **  INITIAL CONDITIONS  **

TIME   0.00000E+00  SEC              AREA   0.00000E+00  SQ CM              AXIAL POSITION   0.00000E+00  CM

   FLOW PROPERTIES                                                  INTEGRATION INDICATORS

     PRESSURE                 1.00000                                  STEPS FROM LAST PRINT              0
      (ATM)
     VELOCITY                 0.00                                     AVERAGE STEP SIZE            0.00000E+00
      (CM/SEC)
     DENSITY             4.05821E-08                                   METHOD ORDER                       0
      (G/CM**3)
     TEMPERATURE              300.00
      (DEG K)
     MASS FLOW RATE      0.00000E+00                                   TOTAL NUMBER OF STEPS              0
      (G/SEC)
     ENTROPY              28563.1484                                   FUNCT EVALUATIONS                  0
      (CAL/G/DEG K)
     MACH NUMBER              0.0000                                   JACOBIAN EVALUATIONS               0

     GAMMA                    1.6596

     ENTHALPY            1.50150E+06
      (CAL/G)
     SP. HEAT (CP)       5.00500E+03
      (CAL/G/DEG K)

                                  CHEMICAL PROPERTIES

SPECIES    CONCENTRATION   MOLE FRACTION   NET SPECIES PRODUCTION  REACTION   RATE CONST   NET REACTION CONV RATE   NET RATE/POSI-
           (MOLES/CM**3)                   RATE (MOLE/CM**3/SEC)   NUMBER     CGS  UNITS   (MOLE-CM**3/G**2/SEC)    TIVE DIR RATE
 SPECA      4.05821E-05     9.99001E-01          -4.05820E-02         1       1.0000E+03        2.46414E+13              1.00000
 SPECB      4.05820E-08     9.99000E-04           4.05820E-02         2       1.0000E+00        2.46414E+07              1.00000

  DERIVATIVES (CGS UNITS): T            0.00000E+00    RHO          0.00000E+00

  MIXTURE MOLECULAR WEIGHT      0.00100     TOTAL ENERGY EXCHANGE RATE    0.00000E+00       MASS FRACTION SUM    1.00000000
                                                (CAL-CM**3/G**2/SEC)

                         CPU TIME FOR INITIALIZATION OF LSENS =      0.490000 S


TIME   2.00000E-02  SEC              AREA   0.00000E+00  SQ CM              AXIAL POSITION   0.00000E+00  CM

   FLOW PROPERTIES                                                  INTEGRATION INDICATORS

     PRESSURE                 1.00000                                  STEPS FROM LAST PRINT            105
      (ATM)
     VELOCITY                 0.00                                     AVERAGE STEP SIZE            0.18141E-03
      (CM/SEC)
     DENSITY             4.05821E-08                                   METHOD ORDER                       5
      (G/CM**3)
     TEMPERATURE              300.00
      (DEG K)
     MASS FLOW RATE      0.00000E+00                                   TOTAL NUMBER OF STEPS            135
      (G/SEC)
     ENTROPY              28563.1484                                   FUNCT EVALUATIONS                153
      (CAL/G/DEG K)
     MACH NUMBER              0.0000                                   JACOBIAN EVALUATIONS              15

     GAMMA                    1.6596

     ENTHALPY            1.50150E+06
      (CAL/G)
     SP. HEAT (CP)       5.00500E+03
      (CAL/G/DEG K)

                                  CHEMICAL PROPERTIES

SPECIES    CONCENTRATION   MOLE FRACTION   NET SPECIES PRODUCTION  REACTION   RATE CONST   NET REACTION CONV RATE   NET RATE/POSI-
           (MOLES/CM**3)                   RATE (MOLE/CM**3/SEC)   NUMBER     CGS  UNITS   (MOLE-CM**3/G**2/SEC)    TIVE DIR RATE
 SPECA      4.05822E-08     9.99004E-04          -1.04065E-10         1       1.0000E+03        2.46415E+10              1.00000
 SPECB      4.05821E-05     9.99001E-01           1.04065E-10         2       1.0000E+00        2.46414E+10              1.00000

  DERIVATIVES (CGS UNITS): T            0.00000E+00    RHO          0.00000E+00

  MIXTURE MOLECULAR WEIGHT      0.00100     TOTAL ENERGY EXCHANGE RATE    0.00000E+00       MASS FRACTION SUM    1.00000000
                                                (CAL-CM**3/G**2/SEC)

_____________________________________________________________________________________________________

  COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP -  2.000000E-01  S     UP TO THIS TIME -  2.599999E-01  S
```

TABLE E.2.—Continued.
(a) Concluded.

```
                                    ***** SENSITIVITY CALCULATIONS *****
                                            TIME =   2.00000D-02
                    SENSITIVITY COEFFICIENTS OF  0-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES

    **** SENSITIVITY TO INITIAL CONDITIONS ****
            DZ(I)/DYZERO(J)*F(J)/Z(I), WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW
                                             F(J)= YZERO(J) FOR YZERO(J) NOT EQUAL TO 0
                                                 = 1.0E-4/(INITIAL MWT)  FOR YZERO(J) = 0

    PARAMETER    SPECA      SPECB

    SPECA       9.990D-01  9.990D-01
    SPECB       9.990D-04  9.990D-04


**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE PREEXPONENTIAL CONSTANTS ****
        DZ(I)/DA(J)*A(J)/Z(I) WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW
        **** NOTE: FOR CONSTANT TEMPERATURE PROBLEMS NORMALIZED SENSITIVITY COEFFICIENTS W.R.T. N(J) AND E(J) ARE
                   THE SAME AS THE NORMALIZED COEFFICIENTS W.R.T. A(J) ****

REAC NUM     SPECA      SPECB

    1      -9.990D-01  9.990D-04
    2       9.990D-01 -9.990D-04


                                    ***** SENSITIVITY CALCULATIONS *****
                                            TIME =   2.00000D-02
                    SENSITIVITY COEFFICIENTS OF  1-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES

    **** SENSITIVITY TO INITIAL CONDITIONS ****
            DZ(I)/DYZERO(J)*F(J)/Z(I), WHERE Z(I)= 1-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW
                                             F(J)= YZERO(J) FOR YZERO(J) NOT EQUAL TO 0
                                                 = 1.0E-4/(INITIAL MWT)  FOR YZERO(J) = 0

    PARAMETER    SPECA      SPECB

    SPECA       9.972D-01  9.972D-01
    SPECB      -9.972D-07 -9.972D-07


**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE PREEXPONENTIAL CONSTANTS ****
        DZ(I)/DA(J)*A(J)/Z(I) WHERE Z(I)= 1-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW
        **** NOTE: FOR CONSTANT TEMPERATURE PROBLEMS NORMALIZED SENSITIVITY COEFFICIENTS W.R.T. N(J) AND E(J) ARE
                   THE SAME AS THE NORMALIZED COEFFICIENTS W.R.T. A(J) ****

REAC NUM     SPECA      SPECB

    1      -1.808D+01 -1.808D+01
    2      -1.908D-02 -1.908D-02


        (LSENS)     END OF THIS CASE


                    SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

                       TOTAL NO. OF STEPS -                        135
                       TOTAL NO. OF DERIVATIVE EVALUATIONS -       153
                       TOTAL NO. OF JACOBIAN EVALUATIONS -          15
                       TOTAL CPU TIME -                       0.260000 S


                    WORK REQUIRED BY SENSITIVITY ROUTINE:

                         NO. STEPS =              135
                         NO. FUNC. EVAL. =        135
                         NO. JAC. EVAL. =         135
                         TOTAL REAL    SPACE USED =        100
                         TOTAL INTEGER SPACE USED =         44


                                TOTAL CPU TIME (INCLUDING I/O) REQUIRED =      0.920000 S


        (LSENS)     READ DATA FOR NEXT CASE
```

TABLE E.2.—Continued.
(b) Case 2

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

SIMPLE TEST CASE A=B=C: HWANG ET AL, J. CHEM PHYS, V69, P5180, 1978. CASE 2

REACTION NUMBER	REACTION			REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1*DUMA	>	1*DUMB	1.00000E+00	0.0000	0.00
2	1*DUMB	>	1*DUMA	1.00000E+02	0.0000	0.00
3	1*DUMB	>	1*DUMC	1.00000E+02	0.0000	0.00
4	1*DUMC	>	1*DUMB	1.00000E+00	0.0000	0.00

** INITIAL CONDITIONS **

TIME 0.00000E+00 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.00000
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	4.06227E-05
TEMPERATURE (DEG K)	300.00
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	28.5189
MACH NUMBER	0.0000
GAMMA	1.6596
ENTHALPY (CAL/G)	1.50000E+03
SP. HEAT (CP) (CAL/G/DEG K)	5.00000E+00

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
DUMA	4.06227E-05	1.00000E+00	-4.06227E-05	1	1.0000E+00	2.46168E+04	1.00000
DUMB	0.00000E+00	0.00000E+00	4.06227E-05	2	1.0000E+02	0.00000E+00	0.00000
DUMC	0.00000E+00	0.00000E+00	0.00000E+00	3	1.0000E+02	0.00000E+00	0.00000
				4	1.0000E+00	0.00000E+00	0.00000

DERIVATIVES (CGS UNITS): T 0.00000E+00 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 1.00000 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 0.00000E+00 MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 0.340000 S

TABLE E.2.—Continued.
(b) Continued.

TIME 2.50000E+00 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.00000
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	4.06227E-05
TEMPERATURE (DEG K)	300.00
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	29.9450
MACH NUMBER	0.0000
GAMMA	1.6596
ENTHALPY (CAL/G)	1.50000E+03
SP. HEAT (CP) (CAL/G/DEG K)	5.00000E+00

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	50
AVERAGE STEP SIZE	0.48681E-01
METHOD ORDER	4
TOTAL NUMBER OF STEPS	120
FUNCT EVALUATIONS	150
JACOBIAN EVALUATIONS	19

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
DUMA	2.18775E-05	5.38555E-01	-1.66726E-06	1	1.0000E+00	1.32575E+04	1.00000
DUMB	2.02103E-07	4.97512E-03	-4.30623E-13	2	1.0000E+02	1.22472E+04	1.00000
DUMC	1.85430E-05	4.56470E-01	1.66726E-06	3	1.0000E+02	1.22472E+04	1.00000
				4	1.0000E+00	1.12368E+04	1.00000

DERIVATIVES (CGS UNITS): T 0.00000E+00 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 1.00000 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 0.00000E+00 MASS FRACTION SUM 1.00000000

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 1.300000E-01 S UP TO THIS TIME - 3.099999E-01 S

***** SENSITIVITY CALCULATIONS *****

TIME = 2.50000D+00

SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES

**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE PREEXPONENTIAL CONSTANTS ****

DZ(I)/DA(J)*A(J)/Z(I) WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW

**** NOTE: FOR CONSTANT TEMPERATURE PROBLEMS NORMALIZED SENSITIVITY COEFFICIENTS W.R.T. N(J) AND E(J) ARE THE SAME AS THE NORMALIZED COEFFICIENTS W.R.T. A(J) ****

REAC NUM	DUMA	DUMB	DUMC
1	-5.217D-01	5.388D-01	6.097D-01
2	4.261D-01	-4.975D-01	-4.973D-01
3	-4.215D-01	-4.975D-01	5.027D-01
4	3.266D-01	4.563D-01	-3.903D-01

TABLE E.2.—Continued.
(b) Concluded.

TIME 4.50000E+00 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.00000
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	4.06227E-05
TEMPERATURE (DEG K)	300.00
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	29.9516
MACH NUMBER	0.0000
GAMMA	1.6596
ENTHALPY (CAL/G)	1.50000E+03
SP. HEAT (CP) (CAL/G/DEG K)	5.00000E+00

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	14
AVERAGE STEP SIZE	0.14637E+00
METHOD ORDER	5
TOTAL NUMBER OF STEPS	134
FUNCT EVALUATIONS	166
JACOBIAN EVALUATIONS	20

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
DUMA	2.04359E-05	5.03067E-01	-2.25653E-07	1	1.0000E+00	1.23839E+04	1.00000
DUMB	2.02103E-07	4.97512E-03	-1.02183E-12	2	1.0000E+02	1.22472E+04	1.00000
DUMC	1.99846E-05	4.91958E-01	2.25654E-07	3	1.0000E+02	1.22472E+04	1.00000
				4	1.0000E+00	1.21104E+04	1.00000

DERIVATIVES (CGS UNITS): T 0.00000E+00 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 1.00000 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 0.00000E+00 MASS FRACTION SUM 1.00000000

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 3.999996E-02 S UP TO THIS TIME - 3.499999E-01 S

***** SENSITIVITY CALCULATIONS *****

TIME = 4.50000D+00

SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES

**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE PREEXPONENTIAL CONSTANTS ****

DZ(I)/DA(J)*A(J)/Z(I) WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW

**** NOTE: FOR CONSTANT TEMPERATURE PROBLEMS NORMALIZED SENSITIVITY COEFFICIENTS W.R.T. N(J) AND E(J) ARE THE SAME AS THE NORMALIZED COEFFICIENTS W.R.T. A(J) ****

REAC NUM	DUMA	DUMB	DUMC
1	-5.163D-01	5.031D-01	5.229D-01
2	4.914D-01	-4.975D-01	-4.975D-01
3	-4.865D-01	-4.975D-01	5.025D-01
4	4.617D-01	4.919D-01	-4.771D-01

(LSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

TOTAL NO. OF STEPS -	134
TOTAL NO. OF DERIVATIVE EVALUATIONS -	166
TOTAL NO. OF JACOBIAN EVALUATIONS -	20
TOTAL CPU TIME -	0.350000 S

WORK REQUIRED BY SENSITIVITY ROUTINE:

NO. STEPS =	134
NO. FUNC. EVAL. =	134
NO. JAC. EVAL. =	134
TOTAL REAL SPACE USED =	144
TOTAL INTEGER SPACE USED =	46

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 0.840000 S

(LSENS) READ DATA FOR NEXT CASE

TABLE E.2.—Continued.

(c) Case 3

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

ETHANE PYROLYSIS: KRAMER ET AL, APPL MATH MODELLING, V5, P432, 1981. CASE 3

REACTION NUMBER	REACTION								REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1			1*C2H6	>	2*CH3				1.20000E+12	0.0000	59218.00
2	1*C2H6	+	1*CH3	>	1*C2H5	+	1*CH4		8.01000E+08	0.0000	11943.00
3			1*C2H5	>	1*C2H4	+	1*H		3.00000E+11	0.0000	34974.00
4	1*H	+	1*C2H6	>	1*C2H5	+	1*H2		1.30000E+11	0.0000	8982.00
5			2*H	>	1*H2				6.99000E+13	0.0000	0.00

** INITIAL CONDITIONS **

TIME 0.00000E+00 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	0.45070
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	1.78937E-04
TEMPERATURE (DEG K)	923.00
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	2.6117
MACH NUMBER	0.0000
GAMMA	1.0762
ENTHALPY (CAL/G)	-2.27762E+02
SP. HEAT (CP) (CAL/G/DEG K)	9.33015E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
C2H6	5.95080E-06	1.00000E+00	-6.79204E-08	1	1.1414E-02	2.12129E+00	1.00000
CH3	0.00000E+00	0.00000E+00	1.35841E-07	2	1.1905E+06	0.00000E+00	0.00000
C2H5	0.00000E+00	0.00000E+00	0.00000E+00	3	1.5700E+03	0.00000E+00	0.00000
CH4	0.00000E+00	0.00000E+00	0.00000E+00	4	9.7088E+08	0.00000E+00	0.00000
C2H4	0.00000E+00	0.00000E+00	0.00000E+00	5	6.9900E+13	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	0.00000E+00				
H2	0.00000E+00	0.00000E+00	0.00000E+00				

DERIVATIVES (CGS UNITS): T 0.00000E+00 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 30.06940 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 1.90244E+05 MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 0.730000 S

TIME 2.00000E+01 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	0.69709
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	1.78937E-04
TEMPERATURE (DEG K)	923.00
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	3.3191
MACH NUMBER	0.0000
GAMMA	1.1225
ENTHALPY (CAL/G)	3.18711E+02
SP. HEAT (CP) (CAL/G/DEG K)	9.36808E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	31
AVERAGE STEP SIZE	0.62654E+00
METHOD ORDER	5
TOTAL NUMBER OF STEPS	93
FUNCT EVALUATIONS	134
JACOBIAN EVALUATIONS	20

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
C2H6	1.91006E-06	2.07526E-01	-9.81539E-08	1	1.1414E-02	6.80881E-01	1.00000
CH3	1.91739E-08	2.08322E-03	-1.46091E-15	2	1.1905E+06	1.36176E+00	1.00000
C2H5	4.86333E-11	5.28396E-06	-2.53404E-12	3	1.5700E+03	2.38474E+00	1.00000
CH4	1.57517E-06	1.71141E-01	4.36015E-08	4	9.7088E+08	1.02290E+00	1.00000
C2H4	3.24352E-06	3.52406E-01	7.63556E-08	5	6.9900E+13	6.80945E-01	1.00000
H	1.76611E-11	1.91886E-06	-1.57847E-12				
H2	2.45595E-06	2.66837E-01	5.45544E-08				

DERIVATIVES (CGS UNITS): T 0.00000E+00 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 19.44135 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 6.68713E+04 MASS FRACTION SUM 0.99999982

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 1.599998E-01 S UP TO THIS TIME - 5.100000E-01 S

TABLE E.2.—Continued.
(c) Concluded.

```
                                    ***** SENSITIVITY CALCULATIONS *****

                                          TIME =   2.00000D+01

                    SENSITIVITY COEFFICIENTS OF  0-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES

**** SENSITIVITY TO INITIAL CONDITIONS ****

        DZ(I)/DYZERO(J)*F(J)/Z(I), WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW
                                         F(J)= YZERO(J) FOR YZERO(J) NOT EQUAL TO 0
                                             = 1.0E-4/(INITIAL MWT)  FOR YZERO(J) = 0

PARAMETER    C2H6        CH3         C2H5        CH4         C2H4        H           H2

C2H6        7.919D-01 -5.490D-08  9.617D-01  9.104D-01  1.147D+00  3.959D-01  1.223D+00
TEMP       -2.849D+01  2.577D+01 -2.620D+01  1.987D+01  1.187D+01  1.900D+00  9.311D+00
```

```
**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE PREEXPONENTIAL CONSTANTS ****

        DZ(I)/DA(J)*A(J)/Z(I) WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW

        **** NOTE: FOR CONSTANT TEMPERATURE PROBLEMS NORMALIZED SENSITIVITY COEFFICIENTS W.R.T. N(J) AND E(J) ARE
                   THE SAME AS THE NORMALIZED COEFFICIENTS W.R.T. A(J) ****

REAC NUM     C2H6        CH3         C2H5        CH4         C2H4        H           H2

     1     -8.196D-01  1.000D+00 -2.099D-01  6.433D-01  3.235D-01  9.020D-02  2.210D-01
     2     -4.718D-03 -1.000D+00 -5.729D-03  6.888D-03  4.061D-03 -2.359D-03  3.155D-03
```

```
(LSENS)     END OF THIS CASE

                SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

                   TOTAL NO. OF STEPS -                        93
                   TOTAL NO. OF DERIVATIVE EVALUATIONS -      134
                   TOTAL NO. OF JACOBIAN EVALUATIONS -         20
                   TOTAL CPU TIME -                      0.510000 S


                WORK REQUIRED BY SENSITIVITY ROUTINE:

                     NO. STEPS =              93
                     NO. FUNC. EVAL. =        93
                     NO. JAC. EVAL. =         93
                     TOTAL REAL    SPACE USED =        424
                     TOTAL INTEGER SPACE USED =         56

                                TOTAL CPU TIME (INCLUDING I/O) REQUIRED =      1.400000 S

(LSENS)     READ DATA FOR NEXT CASE
```

TABLE E.2.—Continued.

(d) Case 4

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

CH4-O2-AR SHOCK IGNITION: BONI & PENNER, COMB SCI & TECH, V15, P99, 1977. CASE 4

REACTION NUMBER	REACTION							REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	M	+	1*CH4	>	1*CH3	+	1*H	4.33700E+07	0.0000	0.00
2	1*H	+	1*CH3	>	1*CH4	+	M	1.10600E+17	0.0000	0.00
3	1*OH	+	1*CH4	>	1*CH3	+	1*H2O	2.59000E+13	0.0000	0.00
4	1*CH3	+	1*H2O	>	1*OH	+	1*CH4	1.04800E+11	0.0000	0.00
5	1*H	+	1*CH4	>	1*CH3	+	1*H2	1.98800E+13	0.0000	0.00
6	1*CH3	+	1*H2	>	1*H	+	1*CH4	8.07100E+11	0.0000	0.00
7	1*O	+	1*CH4	>	1*CH3	+	1*OH	2.16800E+12	0.0000	0.00
8	1*CH3	+	1*OH	>	1*O	+	1*CH4	6.62500E+10	0.0000	0.00
9	1*CH3	+	1*O	>	1*CH2O	+	1*H	1.00000E+14	0.0000	0.00
10	1*CH2O	+	1*H	>	1*CH3	+	1*O	5.30000E+07	0.0000	0.00
11	1*CH3	+	1*O2	>	1*CH2O	+	1*OH	2.00000E+10	0.0000	0.00
12	1*CH2O	+	1*OH	>	1*CH3	+	1*O2	4.33700E+04	0.0000	0.00
13	1*CH2O	+	1*O	>	1*HCO	+	1*OH	1.58400E+13	0.0000	0.00
14	1*HCO	+	1*OH	>	1*CH2O	+	1*O	9.03500E+09	0.0000	0.00
15	1*CH2O	+	1*OH	>	1*HCO	+	1*H2O	1.10800E+14	0.0000	0.00
16	1*HCO	+	1*H2O	>	1*CH2O	+	1*OH	8.55300E+09	0.0000	0.00
17	1*CH2O	+	1*H	>	1*HCO	+	1*H2	5.24000E+12	0.0000	0.00
18	1*HCO	+	1*H2	>	1*CH2O	+	1*H	4.21600E+09	0.0000	0.00
19	M	+	1*CH2O	>	1*HCO	+	1*H	3.84300E+08	0.0000	0.00
20	1*HCO	+	1*H	>	1*CH2O	+	M	1.95900E+16	0.0000	0.00
21	1*HCO	+	1*O	>	1*CO	+	1*OH	1.00000E+14	0.0000	0.00
22	1*CO	+	1*OH	>	1*HCO	+	1*O	1.14400E+05	0.0000	0.00
23	1*HCO	+	1*OH	>	1*CO	+	1*H2O	1.00000E+14	0.0000	0.00
24	1*CO	+	1*H2O	>	1*HCO	+	1*OH	1.26500E+04	0.0000	0.00
25	1*HCO	+	1*H	>	1*CO	+	1*H2	2.00000E+14	0.0000	0.00
26	1*CO	+	1*H2	>	1*HCO	+	1*H	2.77100E+05	0.0000	0.00
27	M	+	1*HCO	>	1*H	+	1*CO	4.21600E+10	0.0000	0.00
28	1*H	+	1*CO	>	1*HCO	+	M	3.62800E+12	0.0000	0.00
29	1*CO	+	1*OH	>	1*CO2	+	1*H	5.36000E+11	0.0000	0.00
30	1*CO2	+	1*H	>	1*CO	+	1*OH	2.28900E+11	0.0000	0.00
31	1*H2	+	1*OH	>	1*H2O	+	1*H	1.80700E+13	0.0000	0.00
32	1*H2O	+	1*H	>	1*H2	+	1*OH	1.80700E+12	0.0000	0.00
33	1*O	+	1*H2	>	1*OH	+	1*H	7.22800E+12	0.0000	0.00
34	1*OH	+	1*H	>	1*O	+	1*H2	6.62500E+12	0.0000	0.00
35	1*H	+	1*O2	>	1*OH	+	1*O	3.21600E+12	0.0000	0.00
36	1*OH	+	1*O	>	1*H	+	1*O2	1.38500E+13	0.0000	0.00
37	1*H	+	1*OH	>	1*H2O	+	M	2.10400E+15	0.0000	0.00
38	M	+	1*H2O	>	1*H	+	1*OH	3.09600E+03	0.0000	0.00
39	1*H	+	1*HO2	>	2*OH			1.55400E+14	0.0000	0.00
40			2*OH	>	1*H	+	1*HO2	6.02300E+08	0.0000	0.00
41	1*H	+	1*O2	>	1*HO2	+	M	1.93000E+15	0.0000	0.00
42	M	+	1*HO2	>	1*H	+	1*O2	2.16800E+10	0.0000	0.00
43			2*OH	>	1*O	+	1*H2O	9.45600E+12	0.0000	0.00
44	1*O	+	1*H2O	>	2*OH			1.20500E+12	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2O , 37) = 16.70000 M(H2O , 38) = 16.70000

TABLE E.2.—Continued.
(d) Continued.

** INITIAL CONDITIONS **

TIME 0.00000E+00 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	6.72900
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	1.48828E-03
TEMPERATURE (DEG K)	2000.00
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	1.3750
MACH NUMBER	0.0000
GAMMA	1.3655
ENTHALPY (CAL/G)	2.71187E+02
SP. HEAT (CP) (CAL/G/DEG K)	2.04545E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	3.76075E-06	9.17200E-02	-6.68765E-03
CH3	0.00000E+00	0.00000E+00	6.68765E-03
H	0.00000E+00	0.00000E+00	6.68765E-03
OH	0.00000E+00	0.00000E+00	0.00000E+00
H2O	0.00000E+00	0.00000E+00	0.00000E+00
H2	1.66035E-24	4.04940E-20	0.00000E+00
O	0.00000E+00	0.00000E+00	0.00000E+00
CH2O	0.00000E+00	0.00000E+00	0.00000E+00
O2	7.52150E-06	1.83440E-01	0.00000E+00
HCO	0.00000E+00	0.00000E+00	0.00000E+00
CO	0.00000E+00	0.00000E+00	0.00000E+00
CO2	1.66035E-24	4.04940E-20	0.00000E+00
HO2	0.00000E+00	0.00000E+00	0.00000E+00
AR	2.97202E-05	7.24840E-01	0.00000E+00

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	4.3370E+07	3.01931E+03	1.00000
2	1.1060E+17	0.00000E+00	0.00000
3	2.5900E+13	0.00000E+00	0.00000
4	1.0480E+11	0.00000E+00	0.00000
5	1.9880E+13	0.00000E+00	0.00000
6	8.0710E+11	0.00000E+00	0.00000
7	2.1680E+12	0.00000E+00	0.00000
8	6.6250E+10	0.00000E+00	0.00000
9	1.0000E+14	0.00000E+00	0.00000
10	5.3000E+07	0.00000E+00	0.00000
11	2.0000E+10	0.00000E+00	0.00000
12	4.3370E+04	0.00000E+00	0.00000
13	1.5840E+13	0.00000E+00	0.00000
14	9.0350E+09	0.00000E+00	0.00000
15	1.1080E+14	0.00000E+00	0.00000
16	8.5530E+09	0.00000E+00	0.00000
17	5.2400E+12	0.00000E+00	0.00000
18	4.2160E+09	0.00000E+00	0.00000
19	3.8430E+08	0.00000E+00	0.00000
20	1.9590E+16	0.00000E+00	0.00000
21	1.0000E+14	0.00000E+00	0.00000
22	1.1440E+05	0.00000E+00	0.00000
23	1.0000E+14	0.00000E+00	0.00000
24	1.2650E+04	0.00000E+00	0.00000
25	2.0000E+14	0.00000E+00	0.00000
26	2.7710E+05	0.00000E+00	0.00000
27	4.2160E+10	0.00000E+00	0.00000
28	3.6280E+12	0.00000E+00	0.00000
29	5.3600E+11	0.00000E+00	0.00000
30	2.2890E+11	0.00000E+00	0.00000
31	1.8070E+13	0.00000E+00	0.00000
32	1.8070E+12	0.00000E+00	0.00000
33	7.2280E+12	0.00000E+00	0.00000
34	6.6250E+12	0.00000E+00	0.00000
35	3.2160E+12	0.00000E+00	0.00000
36	1.3850E+13	0.00000E+00	0.00000
37	2.1040E+15	0.00000E+00	0.00000
38	3.0960E+03	0.00000E+00	0.00000
39	1.5540E+14	0.00000E+00	0.00000
40	6.0230E+08	0.00000E+00	0.00000
41	1.9300E+15	0.00000E+00	0.00000
42	2.1680E+10	0.00000E+00	0.00000
43	9.4560E+12	0.00000E+00	0.00000
44	1.2050E+12	0.00000E+00	0.00000

DERIVATIVES (CGS UNITS): T 0.00000E+00 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 36.29719 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 3.16488E+08 MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 1.140000 S

TABLE E.2.—Continued.
(d) Continued.

TIME 2.50000E-05 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	6.83904
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	1.48828E-03
TEMPERATURE (DEG K)	2000.00
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	1.4038
MACH NUMBER	0.0000
GAMMA	1.3809
ENTHALPY (CAL/G)	2.20707E+02
SP. HEAT (CP) (CAL/G/DEG K)	2.01718E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	92
AVERAGE STEP SIZE	0.28285E-06
METHOD ORDER	3
TOTAL NUMBER OF STEPS	92
FUNCT EVALUATIONS	123
JACOBIAN EVALUATIONS	21

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	2.33149E-06	5.59472E-02	-7.80458E-02
CH3	3.51582E-07	8.43670E-03	-9.61705E-03
H	3.39090E-09	8.13694E-05	2.25868E-04
OH	1.75717E-09	4.21658E-05	1.03282E-04
H2O	1.44637E-06	3.47076E-02	1.37114E-01
H2	4.82428E-07	1.15765E-02	3.94366E-02
O	1.24225E-09	2.98095E-05	8.06246E-05
CH2O	3.82100E-07	9.16900E-03	-6.56945E-03
O2	6.25565E-06	1.50113E-01	-1.12830E-01
HCO	3.41967E-08	8.20597E-04	7.02750E-04
CO	6.59063E-07	1.58151E-02	9.29106E-02
CO2	2.32046E-09	5.56826E-05	6.18934E-04
HO2	1.16503E-09	2.79566E-05	3.96000E-05
AR	2.97202E-05	7.13178E-01	0.00000E+00

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	4.3370E+07	1.90244E+03	1.00000
2	1.1060E+17	2.48077E+03	1.00000
3	2.5900E+13	4.79050E+04	1.00000
4	1.0480E+11	2.40603E+04	1.00000
5	1.9880E+13	7.09575E+04	1.00000
6	8.0710E+11	6.18046E+04	1.00000
7	2.1680E+12	2.83488E+03	1.00000
8	6.6250E+10	1.84783E+01	1.00000
9	1.0000E+14	1.97183E+04	1.00000
10	5.3000E+07	3.10028E-02	1.00000
11	2.0000E+10	1.98592E+04	1.00000
12	4.3370E+04	1.31466E-05	1.00000
13	1.5840E+13	3.39449E+03	1.00000
14	9.0350E+09	2.45110E-01	1.00000
15	1.1080E+14	3.35865E+04	1.00000
16	8.5530E+09	1.90992E+02	1.00000
17	5.2400E+12	3.06519E+03	1.00000
18	4.2160E+09	3.14016E+01	1.00000
19	3.8430E+08	2.76271E+03	1.00000
20	1.9590E+16	4.27388E+01	1.00000
21	1.0000E+14	1.91791E+03	1.00000
22	1.1440E+05	5.98138E-05	1.00000
23	1.0000E+14	2.71289E+03	1.00000
24	1.2650E+04	5.44414E-03	1.00000
25	2.0000E+14	1.04704E+04	1.00000
26	2.7710E+05	3.97768E-02	1.00000
27	4.2160E+10	2.71252E+04	1.00000
28	3.6280E+12	1.52545E-01	1.00000
29	5.3600E+11	2.80246E+02	1.00000
30	2.2890E+11	8.13147E-01	1.00000
31	1.8070E+13	6.91575E+03	1.00000
32	1.8070E+12	4.00116E+03	1.00000
33	7.2280E+12	1.95566E+03	1.00000
34	6.6250E+12	1.78217E+01	1.00000
35	3.2160E+12	3.07991E+04	1.00000
36	1.3850E+13	1.36492E+01	1.00000
37	2.1040E+15	3.64390E-01	1.00000
38	3.0960E+03	1.30158E-01	1.00000
39	1.5540E+14	2.77165E+02	1.00000
40	6.0230E+08	8.39606E-04	1.00000
41	1.9300E+15	7.70253E+02	1.00000
42	2.1680E+10	4.75210E+02	1.00000
43	9.4560E+12	1.31817E+01	1.00000
44	1.2050E+12	9.77482E+02	1.00000

DERIVATIVES (CGS UNITS): T 0.00000E+00 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 35.71319 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) -4.13916E+09 MASS FRACTION SUM 1.00000001

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 5.130000E+00 S UP TO THIS TIME - 5.130000E+00 S

TABLE E.2.—Continued.
(d) Concluded.

```
***** SENSITIVITY CALCULATIONS *****

TIME =   2.50000D-05

SENSITIVITY COEFFICIENTS OF  0-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES


**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE PREEXPONENTIAL CONSTANTS ****

     DZ(I)/DA(J)*A(J)/Z(I) WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW

     **** NOTE: FOR CONSTANT TEMPERATURE PROBLEMS NORMALIZED SENSITIVITY COEFFICIENTS W.R.T. N(J) AND E(J) ARE
                THE SAME AS THE NORMALIZED COEFFICIENTS W.R.T. A(J) ****

REAC NUM     CH4         CH3         H           OH          H2O         H2          O           CH2O        O2          HCO         CO

    1     -3.319D-01 -1.247D-01  8.069D-01  6.898D-01  8.722D-01  8.049D-01  6.668D-01 -1.152D-01 -1.669D-01  3.045D-01  1.283D+00
    2      3.728D-02 -6.432D-02 -1.712D-01 -1.390D-01 -6.647D-02 -8.629D-02 -1.083D-01 -1.042D-03  1.291D-02 -7.517D-02 -9.244D-02
    3     -5.708D-02  2.276D-01  6.977D-02 -5.303D-01  8.713D-03 -1.111D-01 -1.280D-01  4.872D-01 -4.995D-03  7.549D-02 -2.027D-01
    4      2.381D-02 -1.010D-01 -2.376D-02  2.608D-01 -5.333D-03  4.701D-02  5.876D-02 -1.913D-01  2.114D-03  9.591D-03  7.887D-02
    5      8.496D-02  2.603D-01 -5.873D-01 -3.950D-01 -4.300D-01  5.616D-02 -6.936D-01  1.675D-01  7.324D-02 -6.018D-02 -5.296D-01
    6     -4.008D-02 -1.947D-01  4.772D-01  2.912D-01  2.593D-01 -8.890D-02  5.700D-01 -1.167D-01 -4.318D-02  4.350D-02  3.089D-01
    7     -2.685D-02  9.706D-02  4.945D-02  1.261D-01  7.261D-02 -3.955D-02 -1.115D-01 -3.387D-02 -1.071D-02  4.634D-02  5.984D-02
    8      1.063D-04 -5.710D-04 -2.170D-04 -6.599D-04 -2.687D-04  2.526D-04  7.550D-04  2.007D-04  3.500D-05 -2.131D-04 -1.746D-04
    9      3.510D-02 -2.348D-01 -4.920D-02 -3.311D-01 -1.302D-01  1.475D-01 -5.521D-01  2.056D-01  1.517D-02 -4.792D-02 -1.143D-01
   10     -3.299D-08  3.245D-07  4.680D-08  4.470D-07  1.311D-07 -2.015D-07  8.730D-07 -2.910D-07 -1.241D-08  5.746D-08  1.079D-07
   11     -2.627D-01 -4.731D-01  4.115D-01  4.310D-01  7.612D-01  6.661D-01  4.842D-01  1.151D-01 -1.507D-01  4.018D-01  1.087D+00
   12      5.889D-11  1.446D-10 -7.731D-11 -1.391D-10 -1.662D-10 -1.391D-10 -1.033D-10 -1.038D-10  3.435D-11 -1.955D-10 -2.139D-10
   13     -9.422D-03  6.505D-02  2.924D-02  1.200D-01  4.330D-02 -1.805D-02 -1.160D-01 -1.182D-01 -4.972D-03  4.078D-02  6.446D-02
   14      4.210D-07 -3.994D-06 -1.560D-06 -7.329D-06 -2.162D-06  1.086D-06  8.489D-06  7.354D-06  2.180D-07 -3.189D-06 -3.428D-06
   15      4.269D-02 -1.945D-01 -2.603D-02 -3.000D-01  1.409D-02  1.867D-01  1.395D-01 -5.428D-01  8.691D-04  4.694D-02  2.647D-01
   16     -2.053D-04  9.345D-04  1.264D-04  1.886D-03 -8.884D-06 -8.094D-04 -6.080D-04  2.306D-03 -1.124D-05 -8.719D-04 -1.065D-03
   17      7.992D-03 -2.058D-02 -2.840D-02 -9.167D-03 -1.052D-02  2.631D-02 -8.809D-03 -6.272D-02  2.129D-03  8.556D-03  1.857D-02
   18     -7.032D-05  1.941D-04  2.862D-04  1.037D-04  8.944D-05 -2.383D-04  1.111D-04  5.578D-04 -1.802D-05 -1.569D-04 -1.697D-04
   19     -8.995D-02  3.298D-02  3.295D-01  2.907D-01  2.175D-01  2.603D-01  2.565D-01 -1.078D-01 -4.121D-02  1.275D-01  3.541D-01
   20      3.567D-04 -6.411D-04 -2.284D-03 -1.920D-03 -6.806D-04 -1.260D-03 -1.682D-03  7.722D-04  1.282D-04 -1.264D-03 -1.294D-03
   21      9.570D-03  1.365D-02 -6.007D-02 -7.704D-03 -1.067D-02 -5.730D-02 -1.182D-01 -1.973D-02  3.425D-03 -6.290D-02 -2.633D-02
   22     -1.782D-10 -2.795D-10  1.399D-09  4.156D-11  1.352D-10  1.157D-09  3.227D-09  5.044D-10 -5.724D-11  1.703D-09  3.977D-10
   23      2.141D-02 -3.890D-02 -1.047D-01 -1.183D-01 -3.878D-02 -5.702D-02 -6.428D-02  1.712D-02  7.439D-03 -1.148D-01 -5.850D-02
   24     -2.274D-08  5.939D-08  1.379D-07  1.740D-07  3.480D-08  6.156D-08  8.079D-08 -2.376D-08 -6.664D-09  1.949D-07  5.196D-08
   25      7.995D-02 -1.585D-01 -4.490D-01 -3.506D-01 -1.454D-01 -1.495D-01 -2.879D-01  4.087D-03  2.744D-02 -4.176D-01 -1.777D-01
   26     -2.041D-07  4.845D-07  1.366D-06  1.032D-06  3.447D-07  3.618D-07  8.906D-07 -1.012D-08 -6.480D-08  1.370D-06  3.954D-07
   27     -1.298D-01  1.794D-01  6.796D-01  5.260D-01  2.485D-01  3.326D-01  5.241D-01 -1.258D-02 -4.820D-02 -3.714D-01  3.874D-01
   28      3.263D-07 -8.015D-07 -2.598D-06 -1.909D-06 -4.975D-07 -8.700D-07 -2.094D-06  1.397D-08  9.682D-08  2.442D-06 -8.565D-07
   29     -3.352D-04 -3.613D-05  5.231D-03 -1.074D-03 -4.015D-04  3.494D-03  4.733D-03  1.235D-03 -2.028D-04 -2.633D-04 -3.008D-03
   30      5.927D-07 -2.474D-07 -1.257D-05  3.838D-06  1.132D-06 -6.688D-06 -1.147D-05 -2.748D-06  3.296D-07  1.644D-06  6.285D-06
   31     -8.104D-03  7.692D-03  5.921D-02 -4.415D-02  2.086D-02 -2.072D-02  4.822D-02  3.549D-02 -3.705D-03 -5.123D-03  4.355D-03
   32      3.914D-03 -4.533D-03 -3.380D-02  2.608D-02 -9.824D-03  1.161D-02 -2.802D-02 -1.907D-02  1.737D-03  4.728D-03 -6.772D-04
   33     -7.407D-03  3.984D-02  2.860D-02  6.023D-02  2.138D-02 -2.136D-02 -6.034D-02 -1.959D-02 -2.748D-03  1.657D-02  1.526D-02
   34      6.338D-05 -3.640D-04 -2.562D-04 -5.427D-04 -1.820D-04  1.965D-04  5.522D-04  1.790D-04  2.275D-05 -1.465D-04 -1.246D-04
   35     -2.196D-01 -1.163D-02  3.051D-01  8.778D-01  6.709D-01  1.693D-01  1.157D+00 -8.570D-02 -1.194D-01  5.463D-01  7.986D-01
   36      6.190D-05 -7.743D-06 -8.059D-05 -3.234D-04 -1.892D-04 -3.063D-05 -4.715D-04  2.065D-05  3.337D-05 -2.119D-04 -2.143D-04
   37      3.043D-06 -6.511D-06 -1.799D-05 -1.844D-05 -5.111D-06 -8.111D-06 -1.213D-05  1.946D-06  9.838D-07 -8.348D-06 -7.926D-06
   38     -1.898D-06  2.364D-06  8.663D-06  8.522D-06  3.813D-06  4.927D-06  6.029D-06 -9.966D-07 -7.330D-07  3.867D-06  5.788D-06
   39      4.937D-04  5.447D-04 -7.330D-03  1.560D-03  8.949D-04 -5.906D-03 -7.056D-03 -2.149D-03  6.936D-05  6.605D-05 -7.987D-04
   40     -2.175D-09 -2.328D-09  2.502D-08 -3.312D-09 -1.552D-09  2.163D-08  2.407D-08  6.582D-09 -4.901D-10  6.584D-10  5.083D-09
   41      1.997D-03  4.164D-04 -1.542D-02 -1.512D-03 -2.177D-03 -1.222D-02 -1.416D-02 -2.639D-03  4.540D-04 -1.597D-03 -5.648D-03

   42     -1.364D-03 -4.455D-04  9.951D-03  1.083D-03  1.601D-03  8.197D-03  9.182D-03  1.694D-03 -3.387D-04  1.112D-03  4.004D-03
   43      3.958D-05 -2.732D-04 -9.129D-05 -5.145D-04 -1.202D-04  1.147D-04  5.004D-04  2.116D-04  1.371D-05 -1.265D-04 -1.088D-04
   44     -2.420D-03  1.839D-02  5.592D-03  3.570D-02  7.314D-03 -7.596D-03 -3.700D-02 -1.445D-02 -7.868D-04  8.903D-03  6.567D-03


REAC NUM     CO2         HO2

    1      2.403D+00  4.339D-01
    2     -1.772D-01 -9.777D-02
    3     -9.206D-01  2.923D-02
    4      3.300D-01 -8.113D-03        (LSENS)     END OF THIS CASE
    5     -1.062D+00 -3.508D-01
    6      6.225D-01  2.916D-01
    7      1.697D-01  2.248D-02
    8     -6.472D-04 -9.945D-05                SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:
    9     -3.751D-01 -1.632D-02
   10      4.001D-07  1.349D-08                   TOTAL NO. OF STEPS -                    92
   11      1.858D+00  1.671D-01                   TOTAL NO. OF DERIVATIVE EVALUATIONS -   123
   12     -3.396D-10 -2.540D-11                   TOTAL NO. OF JACOBIAN EVALUATIONS -      21
   13      1.626D-01  1.447D-02                   TOTAL CPU TIME -                 5.130000 S
   14     -8.218D-06 -7.706D-07
   15      9.606D-02 -3.899D-03
   16      2.931D-04  1.435D-05
   17      1.585D-02 -1.568D-02
   18     -1.097D-04  1.558D-04
   19      6.817D-01  1.905D-01
   20     -2.211D-03 -1.302D-03                WORK REQUIRED BY SENSITIVITY ROUTINE:
   21     -2.803D-02 -3.582D-02
   22      3.268D-10  7.981D-10                   NO. STEPS =              92
   23     -1.325D-01 -5.979D-02                   NO. FUNC. EVAL. =        92
   24      1.322D-07  7.453D-08                   NO. JAC. EVAL. =         92
   25     -3.599D-01 -2.562D-01                   TOTAL REAL     SPACE USED =       3924
   26      8.419D-07  7.432D-07                   TOTAL INTEGER SPACE USED =          66
   27      7.300D-01  3.909D-01
   28     -1.484D-06 -1.383D-06
   29      9.971D-01  2.895D-03                        TOTAL CPU TIME (INCLUDING I/O) REQUIRED =      6.800000 S
   30     -1.915D-03 -6.484D-06
   31     -2.878D-02  3.344D-02
   32      1.755D-02 -1.903D-02
   33      5.220D-02  1.472D-02
   34     -4.462D-04 -1.331D-04
   35      1.593D+00  1.065D-01        (LSENS)     READ DATA FOR NEXT CASE
   36     -4.344D-04 -2.501D-05
   37     -1.726D-05 -9.929D-06
   38      1.192D-05  4.871D-06
   39      1.068D-03 -3.502D-01
   40      8.026D-10  1.056D-06
   41     -7.250D-03  9.904D-01
   42      5.261D-03 -6.182D-01
   43     -4.557D-04 -4.132D-05
   44      2.877D-02  2.483D-03
```

TABLE E.2.—Continued.
(e) Case 5

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

FORMALDEHYDE OXID.: DOUGHERTY ET AL, J. CHEM PHYS, V71, P1794, 1979. CASE 5

REACTION NUMBER	REACTION							REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1*HCO	+	1*O2	>	1*CO	+	1*HO2	6.02000E+10	0.0000	0.00
2	1*HO2	+	1*CH2O	>	1*H2O2	+	1*HCO	3.43000E+10	0.0000	0.00
3	M	+	1*H2O2	>	2*OH			4.01000E+06	0.0000	0.00
4	1*CH2O	+	1*OH	>	1*HCO	+	1*H2O	9.64000E+13	0.0000	0.00
5	1*OH	+	1*H2O2	>	1*H2O	+	1*HO2	3.07000E+12	0.0000	0.00
6			1*H2O2	>	1*H2O2W			1.05000E+02	0.0000	0.00
7			1*HO2	>	1*HO2W			1.05000E+01	0.0000	0.00
8			2*HO2	>	1*H2O2	+	1*O2	1.81000E+12	0.0000	0.00
9	1*CO	+	1*OH	>	1*CO2	+	1*H	1.99000E+11	0.0000	0.00
10	1*CO	+	1*HO2	>	1*CO2	+	1*OH	7.23000E+08	0.0000	0.00
11	1*CH2O	+	1*H	>	1*HCO	+	1*H2	1.63000E+12	0.0000	0.00
12	1*H	+	1*O2	>	1*OH	+	1*O	3.32000E+10	0.0000	0.00
13	1*H	+	1*O2	>	1*HO2	+	M	3.63000E+15	0.0000	0.00
14	M	+	1*HO2	>	1*H	+	1*O2	2.83000E+05	0.0000	0.00
15	1*O	+	1*H2	>	1*OH	+	1*H	1.82000E+11	0.0000	0.00
16	1*CH2O	+	1*O	>	1*HCO	+	1*OH	6.02000E+13	0.0000	0.00
17	1*H	+	1*H2O2	>	1*HO2	+	1*H2	7.83000E+11	0.0000	0.00
18	1*H	+	1*H2O2	>	1*H2O	+	1*OH	3.55000E+12	0.0000	0.00
19	1*O	+	1*H2O2	>	1*OH	+	1*HO2	6.02000E+10	0.0000	0.00
20			1*HCO	>	1*H	+	1*CO	4.60000E-12	0.0000	0.00
21	1*H2	+	1*OH	>	1*H2O	+	1*H	6.02000E+12	0.0000	0.00
22	1*CH2O	+	1*O2	>	1*HCO	+	1*HO2	1.75000E+04	0.0000	0.00
23	1*H	+	1*HO2	>	2*OH			3.01000E+12	0.0000	0.00
24	1*HO2	+	1*H	>	1*H2O	+	1*O	3.01000E+13	0.0000	0.00
25	1*H	+	1*HO2	>	1*H2	+	1*O2	2.71000E+13	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0

** INITIAL CONDITIONS **

TIME 0.00000E+00 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	0.91807
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	3.37842E-04
TEMPERATURE (DEG K)	952.00
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	2.0112
MACH NUMBER	0.0000
GAMMA	1.3330
ENTHALPY (CAL/G)	-2.07869E+02
SP. HEAT (CP) (CAL/G/DEG K)	2.76737E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
HCO	0.00000E+00	0.00000E+00	4.14841E-09
O2	2.10900E-06	1.79453E-01	-4.14841E-09
CO	4.69900E-06	3.99833E-01	0.00000E+00
HO2	0.00000E+00	0.00000E+00	4.14841E-09
CH2O	1.12400E-07	9.56400E-03	-4.14841E-09
H2O2	0.00000E+00	0.00000E+00	0.00000E+00
OH	0.00000E+00	0.00000E+00	0.00000E+00
H2O	0.00000E+00	0.00000E+00	0.00000E+00
H2O2W	0.00000E+00	0.00000E+00	0.00000E+00
HO2W	0.00000E+00	0.00000E+00	0.00000E+00
CO2	0.00000E+00	0.00000E+00	0.00000E+00
H	0.00000E+00	0.00000E+00	0.00000E+00
H2	0.00000E+00	0.00000E+00	0.00000E+00
O	0.00000E+00	0.00000E+00	0.00000E+00
N2	4.83200E-06	4.11150E-01	0.00000E+00

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	6.0200E+10	0.00000E+00	0.00000
2	3.4300E+10	0.00000E+00	0.00000
3	4.0100E+06	0.00000E+00	0.00000
4	9.6400E+13	0.00000E+00	0.00000
5	3.0700E+12	0.00000E+00	0.00000
6	1.0500E+02	0.00000E+00	0.00000
7	1.0500E+01	0.00000E+00	0.00000
8	1.8100E+12	0.00000E+00	0.00000
9	1.9900E+11	0.00000E+00	0.00000
10	7.2300E+08	0.00000E+00	0.00000
11	1.6300E+12	0.00000E+00	0.00000
12	3.3200E+10	0.00000E+00	0.00000
13	3.6300E+15	0.00000E+00	0.00000
14	2.8300E+05	0.00000E+00	0.00000
15	1.8200E+11	0.00000E+00	0.00000
16	6.0200E+13	0.00000E+00	0.00000
17	7.8300E+11	0.00000E+00	0.00000
18	3.5500E+12	0.00000E+00	0.00000
19	6.0200E+10	0.00000E+00	0.00000
20	4.6000E-12	0.00000E+00	0.00000
21	6.0200E+12	0.00000E+00	0.00000
22	1.7500E+04	3.63458E-02	1.00000
23	3.0100E+12	0.00000E+00	0.00000
24	3.0100E+13	0.00000E+00	0.00000
25	2.7100E+13	0.00000E+00	0.00000

TABLE E.2.—Continued.
(e) Continued.

DERIVATIVES (CGS UNITS): T 0.00000E+00 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 28.74664 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 1.40297E+03 MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 1.040001 S

TIME 5.00000E-03 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	0.91807
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	3.37842E-04
TEMPERATURE (DEG K)	952.00
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	2.0113
MACH NUMBER	0.0000
GAMMA	1.3330
ENTHALPY (CAL/G)	-2.08171E+02
SP. HEAT (CP) (CAL/G/DEG K)	2.76736E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	10
AVERAGE STEP SIZE	0.51495E-03
METHOD ORDER	3
TOTAL NUMBER OF STEPS	13
FUNCT EVALUATIONS	15
JACOBIAN EVALUATIONS	4

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
HCO	5.99396E-12	5.10019E-07	2.49009E-09	1	6.0200E+10	6.66295E+00	1.00000
O2	2.10758E-06	1.79331E-01	-7.61730E-07	2	3.4300E+10	3.23812E+00	1.00000
CO	4.69973E-06	3.99895E-01	3.98642E-07	3	4.0100E+06	2.38579E-01	1.00000
HO2	9.70807E-11	8.26048E-06	3.75318E-08	4	9.6400E+13	3.20526E+00	1.00000
CH2O	1.10992E-07	9.44422E-03	-7.62981E-07	5	3.0700E+12	5.31397E-04	1.00000
H2O2	5.77813E-10	4.91654E-05	2.98456E-07	6	1.0500E+02	5.31556E-01	1.00000
OH	3.41917E-14	2.90933E-09	-1.01196E-10	7	1.0500E+01	8.93089E-03	1.00000
H2O	6.57434E-10	5.59403E-05	3.66366E-07	8	1.8100E+12	1.49457E-01	1.00000
H2O2W	8.91753E-11	7.58782E-06	6.06704E-08	9	1.9900E+11	2.80168E-01	1.00000
HO2W	1.88581E-12	1.60461E-07	1.01935E-09	10	7.2300E+08	2.89013E+00	1.00000
CO2	6.67303E-10	5.67800E-05	3.61849E-07	11	1.6300E+12	1.46432E-01	1.00000
H	9.23807E-14	7.86056E-09	5.21113E-11	12	3.3200E+10	5.66337E-02	1.00000
H2	3.05162E-11	2.59659E-06	1.69919E-08	13	3.6300E+15	7.27731E-02	1.00000
O	1.00921E-15	8.58722E-11	-9.34028E-12	14	2.8300E+05	2.82891E-03	1.00000
N2	4.83200E-06	4.11149E-01	0.00000E+00	15	1.8200E+11	4.91082E-08	1.00000
				16	6.0200E+13	5.90803E-02	1.00000
				17	7.8300E+11	3.66187E-04	1.00000
				18	3.5500E+12	1.66023E-03	1.00000
				19	6.0200E+10	3.07565E-07	1.00000
				20	4.6000E-12	2.41571E-16	1.00000
				21	6.0200E+12	5.50326E-05	1.00000
				22	1.7500E+04	3.58664E-02	1.00000
				23	3.0100E+12	2.36512E-04	1.00000
				24	3.0100E+13	2.36512E-03	1.00000
				25	2.7100E+13	2.12939E-03	1.00000

DERIVATIVES (CGS UNITS): T 0.00000E+00 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 28.74658 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) -4.92865E+05 MASS FRACTION SUM 1.00000000

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 3.199997E-01 S UP TO THIS TIME - 4.099989E-01 S

TABLE E.2.—Continued.

(e) Continued.

***** SENSITIVITY CALCULATIONS *****

TIME = 5.00000D-03

SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES

**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE PREEXPONENTIAL CONSTANTS ****

DZ(I)/DA(J)*A(J)/Z(I) WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW

**** NOTE: FOR CONSTANT TEMPERATURE PROBLEMS NORMALIZED SENSITIVITY COEFFICIENTS W.R.T. N(J) AND E(J) ARE THE SAME AS THE NORMALIZED COEFFICIENTS W.R.T. A(J) ****

REAC NUM	HCO	O2	CO	HO2	CH2O	H2O2	OH	H2O	H2O2W	HO2W	CO2
1	-9.231D-01	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
2	1.236D+00	0.000D+00	0.000D+00	7.054D-01	0.000D+00	1.493D+00	8.297D-01	5.878D-01	1.358D+00	4.858D-01	4.952D-01
3	7.700D-01	0.000D+00	0.000D+00	7.224D-01	0.000D+00	4.922D-01	8.383D-01	6.084D-01	3.565D-01	5.095D-01	5.183D-01
4	-2.137D-01	0.000D+00	0.000D+00	-2.124D-01	0.000D+00	-1.836D-01	-1.162D+00	-1.233D-01	-1.512D-01	-1.736D-01	-2.548D-01
5	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
6	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	-1.827D-01	0.000D+00	0.000D+00	8.576D-01	0.000D+00	0.000D+00
7	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	9.833D-01	0.000D+00
8	-3.056D-01	0.000D+00	0.000D+00	-3.195D-01	0.000D+00	-1.770D-01	-3.016D-01	-1.780D-01	-1.130D-01	-1.862D-01	-1.856D-01
9	2.142D-01	0.000D+00	0.000D+00	2.128D-01	0.000D+00	1.841D-01	1.624D-01	1.238D-01	1.517D-01	1.740D-01	2.552D-01
10	5.976D-01	0.000D+00	0.000D+00	1.662D-01	0.000D+00	1.377D-01	1.027D+00	1.013D+00	1.108D-01	1.325D-01	1.122D+00
11	-1.235D-01	0.000D+00	0.000D+00	-1.227D-01	0.000D+00	-1.065D-01	-1.397D-01	-1.178D-01	0.000D+00	-1.007D-01	-1.022D-01
12	2.034D-01	0.000D+00	0.000D+00	1.915D-01	0.000D+00	1.648D-01	2.164D-01	1.798D-01	1.352D-01	1.554D-01	1.576D-01
13	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
14	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
15	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
16	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
17	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
18	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
19	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
20	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
21	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
22	6.836D-01	0.000D+00	0.000D+00	6.756D-01	0.000D+00	8.101D-01	7.048D-01	8.183D-01	8.805D-01	8.094D-01	8.106D-01
23	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
24	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
25	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00

REAC NUM	H	H2	O
1	0.000D+00	0.000D+00	0.000D+00
2	8.133D-01	5.845D-01	8.527D-01
3	8.255D-01	6.063D-01	8.599D-01
4	-1.149D+00	-1.112D+00	-1.158D+00
5	0.000D+00	0.000D+00	0.000D+00
6	0.000D+00	0.000D+00	0.000D+00
7	0.000D+00	0.000D+00	0.000D+00
8	-2.962D-01	-1.775D-01	-3.109D-01
9	1.150D+00	1.112D+00	1.159D+00
10	1.019D+00	1.005D+00	1.031D+00
11	-6.550D-01	3.487D-01	-6.602D-01
12	0.000D+00	0.000D+00	9.810D-01
13	-3.246D-01	-3.156D-01	-3.273D-01
14	0.000D+00	0.000D+00	0.000D+00
15	0.000D+00	0.000D+00	0.000D+00
16	0.000D+00	0.000D+00	-9.999D-01
17	0.000D+00	0.000D+00	0.000D+00
18	0.000D+00	0.000D+00	0.000D+00
19	0.000D+00	0.000D+00	0.000D+00
20	0.000D+00	0.000D+00	0.000D+00
21	0.000D+00	0.000D+00	0.000D+00
22	6.940D-01	8.176D-01	7.297D-01
23	0.000D+00	0.000D+00	0.000D+00
24	0.000D+00	0.000D+00	0.000D+00
25	0.000D+00	0.000D+00	0.000D+00

TABLE E.2.—Continued.
(e) Concluded.

TIME = 5.00000E-03

*** REACTION IMPORTANCE FOR NORMALIZED SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF Y(I) WRT PREEXPONENTIAL CONSTANTS ***

VARIABLE	REACTION NUMBER / NORMALIZED SENSITIVITY COEFFICIENT									
HCO	2	1	3	22	10	8	9	4	12	11
	1.236E+00	-9.231E-01	7.700E-01	6.836E-01	5.976E-01	-3.056E-01	2.142E-01	-2.137E-01	2.034E-01	-1.235E-01
O2										
CO										
HO2	3	2	22	8	9	4	12	10	11	
	7.224E-01	7.054E-01	6.756E-01	-3.195E-01	2.128E-01	-2.124E-01	1.915E-01	1.662E-01	-1.227E-01	
CH2O										
H2O2	2	22	3	9	4	6	8	12	10	11
	1.493E+00	8.101E-01	4.922E-01	1.841E-01	-1.836E-01	-1.827E-01	-1.770E-01	1.648E-01	1.377E-01	-1.065E-01
OH	4	10	3	2	22	8	12	9	11	
	-1.162E+00	1.027E+00	8.383E-01	8.297E-01	7.048E-01	-3.016E-01	2.164E-01	1.624E-01	-1.397E-01	
H2O	10	22	3	2	12	8	9	4	11	
	1.013E+00	8.183E-01	6.084E-01	5.878E-01	1.798E-01	-1.780E-01	1.238E-01	-1.233E-01	-1.178E-01	
H2O2W	2	22	6	3	9	4	12	8	10	
	1.358E+00	8.805E-01	8.576E-01	3.565E-01	1.517E-01	-1.512E-01	1.352E-01	-1.130E-01	1.108E-01	
HO2W	7	22	3	2	8	9	4	12	10	11
	9.833E-01	8.094E-01	5.095E-01	4.858E-01	-1.862E-01	1.740E-01	-1.736E-01	1.554E-01	1.325E-01	-1.007E-01
CO2	10	22	3	2	9	4	8	12	11	
	1.122E+00	8.106E-01	5.183E-01	4.952E-01	2.552E-01	-2.548E-01	-1.856E-01	1.576E-01	-1.022E-01	
H	9	4	10	3	2	22	11	13	8	
	1.150E+00	-1.149E+00	1.019E+00	8.255E-01	8.133E-01	6.940E-01	-6.550E-01	-3.246E-01	-2.962E-01	
H2	9	4	10	22	3	2	11	13	8	
	1.112E+00	-1.112E+00	1.005E+00	8.176E-01	6.063E-01	5.845E-01	3.487E-01	-3.156E-01	-1.775E-01	
O	9	4	10	16	12	3	2	22	11	13
	1.159E+00	-1.158E+00	1.031E+00	-9.999E-01	9.810E-01	8.599E-01	8.527E-01	7.297E-01	-6.602E-01	-3.273E-01
	8									
	-3.109E-01									

(LSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

TOTAL NO. OF STEPS - 13
TOTAL NO. OF DERIVATIVE EVALUATIONS - 15
TOTAL NO. OF JACOBIAN EVALUATIONS - 4
TOTAL CPU TIME - 0.409999 S

WORK REQUIRED BY SENSITIVITY ROUTINE:

NO. STEPS = 13
NO. FUNC. EVAL. = 13
NO. JAC. EVAL. = 13
TOTAL REAL SPACE USED = 2656
TOTAL INTEGER SPACE USED = 68

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 2.030000 S

(LSENS) READ DATA FOR NEXT CASE

TABLE E.2.—Continued.
(f) Case 6

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

WET CO OXIDATION: YETTER ET AL, COMB & FLAME, V59, P107, 1985. CASE 6

REACTION NUMBER	REACTION							REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1*HCO	+	1*H	>	1*CO	+	1*H2	2.00000E+14	0.0000	0.00
2	1*CO	+	1*H2	>	1*HCO	+	1*H	1.71600E-03	0.0000	0.00
3	1*HCO	+	1*OH	>	1*CO	+	1*H2O	1.00000E+14	0.0000	0.00
4	1*CO	+	1*H2O	>	1*HCO	+	1*OH	3.65600E-06	0.0000	0.00
5	1*HCO	+	1*O	>	1*CO	+	1*OH	3.01200E+13	0.0000	0.00
6	1*CO	+	1*OH	>	1*O	+	1*HCO	2.86700E-04	0.0000	0.00
7	1*HCO	+	1*O2	>	1*CO	+	1*HO2	3.01500E+12	0.0000	0.00
8	1*CO	+	1*HO2	>	1*HCO	+	1*O2	2.59000E+06	0.0000	0.00
9	1*CO	+	1*HO2	>	1*CO2	+	1*OH	3.08400E+09	0.0000	0.00
10	1*CO2	+	1*OH	>	1*CO	+	1*HO2	1.77700E-02	0.0000	0.00
11	1*CO	+	1*OH	>	1*CO2	+	1*H	1.92100E+11	0.0000	0.00
12	1*CO2	+	1*H	>	1*CO	+	1*OH	7.89000E+08	0.0000	0.00
13	1*CO2	+	1*O	>	1*CO	+	1*O2	4.43400E+02	0.0000	0.00
14	1*CO	+	1*O2	>	1*CO2	+	1*O	8.49200E+02	0.0000	0.00
15	1*H	+	1*O2	>	1*OH	+	1*O	1.12600E+11	0.0000	0.00
16	1*OH	+	1*O	>	1*H	+	1*O2	1.38500E+13	0.0000	0.00
17	1*O	+	1*H2	>	1*OH	+	1*H	3.38500E+11	0.0000	0.00
18	1*OH	+	1*H	>	1*O	+	1*H2	3.83100E+11	0.0000	0.00
19	1*O	+	1*H2O	>	2*OH			1.65000E+10	0.0000	0.00
20			2*OH	>	1*O	+	1*H2O	4.10800E+12	0.0000	0.00
21	1*H2O	+	1*H	>	1*OH	+	1*H2	7.70900E+09	0.0000	0.00
22	1*OH	+	1*H2	>	1*H2O	+	1*H	1.83700E+12	0.0000	0.00
23	1*OH	+	1*H2O2	>	1*H2O	+	1*HO2	3.63200E+12	0.0000	0.00
24	1*H2O	+	1*HO2	>	1*OH	+	1*H2O2	7.10700E+06	0.0000	0.00
25	1*O	+	1*HO2	>	1*OH	+	1*O2	2.16800E+13	0.0000	0.00
26	1*OH	+	1*O2	>	1*O	+	1*HO2	2.47500E+02	0.0000	0.00
27	1*H	+	1*HO2	>	2*OH			1.12600E+14	0.0000	0.00
28			2*OH	>	1*H	+	1*HO2	1.38500E+05	0.0000	0.00
29	1*H	+	1*HO2	>	1*H2	+	1*O2	2.50600E+13	0.0000	0.00
30	1*H2	+	1*O2	>	1*H	+	1*HO2	2.48700E+02	0.0000	0.00
31	1*HO2	+	1*OH	>	1*H2O	+	1*O2	1.31300E+13	0.0000	0.00
32	1*H2O	+	1*O2	>	1*HO2	+	1*OH	5.52900E-01	0.0000	0.00
33	1*O2	+	1*H2O2	>	2*HO2			1.34900E+05	0.0000	0.00
34			2*HO2	>	1*O2	+	1*H2O2	6.32400E+12	0.0000	0.00
35	1*HO2	+	1*H2	>	1*H2O2	+	1*H	1.40300E+08	0.0000	0.00
36	1*H2O2	+	1*H	>	1*HO2	+	1*H2	3.05400E+11	0.0000	0.00
37	M	+	1*O2	>	2*O			2.03000E-08	0.0000	0.00
38			2*O	>	1*O2	+	M	1.86100E+14	0.0000	0.00
39	M	+	1*H2	>	2*H			1.85000E-05	0.0000	0.00
40			2*H	>	1*H2	+	M	3.00000E+15	0.0000	0.00
41	M	+	1*OH	>	1*O	+	1*H	1.80700E-04	0.0000	0.00
42	1*O	+	1*H	>	1*OH	+	M	1.00100E+16	0.0000	0.00
43	M	+	1*H2O2	>	2*OH			1.09000E+08	0.0000	0.00
44			2*OH	>	1*H2O2	+	M	9.25100E+15	0.0000	0.00
45	M	+	1*H2O	>	1*H	+	1*OH	3.01200E-05	0.0000	0.00
46	1*H	+	1*OH	>	1*H2O	+	M	1.15700E+17	0.0000	0.00
47	M	+	1*HO2	>	1*H	+	1*O2	1.75300E+06	0.0000	0.00
48	1*H	+	1*O2	>	1*HO2	+	M	2.60500E+15	0.0000	0.00
49	M	+	1*CO2	>	1*CO	+	1*O	3.23400E-08	0.0000	0.00
50	1*CO	+	1*O	>	1*CO2	+	M	9.06900E+14	0.0000	0.00
51	M	+	1*HCO	>	1*H	+	1*CO	2.77700E+10	0.0000	0.00
52	1*H	+	1*CO	>	1*HCO	+	M	3.21000E+14	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0

TABLE E.2.—Continued.
(f) Continued.

```
                                   **  INITIAL CONDITIONS  **

TIME   0.00000E+00  SEC              AREA   0.00000E+00  SQ CM              AXIAL POSITION   0.00000E+00  CM

   FLOW PROPERTIES                                                  INTEGRATION INDICATORS

     PRESSURE                 1.00000                                STEPS FROM LAST PRINT                0
      (ATM)
     VELOCITY                 0.00                                   AVERAGE STEP SIZE              0.00000E+00
      (CM/SEC)
     DENSITY             3.10486E-04                                 METHOD ORDER                         0
      (G/CM**3)
     TEMPERATURE            1100.00
      (DEG K)
     MASS FLOW RATE      0.00000E+00                                 TOTAL NUMBER OF STEPS                0
      (G/SEC)
     ENTROPY                  1.9901                                FUNCT EVALUATIONS                    0
      (CAL/G/DEG K)
     MACH NUMBER              0.0000                                JACOBIAN EVALUATIONS                 0

     GAMMA                    1.3319

     ENTHALPY            1.89467E+02
      (CAL/G)
     SP. HEAT (CP)       2.84564E-01
      (CAL/G/DEG K)

                                   CHEMICAL PROPERTIES

SPECIES    CONCENTRATION   MOLE FRACTION   NET SPECIES PRODUCTION  REACTION   RATE CONST   NET REACTION CONV RATE   NET RATE/POSI-
           (MOLES/CM**3)                    RATE (MOLE/CM**3/SEC)   NUMBER     CGS  UNITS   (MOLE-CM**3/G**2/SEC)    TIVE DIR RATE
 HCO       0.00000E+00     0.00000E+00          8.97491E-21          1        2.0000E+14        0.00000E+00              0.00000
 H         0.00000E+00     0.00000E+00          3.69700E-17          2        1.7160E-03        0.00000E+00              0.00000
 CO        2.21578E-08     2.00000E-03         -5.83703E-12          3        1.0000E+14        0.00000E+00              0.00000
 H2        0.00000E+00     0.00000E+00          0.00000E+00          4        3.6560E-06        9.30990E-14              1.00000
 OH        0.00000E+00     0.00000E+00          1.90389E-14          5        3.0120E+13        0.00000E+00              0.00000
 H2O       1.10789E-07     1.00000E-02         -1.90389E-14          6        2.8670E-04        0.00000E+00              0.00000
 O         0.00000E+00     0.00000E+00          5.83703E-12          7        3.0150E+12        0.00000E+00              0.00000
 O2        3.10209E-07     2.80000E-02         -5.85603E-12          8        2.5900E+06        0.00000E+00              0.00000
 HO2       0.00000E+00     0.00000E+00          1.90020E-14          9        3.0840E+09        0.00000E+00              0.00000
 CO2       0.00000E+00     0.00000E+00          5.83703E-12         10        1.7770E-02        0.00000E+00              0.00000
 H2O2      0.00000E+00     0.00000E+00          0.00000E+00         11        1.9210E+11        0.00000E+00              0.00000
 N2        1.06358E-05     9.60000E-01          5.21113E-11         12        7.8900E+08        0.00000E+00              0.00000
                                                                    13        4.4340E+02        0.00000E+00              0.00000
                                                                    14        8.4920E+02        6.05490E-05              1.00000
                                                                    15        1.1260E+11        0.00000E+00              0.00000
                                                                    16        1.3850E+13        0.00000E+00              0.00000
                                                                    17        3.3850E+11        0.00000E+00              0.00000
                                                                    18        3.8310E+11        0.00000E+00              0.00000
                                                                    19        1.6500E+10        0.00000E+00              0.00000
                                                                    20        4.1080E+12        0.00000E+00              0.00000
                                                                    21        7.7090E+09        0.00000E+00              0.00000
                                                                    22        1.8370E+12        0.00000E+00              0.00000
                                                                    23        3.6320E+12        0.00000E+00              0.00000
                                                                    24        7.1070E+06        0.00000E+00              0.00000
                                                                    25        2.1680E+13        0.00000E+00              0.00000

                                                                    26        2.4750E+02        0.00000E+00              0.00000
                                                                    27        1.1260E+14        0.00000E+00              0.00000
                                                                    28        1.3850E+05        0.00000E+00              0.00000
                                                                    29        2.5060E+13        0.00000E+00              0.00000
                                                                    30        2.4870E+02        0.00000E+00              0.00000
                                                                    31        1.3130E+13        0.00000E+00              0.00000
                                                                    32        5.5290E-01        1.97112E-07              1.00000
                                                                    33        1.3490E+05        0.00000E+00              0.00000
                                                                    34        6.3240E+12        0.00000E+00              0.00000
                                                                    35        1.4030E+08        0.00000E+00              0.00000
                                                                    36        3.0540E+11        0.00000E+00              0.00000
                                                                    37        2.0300E-08        7.23707E-13              1.00000
                                                                    38        1.8610E+14        0.00000E+00              0.00000
                                                                    39        1.8500E-05        0.00000E+00              0.00000
                                                                    40        3.0000E+15        0.00000E+00              0.00000
                                                                    41        1.8070E-04        0.00000E+00              0.00000
                                                                    42        1.0010E+16        0.00000E+00              0.00000
                                                                    43        1.0900E+08        0.00000E+00              0.00000
                                                                    44        9.2510E+15        0.00000E+00              0.00000
                                                                    45        3.0120E-05        3.83498E-10              1.00000
                                                                    46        1.1570E+17        0.00000E+00              0.00000
                                                                    47        1.7530E+06        0.00000E+00              0.00000
                                                                    48        2.6050E+15        0.00000E+00              0.00000
                                                                    49        3.2340E-08        0.00000E+00              0.00000
                                                                    50        9.0690E+14        0.00000E+00              0.00000
                                                                    51        2.7770E+10        0.00000E+00              0.00000
                                                                    52        3.2100E+14        0.00000E+00              0.00000

   DERIVATIVES (CGS UNITS): T          0.00000E+00     RHO          0.00000E+00

   MIXTURE MOLECULAR WEIGHT     28.02500     TOTAL ENERGY EXCHANGE RATE   -4.75754E-01      MASS FRACTION SUM    1.00000000
                                                (CAL-CM**3/G**2/SEC)

                                   CPU TIME FOR INITIALIZATION OF LSENS =     1.150001 S
```

TABLE E.2.—Continued.
(f) Continued.

TIME 1.00000E+02 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	0.99900
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	3.10486E-04
TEMPERATURE (DEG K)	1100.00
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	1.9884
MACH NUMBER	0.0000
GAMMA	1.3313
ENTHALPY (CAL/G)	1.84654E+02
SP. HEAT (CP) (CAL/G/DEG K)	2.84633E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	98
AVERAGE STEP SIZE	0.11394E+01
METHOD ORDER	2
TOTAL NUMBER OF STEPS	183
FUNCT EVALUATIONS	233
JACOBIAN EVALUATIONS	31

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
HCO	1.40292E-30	1.26756E-25	8.48901E-30
H	2.32220E-18	2.09816E-13	1.09046E-19
CO	1.55444E-16	1.40446E-11	-3.18356E-21
H2	7.94032E-16	7.17423E-11	-9.52088E-21
OH	1.35978E-12	1.22859E-07	-1.75355E-17
H2O	1.10788E-07	1.00099E-02	8.60489E-18
O	4.15515E-15	3.75426E-10	4.99908E-18
O2	2.99130E-07	2.70270E-02	1.85412E-18
HO2	1.02866E-15	9.29411E-11	-1.56016E-20
CO2	2.21578E-08	2.00200E-03	3.18356E-21
H2O2	1.56956E-16	1.41813E-11	1.25657E-19
N2	1.06358E-05	9.60961E-01	5.21113E-11

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	2.0000E+14	6.75891E-27	1.00000
2	1.7160E-03	2.19707E-27	1.00000
3	1.0000E+14	1.97886E-21	1.00000
4	3.6560E-06	6.53113E-22	1.00000
5	3.0120E+13	1.82133E-24	1.00000
6	2.8670E-04	6.28613E-25	1.00000
7	3.0150E+12	1.31248E-17	1.00000
8	2.5900E+06	4.29593E-18	1.00000
9	3.0840E+09	5.11531E-15	1.00000
10	1.7770E-02	5.55389E-15	1.00000
11	1.9210E+11	4.21195E-10	1.00000
12	7.8900E+08	4.21133E-10	1.00000
13	4.4340E+02	4.23471E-13	1.00000
14	8.4920E+02	4.09598E-13	1.00000
15	1.1260E+11	8.11360E-07	1.00000
16	1.3850E+13	8.11744E-07	1.00000
17	3.3850E+11	1.15850E-11	1.00000
18	3.8310E+11	1.25486E-11	1.00000
19	1.6500E+10	7.87915E-05	1.00000
20	4.1080E+12	7.87919E-05	1.00000
21	7.7090E+09	2.05735E-08	1.00000
22	1.8370E+12	2.05745E-08	1.00000
23	3.6320E+12	8.04095E-09	1.00000
24	7.1070E+06	8.40167E-09	1.00000
25	2.1680E+13	9.61237E-10	1.00000
26	2.4750E+02	1.04428E-09	1.00000
27	1.1260E+14	2.79012E-12	1.00000
28	1.3850E+05	2.65644E-12	1.00000
29	2.5060E+13	6.20964E-13	1.00000
30	2.4870E+02	6.12758E-13	1.00000
31	1.3130E+13	1.90510E-07	1.00000
32	5.5290E-01	1.90071E-07	1.00000
33	1.3490E+05	6.57000E-11	1.00000
34	6.3240E+12	6.94140E-11	1.00000
35	1.4030E+08	1.18872E-15	1.00000
36	3.0540E+11	1.15468E-15	1.00000
37	2.0300E-08	6.97162E-13	1.00000
38	1.8610E+14	3.68890E-13	1.00000
39	1.8500E-05	1.68650E-18	1.00000
40	3.0000E+15	1.85737E-18	1.00000
41	1.8070E-04	2.82100E-14	1.00000
42	1.0010E+16	1.10891E-14	1.00000
43	1.0900E+08	1.96419E-06	1.00000
44	9.2510E+15	1.96382E-06	1.00000
45	3.0120E-05	3.83113E-10	1.00000
46	1.1570E+17	4.19449E-11	1.00000
47	1.7530E+06	2.07028E-07	1.00000
48	2.6050E+15	2.07752E-07	1.00000
49	3.2340E-08	8.22705E-14	1.00000
50	9.0690E+14	6.72506E-14	1.00000
51	2.7770E+10	4.47286E-18	1.00000
52	3.2100E+14	1.33032E-17	1.00000

DERIVATIVES (CGS UNITS): T 0.00000E+00 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 28.05305 TOTAL ENERGY EXCHANGE RATE -3.89288E-06 (CAL-CM**3/G**2/SEC) MASS FRACTION SUM 1.00000000

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 5.450001E+00 S UP TO THIS TIME - 1.033000E+01 S

TABLE E.2.—Continued.
(f) Concluded.

```
                                    ***** SENSITIVITY CALCULATIONS *****
                                          TIME =    1.00000D+02
                    SENSITIVITY COEFFICIENTS OF  0-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES

**** SENSITIVITY TO INITIAL CONDITIONS ****

        DZ(I)/DYZERO(J)*F(J)/Z(I), WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW
                                         F(J)= YZERO(J) FOR YZERO(J) NOT EQUAL TO 0
                                             = 1.0E-4/(INITIAL MWT)  FOR YZERO(J) = 0

PARAMETER    CO          H2

HCO          5.251D-02  5.630D-03
H            4.574D-03  2.647D-03
OH           2.355D-03  2.604D-03
O            1.645D-03 -2.698D-03
HO2         -1.255D-03  3.517D-03
H2O2         1.232D-03  7.597D-03

                                    TIME =    1.00000E+02

*** REACTION IMPORTANCE FOR NORMALIZED SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF Y(I) WRT PREEXPONENTIAL CONSTANTS ***

                                                  REACTION NUMBER
VARIABLE
                                          NORMALIZED SENSITIVITY COEFFICIENT

          11          12          16          15          20          19          31          32          48          47
CO
     -9.989E-01   9.988E-01   5.121E-01  -5.119E-01   5.104E-01  -5.104E-01  -4.963E-01   4.949E-01  -4.867E-01   4.847E-01
          24          23          43          44          26          25          45          13          14          46
      1.426E-02  -1.366E-02   1.360E-02  -1.359E-02   2.727E-03  -2.511E-03   1.894E-03   1.005E-03  -9.717E-04  -2.077E-04
          49          50          34          33          10           9          27          28          37          22
      1.955E-04  -1.598E-04  -6.284E-05   5.963E-05   1.319E-05  -1.213E-05  -8.980E-06   8.614E-06   3.012E-06  -2.838E-06
          21          29          38          30          41          18          17          42          36          35
      2.762E-06  -1.626E-06  -1.597E-06   1.596E-06   1.397E-07   8.208E-08  -7.433E-08  -5.643E-08  -2.069E-09   2.022E-09
          52          51           7          40           3          39           8           1           5           4
     -1.972E-09   4.891E-10  -4.622E-10  -6.291E-11  -2.144E-11   8.342E-12   4.922E-12  -4.040E-12  -1.261E-12   2.117E-15
           6           2
      2.071E-18   9.892E-21

          22          21          16          15          20          19          31          32          48          47
H2
     -9.994E-01   9.994E-01   5.131E-01  -5.129E-01   5.101E-01  -5.101E-01  -4.966E-01   4.953E-01  -4.868E-01   4.850E-01
          24          23          43          44          26          25          45          18          17          46
      1.426E-02  -1.365E-02   1.359E-02  -1.359E-02   2.728E-03  -2.512E-03   1.896E-03   6.096E-04  -5.628E-04  -2.076E-04
          34          11          33          29          30          27          28          37          38          49
     -6.319E-05  -6.163E-05   5.974E-05   2.855E-05  -2.817E-05  -9.105E-06   8.621E-06   3.013E-06  -1.596E-06   4.074E-07
          50          14          13          12          41          35          36          42           9          10
     -3.636E-07  -2.775E-07   2.673E-07  -2.511E-07   1.398E-07  -5.573E-08   5.420E-08  -5.404E-08  -2.601E-08   1.801E-08
          52          51           7          40          39           3           1           8           5           4
      1.298E-09  -3.190E-10   3.005E-10   1.179E-10  -7.357E-11   1.471E-11   2.775E-12   1.315E-12   8.662E-13   2.090E-15
           6           2
      2.024E-18  -1.012E-19

        (LSENS)     END OF THIS CASE

                    SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

                       TOTAL NO. OF STEPS -                      183
                       TOTAL NO. OF DERIVATIVE EVALUATIONS -     233
                       TOTAL NO. OF JACOBIAN EVALUATIONS -        31
                       TOTAL CPU TIME -                   10.330002 S


                    WORK REQUIRED BY SENSITIVITY ROUTINE:

                         NO. STEPS =              183
                         NO. FUNC. EVAL. =        183
                         NO. JAC. EVAL. =         183
                         TOTAL REAL     SPACE USED =        4204
                         TOTAL INTEGER SPACE USED =          62

                                    TOTAL CPU TIME (INCLUDING I/O) REQUIRED =     12.240001 S

        (LSENS)     READ DATA FOR NEXT CASE
```

TABLE E.2.—Continued.
(g) Case 7

```
                                  **  DATA LINES  **
                   1         2         3         4         5         6         7         8
CC  12345678901234567890123456789012345678901234567890123456789012345678901234567890

      SIMPLE NONISOTHERMAL TEST CASE  R>P                                          CASE 7
NEW
                  DUMR      >   DUMP                                  1.0   1.0        0.0
                                          -  BLANK LINE  -
                                          -  BLANK LINE  -
TIME       PRESSURE
 &prob   pcon=.true., sencal=.true., senstd=.true.,
   print=1.0E-06,1.0E-04,1.0E-02,   &end
 &start t=1000.0, p=1.0,   &end
DUMR       1.00
END
 &solver  emax=1.0E-3, atolsp=1.0E-12, &end
INIT
ALL        END
SENSVAR
ALL        END
REAC
 &senrxn  sensaj=.true., sensnj=.true., sensej=.true., allrxn=.true.,
  &end
FINIS
```

```
                                  **  INITIAL CONDITIONS  **

TIME   0.00000E+00  SEC              AREA   0.00000E+00  SQ CM              AXIAL POSITION   0.00000E+00  CM

   FLOW PROPERTIES                                                  INTEGRATION INDICATORS
     PRESSURE                  1.00000                                STEPS FROM LAST PRINT                0
      (ATM)
     VELOCITY                  0.00                                   AVERAGE STEP SIZE             0.00000E+00
      (CM/SEC)
     DENSITY                1.21868E-05                               METHOD ORDER                         0
      (G/CM**3)
     TEMPERATURE              1000.00
      (DEG K)
     MASS FLOW RATE         0.00000E+00                              TOTAL NUMBER OF STEPS                0
      (G/SEC)
     ENTROPY                   34.5388                               FUNCT EVALUATIONS                    0
      (CAL/G/DEG K)
     MACH NUMBER                0.0000                               JACOBIAN EVALUATIONS                 0

     GAMMA                      1.6596

     ENTHALPY               5.00000E+03
      (CAL/G)
     SP. HEAT (CP)          5.00000E+00
      (CAL/G/DEG K)
```

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
DUMR	1.21868E-05	1.00000E+00	-1.21868E-02	1	1.0000E+03	8.20560E+07	1.00000
DUMP	0.00000E+00	0.00000E+00	1.21868E-02				

```
   DERIVATIVES (CGS UNITS): T            1.00000E+06    RHO          -1.21868E-02

   MIXTURE MOLECULAR WEIGHT       1.00000      TOTAL ENERGY EXCHANGE RATE    -4.10280E+11       MASS FRACTION SUM    1.00000000
                                                  (CAL-CM**3/G**2/SEC)

                        CPU TIME FOR INITIALIZATION OF LSENS =      0.359999 S
```

TABLE E.2.—Continued.
(g) Continued.

```
TIME   1.00000E-02  SEC              AREA   0.00000E+00  SQ CM              AXIAL POSITION   0.00000E+00  CM

    FLOW PROPERTIES                                                  INTEGRATION INDICATORS

      PRESSURE                  1.00000                                STEPS FROM LAST PRINT              69
       (ATM)
      VELOCITY                  0.00                                   AVERAGE STEP SIZE             0.14541E-03
       (CM/SEC)
      DENSITY              6.09842E-06                                 METHOD ORDER                        4
       (G/CM**3)
      TEMPERATURE              2000.00
       (DEG K)
      MASS FLOW RATE       0.00000E+00                                 TOTAL NUMBER OF STEPS              84
       (G/SEC)
      ENTROPY                  38.0045                                 FUNCT EVALUATIONS                 101
       (CAL/G/DEG K)
      MACH NUMBER               0.0000                                 JACOBIAN EVALUATIONS               13

      GAMMA                     1.6596

      ENTHALPY             5.00000E+03
       (CAL/G)
      SP. HEAT (CP)        5.00000E+00
       (CAL/G/DEG K)

                                          CHEMICAL PROPERTIES

SPECIES    CONCENTRATION   MOLE FRACTION   NET SPECIES PRODUCTION  REACTION   RATE CONST   NET REACTION CONV RATE   NET RATE/POSI-
           (MOLES/CM**3)                   RATE (MOLE/CM**3/SEC)   NUMBER     CGS  UNITS   (MOLE-CM**3/G**2/SEC)     TIVE DIR RATE
 DUMR       2.47386E-14     4.05656E-09          -4.94773E-11        1        2.0000E+03        1.33036E+00                1.00000
 DUMP       6.09842E-06     1.00000E+00           4.94773E-11

   DERIVATIVES (CGS UNITS): T            8.11312E-03    RHO          -2.47386E-11

   MIXTURE MOLECULAR WEIGHT      1.00000     TOTAL ENERGY EXCHANGE RATE   -6.65182E+03       MASS FRACTION SUM    1.00000000
                                                (CAL-CM**3/G**2/SEC)
```

```
COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP -  3.199997E-01  S     UP TO THIS TIME -  4.000015E-01  S

                                                  ***** SENSITIVITY CALCULATIONS *****
                                                          TIME =   1.00000D-02
                                  SENSITIVITY COEFFICIENTS OF  0-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES

**** SENSITIVITY TO INITIAL CONDITIONS ****

        DZ(I)/DYZERO(J)*F(J)/Z(I), WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW
                                          F(J)= YZERO(J) FOR YZERO(J) NOT EQUAL TO 0
                                              = 1.0E-4/(INITIAL MWT)  FOR YZERO(J) = 0

PARAMETER    DUMR        DUMP        TEMP        DENSITY

DUMR        1.002D+00  1.000D+00 -2.952D-05  2.976D-05
DUMP        9.553D-04  1.000D-04 -5.000D-05  4.990D-05
TEMP       -1.054D+01  4.275D-08  5.000D-01  4.985D-01
DENSITY     0.000D+00  0.000D+00  0.000D+00  1.000D+00

**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE PREEXPONENTIAL CONSTANTS ****
          DZ(I)/DA(J)*A(J)/Z(I) WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW

REAC NUM     DUMR        DUMP        TEMP        DENSITY
     1     -2.009D+01  8.150D-08  4.075D-08 -4.520D-04

**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE TEMPERATURE EXPONENTS ****
          DZ(I)/DN(J)/[Z(I)*LN(T0)] WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW

REAC NUM     DUMR        DUMP        TEMP        DENSITY
     1     -2.199D+01  8.920D-08  4.460D-08 -3.899D-04

**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE ACTIVATION ENERGIES ****
          DZ(I)/DE(J)*[-R*T0/Z(I)], WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW

REAC NUM     DUMR        DUMP        TEMP        DENSITY
     1     -1.054D+01  4.275D-08  2.138D-08 -7.495D-04
```

TABLE E.2.—Continued.
(g) Concluded.

```
                    ***** SENSITIVITY CALCULATIONS *****
                              TIME =   1.00000D-02
          SENSITIVITY COEFFICIENTS OF  1-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES

**** SENSITIVITY TO INITIAL CONDITIONS ****
      DZ(I)/DYZERO(J)*F(J)/Z(I), WHERE Z(I)= 1-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW
                                       F(J)= YZERO(J) FOR YZERO(J) NOT EQUAL TO 0
                                           = 1.0E-4/(INITIAL MWT)  FOR YZERO(J) = 0

PARAMETER    DUMR        DUMP        TEMP        DENSITY

DUMR        1.002D+00  1.002D+00  1.635D-03  1.694D-03
DUMP        9.037D-04  9.037D-04  8.037D-04  9.036D-04
TEMP       -1.002D+01 -1.002D+01 -1.002D+01 -1.002D+01
DENSITY     0.000D+00  0.000D+00  0.000D+00  1.000D+00


     **** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE PREEXPONENTIAL CONSTANTS ****
          DZ(I)/DA(J)*A(J)/Z(I) WHERE Z(I)= 1-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW

     REAC NUM     DUMR        DUMP        TEMP        DENSITY
        1      -1.906D+01 -1.906D+01 -1.906D+01 -1.906D+01


    **** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE TEMPERATURE EXPONENTS ****
         DZ(I)/DN(J)/[Z(I)*LN(T0)] WHERE Z(I)= 1-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW

    REAC NUM     DUMR        DUMP        TEMP        DENSITY
        1      -2.086D+01 -2.086D+01 -2.086D+01 -2.086D+01


     **** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE ACTIVATION ENERGIES ****
          DZ(I)/DE(J)*[-R*T0/Z(I)], WHERE Z(I)= 1-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW

     REAC NUM     DUMR        DUMP        TEMP        DENSITY
        1      -1.002D+01 -1.002D+01 -1.002D+01 -1.002D+01


     (LSENS)     END OF THIS CASE

                 SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:
                    TOTAL NO. OF STEPS -                        84
                    TOTAL NO. OF DERIVATIVE EVALUATIONS -      101
                    TOTAL NO. OF JACOBIAN EVALUATIONS -         13
                    TOTAL CPU TIME -                      0.400002 S


                 WORK REQUIRED BY SENSITIVITY ROUTINE:
                      NO. STEPS =                84
                      NO. FUNC. EVAL. =          84
                      NO. JAC. EVAL. =           84
                      TOTAL REAL     SPACE USED =          264
                      TOTAL INTEGER SPACE USED =            48

                              TOTAL CPU TIME (INCLUDING I/O) REQUIRED =       0.980000 S


     (LSENS)     READ DATA FOR NEXT CASE
```

TABLE E.2.—Continued.

(h) Case 8

TIME-PRESSURE VERSION LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

HYDROGEN COMBUSTION IN STANDARD AIR AT 3.10 ATM. CASE 8

REACTION NUMBER	REACTION							REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1*CO	+	1*O	=	1*CO2	+	M	5.88800E+15	0.0000	4100.00
2	1*CO	+	1*O2	=	1*CO2	+	1*O	2.51200E+12	0.0000	47690.00
3	1*CO	+	1*OH	=	1*CO2	+	1*H	4.16900E+11	0.0000	1000.00
4	1*CO	+	1*HO2	=	1*CO2	+	1*OH	5.75400E+13	0.0000	22930.00
5	1*O	+	1*H2O	=	2*OH			6.80000E+13	0.0000	18365.00
6	1*H	+	1*O2	=	1*OH	+	1*O	1.89000E+14	0.0000	16400.00
7	1*O	+	1*H2	=	1*OH	+	1*H	4.20000E+14	0.0000	13750.00
8	1*H	+	1*HO2	=	1*H2	+	1*O2	7.28000E+13	0.0000	2126.00
9	1*O	+	1*HO2	=	1*OH	+	1*O2	5.00000E+13	0.0000	1000.00
10	1*HO2	+	1*OH	=	1*H2O	+	1*O2	8.00000E+12	0.0000	0.00
11	1*H	+	1*HO2	=	2*OH			1.34000E+14	0.0000	1070.00
12	1*H2	+	1*HO2	=	1*H2O2	+	1*H	7.91000E+13	0.0000	25000.00
13	1*OH	+	1*H2O2	=	1*H2O	+	1*HO2	6.10000E+12	0.0000	1430.00
14			2*HO2	=	1*H2O2	+	1*O2	1.80000E+12	0.0000	0.00
15	1*H	+	1*H2O2	=	1*OH	+	1*H2O	7.80000E+11	0.0000	0.00
16	M	+	1*H2O2	=	2*OH			1.44000E+17	0.0000	45510.00
17	1*H2	+	1*OH	=	1*H2O	+	1*H	4.74000E+13	0.0000	6098.00
18	1*H	+	1*O2	=	1*HO2	+	M	1.46000E+15	0.0000	-1000.00
19	M	+	1*H2O	=	1*H	+	1*OH	1.30000E+15	0.0000	105140.00
20	1*H	+	1*O	=	1*OH	+	M	7.10000E+18	-1.0000	0.00
21	M	+	1*H2	=	2*H			2.20000E+14	0.0000	96000.00
22	M	+	1*O2	=	2*O			1.80000E+18	-1.0000	118020.00
23	1*HO2	+	1*NO	=	1*NO2	+	1*OH	2.09000E+12	0.0000	-477.00
24	1*O	+	1*NO2	=	1*NO	+	1*O2	1.00000E+13	0.0000	596.00
25	1*NO	+	1*O	=	1*NO2	+	M	5.62000E+15	0.0000	-1160.00
26	1*NO2	+	1*H	=	1*NO	+	1*OH	3.47000E+14	0.0000	1470.00
27	1*NO	+	1*O	=	1*N	+	1*O2	3.80000E+09	1.0000	41370.00
28	1*O	+	1*N2	=	1*NO	+	1*N	1.80000E+14	0.0000	76250.00
29	1*NO	+	1*H	=	1*N	+	1*OH	2.63000E+14	0.0000	50410.00
30	M	+	1*N2O	=	1*N2	+	1*O	6.92000E+23	-2.5000	65000.00
31	1*O	+	1*N2O	=	1*N2	+	1*O2	1.00000E+14	0.0000	28020.00
32	1*O	+	1*N2O	=	2*NO			6.92000E+13	0.0000	26630.00
33	1*N	+	1*NO2	=	2*NO			4.00000E+12	0.0000	0.00
34	1*N2O	+	1*H	=	1*N2	+	1*OH	7.59000E+13	0.0000	15100.00
35	1*NO2	+	1*H2	=	1*HNO2	+	1*H	2.40000E+13	0.0000	29000.00
36	1*OH	+	1*NO2	=	1*HNO3	+	M	3.00000E+15	0.0000	-3800.00
37	1*OH	+	1*NO	=	1*HNO2	+	M	5.60000E+15	0.0000	-1700.00
38	1*HNO	+	1*H	=	1*H2	+	1*NO	5.00000E+12	0.0000	0.00
39	1*H	+	1*NO	=	1*HNO	+	M	5.40000E+15	0.0000	-600.00
40	1*HNO	+	1*OH	=	1*H2O	+	1*NO	3.60000E+13	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2 , 16) =	2.30000	M(O2 , 16) =	0.78000	M(H2O , 16) =	6.00000	M(H2O2 , 16) =	6.60000
M(O2 , 18) =	1.30000	M(N2 , 18) =	1.30000	M(H2O , 18) =	21.30000	M(H2 , 18) =	5.00000
M(H2 , 19) =	4.00000	M(O2 , 19) =	1.50000	M(H2O , 19) =	20.00000	M(N2 , 19) =	1.50000
M(H2 , 21) =	4.10000	M(O2 , 21) =	2.00000	M(H2O , 21) =	15.00000	M(N2 , 21) =	2.00000
M(O2 , 36) =	0.70000	M(H2 , 36) =	1.40000				

** INITIAL CONDITIONS **

TIME 0.00000E+00 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	3.10000
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	8.35179E-04
TEMPERATURE (DEG K)	950.66
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	2.3811
MACH NUMBER	0.0000
GAMMA	1.3514
ENTHALPY (CAL/G)	2.28819E+02
SP. HEAT (CP) (CAL/G/DEG K)	3.63657E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

TABLE E.2.—Continued.
(h) Continued.

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CO	0.00000E+00	0.00000E+00	9.55759E-25
O	0.00000E+00	0.00000E+00	4.21098E-11
CO2	8.40100E-09	2.11400E-04	-9.55759E-25
O2	5.86721E-06	1.47640E-01	-3.39182E-09
OH	0.00000E+00	0.00000E+00	0.00000E+00
H	0.00000E+00	0.00000E+00	3.35098E-09
HO2	0.00000E+00	0.00000E+00	3.34971E-09
H2O	0.00000E+00	0.00000E+00	0.00000E+00
H2	1.17341E-05	2.95273E-01	-3.35098E-09
H2O2	0.00000E+00	0.00000E+00	0.00000E+00
NO	1.78829E-07	4.50000E-03	-4.33823E-11
NO2	0.00000E+00	0.00000E+00	4.21096E-11
N	0.00000E+00	0.00000E+00	7.51490E-21
N2	2.16903E-05	5.45807E-01	-6.35262E-22
N2O	0.00000E+00	0.00000E+00	1.21953E-16
HNO2	0.00000E+00	0.00000E+00	0.00000E+00
HNO3	0.00000E+00	0.00000E+00	0.00000E+00
HNO	0.00000E+00	0.00000E+00	1.27237E-12
AR	2.61015E-07	6.56810E-03	0.00000E+00

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	6.7206E+14	-1.37022E-18	1.00000
2	2.7317E+01	0.00000E+00	0.00000
3	2.4555E+11	0.00000E+00	0.00000
4	3.0799E+08	0.00000E+00	0.00000
5	4.0788E+09	0.00000E+00	0.00000
6	3.2079E+10	0.00000E+00	0.00000
7	2.8988E+11	0.00000E+00	0.00000
8	2.3625E+13	-4.80228E-03	1.00000
9	2.9449E+13	0.00000E+00	0.00000
10	8.0000E+12	0.00000E+00	0.00000
11	7.6054E+13	0.00000E+00	0.00000
12	1.4153E+08	0.00000E+00	0.00000
13	2.8614E+12	0.00000E+00	0.00000
14	1.8000E+12	0.00000E+00	0.00000
15	7.8000E+11	0.00000E+00	0.00000
16	4.9653E+06	0.00000E+00	0.00000
17	1.8789E+12	0.00000E+00	0.00000
18	2.4788E+15	0.00000E+00	0.00000
19	8.7705E-10	0.00000E+00	0.00000
20	7.4685E+15	0.00000E+00	0.00000
21	1.8738E-08	3.26799E-11	1.00000
22	1.3974E-12	4.67100E-16	1.00000
23	2.6903E+12	0.00000E+00	0.00000
24	7.2943E+12	-6.03702E-05	1.00000
25	1.0385E+16	0.00000E+00	0.00000
26	1.5936E+14	0.00000E+00	0.00000
27	1.1147E+03	0.00000E+00	0.00000
28	5.3205E-04	0.00000E+00	0.00000
29	6.7774E+02	0.00000E+00	0.00000
30	2.8315E+01	0.00000E+00	0.00000
31	3.6175E+07	-9.10738E-16	1.00000
32	5.2247E+07	-1.74836E-10	1.00000
33	4.0000E+12	-1.07737E-14	1.00000
34	2.5637E+10	0.00000E+00	0.00000
35	5.1680E+06	0.00000E+00	0.00000
36	2.2424E+16	0.00000E+00	0.00000
37	1.3772E+16	0.00000E+00	0.00000
38	5.0000E+12	-1.82412E-06	1.00000
39	7.4187E+15	0.00000E+00	0.00000
40	3.6000E+13	0.00000E+00	0.00000

DERIVATIVES (CGS UNITS): T -5.88487E-01 RHO 5.17001E-07

MIXTURE MOLECULAR WEIGHT 21.01616 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 2.55482E+02 MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 1.260000 S

TIME 2.00000E-04 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	3.10000
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	3.51245E-04
TEMPERATURE (DEG K)	2541.16
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	2.6303
MACH NUMBER	0.0000
GAMMA	1.2550
ENTHALPY (CAL/G)	2.28818E+02
SP. HEAT (CP) (CAL/G/DEG K)	4.13930E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	132
AVERAGE STEP SIZE	0.15001E-06
METHOD ORDER	3
TOTAL NUMBER OF STEPS	228
FUNCT EVALUATIONS	379
JACOBIAN EVALUATIONS	39

TABLE E.2.—Continued.

(h) Continued.

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
CO	1.67166E-09	1.12439E-04	6.63430E-06	1	2.6143E+15	4.41273E+01	0.95189
O	8.80256E-08	5.92079E-03	-4.92577E-03	2	1.9883E+08	-3.58042E-02	0.05288
CO2	1.86148E-09	1.25207E-04	-6.63430E-06	3	3.4200E+11	-9.94751E+01	0.05779
O2	2.38044E-07	1.60113E-02	-6.95371E-03	4	6.1362E+11	1.60922E+00	0.76161
OH	3.50002E-07	2.35419E-02	-4.81197E-03	5	1.7908E+12	-2.91878E+03	0.00057
H	2.40937E-07	1.62060E-02	-1.48576E-02	6	7.3451E+12	1.77058E+04	0.00519
HO2	2.54128E-10	1.70932E-05	-9.33737E-06	7	2.7586E+13	4.27096E+04	0.00352
H2O	4.02200E-06	2.70528E-01	2.36563E-02	8	4.7784E+13	1.83418E+04	0.77342
H2	6.17267E-07	4.15187E-02	-1.38113E-02	9	4.1017E+13	5.75800E+03	0.77422
H2O2	3.08090E-11	2.07228E-06	-3.37934E-06	10	8.0000E+12	4.46611E+03	0.77435
NO	7.51649E-08	5.05575E-03	2.46971E-05	11	1.0841E+14	4.17194E+04	0.77539
NO2	1.68514E-11	1.13346E-06	3.36730E-07	12	5.5986E+11	-2.73562E+03	0.79352
N	1.14996E-11	7.73489E-07	2.63812E-07	13	4.5956E+12	3.19073E+02	0.79436
N2	9.12211E-06	6.13572E-01	-1.07127E-05	14	1.8000E+12	-9.16922E-02	0.08868
H2O	4.13216E-12	2.77938E-07	1.75265E-07	15	7.8000E+11	4.47630E+01	0.95381
HNO2	4.34027E-12	2.91936E-07	-3.94736E-07	16	1.7552E+13	-3.07215E+03	0.01924
HNO3	1.74341E-16	1.17265E-11	-1.69994E-11	17	1.4169E+13	1.01255E+05	0.00408
HNO	3.67249E-11	2.47019E-06	-3.82810E-06	18	1.7797E+15	6.73114E+04	0.79925
AR	1.09773E-07	7.38358E-03	0.00000E+00	19	1.1789E+06	-7.92304E+04	0.95470
				20	2.7940E+15	6.81717E+03	0.95467
				21	1.2191E+06	-1.05533E+04	0.95451
				22	5.0125E+04	-3.01206E+01	0.95444
				23	2.2970E+12	1.55124E+02	0.43618
				24	8.8867E+12	6.40614E+01	0.59956
				25	7.0713E+15	4.99663E+03	0.88622
				26	2.5936E+14	5.13517E+03	0.60163
				27	2.6720E+09	-6.85876E+00	0.04568
				28	4.9828E+07	8.46624E+01	0.26106
				29	1.2148E+10	-7.56614E+01	0.04070
				30	5.4610E+09	-2.13127E+01	0.88685
				31	3.8920E+11	6.85923E-01	0.59734
				32	3.5467E+11	7.48739E-01	0.71605
				33	4.0000E+12	3.88187E-03	0.61785
				34	3.8158E+12	1.84579E+01	0.59943
				35	7.6930E+10	-5.02127E+01	0.88560
				36	6.3670E+15	-1.37789E-04	0.00003
				37	7.8414E+15	4.70131E+01	0.00189
				38	5.0000E+12	3.35707E+02	0.93615
				39	6.0813E+15	3.81689E+03	0.28760
				40	3.6000E+13	3.51221E+03	0.93641

DERIVATIVES (CGS UNITS): T 1.77523E+07 RHO -1.94094E+00

MIXTURE MOLECULAR WEIGHT 23.62546 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) -2.00893E+10 MASS FRACTION SUM 1.00000010

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 9.860001E+00 S UP TO THIS TIME - 1.659000E+01 S

***** SENSITIVITY CALCULATIONS *****

TIME = 2.00000D-04

SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES

**** SENSITIVITY TO INITIAL CONDITIONS ****

DZ(I)/DYZERO(J)*F(J)/Z(I), WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW
F(J)= YZERO(J) FOR YZERO(J) NOT EQUAL TO 0
= 1.0E-4/(INITIAL MWT) FOR YZERO(J) = 0

PARAMETER	CO	CO2	OH	H2O	H2	NO	TEMP
CO	5.195D-01	4.313D-01	1.378D-04	-2.015D-04	9.540D-04	-9.365D-06	-1.229D-04
H2	1.336D+00	-1.199D+00	8.467D-01	1.506D-01	5.383D+00	-3.852D-02	-3.705D-01
O2	-8.292D-01	7.447D-01	3.077D-01	9.769D-01	-4.887D+00	6.952D-02	8.772D-01
HO2	2.138D+03	-1.920D+03	-7.454D+03	3.176D+03	-1.209D+04	1.767D+02	3.770D+03
H2O2	1.562D+01	-1.403D+01	-5.446D+01	2.321D+01	-8.834D+01	1.291D+00	2.755D+01
NO	2.729D-01	-2.451D-01	-9.933D-01	4.218D-01	-1.605D+00	1.012D+00	4.977D-01
TEMP	1.108D+01	-9.946D+00	-3.656D+01	1.577D+01	-6.004D+01	8.958D-01	1.906D+01
DENSITY	-8.695D-02	7.808D-02	-2.351D-01	9.916D-02	-3.758D-01	4.545D-03	1.181D-01

TIME = 2.00000E-04

*** REACTION IMPORTANCE FOR NORMALIZED SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF Y(I) WRT PREEXPONENTIAL CONSTANTS ***

VARIABLE	REACTION NUMBER					
	NORMALIZED SENSITIVITY COEFFICIENT					
CO	6	18	8	11	17	5
	1.018E+00	-6.199E-01	-1.402E-01	1.182E-01	6.086E-02	6.243E-05
CO2	6	18	8	11	17	5
	-9.145E-01	5.567E-01	1.259E-01	-1.062E-01	-5.465E-02	-5.606E-05
OH	6	18	8	11	17	5
	-3.553E+00	1.982E+00	4.869E-01	-4.191E-01	-2.056E-01	1.257E-05

TABLE E.2.—Continued.
(h) Concluded.

H2O	6	18	8	11	17	5
	1.515E+00	-8.443E-01	-2.079E-01	1.794E-01	8.754E-02	-3.079E-05
H2	6	18	8	11	17	5
	-5.766E+00	3.213E+00	7.919E-01	-6.835E-01	-3.338E-01	1.283E-04
NO	6	18	8	11	17	5
	8.430E-02	-4.704E-02	-1.159E-02	9.979E-03	4.847E-03	-2.308E-06
TEMP	6	18	8	11	17	5
	1.798E+00	-1.002E+00	-2.467E-01	2.128E-01	1.038E-01	-3.873E-05

*** REACTION IMPORTANCE FOR NORMALIZED SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF Y(I) WRT ACTIVATION ENERGIES ***

VARIABLE	REACTION NUMBER NORMALIZED SENSITIVITY COEFFICIENT					
CO	6	18	8	11	17	5
	9.973E-01	-5.887E-01	-1.316E-01	1.120E-01	5.767E-02	2.268E-05
CO2	6	18	8	11	17	5
	-8.956E-01	5.286E-01	1.181E-01	-1.006E-01	-5.179E-02	-2.037E-05
OH	6	18	8	11	17	5
	-3.478E+00	1.977E+00	4.579E-01	-3.933E-01	-1.981E-01	3.077E-05
H2O	6	18	8	11	17	5
	1.482E+00	-8.421E-01	-1.953E-01	1.679E-01	8.438E-02	-2.263E-05
H2	6	18	8	11	17	5
	-5.643E+00	3.205E+00	7.436E-01	-6.393E-01	-3.214E-01	9.026E-05
NO	6	18	8	11	17	5
	8.249E-02	-4.686E-02	-1.087E-02	9.341E-03	4.685E-03	-1.573E-06
TEMP	6	18	8	11	17	5
	1.759E+00	-9.995E-01	-2.318E-01	1.992E-01	1.001E-01	-2.767E-05

(LSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

TOTAL NO. OF STEPS - 228
TOTAL NO. OF DERIVATIVE EVALUATIONS - 379
TOTAL NO. OF JACOBIAN EVALUATIONS - 39
TOTAL CPU TIME - 16.590000 S

WORK REQUIRED BY SENSITIVITY ROUTINE:

NO. STEPS = 228
NO. FUNC. EVAL. = 228
NO. JAC. EVAL. = 228
TOTAL REAL SPACE USED = 3424
TOTAL INTEGER SPACE USED = 80

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 18.650002 S

(LSENS) READ DATA FOR NEXT CASE

TABLE E.2.—Continued.

(i) Case 9

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

BENZENE-OXYGEN-AR SHOCK IGNITION - WITH SENSITIVITY MECHANISM K-70 CASE 9

REACTION NUMBER	REACTION								REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1*C6H6	+	1*O2	=	1*C6H5O	+	1*OH		4.00000E+13	0.0000	34000.00
2	1*C6H6	+	1*C6H5	=	1*C12H10	+	1*H		4.00000E+11	0.0000	4000.00
3			1*C6H6	=	1*C6H5	+	1*H		1.00000E+16	0.0000	108000.00
4	1*C6H6	+	1*H	=	1*C6H5	+	1*H2		2.50000E+14	0.0000	16000.00
5	1*C6H6	+	1*O	=	1*C6H5O	+	1*H		2.78300E+13	0.0000	4910.00
6	1*C6H6	+	1*OH	=	1*C6H5	+	1*H2O		2.13200E+13	0.0000	4580.00
7	M	+	1*C4H3	=	1*C4H2	+	1*H		1.00000E+16	0.0000	60000.00
8			1*C6H5O	=	1*C5H5	+	1*CO		2.51000E+11	0.0000	43900.00
9	1*C6H5	+	1*O2	=	1*C6H5O	+	1*O		2.10000E+12	0.0000	7470.00
10	1*C6H5	+	1*HO2	=	1*C6H5O	+	1*OH		2.00000E+13	0.0000	1000.00
11			1*C6H5	=	1*C4H3	+	1*C2H2		4.50000E+13	0.0000	72530.00
12			1*C6H5OH	=	1*C6H5O	+	1*H		2.00000E+16	0.0000	88000.00
13	1*C6H5OH	+	1*H	=	1*C6H6	+	1*OH		2.20000E+13	0.0000	7910.00
14	1*C6H5OH	+	1*H	=	1*C6H5O	+	1*H2		1.15000E+14	0.0000	12405.00
15	1*C5H5	+	1*C6H5OH	=	1*C6H5O	+	1*C5H6		2.67000E+14	0.0000	25227.00
16			1*C5H6	=	1*C5H5	+	1*H		8.13000E+24	-2.9810	78682.00
17	1*C5H6	+	1*O2	=	1*C5H5O	+	1*OH		1.00000E+13	0.0000	20712.00
18	1*C6H5OH	+	1*OH	=	1*C6H5O	+	1*H2O		3.00000E+13	0.0000	0.00
19	1*C6H5OH	+	1*HO2	=	1*C6H5O	+	1*H2O2		3.00000E+13	0.0000	1500.00
20			1*C5H5O	=	1*C4H5	+	1*CO		3.00000E+16	0.0000	15000.00
21	1*C5H5	+	1*O	=	1*C5H5O				1.00000E+13	0.0000	0.00
22	1*C5H5	+	1*OH	=	1*C5H4OH	+	1*H		1.00000E+13	0.0000	0.00
23			1*C5H4OH	=	1*C4H4	+	1*HCO		1.00000E+15	0.0000	22000.00
24	1*C5H5	+	1*HO2	=	1*C5H5O	+	1*OH		2.00000E+13	0.0000	0.00
25			2*C6H5	=	1*C12H10				3.10000E+12	0.0000	0.00
26			1*C4H5	=	1*C2H3	+	1*C2H2		1.40000E+13	0.0000	32900.00
27	1*C4H2	+	1*O	=	1*C2HO	+	1*C2H		1.00000E+13	0.0000	0.00
28	1*C4H2	+	1*OH	=	1*HCO	+	1*C3H2		3.00000E+13	0.0000	0.00
29	1*C4H2	+	1*O	=	1*CO	+	1*C3H2		1.20000E+12	0.0000	0.00
30	M	+	1*C2H4	=	1*C2H2	+	1*H2		9.33000E+16	0.0000	77200.00
31	1*C2H4	+	1*OH	=	1*C2H3	+	1*H2O		4.78600E+12	0.0000	1230.00
32	1*C2H4	+	1*O	=	1*CH3	+	1*HCO		3.31100E+12	0.0000	1130.00
33	1*C2H4	+	1*O	=	1*CH2O	+	1*CH2		2.51200E+13	0.0000	5000.00
34	1*C2H4	+	1*OH	=	1*CH3	+	1*CH2O		1.99500E+12	0.0000	960.00
35	M	+	1*C2H3	=	1*C2H2	+	1*H		3.00000E+15	0.0000	32000.00
36	1*C2H3	+	1*O2	=	1*CH2O	+	1*HCO		3.98000E+12	0.0000	-250.00
37	1*C2H3	+	1*H	=	1*C2H2	+	1*H2		6.00000E+12	0.0000	0.00
38	1*C2H3	+	1*OH	=	1*C2H2	+	1*H2O		5.01200E+12	0.0000	0.00
39	1*C2H3	+	1*CH2	=	1*C2H2	+	1*CH3		3.02000E+13	0.0000	0.00
40	1*C2H3	+	1*C2H	=	2*C2H2				3.02000E+13	0.0000	0.00
41	1*C2H3	+	1*O	=	1*C2H2O	+	1*H		3.30000E+13	0.0000	0.00
42			2*CH2	=	1*C2H2	+	1*H2		4.00000E+13	0.0000	0.00
43			2*CH2	=	1*C2H3	+	1*H		5.01200E+12	0.0000	0.00
44	1*CH2	+	1*OH	=	1*CH	+	1*H2O		2.51000E+11	0.6700	25700.00
45	1*CH2	+	1*O	=	1*CH	+	1*OH		2.00000E+11	0.6800	25000.00
46	1*CH2	+	1*O2	=	1*CO2	+	2*H		1.59000E+12	0.0000	1000.00
47	M	+	1*C2H2	=	1*C2H	+	1*H		4.16900E+16	0.0000	107000.00
48			2*C2H2	=	1*C4H3	+	1*H		2.00000E+12	0.0000	45900.00
49	1*C2H2	+	1*O	=	1*CH2	+	1*CO		1.60000E+14	0.0000	9890.00
50	1*C2H2	+	1*O	=	1*C2HO	+	1*H		4.00000E+14	0.0000	10660.00
51	1*C2H2	+	1*OH	=	1*C2H	+	1*H2O		6.31000E+12	0.0000	7000.00

TABLE E.2.—Continued.

(i) Continued.

52	1*C2H2	+	1*OH	=	1*C2H2O	+	1*H	3.20000E+11	0.0000	200.00
53	1*C2H2	+	1*C2H	=	1*C4H2	+	1*H	3.00000E+13	0.0000	0.00
54	1*C2H2	+	1*CH2	=	1*C3H3	+	1*H	1.20000E+13	0.0000	6600.00
55	M	+	1*C3H4	=	1*C3H3	+	1*H	2.00000E+17	0.0000	65000.00
56	1*C2H2O	+	1*OH	=	1*CH2O	+	1*HCO	2.80000E+13	0.0000	0.00
57	1*C2H2O	+	1*OH	=	1*C2HO	+	1*H2O	7.50000E+12	0.0000	3000.00
58	1*C2H2O	+	1*H	=	1*CH3	+	1*CO	1.13000E+13	0.0000	3428.00
59	1*C2H2O	+	1*H	=	1*C2HO	+	1*H2	7.50000E+13	0.0000	8000.00
60	1*C2H2O	+	1*O	=	1*C2HO	+	1*OH	5.00000E+13	0.0000	8000.00
61	1*C2H2O	+	1*O	=	1*CH2O	+	1*CO	2.00000E+13	0.0000	0.00
62	M	+	1*C2H2O	=	1*CH2	+	1*CO	2.00000E+16	0.0000	60000.00
63	1*C2HO	+	1*O2	=	2*CO	+	1*OH	1.46000E+12	0.0000	2500.00
64	1*C2HO	+	1*O	=	2*CO	+	1*H	1.20200E+12	0.0000	0.00
65	1*C2HO	+	1*OH	=	2*HCO			1.00000E+13	0.0000	0.00
66	1*C2HO	+	1*H	=	1*CH2	+	1*CO	5.00000E+13	0.0000	0.00
67	1*C2HO	+	1*CH2	=	1*C2H3	+	1*CO	3.00000E+13	0.0000	0.00
68	1*C2HO	+	1*CH2	=	1*CH2O	+	1*C2H	1.00000E+13	0.0000	2000.00
69			2*C2HO	=	1*C2H2	+	2*CO	1.00000E+13	0.0000	0.00
70	1*C2H	+	1*OH	=	1*C2HO	+	1*H	2.00000E+13	0.0000	0.00
71	1*C2H	+	1*O2	=	1*C2HO	+	1*O	5.00000E+13	0.0000	1500.00
72	1*C2H	+	1*O	=	1*CO	+	1*CH	5.01200E+13	0.0000	0.00
73	M	+	1*CH4	=	1*CH3	+	1*H	2.00000E+17	0.0000	88000.00
74	1*CH4	+	1*O2	=	1*CH3	+	1*HO2	7.94300E+13	0.0000	56000.00
75	1*CH4	+	1*H	=	1*CH3	+	1*H2	1.26000E+14	0.0000	11900.00
76	1*OH	+	1*CH4	=	1*CH3	+	1*H2O	2.50000E+13	0.0000	5010.00
77	1*O	+	1*CH4	=	1*CH3	+	1*OH	1.90000E+14	0.0000	11720.00
78	1*CH3	+	1*O2	=	1*CH3O	+	1*O	4.78600E+13	0.0000	29000.00
79	1*CH3	+	1*OH	=	1*CH3O	+	1*H	6.30000E+12	0.0000	0.00
80	M	+	1*CH3O	=	1*CH2O	+	1*H	5.00000E+13	0.0000	21000.00
81	1*CH3O	+	1*O2	=	1*CH2O	+	1*HO2	1.00000E+12	0.0000	6000.00
82	1*CH3O	+	1*H	=	1*CH2O	+	1*H2	2.00000E+13	0.0000	0.00
83			2*CH3	=	1*C2H4	+	1*H2	1.00000E+16	0.0000	32000.00
84	1*CH3	+	1*O	=	1*CH2O	+	1*H	1.28800E+14	0.0000	2000.00
85	1*CH3	+	1*CH2O	=	1*CH4	+	1*HCO	1.00000E+10	0.5000	6000.00
86	1*CH3	+	1*HCO	=	1*CH4	+	1*CO	3.02000E+11	0.5000	0.00
87	1*CH3	+	1*HO2	=	1*CH3O	+	1*OH	2.00000E+13	0.0000	0.00
88	M	+	1*CH2O	=	1*HCO	+	1*H	5.00000E+16	0.0000	81000.00
89	1*CH2O	+	1*OH	=	1*HCO	+	1*H2O	3.00000E+13	0.0000	1200.00
90	1*CH2O	+	1*H	=	1*HCO	+	1*H2	2.50000E+13	0.0000	3990.00
91	1*CH2O	+	1*O	=	1*HCO	+	1*OH	3.50000E+13	0.0000	3510.00
92	1*HCO	+	1*HO2	=	1*CH2O	+	1*O2	1.00000E+14	0.0000	3000.00
93	M	+	1*HCO	=	1*H	+	1*CO	2.94000E+14	0.0000	15569.00
94	1*HCO	+	1*O2	=	1*CO	+	1*HO2	3.31100E+12	0.0000	7000.00
95	1*HCO	+	1*OH	=	1*CO	+	1*H2O	1.00000E+14	0.0000	0.00
96	1*HCO	+	1*H	=	1*CO	+	1*H2	1.99500E+14	0.0000	0.00
97	1*HCO	+	1*O	=	1*CO	+	1*OH	1.00000E+14	0.0000	0.00
98	1*CH	+	1*O2	=	1*HCO	+	1*O	1.00000E+13	0.0000	0.00
99	1*CO	+	1*O	=	1*CO2	+	M	5.90000E+15	0.0000	4100.00
100	1*CO	+	1*O2	=	1*CO2	+	1*O	2.50000E+12	0.0000	47690.00
101	1*CO	+	1*OH	=	1*CO2	+	1*H	4.17000E+11	0.0000	1000.00
102	1*CO	+	1*HO2	=	1*CO2	+	1*OH	5.75000E+13	0.0000	22930.00
103	1*O	+	1*H2O	=	2*OH			6.80000E+13	0.0000	18365.00
104	1*H	+	1*O2	=	1*OH	+	1*O	1.89000E+14	0.0000	16400.00
105	1*O	+	1*H2	=	1*OH	+	1*H	4.20000E+14	0.0000	13750.00
106	1*H	+	1*HO2	=	1*H2	+	1*O2	7.28000E+13	0.0000	2126.00
107	1*O	+	1*HO2	=	1*OH	+	1*O2	5.00000E+13	0.0000	1000.00
108	1*HO2	+	1*OH	=	1*H2O	+	1*O2	8.00000E+12	0.0000	0.00
109	1*H	+	1*HO2	=	2*OH			1.34000E+14	0.0000	1070.00
110	1*H2	+	1*HO2	=	1*H2O2	+	1*H	7.91000E+13	0.0000	25000.00
111	1*OH	+	1*H2O2	=	1*H2O	+	1*HO2	6.10000E+12	0.0000	1430.00
112			2*HO2	=	1*H2O2	+	1*O2	1.80000E+12	0.0000	0.00
113	1*H	+	1*H2O2	=	1*OH	+	1*H2O	7.80000E+11	0.0000	0.00
114	M	+	1*H2O2	=	2*OH			1.44000E+17	0.0000	45510.00
115	1*H2	+	1*OH	=	1*H2O	+	1*H	4.74000E+13	0.0000	6098.00
116	1*H	+	1*O2	=	1*HO2	+	M	1.46000E+15	0.0000	-1000.00
117	M	+	1*H2O	=	1*H	+	1*OH	1.30000E+15	0.0000	105140.00
118	1*H	+	1*O	=	1*OH	+	M	7.10000E+18	-1.0000	0.00
119	M	+	1*H2	=	2*H			2.20000E+14	0.0000	96000.00
120	M	+	1*O2	=	2*O			1.80000E+18	-1.0000	118020.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2	,114) =	2.30000	M(O2	,114) =	0.78000	M(H2O	,114) =	6.00000	M(H2O2	,114) =	6.60000
M(O2	,116) =	1.30000	M(CO2	,116) =	7.00000	M(H2O	,116) =	21.30000	M(H2	,116) =	3.00000
M(C6H6	,116) =	20.00000	M(CH4	,116) =	5.00000	M(H2	,117) =	4.00000	M(O2	,117) =	1.50000
M(H2O	,117) =	20.00000	M(C6H6	,117) =	20.00000	M(CO2	,117) =	4.00000	M(H2	,119) =	4.10000
M(O2	,119) =	2.00000	M(H2O	,119) =	15.00000						

TABLE E.2.—Continued.
(i) Continued.

** INITIAL CONDITIONS **

TIME 0.00000E+00 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	2.38680
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	8.19683E-04
TEMPERATURE (DEG K)	1405.00
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	1.1945
MACH NUMBER	0.0000
GAMMA	1.4607
ENTHALPY (CAL/G)	1.76459E+02
SP. HEAT (CP) (CAL/G/DEG K)	1.59128E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSI-TIVE DIR RATE
C6H6	3.49878E-07	1.69000E-02	-1.87557E-04	1	2.0574E+08	2.79071E+02	1.00000
O2	2.60483E-06	1.25820E-01	-1.87502E-04	2	9.5467E+10	0.00000E+00	0.00000
C6H5O	0.00000E+00	0.00000E+00	1.87502E-04	3	1.5865E-01	8.26167E-02	1.00000
OH	0.00000E+00	0.00000E+00	1.87502E-04	4	8.1118E+11	0.00000E+00	0.00000
C6H5	0.00000E+00	0.00000E+00	5.55085E-08	5	4.7946E+12	0.00000E+00	0.00000
C12H10	0.00000E+00	0.00000E+00	0.00000E+00	6	4.1339E+12	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	5.55085E-08	7	4.6442E+06	0.00000E+00	0.00000
H2	0.00000E+00	0.00000E+00	0.00000E+00	8	3.7236E+04	0.00000E+00	0.00000
O	0.00000E+00	0.00000E+00	6.05693E-14	9	1.4463E+11	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	0.00000E+00	10	1.3979E+13	0.00000E+00	0.00000
C4H3	0.00000E+00	0.00000E+00	0.00000E+00	11	2.3500E+02	0.00000E+00	0.00000
C4H2	0.00000E+00	0.00000E+00	0.00000E+00	12	4.0973E+02	0.00000E+00	0.00000
C5H5	0.00000E+00	0.00000E+00	0.00000E+00	13	1.2942E+12	0.00000E+00	0.00000
CO	0.00000E+00	0.00000E+00	0.00000E+00	14	1.3523E+12	0.00000E+00	0.00000
HO2	0.00000E+00	0.00000E+00	0.00000E+00	15	3.1799E+10	0.00000E+00	0.00000
C2H2	0.00000E+00	0.00000E+00	0.00000E+00	16	1.9399E+03	0.00000E+00	0.00000
C6H5OH	0.00000E+00	0.00000E+00	0.00000E+00	17	6.0009E+09	0.00000E+00	0.00000
C5H6	0.00000E+00	0.00000E+00	0.00000E+00	18	3.0000E+13	0.00000E+00	0.00000
C5H5O	0.00000E+00	0.00000E+00	0.00000E+00	19	1.7530E+13	0.00000E+00	0.00000
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	20	1.3927E+14	0.00000E+00	0.00000
C4H5	0.00000E+00	0.00000E+00	0.00000E+00	21	1.0000E+13	0.00000E+00	0.00000
C5H4OH	0.00000E+00	0.00000E+00	0.00000E+00	22	1.0000E+13	0.00000E+00	0.00000
C4H4	0.00000E+00	0.00000E+00	0.00000E+00	23	3.7833E+11	0.00000E+00	0.00000
HCO	0.00000E+00	0.00000E+00	0.00000E+00	24	2.0000E+13	0.00000E+00	0.00000
C2H3	0.00000E+00	0.00000E+00	0.00000E+00	25	3.1000E+12	0.00000E+00	0.00000

TABLE E.2.—Continued.

(i) Continued.

C2HO	0.00000E+00	0.00000E+00	0.00000E+00
C2H	0.00000E+00	0.00000E+00	0.00000E+00
C3H2	0.00000E+00	0.00000E+00	0.00000E+00
C2H4	0.00000E+00	0.00000E+00	0.00000E+00
CH3	0.00000E+00	0.00000E+00	0.00000E+00
CH2O	0.00000E+00	0.00000E+00	0.00000E+00
CH2	0.00000E+00	0.00000E+00	0.00000E+00
C2H2O	0.00000E+00	0.00000E+00	0.00000E+00
CH	0.00000E+00	0.00000E+00	0.00000E+00
CO2	0.00000E+00	0.00000E+00	0.00000E+00
C3H3	0.00000E+00	0.00000E+00	0.00000E+00
C3H4	0.00000E+00	0.00000E+00	0.00000E+00
CH4	0.00000E+00	0.00000E+00	0.00000E+00
CH3O	0.00000E+00	0.00000E+00	0.00000E+00
AR	1.77481E-05	8.57280E-01	0.00000E+00

26	1.0678E+08	0.00000E+00	0.00000
27	1.0000E+13	0.00000E+00	0.00000
28	3.0000E+13	0.00000E+00	0.00000
29	1.2000E+12	0.00000E+00	0.00000
30	9.1477E+04	0.00000E+00	0.00000
31	3.0807E+12	0.00000E+00	0.00000
32	2.2090E+12	0.00000E+00	0.00000
33	4.1905E+12	0.00000E+00	0.00000
34	1.4145E+12	0.00000E+00	0.00000
35	3.1585E+10	0.00000E+00	0.00000
36	4.3528E+12	0.00000E+00	0.00000
37	6.0000E+12	0.00000E+00	0.00000
38	5.0120E+12	0.00000E+00	0.00000
39	3.0200E+13	0.00000E+00	0.00000
40	3.0200E+13	0.00000E+00	0.00000
41	3.3000E+13	0.00000E+00	0.00000
42	4.0000E+13	0.00000E+00	0.00000
43	5.0120E+12	0.00000E+00	0.00000
44	3.2430E+09	0.00000E+00	0.00000
45	3.5700E+09	0.00000E+00	0.00000
46	1.1113E+12	0.00000E+00	0.00000
47	9.4630E-01	0.00000E+00	0.00000
48	1.4495E+05	0.00000E+00	0.00000
49	4.6314E+12	0.00000E+00	0.00000
50	8.7878E+12	0.00000E+00	0.00000
51	5.1424E+11	0.00000E+00	0.00000
52	2.9788E+11	0.00000E+00	0.00000
53	3.0000E+13	0.00000E+00	0.00000
54	1.1286E+12	0.00000E+00	0.00000
55	1.5495E+07	0.00000E+00	0.00000
56	2.8000E+13	0.00000E+00	0.00000
57	2.5610E+12	0.00000E+00	0.00000
58	3.3102E+12	0.00000E+00	0.00000
59	4.2722E+12	0.00000E+00	0.00000
60	2.8481E+12	0.00000E+00	0.00000
61	2.0000E+13	0.00000E+00	0.00000
62	9.2884E+06	0.00000E+00	0.00000
63	5.9631E+11	0.00000E+00	0.00000
64	1.2020E+12	0.00000E+00	0.00000
65	1.0000E+13	0.00000E+00	0.00000
66	5.0000E+13	0.00000E+00	0.00000
67	3.0000E+13	0.00000E+00	0.00000
68	4.8854E+12	0.00000E+00	0.00000
69	1.0000E+13	0.00000E+00	0.00000
70	2.0000E+13	0.00000E+00	0.00000
71	2.9217E+13	0.00000E+00	0.00000
72	5.0120E+13	0.00000E+00	0.00000
73	4.0973E+03	0.00000E+00	0.00000
74	1.5456E+05	0.00000E+00	0.00000
75	1.7754E+12	0.00000E+00	0.00000
76	4.1555E+12	0.00000E+00	0.00000
77	2.8556E+12	0.00000E+00	0.00000
78	1.4756E+09	0.00000E+00	0.00000
79	6.3000E+12	0.00000E+00	0.00000
80	2.7064E+10	0.00000E+00	0.00000
81	1.1660E+11	0.00000E+00	0.00000
82	2.0000E+13	0.00000E+00	0.00000
83	1.0528E+11	0.00000E+00	0.00000
84	6.2924E+13	0.00000E+00	0.00000
85	4.3705E+10	0.00000E+00	0.00000
86	1.1320E+13	0.00000E+00	0.00000
87	2.0000E+13	0.00000E+00	0.00000
88	1.2569E+04	0.00000E+00	0.00000
89	1.9519E+13	0.00000E+00	0.00000
90	5.9881E+12	0.00000E+00	0.00000
91	9.9559E+12	0.00000E+00	0.00000
92	3.4146E+13	0.00000E+00	0.00000
93	1.1132E+12	0.00000E+00	0.00000
94	2.6984E+11	0.00000E+00	0.00000
95	1.0000E+14	0.00000E+00	0.00000
96	1.9950E+14	0.00000E+00	0.00000
97	1.0000E+14	0.00000E+00	0.00000
98	1.0000E+13	0.00000E+00	0.00000
99	1.3586E+15	0.00000E+00	0.00000
100	9.5431E+04	0.00000E+00	0.00000
101	2.9146E+11	0.00000E+00	0.00000
102	1.5591E+10	0.00000E+00	0.00000
103	9.4582E+10	0.00000E+00	0.00000
104	5.3140E+11	0.00000E+00	0.00000
105	3.0508E+12	0.00000E+00	0.00000
106	3.3996E+13	0.00000E+00	0.00000
107	3.4948E+13	0.00000E+00	0.00000
108	8.0000E+12	0.00000E+00	0.00000
109	9.1341E+13	0.00000E+00	0.00000
110	1.0219E+10	0.00000E+00	0.00000
111	3.6550E+12	0.00000E+00	0.00000
112	1.8000E+12	0.00000E+00	0.00000
113	7.8000E+11	0.00000E+00	0.00000
114	1.2001E+10	0.00000E+00	0.00000
115	5.3361E+12	0.00000E+00	0.00000
116	2.0888E+15	0.00000E+00	0.00000
117	5.7447E-02	0.00000E+00	0.00000
118	5.0534E+15	0.00000E+00	0.00000
119	2.5673E-01	0.00000E+00	0.00000
120	5.6158E-04	4.50745E-08	1.00000

DERIVATIVES (CGS UNITS): T -5.10692E+03 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 39.59283 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 2.68773E+05 MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 2.129997 S

TABLE E.2.—Continued.

(i) Continued.

TIME 3.02811E-04 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	3.63501
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	8.19683E-04
TEMPERATURE (DEG K)	2068.59
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	1.2812
MACH NUMBER	0.0000
GAMMA	1.4813
ENTHALPY (CAL/G)	2.13338E+02
SP. HEAT (CP) (CAL/G/DEG K)	1.59794E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	50
AVERAGE STEP SIZE	0.81053E-06
METHOD ORDER	3
TOTAL NUMBER OF STEPS	200
FUNCT EVALUATIONS	305
JACOBIAN EVALUATIONS	36

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
C6H6	1.95706E-08	9.13868E-04	-1.16032E-02
O2	1.67348E-06	7.81449E-02	-1.40865E-01
C6H5O	3.77703E-09	1.76372E-04	-1.37938E-03
OH	6.27174E-08	2.92865E-03	3.07656E-02
C6H5	3.50165E-09	1.63513E-04	-1.30945E-03
C12H10	4.41770E-09	2.06289E-04	-4.90881E-04
H	2.46542E-08	1.15125E-03	1.20295E-02
H2	2.52278E-08	1.17804E-03	4.91811E-03
O	4.92998E-08	2.30210E-03	2.83327E-02
H2O	4.92184E-07	2.29830E-02	4.89969E-02
C4H5	7.15460E-09	3.34091E-04	1.77918E-03
C4H2	2.33546E-10	1.09057E-05	7.05050E-05
C5H5	3.16265E-08	1.47683E-03	-1.03612E-02
CO	9.92200E-07	4.63318E-02	1.11641E-01
HO2	4.94453E-10	2.30890E-05	-4.81231E-05
C2H2	2.03938E-08	9.52311E-04	-7.68259E-03
C6H5OH	1.67321E-08	7.81323E-04	-9.96410E-03
C5H6	7.93748E-09	3.70649E-04	-4.42616E-03
C5H5O	2.16902E-17	1.01284E-12	3.29176E-07
H2O2	1.13976E-11	5.32223E-07	1.00283E-06
C4H5	3.58781E-12	1.67536E-07	-1.77523E-06
C5H4OH	7.07076E-15	3.30176E-10	-3.12696E-07
C4H4	9.27112E-08	4.32924E-03	1.98356E-02
HCO	2.71147E-10	1.26615E-05	2.06916E-05
C2H3	5.31954E-10	2.48401E-05	3.36206E-06
C2HO	8.48947E-09	3.96424E-04	6.98143E-04
C2H	3.21462E-11	1.50110E-06	1.12092E-05
C3H2	6.91686E-10	3.22990E-05	4.52965E-04
C2H4	4.51217E-12	2.10700E-07	-5.34455E-07
CH3	5.07427E-11	2.36948E-06	-5.01826E-06
CH2O	2.67723E-09	1.25016E-04	-1.05448E-03
CH2	7.02250E-09	3.27923E-04	2.79024E-03
C2H2O	6.55580E-10	3.06130E-05	-3.48518E-05
CH	8.02821E-12	3.74885E-07	8.95177E-06
CO2	1.16338E-07	5.43252E-03	3.69010E-02
C3H3	1.41642E-09	6.61411E-05	2.48428E-04
C3H4	4.73461E-10	2.21087E-05	7.81681E-05
CH4	5.71018E-12	2.66643E-07	-9.54263E-07
CH3O	1.40651E-13	6.56784E-09	-4.75547E-09
AR	1.77481E-05	8.28766E-01	0.00000E+00

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	1.0231E+10	4.98496E+02	0.99958
2	1.5117E+11	-5.82333E+02	0.97421
3	3.8873E+04	-1.09910E+04	0.90660
4	5.0994E+12	3.60007E+03	0.98308
5	8.4288E+12	1.20854E+04	0.99848
6	6.9969E+12	1.25907E+04	0.98502
7	4.5805E+09	1.04350E+03	0.99899
8	5.7753E+06	3.24665E+04	1.00000
9	3.4120E+11	2.89061E+03	0.97137
10	1.5681E+13	4.03808E+01	0.99929
11	9.7795E+05	5.09657E+03	0.99996
12	1.0086E+07	-3.54713E+04	0.12375
13	3.2116E+12	-6.84638E+01	0.03356
14	5.6246E+12	3.44714E+03	0.99820
15	5.7709E+11	-1.12432E+02	0.19831
16	5.1665E+06	5.19366E+03	0.08509
17	6.4826E+10	1.28162E+03	1.00000
18	3.0000E+13	4.67815E+04	0.99840
19	2.0828E+13	2.53738E+02	0.98937
20	7.8046E+14	2.49529E+04	0.99037
21	1.0000E+13	2.32062E+04	1.00000
22	1.0000E+13	2.95221E+04	1.00000
23	4.7388E+12	2.95225E+04	0.59198
24	2.0000E+13	4.65495E+02	1.00000
25	3.1000E+12	-1.48276E+02	0.72383
26	4.6795E+09	2.49555E+04	0.99869
27	1.0000E+13	1.71315E+02	0.99970
28	3.0000E+13	6.53612E+02	0.99938
29	1.2000E+12	2.05640E+01	1.00000
30	6.5102E+08	8.60995E-02	0.91959
31	3.5483E+12	-2.18709E+00	0.59406
32	2.5152E+12	8.32743E-01	1.00000
33	7.4433E+12	1.41809E+00	0.57544
34	1.5795E+12	6.61514E-01	0.99435
35	1.2482E+12	2.05514E+04	0.97110
36	4.2296E+12	5.60402E+03	1.00000
37	6.0000E+12	1.17113E+02	0.99995
38	5.0120E+12	2.48865E+02	0.99996
39	3.0200E+13	1.67912E+02	1.00000
40	3.0200E+13	7.67487E-01	0.99851
41	3.3000E+13	1.28808E+03	1.00000
42	4.0000E+13	2.93597E+03	1.00000
43	5.0120E+12	3.67877E+02	1.00000
44	8.0526E+10	5.27685E+01	0.99966
45	8.2111E+10	4.22963E+01	0.99966
46	1.2467E+12	2.18055E+04	1.00000
47	2.0670E+05	-2.46745E+00	0.94836
48	2.8290E+07	-1.40501E+03	0.99999
49	1.4429E+13	2.15912E+04	0.99999
50	2.9910E+13	4.47018E+04	0.99875
51	1.1494E+12	2.12881E+03	0.97291
52	3.0480E+11	5.79690E+02	0.99904
53	3.0000E+13	-9.30694E+01	0.76073
54	2.4093E+12	4.86093E+02	0.94654
55	2.7145E+10	-1.16342E+02	0.22119
56	2.8000E+13	1.71317E+03	0.99982
57	3.6150E+12	-6.91095E+01	0.23804
58	4.9080E+12	1.18059E+02	0.99993
59	1.0711E+13	-1.24257E+02	0.32534
60	7.1410E+12	-1.01311E+02	0.22776
61	2.0000E+13	9.62074E+02	1.00000
62	9.1611E+09	-5.78988E+02	0.75153
63	7.9474E+11	1.68048E+04	1.00000
64	1.2020E+12	7.48752E+02	1.00000
65	1.0000E+13	7.92459E+03	1.00000
66	5.0000E+13	1.55090E+04	0.99571
67	3.0000E+13	2.66196E+03	1.00000
68	6.1475E+12	5.45476E+02	1.00000
69	1.0000E+13	1.07268E+03	1.00000
70	2.0000E+13	5.72112E+01	0.95329
71	3.4713E+13	2.74332E+03	0.98702
72	5.0120E+13	1.18221E+02	1.00000
73	1.0086E+08	-4.65289E+00	0.99607
74	9.6273E+07	-1.80108E-02	0.92935
75	6.9682E+12	8.73049E-01	0.59796
76	7.3897E+12	2.53672E+00	0.64402
77	1.0978E+13	2.98404E+00	0.64876
78	4.1313E+10	3.63130E+00	0.69547
79	6.3000E+12	-2.85430E+00	0.08730
80	3.0220E+11	1.34073E+00	0.98964
81	2.3232E+11	8.13418E-02	0.99942
82	2.0000E+13	1.03220E-01	0.99998
83	4.1606E+12	1.58939E-02	0.99683
84	7.9180E+13	2.94804E+02	0.99998
85	1.0566E+11	2.13530E-02	0.99945
86	1.3736E+13	2.81270E-01	0.99998
87	2.0000E+13	7.41212E-01	0.99244

TABLE E.2.—Continued.

(i) Continued.

88	1.3842E+08	1.01607E+01	0.86021
89	2.2405E+13	5.59804E+03	0.99980
90	9.4709E+12	9.30207E+02	0.99978
91	1.4902E+13	2.92676E+03	0.99981
92	4.8200E+13	-1.22740E+03	0.99222
93	6.6598E+12	5.72921E+04	0.99541
94	6.0311E+11	4.07214E+02	0.99974
95	1.0000E+14	2.53104E+03	0.99999
96	1.9950E+14	1.98492E+03	0.99999
97	1.0000E+14	1.98955E+03	0.99999
98	1.0000E+13	1.99962E+02	1.00000
99	2.1761E+15	3.39264E+03	0.99996
100	2.2878E+07	5.61387E+01	0.99291
101	3.2695E+11	2.95091E+04	0.97449
102	2.1731E+11	1.58649E+02	0.99982
103	7.8023E+11	3.75030E+02	0.01331
104	3.4977E+12	1.55084E+05	0.72205
105	1.4810E+13	3.46399E+03	0.12636
106	4.3403E+13	7.65113E+02	0.97159
107	3.9203E+13	1.38702E+03	0.97518
108	8.0000E+12	3.59955E+02	0.97485
109	1.0329E+14	1.86113E+03	0.99310
110	1.8067E+11	-1.64242E+01	0.83041
111	4.3077E+12	3.89488E+00	0.84984
112	1.8000E+12	5.45280E-01	0.83251
113	7.8000E+11	3.25880E-01	0.99896
114	2.2396E+12	2.32146E+02	0.25957
115	1.0753E+13	2.90117E+03	0.11457
116	1.8621E+15	3.56669E+03	0.94438
117	1.0133E+04	-1.71692E+02	0.99860
118	3.4323E+15	1.32785E+02	0.99862
119	1.5845E+04	-1.13010E+01	0.99842
120	2.9554E+02	-3.15872E+00	0.99503

DERIVATIVES (CGS UNITS): T 7.54742E+07 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 38.27592 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) -8.88370E+09 MASS FRACTION SUM 1.00000002

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 2.054000E+01 S UP TO THIS TIME - 8.349001E+01 S

***** SENSITIVITY CALCULATIONS *****

TIME = 3.02811D-04

SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES

**** SENSITIVITY TO INITIAL CONDITIONS ****

DZ(I)/DYZERO(J)*F(J)/Z(I), WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW
F(J)= YZERO(J) FOR YZERO(J) NOT EQUAL TO 0
= 1.0E-4/(INITIAL MWT) FOR YZERO(J) = 0

PARAMETER	C6H6	C6H5	H2O	CO	C2H2	C6H5OH	C5H6	TEMP	PRESSURE
C6H6	-4.595D+01	-2.848D+01	8.699D+00	9.844D+00	-2.875D+01	-4.749D+01	-4.410D+01	3.063D+00	3.524D+00
OH	-6.884D+00	-4.338D+00	1.157D+00	1.306D+00	-4.376D+00	-6.901D+00	-6.474D+00	4.239D-01	4.838D-01
AR	6.824D+01	4.281D+01	-1.129D+01	-1.290D+01	4.337D+01	6.916D+01	6.481D+01	-4.301D+00	-4.069D+00
TEMP	-2.049D+03	-1.291D+03	3.432D+02	3.882D+02	-1.303D+03	-2.056D+03	-1.928D+03	1.264D+02	1.442D+02
DENSITY	-1.173D+02	-7.382D+01	1.972D+01	2.223D+01	-7.451D+01	-1.171D+02	-1.103D+02	7.238D+00	9.254D+00

TABLE E.2.—Concluded.

(i) Concluded.

```
**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE PREEXPONENTIAL CONSTANTS ****

        DZ(I)/DA(J)*A(J)/Z(I) WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW

REAC NUM     C6H6        C6H5        H2O         CO          C2H2        C6H5OH      C5H6        TEMP        PRESSURE

    1     -5.692D+01 -3.593D+01  9.534D+00  1.078D+01 -3.610D+01 -5.691D+01 -5.337D+01  3.494D+00  3.988D+00
    2      2.059D+00  1.345D+00 -3.488D-01 -4.016D-01  1.283D+00  2.045D+00  1.904D+00 -1.283D-01 -1.466D-01
    3      1.759D+00  5.978D-01 -2.539D-01 -2.868D-01  9.145D-01  1.413D+00  1.327D+00 -9.098D-02 -1.042D-01
    4     -7.968D-01 -3.372D-01  1.145D-01  1.345D-01 -4.102D-01 -7.069D-01 -6.318D-01  4.205D-02  4.824D-02
    5      1.277D+01  7.873D+00 -2.256D+00 -2.527D+00  8.691D+00  1.368D+01  1.290D+01 -8.285D-01 -9.445D-01
    6     -2.174D+01 -1.315D+01  3.600D+00  4.073D+00 -1.337D+01 -2.139D+01 -1.989D+01  1.316D+00  1.502D+00
    7     -1.162D-02 -8.334D-03  2.378D-03  3.055D-03 -1.203D-02 -5.860D-03 -8.083D-03  8.672D-04  1.010D-03
    8     -6.044D+01 -3.803D+01  1.015D+01  1.150D+01 -3.853D+01 -6.101D+01 -5.643D+01  3.722D+00  4.249D+00
   10      2.765D-01  1.708D-01 -4.691D-02 -5.283D-02  1.771D-01  2.811D-01  2.641D-01 -1.720D-02 -1.962D-02
   11      1.364D-01 -1.754D-01 -3.387D-02 -4.276D-02  2.247D-01  2.255D-01  2.246D-01 -1.524D-02 -1.692D-02
   12      4.142D+01  2.609D+01 -6.954D+00 -7.862D+00  2.635D+01  4.157D+01  3.890D+01 -2.551D+00 -2.911D+00
   13      1.500D+00  9.419D-01 -2.518D-01 -2.830D-01  9.628D-01  1.513D+00  1.424D+00 -9.217D-02 -1.051D-01
   14      7.860D-01  5.001D-01 -1.329D-01 -1.462D-01  5.060D-01  7.250D-01  7.140D-01 -4.803D-02 -5.471D-02
   15      2.395D+00  1.508D+00 -4.029D-01 -4.553D-01  1.523D+00  2.404D+00  2.253D+00 -1.478D-01 -1.687D-01
   16     -1.962D+01 -1.235D+01  3.306D+00  3.735D+00 -1.248D+01 -1.971D+01 -1.857D+01  1.213D+00  1.384D+00
   17     -3.337D+01 -2.097D+01  5.645D+00  6.378D+00 -2.122D+01 -3.367D+01 -3.168D+01  2.071D+00  2.363D+00
   18      1.903D+01  1.203D+01 -3.093D+00 -3.509D+00  1.218D+01  1.799D+01  1.738D+01 -1.142D+00 -1.303D+00
   19      2.322D+00  1.459D+00 -3.969D-01 -4.502D-01  1.473D+00  2.352D+00  2.207D+00 -1.464D-01 -1.670D-01
   20      0.000D+00  0.000D+00  0.000D+00  0.000D+00  0.000D+00  0.000D+00  0.000D+00  0.000D+00  0.000D+00
   21     -6.941D+00 -4.292D+00  1.251D+00  1.428D+00 -3.922D+00 -7.355D+00 -7.247D+00  4.655D-01  5.305D-01
  101     -1.206D+00 -8.037D-01  1.901D-01  1.869D-01 -7.953D-01 -1.162D+00 -1.120D+00  8.560D-02  9.564D-02
  104     -2.728D+01 -1.694D+01  4.551D+00  5.117D+00 -1.734D+01 -2.693D+01 -2.555D+01  1.656D+00  1.890D+00
  116     -2.016D+00 -1.259D+00  3.413D-01  3.846D-01 -1.266D+00 -2.070D+00 -1.938D+00  1.251D-01  1.427D-01


**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE ACTIVATION ENERGIES ****

        DZ(I)/DE(J)*[-R*T0/Z(I)], WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW

REAC NUM     C6H6        C6H5        H2O         CO          C2H2        C6H5OH      C5H6        TEMP        PRESSURE

    1     -5.600D+01 -3.534D+01  9.382D+00  1.061D+01 -3.553D+01 -5.601D+01 -5.252D+01  3.439D+00  3.925D+00
    2      2.026D+00  1.315D+00 -3.443D-01 -3.963D-01  1.265D+00  2.019D+00  1.881D+00 -1.266D-01 -1.447D-01
    3      1.517D+00  6.089D-01 -2.249D-01 -2.543D-01  8.174D-01  1.269D+00  1.189D+00 -8.098D-02 -9.270D-02
    4     -7.708D-01 -3.742D-01  1.152D-01  1.341D-01 -4.206D-01 -7.035D-01 -6.374D-01  4.233D-02  4.850D-02
    5      1.200D+01  7.427D+00 -2.095D+00 -2.350D+00  8.043D+00  1.266D+01  1.193D+01 -7.693D-01 -8.771D-01
    6     -2.062D+01 -1.263D+01  3.425D+00  3.876D+00 -1.277D+01 -2.036D+01 -1.897D+01  1.253D+00  1.430D+00
    7     -9.325D-03 -6.572D-03  1.876D-03  2.380D-03 -9.269D-03 -5.282D-03 -6.825D-03  6.852D-04  7.957D-04
    8     -5.752D+01 -3.620D+01  9.658D+00  1.094D+01 -3.665D+01 -5.796D+01 -5.382D+01  3.543D+00  4.044D+00
   10      2.589D-01  1.607D-01 -4.382D-02 -4.938D-02  1.655D-01  2.624D-01  2.465D-01 -1.607D-02 -1.833D-02
   11      1.394D-01 -9.194D-02 -3.102D-02 -3.853D-02  1.857D-01  2.022D-01  1.980D-01 -1.343D-02 -1.499D-02
   12      3.966D+01  2.498D+01 -6.659D+00 -7.527D+00  2.523D+01  3.979D+01  3.726D+01 -2.442D+00 -2.787D+00
   13      1.497D+00  9.403D-01 -2.512D-01 -2.824D-01  9.596D-01  1.508D+00  1.419D+00 -9.193D-02 -1.049D-01
   14      6.766D-01  4.302D-01 -1.142D-01 -1.261D-01  4.331D-01  6.332D-01  6.167D-01 -4.135D-02 -4.711D-02
   15      2.290D+00  1.442D+00 -3.852D-01 -4.353D-01  1.456D+00  2.299D+00  2.155D+00 -1.413D-01 -1.613D-01
   16     -1.901D+01 -1.197D+01  3.202D+00  3.618D+00 -1.209D+01 -1.909D+01 -1.797D+01  1.175D+00  1.341D+00
   17     -3.128D+01 -1.967D+01  5.286D+00  5.973D+00 -1.990D+01 -3.153D+01 -2.966D+01  1.940D+00  2.213D+00
   18      1.736D+01  1.098D+01 -2.836D+00 -3.213D+00  1.107D+01  1.659D+01  1.591D+01 -1.045D+00 -1.192D+00
   19      2.121D+00  1.332D+00 -3.620D-01 -4.105D-01  1.345D+00  2.147D+00  2.013D+00 -1.335D-01 -1.522D-01
   20      0.000D+00  0.000D+00  0.000D+00  0.000D+00  0.000D+00  0.000D+00  0.000D+00  0.000D+00  0.000D+00
   21     -6.596D+00 -4.092D+00  1.172D+00  1.335D+00 -3.860D+00 -6.916D+00 -6.737D+00  4.349D-01  4.958D-01
  101     -1.035D+00 -6.820D-01  1.647D-01  1.651D-01 -6.770D-01 -1.007D+00 -9.656D-01  7.220D-02  8.086D-02
  104     -2.491D+01 -1.553D+01  4.158D+00  4.680D+00 -1.582D+01 -2.465D+01 -2.333D+01  1.515D+00  1.730D+00
  116     -1.955D+00 -1.224D+00  3.305D-01  3.726D-01 -1.233D+00 -1.996D+00 -1.871D+00  1.212D-01  1.382D-01


        (LSENS)     END OF THIS CASE

                    SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

                       TOTAL NO. OF STEPS -                          247
                       TOTAL NO. OF DERIVATIVE EVALUATIONS -         385
                       TOTAL NO. OF JACOBIAN EVALUATIONS -            44
                       TOTAL CPU TIME -                     103.389999 S


                    WORK REQUIRED BY SENSITIVITY ROUTINE:

                        NO. STEPS =                 247
                        NO. FUNC. EVAL. =           247
                        NO. JAC. EVAL. =            247
                        TOTAL REAL     SPACE USED =       16824
                        TOTAL INTEGER SPACE USED =          124


                                  TOTAL CPU TIME (INCLUDING I/O) REQUIRED =    108.609993 S


        (LSENS)     READ DATA FOR NEXT CASE
```

References

1. Mirels, H.: Test Time in Low-Pressure Shock Tubes. Phys. Fluids, vol. 6, no. 9, 1963, pp. 1201–1214.
2. Mirels, H.: Shock Tube Test Time Limitation Due to Turbulent-Wall Boundary Layer. AIAA J., vol. 2, no. 1, 1964, pp. 84–93.
3. Mirels, H.: Flow Nonuniformity in Shock Tubes Operating at Maximum Test Times. Phys. Fluids, vol. 9, no. 10, 1966, pp. 1907–1912.
4. Warshay, M.: Shock Tube Investigation of Bromine Dissociation Rates in Presence of Helium, Neon, Argon, Krypton and Xenon. J. Chem. Phys., vol. 54, May 1971, pp. 4060–4071.
5. Brabbs, T.A.; and Musiak, J.D.: Ignition Delay Measurements and Proposed Kinetic Model for Hydrogen-Oxygen. NASP CR–1030, 1988.
6. Brabbs, T.A.; Lezberg, E.A.; Bittker, D.A.; and Robertson, T.F., et al.: Hydrogen Oxidation Mechanism With Applications to (1) Chaperon Efficiency of Carbon Dioxide and (2) Vitiated Air Testing. NASA TM–100186, 1987.
7. Westbrook, C.K.; and Dryer, F.L.: Chemical Kinetic Modeling of Hydrocarbon Combustion. Prog. Energy Combust. Sci., vol. 10, 1984, pp. 1–57.
8. Warnatz, J.: Rate Coefficients in the C/H/O System. Combustion Chemistry, W.C. Gardiner, ed., Springer-Verlag, New York, 1984, pp. 197–360.
9. Westbrook, C.K.; and Dryer, F.L.: A Comprehensive Mechanism for Methanol Oxidation. Comb. Sci. Technol., vol. 20, no. 3–4, 1979, pp. 125–140.
10. Westley, F.: Table of Recommended Rate Constants for Chemical Reactions Occurring in Combustion. Report NSRDS–NBS 67, National Bureau of Standards, Washington, DC, 1980.
11. Bortner, M.H.: A Review of Rate Constants of Selected Reactions of Interest in Re-entry Flow Fields in the Atmosphere. NBS Technical Note 484, National Bureau of Standardards, Washington, DC, 1969.
12. Hwang, J.T.: The Scaled Green's Function Method of Sensitivity Analysis and Its Application to Chemical Reaction Systems. Proc. Nat. Sci. Council Republic of China, Pt. B, vol. 6, no. 1, 1982, pp. 37–44.
13. Radhakrishnan, K.: Decoupled Direct Method for Sensitivity Analysis in Combustion Kinetics. Advances in Computer Methods for Partial Differential Equations—VI, R. Vichnevetsky and R.S. Stepleman, eds., IMACS, New Brunswick, NJ, 1987, pp. 479–486. (Also NASA CR–179636, 1987.)
14. Hwang, J.T. et al.: The Green's Function Method of Sensitivity Analysis in Chemical Kinetics. J. Chem. Phys., vol. 69, 1978, pp. 5180–5191.
15. Kramer, M.A.; Calo, J.M.; and Rabitz, H.: An Improved Computational Method for Sensitivity Analysis: the Green's Function Method With 'AIM.' Appl. Math. Modelling, vol. 5, 1981, pp. 432–441.
16. Dunker, A. M.: The Decoupled Direct Method for Calculating Sensitivity Coefficients in Chemical Kinetics. J. Chem. Phys., vol. 81, 1984, pp. 2385–2393.
17. Radhakrishnan, K.: Combustion Kinetics and Sensitivity Analysis Computations. Numerical Approaches to Combustion Modeling, E.S. Oran and J.P. Boris, eds., AIAA, Washington, DC, 1991, pp. 83–128.
18. Boni, A.A.; and Penner, R.C.: Sensitivity Analysis of a Mechanism for Methane Oxidation Kinetics. Combust. Sci. Technol., vol. 15, Mar. 1977, pp. 99–106.
19. Dougherty E.P.; Hwang, J-T.; and Rabitz, H.: Further Developments and Applications of the Green's Function Method of Sensitivity Analysis in Chemical Kinetics. J. Chem. Phys., vol. 71, 1979, pp. 1794–1808.
20. Yetter, R.A.; Dryer, F.L.; and Rabitz, H.: Some Interpretive Aspects of Elementary Sensitivity Gradients in Combustion Kinetics Modeling. Combust. Flame, vol. 59, Feb. 1985, pp. 107–133.
21. Bittker, D.A.: Detailed Mechanism for Oxidation of Benzene. Combust. Sci. Technol., vol. 79, no. 1, 1991, pp. 49–72.

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.

1. AGENCY USE ONLY (*Leave blank*)

2. REPORT DATE
March 1994

3. REPORT TYPE AND DATES COVERED
Reference Publication

4. TITLE AND SUBTITLE
LSENS, A General Chemical Kinetics and Sensitivity Analysis Code for Homogeneous Gas-Phase Reactions
III. Illustrative Test Problems

5. FUNDING NUMBERS
WU–505–62–52

6. AUTHOR(S)
David A. Bittker and Krishnan Radhakrishnan

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
National Aeronautics and Space Administration
Lewis Research Center
Cleveland, Ohio 44135–3191

8. PERFORMING ORGANIZATION REPORT NUMBER
E–5140–3

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
National Aeronautics and Space Administration
Washington, D.C. 20546–0001

10. SPONSORING/MONITORING AGENCY REPORT NUMBER
NASA RP–1330

11. SUPPLEMENTARY NOTES
David A. Bittker, NASA Lewis Research Center; and Krishnan Radhakrishnan, NYMA, Inc., Lewis Research Center Group, 2001 Aerospace Parkway, Brook Park, Ohio 44142. Responsible person, Edward J. Mularz, organization code 2650, (216) 433–5850.

12a. DISTRIBUTION/AVAILABILITY STATEMENT
Unclassified - Unlimited
Subject Categories 25 and 64

12b. DISTRIBUTION CODE

13. ABSTRACT ***(Maximum 200 words)***

LSENS, the Lewis General Chemical Kinetics and Sensitivity Analysis Code, has been developed for solving complex, homogeneous, gas-phase chemical kinetics problems and contains sensitivity analysis for a variety of problems, including nonisothermal situations. This report is part III of a series of three reference publications that describe LSENS, provide a detailed guide to its usage, and present many example problems. Part III explains the kinetics and kinetics-plus-sensitivity-analysis problems supplied with LSENS and presents sample results. These problems illustrate the various capabilities of, and reaction models that can be solved by, the code and may provide a convenient starting point for the user to construct the problem data file required to execute LSENS.

LSENS is a flexible, convenient, accurate, and efficient solver for chemical reaction problems such as static system; steady, one-dimensional, inviscid flow; reaction behind incident shock wave, including boundary layer correction; and perfectly stirred (highly backmixed) reactor. In addition, the chemical equilibrium state can be computed for the following assigned states: temperature and pressure, enthalpy and pressure, temperature and volume, and internal energy and volume. For static problems the code computes the sensitivity coefficients of the dependent variables and their temporal derivatives with respect to the initial values of the dependent variables and/or the three rate coefficient parameters of the chemical reactions.

Part I (NASA RP–1328) derives the governing equations and describes the numerical solution procedures for the types of problems that can be solved by LSENS. Part II (NASA RP–1329) describes LSENS, its usage, illustrated by example problems, and how to modify it.

14. SUBJECT TERMS
Chemical kinetics computation; Sensitivity analysis; Gas-phase chemical kinetics

15. NUMBER OF PAGES
150

16. PRICE CODE
A07

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
Unclassified	Unclassified	Unclassified	