NASA Reference Publication 1362

March 1996

GLSENS, A Generalized Extension of LSENS Including Global Reactions and Added Sensitivity Analysis for the Perfectly Stirred Reactor

David A. Bittker



National Aeronautics and Space Administration

Lewis Research Center Cleveland, Ohio 44135

NASA Reference Publication 1362

1996

GLSENS, A Generalized Extension of LSENS Including Global Reactions and Added Sensitivity Analysis for the Perfectly Stirred Reactor

David A. Bittker Lewis Research Center Cleveland, Ohio



National Aeronautics and Space Administration

Office of Management Scientific and Technical Information Program

Preface

The NASA Lewis general chemical kinetics and sensitivity analysis code, LSENS, has been described in a recent series of three NASA reference publications. This code computes the progress of complex (multistep) molecular processes in a homogeneous gas mixture for several reaction models. For a static (nonflow) chemical reaction it also lets the user perform a sensitivity analysis of the reacting system simultaneously with the chemical kinetics computation. Sensitivity analysis gives the user the ability to rapidly determine the relatively few individual reactions that are rate controlling in a system where many simultaneous steps are occurring. This ability is very useful in the task of mechanism development, especially for the complicated reactions occurring during the oxidation of hydrocarbon fuels. The significant effort now being given to modeling gas turbine and ramjet combustors has made it necessary to understand these oxidation processes so that realistic heat-release models can be developed. These models are needed as part of the numerous comprehensive computational fluid dynamics (CFD) computer codes that are being developed to model practical combustors.

Even if detailed oxidation mechanisms (typically containing 100 or more molecular steps) were known for even simple hydrocarbon fuels, they could not be used directly in the present-day CFD codes because execution times would become impractically long. Therefore, smaller mechanisms have been developed in recent years for many hydrocarbon oxidations. A common technique is to combine several molecular steps into a single overall, or global, reaction. The rate expression for a global step is developed empirically from analysis of experimental data and differs from that for a molecular step. Mechanisms containing only global reactions or both global and molecular reactions have been developed. They give good temperature and heat-release profiles and also a limited number of realistic speciescomposition profiles over a limited range of experimental conditions. However, they lack all the details of a complete molecular mechanism. Of course, the applicability of such all-global or quasi-global (global plus molecular reactions) mechanisms is limited to the range of experimental conditions used to develop them.

So that the LSENS code can be more useful in heat-release computations for practical combustion systems, two new capabilities have been added to it. The first is the ability to use both molecular and global reactions in a chemical mechanism. As far as is known, no other general chemical kinetics code in use today has this ability. Second, the ability to perform rapid and convenient sensitivity analysis has been extended to a second chemical model contained in the original LSENS, namely the perfectly stirred reactor (PSR) model, which is often used to simulate the backmixing type of reaction in a practical gas turbine combustor. This reference

publication documents the new code GLSENS, which incorporates both these additions to the original LSENS code. Chapter 2 discusses the rate equations for both molecular and global reactions and also presents the derivation of the equations used to compute sensitivity coefficients for the PSR reaction model. Chapter 3 describes the coding modifications and new subroutines needed to incorporate the PSR sensitivity analysis equations into GLSENS. It also gives a detailed description of the modified input for global reactions. Chapter 4 presents nine example problems that use global and quasi-global mechanisms to compute the course of PSR and integration problems. Several of the PSR problems illustrate the computation of sensitivity coefficients using the newly encoded equations. These results are verified by comparison with sensitivity coefficients obtained by the direct approach of increasing and decreasing a given parameter and computing the effect on all dependent variables.

For users who wish to execute several problems in one problem data file, the appendix presents a set of seven additional test cases set up in a single data file. These cases illustrate the multiple-case ability of GLSENS, which allows the user to conveniently perform several computations with the same mechanism in a single computer run or to easily modify the reaction mechanism and repeat a calculation.

The user will very likely be able to use the test-case files presented in this report as models in preparing any desired problem data file.

Information about code availability can be obtained from COSMIC, University of Georgia, 328 East Broad Street, Athens, GA 30602; telephone, (706) 542–3265.

Contents

| List of Tables vii |
|---|
| Symbols 1 |
| Chapter 1. Introduction 3 |
| Chapter 2. Molecular and Global Rates and Sensitivity |
| Equations for Perfectly Stirred Reactor |
| 2.1 Molecular and Global Rate Equations 5 |
| 2.2 Equations for Perfectly Stirred Reactor Combustion |
| and Sensitivity Analysis 6 |
| 2.2.1 Sensitivity Coefficients With Respect to Rate Parameters 7 |
| 2.2.1.1 Derivatives of net species formation rate |
| 2.2.1.2 Derivatives of net reaction rate |
| 2.2.1.3 Temperature derivatives of rate coefficient |
| and equilibrium constant |
| 2.2.1.4 Derivatives of rate coefficient equations with |
| respect to rate parameters |
| 2.2.2 Sensitivity Coefficients With Respect to Initial Temperature 10 |
| 2.2.3 Normalized Sensitivity Coefficients |
| 2.2.3.1 Rate coefficient parameters |
| 2.2.3.2 Initial temperature 11 |
| Chapter 3. Description of New GLSENS Coding |
| 3.1 New Subroutines |
| 3.2 Modifications to Problem Data File 13 |
| 3.2.1 Chemical Reaction Input 13 |
| 3.2.2 PSR Sensitivity Coefficient Calculations |
| Chapter 4. Kinetics and Sensitivity Test Cases and Example |
| Problems for Global Reactions and PSR Sensitivity 17 |
| 4.1 Kinetics and Sensitivity Analysis Test Cases |
| 4.2 Global Reaction Example Problems 17 |
| 4.2.1 Example Problem 1 17 |
| 4.2.2 Example Problem 2 18 |
| 4.2.3 Example Problem 3 18 |
| 4.2.4 Example Problem 4 18 |
| 4.3 Perfectly Stirred Reactor Sensitivity Calculations |
| 4.3.1 Error Control for PSR Problems 19 |

| 4.3.2 PSR Sensitivity Analysis Problems and Comparisons | |
|--|----|
| With Brute-Force Results | 19 |
| 4.3.2.1 Example problem 5 | 19 |
| 4.3.2.2 Example problem 6 | 19 |
| 4.3.2.3 Example problem 7 | 20 |
| 4.3.2.4 Example problem 8 | 20 |
| 4.3.2.5 Example problem 9 | 21 |
| Chapter 5. Concluding Remarks | 45 |
| Appendix—Multiple-Case File Setup Showing Changing and Adding of Global and Molecular Reactions | 46 |
| | |
| References | 84 |

List of Tables

| Table 2.1 — Normalization factors for rate coefficient parameter | |
|---|----|
| sensitivity coefficients | 11 |
| Table 3.1.—Description of logical variables in namelist RTYPE | 14 |
| Table 3.2.—Logical variable settings in namelist RTYPE for multiple-case situations | 15 |
| Table 3.3.—Formats of two reaction lines for each global reaction | 16 |
| Table 4.1.—Data file for example problem 1 (all global reactions; perfectly stirred reactor problem) | 22 |
| Table 4.2. —Computed results for example problem 1 (propane-air combustion in perfectly stirred reactor) | 22 |
| Table 4.3. —Data file for example problem 2 (all global reactions) | 23 |
| Table 4.4. —Computed results for example problem 2 (propane-air combustion in perfectly stirred reactor) | 23 |
| Table 4.5. —Data file for example problem 3 (global and molecular reactions; perfectly stirred reactor problem) | 24 |
| Table 4.6. —Computed results for example problem 3 (propane-air combustion in perfectly stirred reactor) | 25 |
| Table 4.7. —Data file for example problem 4 (integration case for mechanism with global and molecular reactions) | 26 |
| Table 4.8. —Computed results for example problem 4 (propane-air combustion at constant volume) | 26 |
| Table 4.9. —Data file for example problem 5 (hydrogen-oxygen PSR sensitivity) | 27 |
| Table 4.10. —Comparison of GLSENS and brute-force sensitivity coefficients for example problem 5 (reaction of hydrogen and oxygen) | 28 |

| Table 4.11. —Data file for example problem 6 (PSR sensitivity with global and molecular reactions) | 29 |
|---|----|
| Table 4.12. —Comparison of GLSENS and brute-force sensitivity coefficients for example problem 6 (reaction of propane and air | |
| with global reactions) | 30 |
| Table 4.13.—Data file for example problem 7 (propane-air PSR) | 31 |
| Table 4.14. —Comparison of GLSENS and brute-force sensitivity coefficients for example problem 7 (propane-air PSR) | 34 |
| Table 4.15.—Data file for example problem 8 (benzene-oxygen PSR) | 36 |
| Table 4.16. —Comparison of GLSENS and brute-force sensitivity coefficients for example problem 8 (reaction of benzene and oxygen) | 39 |
| Table 4.17. —Data file for example problem 9 (benzene-oxygen- nitrogen-argon PSR) | 40 |
| Table 4.18. —Comparison of GLSENS and brute-force sensitivity coefficients for PSR example problem 9 (reaction of benzene, O2, N2, and Ar) | 43 |
| Table 4.19. —Comparison of brute-force and GLSENS sensitivity coefficients with respect to initial temperature for example problems 8 and 9 | 44 |
| Table A.1.—Data file for multiple cases with global code | 49 |
| Table A.2. —Computed results for test case 1 (hydrogen-oxygen PSR problem using all molecular reactions) | 52 |
| Table A.3. —Computed results for test case 2 (propane-air PSR problem using global and molecular reactions) | 55 |
| Table A.4. —Computed results for test case 3 (propane-air PSR problem of case 2 with added molecular reactions in mechanism) | 60 |
| Table A.5. —Computed results for test case 4 (propane-hydrogen-air, constant-volume combustion with mechanism of case 3) | 65 |
| Table A.6. —Computed results for test case 5 (propane-air PSR problem using all global reactions) | 70 |
| Table A.7. —Computed results for test case 6 (propane-air PSR problem with global reaction mechanism modified from case 5) | 75 |
| Table A.8. —Computed results for test case 7 (propane-air PSR problem with molecular reactions added to global mechanism of case 6) | 79 |

Symbols

| A_{j} | preexponential factor in rate coefficient equations (2.6) and (2.7) for reaction <i>j</i> | GLUBAL | glol |
|--------------------|---|----------------|--------------------|
| A _s | preexponential factor for reaction s (eq. (2.43)) | GRONLY | logi mec |
| a_j | sum of all a_{lj} values over all rate-controlling species for reaction j | H_i | mol |
| a _{ij} | empirically determined power of $\rho \sigma_i$ in global reaction rate equation (2.9) for reaction <i>j</i> | H_i° | star |
| <i>a.</i> . | empirical global rate equation exponent for | ΔH_{j} | entł |
| ulj | species l in reaction j (eq. (2.35)) | H_l | mol ture |
| C_{pl} | molar heat capacity of species l | H., | mol |
| c_j | exponential constant in special rate coefficient equation (2.7) for reaction j | 11,0 | tem |
| c _p | mass specific heat of reacting mixture | K_{j} | equ in c |
| c _s | exponential constant for reaction s (eq. (2.46)) | k_j | read che |
| E_j | activation energy in rate coefficient equation for reaction j | $k_{j}(T)$ | read |
| Es | activation energy for reaction s (eq. (2.45)) | | reac |
| ΔG_j° | Gibbs function change for reaction <i>j</i> | k _s | read read |
| GLADD | logical variable which, if true, indicates that global reactions are being added when multiple cases are being performed | MRADD | logi mol mul |
| GLCHNG | logical variable which, if true, indicates that global reaction rates are being changed when multiple cases are being performed | MRCHNG | logi mol mul |

| GLOBAL | logical variable which, if true, indicates that global reactions are in reaction mechanism |
|--------------------------------|--|
| GRONLY | logical variable which, if true, indicates that mechanism contains only global reactions |
| H_{i} | molar enthalpy of species <i>i</i> in reacting mixture |
| H_i° | standard molar enthalpy of species i (298.15 K) |
| ΔH_{j}° | enthalpy change for reaction <i>j</i> at 298.15 K |
| H_l | molar enthalpy of species l at reactor temperature T |
| <i>H</i> _{<i>l</i>,0} | molar enthalpy of species l at initial reactor temperature T_0 |
| K _j | equilibrium constant for <i>j</i> th chemical reaction, in concentration units |
| k _j | reaction rate coefficient for <i>j</i> th molecular chemical reaction (eqs. (2.6) and (2.7)) |
| $k_{j}\left(T ight)$ | reaction rate coefficient for j th global chemical reaction (eq. (2.9)) |
| k _s | reaction rate coefficient for <i>s</i> th chemical reaction (eqs. (2.43) to (2.46)) |
| MRADD | logical variable which, if true, indicates that molecular reactions are being added when multiple cases are being performed |
| MRCHNG | logical variable which, if true, indicates that molecular reaction rates are being changed when multiple cases are being performed |

| MRPREV | logical variable which, if true, indicates that pre- vious case mechanism contains only molecular reactions when multiple cases are being | W _i | net molar formation rate of species <i>i</i> per unit volume |
|--------------------------|---|------------------|--|
| | performed | y _i | <i>i</i> th dependent variable (species concentration or temperature) of PSR problem |
| M_{j} | collisional efficiency factor for collisionally | _ | |
| | catalyzed reaction <i>J</i> (eq. (2.8)) | y_i | value of <i>i</i> th dependent variable for standard value |
| M_W | molecular weight of mixture | | coefficient calculation |
| m _{ij} | relative collisional efficiency of species <i>i</i> in collisionally catalyzed reaction <i>j</i> | η_j | rate coefficient parameter of <i>j</i> th chemical reaction |
| | | v'_j | sum of stoichiometric coefficients for reactants |
| ṁ | mass flow rate through reactor | | in reaction <i>j</i> |
| NR | number of reactions in chemical mechanism | \mathbf{v}_j'' | sum of stoichiometric coefficients for products in reaction <i>j</i> |
| NRS | number of reacting species in reacting mixture | , | |
| | | v'_{ij} | stoichiometric coefficient of reactant species <i>i</i> |
| NS | total number of species (including inert ones) in | | in reaction j |
| | reacting mixture | v_{ii}'' | stoichiometric coefficient of product species <i>i</i> in |
| 11 | temperature exponent in rate coefficient | •) | reaction <i>j</i> |
| nj | equations (2.6) and (2.7) for reaction <i>j</i> | , | |
| | | v'_{lj} | stoichiometric coefficient of reactant species l |
| n _s | temperature exponent in rate coefficient equa- | | In reaction j |
| | tion for reaction s (eq. (2.44)) | v_{li}'' | stoichiometric coefficient of product species l |
| n | nrecure | ·J | in reaction <i>j</i> |
| P | pressure | A | |
| Ż | rate of heat transfer from reactor | ΔV_j | change in number of molecules (products minus reactants) for reaction j |
| R | universal gas constant | ρ | mass density of gas mixture |
| R_j | forward rate of molecular chemical reaction <i>j</i> | σ_i | mole number (moles per unit mass of mixture) |
| | per unit volume | | of species <i>i</i> |
| <i>Rj</i> | backward rate of molecular chemical reaction <i>j</i> per unit volume | σ_l | mole number of species l |
| | | φ | equivalence ratio |
| r_j | <i>i</i> per unit volume | | |
| | j per unit volume | ω_{ij} | net rate of formation of species <i>i</i> by reaction <i>j</i> |
| S_{ii} | unnormalized sensitivity coefficient | | per unit volume |
| . <u>j</u> | | ω_{is} | rate of formation of species <i>i</i> by reaction <i>s</i> |
| $\langle S_{ij} \rangle$ | normalized sensitivity coefficient (eq. (2.54)) | | |
| 0 | symbol for appoint is reactant or product in | Subscript: | |
| ^S i | chemical reaction | 0 | initial-mixture condition |
| Т | absolute temperature | Superscript | : |
| v | volume of reactor | 0 | standard state for thermodynamic property |

Chapter 1 Introduction

This reference publication describes a new computer code, GLSENS, which adds two new capabilities to the general chemical kinetics and sensitivity code LSENS developed at NASA Lewis Research Center. LSENS performs complex chemical kinetics computations for any chemical system and several different reaction types, including static and onedimensional flow reaction, shock-initiated chemical reaction, and the fully backmixed perfectly stirred reactor. All chemical reactions are molecular processes whose rates are calculated from the law of mass action. For static (nonflow) reactions LSENS also computes, at the user's option, linear normalized sensitivity coefficients. These coefficients measure, approximately, the percent change in any dependent variable caused by a 1-percent change in either a reaction rate coefficient or the initial conditions of the problem (e.g., temperature or mixture composition). In the documentation reports for LSENS (refs. 1 to 3) two sets of ordinary differential equations (ODE's) are derived. Solving the first set gives the kinetics solution (i.e., the temporal variation of all dependent variables). These results may then be used to solve the second set of ODE's for the sensitivity coefficients of the dependent variables in a static, nonisothermal chemical reaction. Details of the solution of these equations, as incorporated into LSENS, are also given.

The first enhancement in GLSENS is the ability to use mechanism reactions that are not individual molecular steps but combinations of several of these steps. Using these "global" reactions loses the fine details of the molecular steps but can give reasonably accurate predictions of the temperature profile and heat-release rate as well as important pollutant species profiles in a practical combustion system. A major effort today in combustion research is the theoretical modeling of such gas turbine and ramjet systems. This task often requires the numerical solution of the Navier-Stokes flow equations coupled with models of turbulence generation and heat release in the flow. For many years oversimplified, unrealistic chemical oxidation mechanisms have been used in the heat-release terms of these complicated computational fluid dynamics (CFD) codes. A detailed fuel oxidation mechanism contains a large number of molecular steps, and a numerical analysis code such as LSENS was required for accurate modeling of the heatrelease process. Because coupling a complete complex kinetics code to most CFD codes is impractical, there has been significant use in recent years of simplified oxidation mechanisms containing global reactions, which are computationally rapid and still realistic. A recent paper by Bittker (ref. 4) surveys the present status of this work. The important difference between molecular and global reactions is in the method used to calculate the global reaction rate. A global reaction rate is determined empirically by least-squares fitting of experimental data to an assumed formula. To make the GLSENS code useful in performing practical kinetics computations, the ability to use global reactions along with molecular processes has been added. This reference publication discusses the form of the global reaction rate equation and gives details of its addition to the GLSENS code. Input changes needed to use global reactions are discussed, and several test cases using this type of reaction are presented.

A second new ability in GLSENS is the computation of sensitivity coefficients for the PSR combustion model, which is often used as an approximate model of the highly turbulent gas turbine combustion. The sensitivity analysis method for nonflow processes, which is part of LSENS, does not apply to the PSR model. Previous work has shown how sensitivity analysis is an important tool in developing detailed chemical mechanisms for the ignition and oxidation of pure hydrocarbon components of practical fuels. Early computations by Bittker (ref. 5) on the lower temperature (~1100 K) ignition of benzene and toluene mixtures with oxygen first applied the LSENS technique of nonisothermal sensitivity analysis to understanding the complex oxidation mechanisms of these aromatic components of real fuels. More recent work by Bittker (ref. 6) and by Emdee et al. (ref. 7) has resulted in significantly improved benzene and toluene oxidation mechanisms that give the important molecular steps during the ignition and early heatrelease phases of the reactions. The results of static-reaction sensitivity analysis can be expected to also give useful information about the important reactions in a similar onedimensional plug flow process in which there is no backmixing. It would be expected that different reactions are rate controlling for the higher temperature, completely backmixed PSR. To develop oxidation mechanisms valid for the PSR, a convenient method of calculating sensitivity coefficients for this type of combustion model is needed.

The combustion of several hydrocarbon fuels in a stirred reactor has been studied both experimentally and theoretically by several investigators (refs. 8 to 11). In all these papers sensitivity analysis was performed on the chemical mechanism by the brute-force method. That is, each reaction rate coefficient was increased and decreased by a fixed small percentage, and the kinetics modeling computations were repeated to determine the quantitative effect on the computed values of the dependent variables as the ratio $\delta y_i/\delta k_j$, where y_i is the dependent variable of interest and k_j is the reaction rate coefficient that is being changed. The quantity δy_i is the change in y_i caused by the change δk_j in k_j . The computed ratio is a close approximation to the actual unnormalized sensitivity coefficient, the partial derivative $S_{ij} = \partial y_i/\partial k_j$. To avoid these

tedious brute-force computations, a set of simultaneous linear equations can be derived that is easily and rapidly solved for the S_{ii} values of all dependent variables. If there are N dependent variables in the problem, a set of N linear equations can be obtained in the variables S_{ij} , i = 1, 2,...,N. Of course, the value of j is fixed for any set of equations. This reference publication presents the derivation of the equations for the unnormalized sensitivity coefficients and all formulas for the matrix elements needed in the solution. A similar set of equations was also derived that can be solved for sensitivity coefficients with respect to changes in the initial temperature of the reacting mixture. The programming changes required to add this sensitivity coefficient calculation to the direct PSR solution in the GLSENS code are then described. The results of several sensitivity analysis test cases are also given and are compared with results of the brute-force method of calculating the sensitivity coefficients. Also shown are the differences found in rate-controlling reactions when the perfectly stirred reactor is compared with a lower temperature static ignition reaction for the same chemical system.

Chapter 2 Molecular and Global Rates and Sensitivity Equations for Perfectly Stirred Reactor

This chapter presents the equations for the net rate of a molecular reaction as used in the original LSENS code (ref. 1). The global reaction concept is then introduced and the rate equation for this type of reaction is given. The second part of the chapter describes the new equations used in GLSENS to compute sensitivity coefficients for a perfectly stirred reactor process. These are linear algebraic equations, whereas the equations for sensitivity analysis in a static chemical reaction are linear differential equations. The sensitivity analysis theory for static chemical reactions is not discussed here because it applies to both molecular and global reactions. One must only take care to use the appropriate formulas for the rate of a global reaction and its derivatives when calculating the Jacobian elements in the numerical kinetics and sensitivity analysis solutions. These formulas, for both molecular and global reactions, are derived in sections 2.2.1.2 to 2.2.1.4 after the derivation of the PSR sensitivity equations. They are used in all kinetics and sensitivity coefficient calculations involving both types of chemical reaction.

2.1 Molecular and Global Rate Equations

In the usual complex chemical reaction a system of NRS reacting species participates in NR reversible molecular reactions, which are written in the general form

$$M + \sum_{i=1}^{\text{NRS}} v'_{ij} S_i = \sum_{i=1}^{\text{NRS}} v''_{ij} S_i + M \qquad j = 1, 2, ..., \text{NR} \quad (2.1)$$

Here *M* represents any collision partner if the reaction is a collisionally catalyzed decomposition or recombination process and is not written for regular types of reactions, S_i is the name of species *i*, and v'_{ij} and v''_{ij} are its stoichiometric coefficients as reactant and product, respectively. The net molar formation rate of species *i* per unit volume is then given by

$$W_{i} = \sum_{j=1}^{NR} \omega_{ij} = \sum_{j=1}^{NR} \left(\mathbf{v}_{ij}'' - \mathbf{v}_{ij}' \right) r_{j}$$
(2.2)

where

$$r_j = R_j - R_{-j} \tag{2.3}$$

is the net molar rate per unit volume of reaction *j*. The forward and reverse molar rates, R_j and R_{-j} , are written by using the laws of mass action and of microscopic reversibility (see ref. 1) as

$$R_j = M_j k_j \prod_{i=1}^{\text{NRS}} \left(\rho \sigma_i \right)^{\mathbf{v}'_i}$$
(2.4)

$$R_{-j} = \frac{M_j k_j}{K_j} \prod_{i=1}^{\text{NRS}} \left(\rho \sigma_i \right)^{\mathbf{v}_i''}$$
(2.5)

The forward rate coefficient k_j for reaction *j* is given by the modified Arrhenius expression

$$k_j = A_j T^{n_j} \exp \frac{-E_j}{RT}$$
(2.6)

or, for a few reactions, by the equation

$$k_j = A_j T^{n_j} \exp(c_j T)$$
(2.7)

In the above equations K_j is the equilibrium constant of reaction *j* in concentration units and M_j is the collisional efficiency factor given by

$$M_j = \rho \sum_{i=1}^{NS} m_{ij} \sigma_i$$
 (2.8)

where m_{ij} is the collisional efficiency of species *i* in the *j*th reaction as a collision partner. In the above equations ρ is the mass density of the mixture, σ_i is the mole number (moles per unit mass) of species *i*, and NS is the total number of species, including inerts. If the collisional efficiencies for all species are unity for a collisionally catalyzed reaction, M_j is just the total molar concentration of all species in the mixture. If the reaction is a regular type, M_j is equal to 1.0 and does not appear in equations (2.4) and (2.5).

A global reaction summarizes the net effect of several molecular steps. It is selected to show the formation or destruction of a stable species without considering the actual molecular steps that involve the reactions of free-radical and atomic species. This type of reaction differs from a molecular reaction in the following ways: it is always irreversible, and its rate expression does not obey the law of mass action used for molecular steps. Because the reaction includes effects of species other than the actual reactants, its rate can, in general, depend on the concentration of any species present in the mixture. The general rate expression for a global reaction is, therefore, written as

$$r_j = k_j(T) \prod_{i=1}^{NS} \left(\rho \sigma_i \right)^{a_{ij}}$$
(2.9)

where $\rho\sigma_i$ is the molar concentration of any species in the mixture, not only a reactant, and $k_j(T)$ is a temperature-dependent rate coefficient in the form of equation (2.6). The constants $\{a_{ij}\}$ and the three constants in $k_j(T)$ are obtained by multivariate curve fitting of experimental data taken over as wide a range of conditions as possible. Each global reaction in GLSENS may have a maximum of three species on the reactant side and three species on the product side. On both sides of equation (2.1) each species may be either an actual participant in the process or a species whose concentration appears in equation (2.9) but is not changed by the reaction. An example of a molecular reaction is the collision of two ketyl radicals to form acetylene and two carbon monoxide molecules:

$$C_2HO + C_2HO = C_2H_2 + 2CO$$

This is one of the steps in the oxidation of the fuel benzene, which is discussed in detail in section 4.3.2.4. The code interprets the left side of this reaction as two molecules of C_2HO and uses the rate expression

$$r_j = k_j \left\{ \left[C_2 HO \right]^2 - \frac{\left[C_2 H_2 \right] \left[CO \right]^2}{K_j} \right\}$$

where the square brackets indicate molar concentration and *j* is the reaction index number.

An example of a global step is the reaction

$$OH + H_2 + O_2 \rightarrow H_2O + O + OH$$

which is the conversion of a molecule of hydrogen and oxygen to water and an oxygen atom. A hydroxyl radical is written on both sides of the reaction because the experimentally determined rate expression for this reaction is

$$r_j = k_j [O_2] [OH]$$

This rate is independent of the concentration of hydrogen and is proportional to the concentration of OH radical, which is not changed by the reaction. The exponent of the oxygen concentration was determined by least-squares fitting of experimental data and is not related to the stoichiometric coefficient of oxygen, which has the same value. The code allows the use of as many as three rate-determining species concentrations and their empirically determined concentration exponents in equation (2.9) for each reaction. The latter are read in separately from the reactants and products of the reaction. Program details for using global reactions are given in chapter 3.

2.2 Equations for Perfectly Stirred Reactor Combustion and Sensitivity Analysis

The equations describing combustion reaction in the perfectly stirred reactor have been written and described in reference 1. For this completely backmixed system each reacting species mole number σ_i obeys the continuity equation

$$\frac{\dot{m}}{v} (\sigma_{i,0} - \sigma_i) + W_i = 0$$
 $i = 1, 2, ..., NRS$ (2.10)

where *v* is the reactor volume, \dot{m} is the mass flow rate through the reactor, and W_i , the net molar rate of formation of species *i*, is given by equation (2.2). Each reaction rate r_j in this equation is calculated from either equations (2.3) to (2.5) or equation (2.9), depending on whether the process is molecular or global. The reactor also obeys the energy conservation equation

$$\sum_{l=1}^{NS} \left(\sigma_l H_l - \sigma_{l,0} H_{l,0} \right) + \frac{\dot{Q}}{\dot{m}} = 0$$
 (2.11)

where H_l is the molar enthalpy of species *l* at the reactor temperature *T*, $H_{l,0}$ is the molar enthalpy of species *l* at the initial reactor temperature T_0 , and \dot{Q} is the heat transfer rate from the reactor and is a function of temperature only. Equations (2.10) and (2.11) constitute a system of NRS+1 nonlinear algebraic equations in the variables σ_1 , σ_2 , ..., σ_{NRS} and temperature that are valid for a chemical mechanism containing any mix of molecular and global reactions. These equations are solved by the Newton-Raphson numerical method as described in chapter 7 of reference 1. The iteration procedure solves sets of linear equations involving the logarithms of the increments of the dependent variables.

The present task is to compute the sensitivity coefficients of these NRS+1 dependent variables with respect to changes or uncertainties in the rate coefficient parameters A_j , n_j , and either E_j or c_j in equations (2.6) and (2.7). The sensitivity coefficients of these dependent variables with respect to initial temperature T_0 are also computed. For clarity of presentation the dependent variables are redefined in terms of an array $\{y_i\}$ having NRS+1 elements, where

$$y_i = \sigma_i$$
 $i = 1, 2, 3, ..., NRS$

and

$$y_{\text{NRS}+1} = T$$

2.2.1 Sensitivity Coefficients With Respect to Rate Parameters

The following unnormalized sensitivity coefficients are defined:

$$S_{ij} = \frac{\partial y_i}{\partial \eta_j}$$
 $j = 1, 2..., NR$
 $i = 1, 2, ..., NRS + 1$ (2.12)

where η_j represents any of the rate coefficient parameters of the *j*th chemical reaction, namely A_j , n_j , and E_j or c_j in equations (2.6) and (2.7). Sets of equations that can be solved for these sensitivity coefficients are now derived.

First, equations (2.10) can be differentiated with respect to rate parameter η_s to obtain the equation

$$-\frac{\dot{m}}{v}\frac{\partial\sigma_i}{\partial\eta_s} + \frac{\partial W_i}{\partial\eta_s} + \sum_{l=1}^{\text{NRS}} \left.\frac{\partial W_l}{\partial\sigma_l}\right|_T \frac{\partial\sigma_l}{\partial\eta_s} + \frac{\partial W_l}{\partial T}\Big|_{\sigma_i} \frac{\partial T}{\partial\eta_s} = 0$$

 $i = 1, 2, \dots, NRS$ (2.13)

The quantity η_s represents any of the three rate parameters of reaction *s*. The first and third terms of this equation can be combined by using the Kroneker delta function and the expression rewritten as

$$\sum_{l=1}^{\text{NRS}} \left(\frac{\partial W_i}{\partial \sigma_l} \Big|_T - \frac{\dot{m}}{v} \delta_{il} \right) \frac{\partial \sigma_l}{\partial \eta_s} + \frac{\partial W_i}{\partial T} \Big|_{\sigma_i}^{\text{all}} \frac{\partial T}{\partial \eta_s} = -\frac{\partial W_i}{\partial \eta_s}$$
$$i = 1, 2, ..., \text{NRS} \qquad (2.14)$$

where δ_{il} is defined by

$$\delta_{il} = \begin{cases} 0 & \text{if } i \neq l \\ \\ 1 & \text{if } i = l \end{cases}$$

There are now NRS linear equations in the NRS+1 unnormalized sensitivity coefficients just defined. To obtain an additional equation, equation (2.11) is differentiated with respect to η_s to get

$$\sum_{l=1}^{NS} \left\{ \sigma_l \frac{\partial H_l}{\partial T} \frac{\partial T}{\partial \eta_s} + H_l \frac{\partial \sigma_l}{\partial \eta_s} \right\} + \frac{\partial (\dot{Q} / \dot{m})}{\partial T} \frac{\partial T}{\partial \eta_s} = 0 \qquad (2.15)$$

This equation can be rewritten using the fact that $\partial H_l/\partial T$ is just C_{pl} , the molar heat capacity of species *l*, and that the mixture specific heat per unit mass is given by the summation

$$c_p = \sum_{l=1}^{NS} \sigma_l C_{pl} \tag{2.16}$$

The result is

$$\sum_{l=1}^{\text{NRS}} H_l \frac{\partial \sigma_l}{\partial \eta_s} + \left(c_p + \frac{1}{\dot{m}} \frac{\partial \dot{Q}}{\partial T}\right) \frac{\partial T}{\partial \eta_s} = 0 \qquad (2.17)$$

The limit on the summation is now NRS because all derivatives of inert-species mole numbers are equal to zero.

After equations (2.14) and (2.17) have been rewritten using the definitions of the sensitivity coefficients (eq. (2.12)), the following set of NRS+1 independent linear equations in the NRS+1 sensitivity coefficients of the dependent variables $\{y_i\}$ is obtained:

$$\sum_{l=1}^{NRS} \left(\frac{\partial W_i}{\partial \sigma_l} \bigg|_T - \frac{\dot{m}}{v} \delta_{il} \right) S_{ls} + \frac{\partial W_i}{\partial T} \bigg|_{\substack{\text{all} \\ \sigma_i}} S_{NRS+1,s} = -\frac{\partial W_i}{\partial \eta_s} \bigg|_{i=1,2,3,...,NRS}$$
(2.18)
$$\sum_{l=1}^{NRS} H_l S_{ls} + \left(c_p + \frac{1}{\dot{m}} \frac{\partial \dot{Q}}{\partial T} \right) S_{NRS+1,s} = 0$$

2.2.1.1 Derivatives of net species formation rate.—To solve the system equation (2.18), the derivatives of each species formation rate W_i must be calculated. For the rate coefficient parameter derivatives, $\partial W_i / \partial \eta_s$, equation (2.2) is differentiated to obtain

$$\frac{\partial W_i}{\partial \eta_s} = \left(\mathbf{v}_{is}'' - \mathbf{v}_{is}' \right) \frac{\partial r_s}{\partial \eta_s} \tag{2.19}$$

where the derivative on the right-hand side can be obtained from equations (2.3) to (2.5) as

$$\frac{\partial r_s}{\partial \eta_s} = r_s \frac{\partial \ln k_s}{\partial \eta_s} \tag{2.20}$$

When equation (2.20) has been substituted into equation (2.19), the result can be written as

$$\frac{\partial W_i}{\partial \eta_s} = \omega_{is} \frac{\partial \ln k_s}{\partial \eta_s}$$
(2.21)

where ω_{is} , the rate of formation of species *i* by reaction *s*, is defined in equation (2.2).

Next, the derivatives of W_i with respect to σ_l and T are calculated from equations (2.2) to (2.5). These equations present W_i as an explicit function of gas density ρ , which is, however, a function of T and the { σ_i } through the ideal-gas law.

$$\rho = \frac{p}{RT \sum_{i=1}^{NS} \sigma_i}$$
(2.22)

Therefore, implicit differentiation of equation (2.2) gives the following expressions for the partial derivatives of W_i with respect to σ_l and T:

$$\frac{\partial W_i}{\partial \sigma_l}\Big|_T = \frac{\partial W_i}{\partial \sigma_l}\Big|_{\substack{\text{other } \sigma_i, \\ \rho, T}} - \rho M_w \frac{\partial W_i}{\partial \rho}\Big|_{\substack{\text{all } \sigma_i, \\ T}}$$
(2.23)

$$\frac{\partial W_i}{\partial T}\Big|_{\substack{\text{all} \\ \sigma_i}} = \frac{\partial W_i}{\partial T}\Big|_{\substack{\text{all} \\ \rho}}, -\frac{\rho}{T}\frac{\partial W_i}{\partial \rho}\Big|_{\substack{\text{all} \\ \sigma_i}}, \qquad (2.24)$$

In these equations the following derivatives of density from equation (2.22) were used:

$$\frac{\partial \rho}{\partial \sigma_I} = -\rho M_w \tag{2.25}$$

$$\frac{\partial \rho}{\partial T} = \frac{-\rho}{T} \tag{2.26}$$

The necessary equations for the derivatives of W_i on the right sides of equations (2.23) and (2.24) are obtained from equation (2.2) as

$$\frac{\partial W_i}{\partial \sigma_l} = \sum_{j=1}^{NR} \left(\mathbf{v}_{ij}'' - \mathbf{v}_{ij}' \right) \frac{\partial r_j}{\partial \sigma_l}$$
(2.27)

$$\frac{\partial W_i}{\partial T} = \sum_{j=1}^{\text{NR}} \left(\mathbf{v}_{ij}'' - \mathbf{v}_{ij}' \right) \frac{\partial r_j}{\partial T}$$
(2.28)

$$\frac{\partial W_i}{\partial \rho} = \sum_{j=1}^{NR} \left(\mathbf{v}_{ij}'' - \mathbf{v}_{ij}' \right) \frac{\partial r_j}{\partial \rho}$$
(2.29)

2.2.1.2 Derivatives of net reaction rate.—The derivatives of r_j needed in equations (2.27) to (2.29) are obtained from equations (2.3) to (2.5) for molecular reactions and from equation (2.9) for global reactions. These derivatives are used not only for the PSR sensitivity calculations, but also for the general kinetics calculations and the static-reaction sensitivity analysis computations. For molecular reactions regular and third-body collisional processes must be treated separately when differentiating with respect to a species concentration or density. Consider the temperature derivatives first. For a molecular reaction rate, differentiating equations (2.4) and (2.5) and substituting into equation (2.3) give, after simplification,

$$\frac{\partial r_j}{\partial T} = r_j \frac{d \ln k_j}{dT} + R_{-j} \frac{d \ln K_j}{dT}$$
(2.30)

Differentiating equation (2.9) for a global reaction rate gives the same expression for the temperature derivative without the reverse rate term, since a global reaction is always irreversible. To obtain the σ_l and ρ derivatives of the molecular reaction rate, two cases are considered separately. For regular (noncollisionally catalytic) reactions M_j is set equal to 1.0 in equations (2.3) to (2.5), and differentiating with respect to σ_l gives, after some simplifying, the following expression for the σ_l derivatives of r_j :

$$\frac{\partial r_j}{\partial \sigma_l} = \frac{\mathbf{v}_{lj}' R_j}{\sigma_l} - \frac{\mathbf{v}_{lj}'' R_{-j}}{\sigma_l}$$
(2.31)

In most situations a species is either a reactant or a product, so either v'_{lj} or v''_{lj} will be zero. For the derivative with respect to density, equations (2.3) to (2.5) give the result

$$\frac{\partial r_j}{\partial \rho} = \frac{\nu'_j R_j}{\rho} - \frac{\nu''_j R_{-j}}{\rho}$$
(2.32)

where v'_j is the sum of the reactant stoichiometric coefficients in the *j*th reaction and v''_j is the sum of product stoichiometric coefficients in that reaction. In the case of collisionally catalytic (third body) reactions, differentiating equations (2.3) to (2.5) with respect to σ_l and using the appropriate derivative of M_j obtained from equation (2.8) give, after simplification,

$$\frac{\partial r_j}{\partial \sigma_l} = \frac{v_{lj}' R_j}{\sigma_l} - \frac{v_{lj}'' R_{-j}}{\sigma_l} + \frac{r_j \rho m_{lj}}{M_j}$$
(2.33)

Differentiating with respect to density and using equation (2.8) for $\partial M_j / \partial \rho$ give the expression

$$\frac{\partial r_j}{\partial \rho} = \frac{\nu'_j R_j}{\rho} - \frac{\nu''_j R_{-j}}{\rho} + \frac{r_j}{\rho}$$
(2.34)

For the σ_l and ρ derivatives of a global reaction rate, differentiating equation (2.9) gives the following results:

$$\frac{\partial r_j}{\partial \sigma_l} = \frac{a_{lj}r_j}{\sigma_l} \tag{2.35}$$

and

$$\frac{\partial r_j}{\partial \rho} = \frac{\mathbf{a}_j r_j}{\rho} \tag{2.36}$$

where a_i is the sum of all the a_{li} values for reaction j.

2.2.1.3 Temperature derivatives of rate coefficient and equilibrium constant.—Two quantities that appear in the r_j derivative expressions of the previous section need to be cal-

culated. These are the temperature derivatives of the rate coefficient and the equilibrium constant in equation (2.30). These equations also apply to more general situations than PSR sensitivity analysis (see ref. 1). Logarithmic differentiation of the usual modified Arrhenius rate expression (eq. (2.6)) gives

$$\frac{d\ln k_j}{dT} = \frac{n_j}{T} + \frac{E_j}{RT^2}$$
(2.37)

Similar differentiation of the special rate coefficient formula (eq. (2.7)) gives

$$\frac{d\ln k_j}{dT} = \frac{n_j}{T} + c_j \tag{2.38}$$

The equilibrium constant K_j for any reaction is expressed in concentration units by the relation

$$K_j = (RT)^{-\Delta v_j} \exp \frac{-\Delta G_j^{\circ}}{RT}$$
(2.39)

where ΔG_j° is the Gibbs function change for the reaction and Δv_j is the change in number of molecules for the reaction (i.e., number of products minus number of reactants.) Differentiating equation (2.39) and using the Gibbs-Helmholtz equation for $\partial(\Delta G_j^{\circ})/\partial T$ (ref. 12) give

$$\frac{d\ln K_j}{dT} = \frac{-\Delta v_j}{T} + \frac{\Delta H_j^\circ}{RT^2}$$
(2.40)

where ΔH_{j}° is the heat of reaction given by

$$\Delta H_{j}^{\circ} = \sum_{i=1}^{\text{NRS}} \left(\mathbf{v}_{ij}'' - \mathbf{v}_{ij}' \right) H_{i}^{\circ}$$
(2.41)

Equation (2.40) is rewritten for ease of computation in GLSENS by substituting equation (2.41) and the definition of Δv_j into it and rearranging terms to obtain the expression

$$\frac{d\ln K_j}{dT} = \frac{1}{T} \sum_{i=1}^{\text{NRS}} \left(\mathbf{v}_{ij}'' - \mathbf{v}_{ij}' \right) \left(\frac{H_i}{RT} - 1 \right)$$
(2.42)

2.2.1.4 Derivatives of rate coefficient equations with respect to rate parameters.—To complete the computation of all matrix coefficients in the system of equations (eq. (2.18)), the specific formulas for the right-hand-side coefficients (eq. (2.21)) have to be calculated. To obtain the logarithmic derivatives of k_j with respect to each rate parameter, the logarithmic forms of equations (2.6) and (2.7) are differentiated. From either of these equations the following formulas are obtained for the derivatives with respect to the preexponential factor and temperature exponent:

$$\frac{\partial \ln k_s}{\partial A_s} = \frac{1}{A_s}$$
(2.43)

$$\frac{\partial \ln k_s}{\partial n_s} = \ln T \tag{2.44}$$

The derivative with respect to E_j , from equation (2.6), is

$$\frac{\partial \ln k_s}{\partial E_s} = -\frac{1}{RT} \tag{2.45}$$

From equation (2.7) the derivative with respect to c_s is

$$\frac{\partial \ln k_s}{\partial c_s} = T \tag{2.46}$$

2.2.2 Sensitivity Coefficients With Respect to Initial Temperature

A set of linear equations that can be solved for the sensitivity coefficients of the dependent variables with respect to the initial temperature of the reacting mixture can be obtained by differentiating equations (2.10) and (2.11) with respect to the initial temperature T_0 . From equation (2.10)

$$\frac{\dot{m}}{v} \left(-\frac{\partial \sigma_i}{\partial T_0} \right) + \frac{\partial W_i}{\partial T_0} = 0$$
(2.47)

The second term can be written out as follows:

N TR G

$$\frac{\partial W_i}{\partial T_0} = \sum_{l=1}^{\text{NRS}} \left. \frac{\partial W_i}{\partial \sigma_l} \right|_T \frac{\partial \sigma_l}{\partial T_0} + \frac{\partial W_i}{\partial T} \bigg|_{\substack{\text{all} \\ \sigma_i}} \frac{\partial T}{\partial T_0}$$
(2.48)

Using equation (2.48) in equation (2.47) gives a set of NRS equations in the required NRS+1 sensitivity coefficients:

$$\sum_{l=1}^{\text{NRS}} \left\{ \frac{\partial W_i}{\partial \sigma_l} \bigg|_T - \frac{\dot{m}}{v} \delta_{il} \right\} \frac{\partial \sigma_l}{\partial T_0} + \frac{\partial W_i}{\partial T} \bigg|_{\substack{\text{all} \\ \sigma_i}} \frac{\partial T}{\partial T_0} = 0 \quad (2.49)$$

The last equation results from differentiating equation (2.11) with respect to T_0 , which gives, first,

$$\sum_{l=1}^{NS} \left\{ \sigma_l \frac{\partial H_l}{\partial T_0} + H_l \frac{\partial \sigma_l}{\partial T_0} - \sigma_{l,0} \frac{\partial H_{l,0}}{\partial T_0} - H_{l,0} \frac{\partial \sigma_{l,0}}{\partial T_0} \right\} + \frac{\partial (\dot{Q}/\dot{m})}{\partial T} \frac{\partial T}{\partial T_0} = 0 \quad (2.50)$$

To rewrite this equation in more useful form, first note that all the derivatives $\partial \sigma_{l,0} / \partial T_0$ are equal to zero and also that $\partial H_{l,0} / \partial T_0$ is $C_{pl,0}$, the molar heat capacity of species *l* at temperature T_0 . Finally,

$$\frac{\partial H_l}{\partial T_0} = \frac{\partial H_l}{\partial T} \frac{\partial T}{\partial T_0} = C_{pl} \frac{\partial T}{\partial T_0}$$

Using this information in equation (2.50) gives

$$\sum_{l=1}^{\text{NRS}} H_l \frac{\partial \sigma_l}{\partial T_0} + \left(c_p + \frac{1}{\dot{m}} \frac{\partial \dot{Q}}{\partial T}\right) \frac{\partial T}{\partial T_0} = c_{p,0} \qquad (2.51)$$

where $c_{p,0}$ is the initial mass specific heat of the mixture (see eq. (2.16)).

Equations (2.49) and (2.51) make up a set of NRS+1 independent linear equations in NRS+1 sensitivity coefficients that can be defined by

$$S_{i,T_0} = \frac{\partial y_i}{\partial T_0}$$
 $i = 1, 2, ..., \text{NRS} + 1$ (2.52)

where $y_i = \sigma_i$ for $i \le NRS$ and $y_i = T$ for i = NRS+1. The set of equations to be solved for these initial-temperature sensitivity coefficients can then be written as

$$\sum_{l=1}^{\text{NRS}} \left\{ \frac{\partial W_i}{\partial \sigma_l} \Big|_T - \frac{\dot{m}}{v} \delta_{il} \right\} S_{l,T_0} + \frac{\partial W_i}{\partial T} \Big|_{\substack{\text{all} \\ \sigma_i}} S_{\text{NRS}+1,T_0} = 0$$

$$i = 1, 2, ..., \text{NRS} \left\{ \begin{array}{l} (2.53) \\ \sum_{l=1}^{\text{NRS}} H_l S_{l,T_0} + \left(c_p + \frac{1}{\dot{m}} \frac{\partial \dot{Q}}{\partial T} \right) S_{\text{NRS}+1,T_0} = c_{p,0} \end{array} \right\}$$

Comparing this set of equations with the set solved for the sensitivity coefficients with respect to rate parameters (eqs. (2.18)) shows that each set has the same left-hand-side matrix of coefficients. Only the right-hand-side constant vector is different. Thus, the computational cost of obtaining the initial-temperature sensitivity coefficients is very small after the rate coefficient sensitivities have been calculated.

2.2.3 Normalized Sensitivity Coefficients

2.2.3.1 Rate coefficient parameters.—The GLSENS code normalizes all sensitivity coefficients calculated by solving the set of equations (2.18) by exactly the same method used for sensitivity coefficients in integration problems. The normalization factors used are discussed in detail in chapter 4 of part I of the LSENS code documentation (ref. 1). A brief summary of the formulas for normalized coefficients is given here for the reader's convenience. Again, using η_j to represent any of the rate parameters of the *j*th chemical reaction, the normalized sensitivity coefficient of any y_i with respect to η_j can be defined by

$$\left\langle S_{ij} \right\rangle = \frac{\partial \ln y_i}{\partial \ln \eta_j} = \left(\frac{\eta_j}{y_i}\right) \left(\frac{\partial y_i}{\partial \eta_j}\right)$$
 (2.54)

This coefficient is the percent change in y_i due to a change in η_j that causes a 1-percent change in the rate coefficient k_j . In practice the correct normalization factor η_j , multiplying the unnormalized coefficient $\partial y_i / \partial \eta_j$ on the right-hand side of equation (2.54), has to be properly chosen for the type of input quantity whose sensitivity is being computed. In the case of the preexponential factor A_j the choice is very simple, namely A_j itself. Because A_j is always nonzero (unlike the other rate parameters), it can be used as the normalization factor. For the other rate parameters assumptions are made to express the normalization factors in terms of the initial temperature. Consult reference 1 for additional details on the derivation of normalization factors for these rate coefficient parameters. The exact factors used in LSENS and GLSENS are listed for reference in table 2.1.

For the perfectly stirred reactor the sensitivity coefficients with respect to all three rate parameters should be the same because the reaction is really occurring at a constant temperature, namely the converged temperature for any assigned mass flow rate. To verify this fact, sensitivity coefficients were calculated for all three rate parameters separately for each reaction and were always found to be identical when the normalization factors of table 2.1 were used. Therefore, only sensitivity to a 1-percent change in the rate coefficient k_j , which is the normalized quantity defined by equation (2.54) for any of the individual rate parameters, needs to be discussed here.

For computing the brute-force sensitivity coefficients the partial derivative in equation (2.54) is replaced by the ratio $\delta y_i / \delta \eta_i$, where δy_i is the small change in y_i caused by the small



change $\delta \eta_j$. Also, the quantity y_i becomes \bar{y}_i , the value of the dependent variable for the standard or unchanged value of η_j . It is most convenient to change the A_j parameter, inasmuch as both equations (2.6) and (2.7) show that a given percent change in the preexponential factor causes the same percent change in the rate coefficient. For a change in any A_j of ±1 percent the approximation formula to equation (2.54) for the normalized brute-force sensitivity coefficient with respect to k_j is then given by

$$\left\langle S_{ij} \right\rangle = \frac{y_i \left(A_j + \Delta \right) - y_i \left(A_j - \Delta \right)}{0.02 \bar{y}_i}$$
(2.55)

where

 \overline{y}_i y_i value for standard value of A_j

 $y_i(A_j + \Delta)$ y_i value when A_j is increased by Δ

 $y_i(A_i - \Delta)$ y_i value when A_i is decreased by Δ

and

$$\Delta = 0.01A_{\perp}$$

This equation was used to calculate the brute-force sensitivity coefficients with respect to the rate coefficients inasmuch as the change in any y_i caused by the change in A_j was found to be small enough to give a good approximation to the sensitivity coefficient derivative.

2.2.3.2 *Initial temperature.*—For the normalized sensitivity with respect to initial temperature, T_0 is used as the normalization factor, the unnormalized coefficient (eq. (2.52)) is multiplied by the factor T_0/y_i , and they are combined to obtain

$$\left\langle S_{i,T_0} \right\rangle = \frac{T_0}{y_i} \left\{ \frac{\partial y_i}{\partial T_0} \right\}$$
 $i = 1, 2, ..., \text{NRS} + 1$ (2.56)

of ± 2 K is used for the initial temperature. The δT_0 becomes just 4 K and the brute-force approximation formula becomes

$$\left\langle S_{i,T_{0}} \right\rangle = \frac{T_{0} \left[y_{i} \left(T_{0} + 2\mathbf{K} \right) - y_{i} \left(T_{0} - 2\mathbf{K} \right) \right]}{4 \overline{y}_{i}}$$
 (2.57)

In performing the brute-force sensitivity calculations a 1-percent change in initial temperature cannot be used because it would result in too large changes in the dependent variables δy_i , thus making the difference approximation to the derivative in equation (2.56) quite inaccurate. Instead a change

Chapter 4 gives the results of several GLSENS test-case computations of sensitivity coefficients for the perfectly stirred reactor and compares them with the results of brute-force computations using equations (2.55) and (2.57).

Chapter 3 Description of New GLSENS Coding

3.1 New Subroutines

In the following description of GLSENS coding, which incorporates the additional abilities described previously, it is assumed that the reader is familiar with the structure of and input to the original LSENS code described in reference 2, the usage manual. GLSENS keeps all the subroutines of LSENS with necessary small modifications and adds four new subroutines. Three of these are needed for reading in global reactions and calculating their rates. The fourth contains the computation of sensitivity coefficients for a PSR problem. The first global reaction subroutine, GLOBIN, is called by subroutine KINP to read in and process the input data for all global reactions after it has read in any data for molecular reactions that may be present. The second new subroutine, GLBCHG, reads in any rate coefficient changes for global reactions in a multiple-case situation. The third global reaction subroutine, GLBRAT, is called by DIFFUN to calculate the molar rates per unit volume of all global reactions after the molar rates for the molecular reactions present have been calculated. A new common block, REAC3, which contains necessary global reaction variables, was added to these subroutines and to subroutine KINP and the main program.

The fourth new subroutine, PSENS, manages the calculation of all sensitivity coefficients for a PSR problem. This subroutine, which is called from subroutine WSR after completion of each incremental assigned mass-flow-rate PSR calculation, first calculates the elements of the left-hand-side coefficient matrix of equations (2.18) and (2.53). To do this, PSENS calls subroutine PEDERV, where many of the same partial derivatives of W_i are calculated as part of the Jacobian elements for the Newton-Raphson iteration that solves the PSR problem itself. After completing the appropriate right-hand-side vector, PSENS calls subroutine GAUSS to solve for the unnormalized sensitivity coefficients. Subroutine SNSOUT is then called to normalize and print only the coefficients that were asked for in the problem data file. Logic changes are made in subroutine SNSOUT and in subroutine SNSTAB to accommodate PSR sensitivity analysis computations. A new common block, PSRSEN, was added to subroutines PEDERV, PSENS, WSR, and SNSTAB as well as to the main program. This common block contains the logical variable WELSEN.

Two changes to the original LSENS subroutines should be mentioned. One is in the output routine OUT1, which was changed to print out the additional input data for global reactions. In addition, the dimensions of many arrays were increased to allow a maximum of 80 species to be used in a single problem. These changes are described in appendix C (table C.3) of reference 2.

3.2 Modifications to Problem Data File

3.2.1 Chemical Reaction Input

For all cases the code must now be told what kind of reaction mechanism is to be used for the computation. GLSENS gives complete flexibility as to the type of mechanism that may be used. All molecular reactions or all global steps or a mixture of the two types may be used. In the last case any number of reactions of each type may be used (up to the maximum number allowed, LRMAX), and the molecular reactions must be listed first. A new namelist called RTYPE must be added to each case. The seven logical variables in this namelist are listed and their usage described in table 3.1. The first two logical variables must be set for all cases. If any global reactions are in the mechanism, the variable GLOBAL must be set equal to TRUE. If the mechanism contains global reactions exclusively, the variable GRONLY must be set equal to TRUE. Both variables are initialized to the value FALSE so that they do not have to be set if a mechanism consists of molecular reactions only. The remaining five logical variables in RTYPE must be set for any cases that use the REPEAT, CHANGE, or ADD settings of the ACTION switch in a multiple-case file. All of these variables except MRPREV are initialized to FALSE. The latter variable is initialized to TRUE, which tells LSENS that the previous

| Variable | Value ^a | Explanation |
|----------|--------------------|---|
| manie | | |
| GLOBAL | TRUE | Global reactions are present in current case mechanism. |
| | <u>FALSE</u> | Global reactions are NOT present in current case mechanism. |
| GRONLY | TRUE | Molecular reactions are NOT present in current case mechanism. |
| | FALSE | Molecular reactions are present in current case mechanism. |
| GLCHNG | TRUE | Some global reaction rate coefficients are to be changed from previous case. |
| | FALSE | No global reaction rate coefficients are to be changed from previous case. |
| GLADD | TRUE | Global reactions are to be added to mechanism of previous case. |
| | FALSE | No global reactions are to be added to mechanism of previous case. |
| MRPREV | TRUE | Mechanism of previous case consists of only molecular reactions. |
| | FALSE | Mechanism of previous case has some global reactions. |
| MRCHNG | TRUE | Some molecular reaction rate coefficients are to be changed from previous case. |
| | FALSE | No molecular reaction rate coefficients are to be changed from previous case. |
| MRADD | TRUE | Molecular reactions are to be added to mechanism of previous case. |
| | FALSE | No molecular reactions are to be added to mechanism of previous case. |

TABLE 3.1.—DESCRIPTION OF LOGICAL VARIABLES IN NAMELIST RTYPE

^aDefault value is underlined.

case's mechanism contained only molecular reactions. Table 3.2 lists the values of the four variables GLCHNG, GLADD, MRCHNG, and MRADD for all possible situations of modifying a mechanism by using the CHANGE and ADD options. Test-case files presented in chapter 4 give examples using the information in tables 3.1 and 3.2. Note that the namelist RTYPE follows the title line in a single case or in the first case of a multiple-case file. However, in any case after the first in a multiple-case file, RTYPE follows the ACTION line.

When both molecular and global reactions are used in a mechanism, the global reactions follow the list of molecular reactions (which ends with a blank line or the word END beginning in column 4). Each global reaction requires two input lines, whose formats are given in table 3.3. The first line gives the names of as many as three reactant and/or rate-controlling species as well as up to three products along with their stoichiometric coefficients, if different from 1. Note that if a global step has a single reactant, it must be placed in the third (rightmost) reactant field. It is called the first or only reactant in table 3.3. If the step has two reactants only, they must be placed in the second and third reactant fields. Likewise, a single product must be listed in the first (leftmost) product field and two products only must be listed on this line include all whose concentra-

tions are to be used in equation (2.9). If the rate expression contains the concentration of a species that is not a participant in the reaction, this species must be listed both as a reactant and a product, so that its net change in concentration will be zero. Note that column 40 must either be blank or have any character except an equal sign, to indicate that the reaction is irreversible. The ">" symbol is the most logical choice. The second line lists first the exponent a_{ii} to be used with each concentration c_i for each reactant species on the previous line. The last half of this line lists the three parameters A_i , n_i , and E_i of the rate coefficient expression (eq. (2.6)). The global reaction list ends with either a blank line or one with the word END starting in column 5. If the reaction mechanism contains only global reactions, this list starts immediately after the namelist RTYPE line. Chapter 4 gives example problems that illustrate problem data files containing mechanisms of all-global and molecular-plus-global reactions.

3.2.2 PSR Sensitivity Coefficient Calculations

No change from the input data for an integration sensitivity problem was required for the PSR sensitivity calculations. For detailed information on setting up the problem data file for a

| Next-case situation | Variable name ^a and value | | | | | |
|---|--------------------------------------|--------------------|--------------------|--------------------|--|--|
| | GLCHNG | GLADD | MRCHNG | MRADD | | |
| Change molecular rate coefficients only. | FALSE ^b | FALSE ^b | TRUE | FALSE ^b | | |
| Change global rate coefficients only. | TRUE | FALSE ^b | FALSE ^b | FALSE ^b | | |
| Change global and molecular rate coefficients. | TRUE | FALSE ^b | TRUE | FALSE ^b | | |
| Change molecular rate coeffi- cients and add molecular reactions. | FALSE ^b | FALSE ^b | TRUE | TRUE | | |
| Change molecular rate coef- ficients and add global reactions. | FALSE ^b | TRUE | TRUE | FALSE ^b | | |
| Change molecular rate coeffi- cients and add global and molecular reactions. | FALSE ^b | TRUE | TRUE | TRUE | | |
| Change global rate coefficients and add molecular reactions. | TRUE | FALSE ^b | FALSE ^b | TRUE | | |
| Change global rate coefficients and add global reactions. | TRUE | TRUE | FALSE ^b | FALSE ^b | | |
| Change global rate coefficients and add global and molecular reactions. | TRUE | TRUE | FALSE ^b | TRUE | | |
| Change global and molecular rate coefficients and add molecular reactions. | TRUE | FALSE ^b | TRUE | TRUE | | |
| Change global and molecular rate coefficients and add global reactions. | TRUE | TRUE | TRUE | FALSE ^b | | |
| Change global and molecular rate coefficients and add global and molecular reactions. | TRUE | TRUE | TRUE | TRUE | | |
| Add molecular reactions only. | FALSE ^b | FALSE ^b | FALSE ^b | TRUE | | |
| Add global reactions only. | FALSE ^b | TRUE | FALSE ^b | FALSE ^b | | |
| Add molecular and global reactions. | FALSE ^b | TRUE | FALSE ^b | TRUE | | |

TABLE 3.2.—LOGICAL VARIABLE SETTINGS IN NAMELIST RTYPE FOR MULTIPLE-CASE SITUATIONS

^aThe variables GLOBAL, GRONLY, and MRPREV are set according to the makeup of the mechanisms of the previous and current cases; see table 3.1.

^bDefault value.

| Columns | Variable type | Format | Content and explanation | | | |
|-------------------|------------------|------------|---|--|--|--|
| 1_4 | Real | F4 2 | Stoichiometric coefficient of left reactant (default value -1) | | | |
| 5_12 | Character | 14.2 | Name of left reactant (third one) | | | |
| $\frac{3-12}{14}$ | Deel | E4.2 | Name of left reactant (till one) Staighteen reactant (default value -1) | | | |
| 14-17 | Character | Г4.2 ло | Storemometric coefficient of center feactant (default value = 1) Norma of center reactant (accord and) | | | |
| 16-23 | Character | Að | Name of center reactant (second one) | | | |
| 27-30 | Real | F4.2 | Stoichiometric coefficient of right reactant (default value = 1) | | | |
| 31–38 | Character | A8 | Name of right reactant (first or only one) | | | |
| 40 | Character | A1 | ">" or any symbol except "="; indicates irreversible reaction | | | |
| 41-44 | Real | F4.2 | Stoichiometric coefficient of left product (default value = 1) | | | |
| 45-52 | Character | A8 | Name of left product (first or only one) | | | |
| 54–57 | Real | F4.2 | Stoichiometric coefficient of center product (default value = 1) | | | |
| 58-65 | Character | A8 | Name of center product (second one) | | | |
| 67–70 | Real | F4.2 | Stoichiometric coefficient of right product (default value = 1) | | | |
| 71–78 | Character | A8 | Name of right product (third one) | | | |
| | | | (b) Line 2. | | | |
| 1-10 | Double | F10.4 | Concentration exponent of left (third) reactant | | | |
| 11-20 | precision | F10.4 | Concentration exponent of center (second) reactant | | | |
| 21-30 | | F10.4 | Concentration exponent of right (first or only) reactant | | | |
| 31-40 | | E10.4 | Preexponential factor A_i in eq. (2.6) | | | |
| 41-50 | | F10.4 | Temperature exponent n_i in eq. (2.6) | | | |
| 51-60 | ↓ | F10.4 | Activation energy E_i in eq. (2.6) | | | |

TABLE 3.3.—FORMATS OF TWO REACTION LINES FOR EACH GLOBAL REACTION (a) Line 1.

sensitivity analysis calculation, consult chapter 11 of reference 2. In the previous LSENS version setting the logical variable SENCAL equal to TRUE for a PSR problem resulted in an error exit. This restriction has been removed by logic changes in the main program and in subroutines KINP and SENSIN. The user places the usual sensitivity analysis key words, SENSVAR, REAC, and INIT (followed by appropriate data lines), directly after the initial-mixture composition data for a PSR problem, inasmuch as namelist SOLVER is not required for this type of problem. Remember, however, that the key word INIT (requesting sensitivity coefficients with respect to initial values of dependent variables) may only be used with the name TEMP on the following line. GLSENS does not compute sensitivity coefficients with respect to initial species concentrations for PSR sensitivity analysis. Note that the user has the same choice of two tabular output formats for sensitivity coefficients with respect to rate parameters as for an integration problem. They are described in reference 2 and illustrated in the several examples of problem data files for PSR sensitivity computations given in chapter 4.

Chapter 4 Kinetics and Sensitivity Test Cases and Example Problems for Global Reactions and PSR Sensitivity

4.1 Kinetics and Sensitivity Analysis Test Cases

Part III of the documentation for the original LSENS code (ref. 3) describes two sets of test cases that illustrate the code's ability to perform many types of chemical kinetics computations as well as sensitivity analysis for static chemical reactions. The GLSENS code, of course, also retains all those abilities. All original LSENS test cases give identical results when executed with the GLSENS code and may be used to verify the performance of this new code. The LSENS test cases are supplied with the new code, GLSENS. Also supplied with the code is the same thermodynamic data file used with LSENS. It contains species coefficients from the thermodynamic data base of the CET computer code (ref. 13) and is described in detail in the LSENS documentation (ref. 2). These coefficients for species not included in the GLSENS file can be computed by using the code of McBride and Gordon (ref. 14).

4.2 Global Reaction Example Problems

The four example problems presented here show the use of quasi-global (global and molecular) reaction mechanisms as well as all-global mechanisms in three perfectly stirred reactor problems and one integration problem. As part of the integration problem the usual sensitivity coefficients calculated by the original LSENS code are computed for both molecular and global reactions to illustrate that the fundamental technique is the same for both types of reaction. Only the details of computing the reaction rate and its derivatives differ.

4.2.1 Example Problem 1

In this problem a mechanism of all global reactions is used to describe the perfectly stirred reactor combustion of a rich propane-air mixture (fuel equivalence ratio $\varphi = 2.0$) at a pressure of 5.5 atmospheres. The initial-mixture temperature is 800 K and the reactor volume is 2500 cm³. The complete problem data file is shown in table 4.1 (see end of chapter for tables) and, except for the use of global reactions, is set up exactly as described in the LSENS code description and usage report (ref. 2). All mechanisms used in these example problems are modifications of those developed by Dr. K. Kundu for simplified description of the combustion of propane and the attendant formation and destruction of oxides of nitrogen (NO_x) . See, for example, reference 15. The last reaction in the mechanism (reaction 13) illustrates two characteristics of a global reaction. First, the concentration exponent of reactant H₂ is zero, which indicates that hydrogen concentration has no effect on the rate of this reaction. Second, the reaction rate depends on the concentration of the hydroxyl radical, which is not a participant in the reaction. This species is written on both sides of the reaction and, on the next line, is given the concentration exponent value 1.0. Reaction 12 illustrates a global step in which a reactant (OH) concentration has an exponent (1.0) in the rate equation that is different from its stoichiometric coefficient of 2.0. The rate of this reaction also depends on propane (C_3H_8) concentration to the power 0.15, but the fuel does not participate in this reaction. The name C3H8 is written as a reactant and a product to indicate that its concentration is unchanged by the reaction. Note that the PSR calculation is controlled by the variables in namelist WSPROB. This is an assigned-mass-flow-rate problem with a desired flow rate of 1600 g/s that is to be reached with increments of 200 g/s from a starting value of 100 g/s assigned in namelist START.

Some of the computed results for this case are listed in table 4.2, which shows partial results for the first, second, fourth, and final convergences. The code had to increase the assigned mass flow rate to 800 g/s to obtain the first successful convergence because lower mass flow rates gave convergence to false solutions of the real combustion problem. The false solutions gave converged temperatures higher than the computed equilibrium temperature of 2020.68 K, which was used as the first estimate for the correct converged temperature. The first converged temperature was about 80 K below the equilibrium temperature and required 14 iterations. Each subsequent convergence required only between three and six iterations and gave much smaller decrements of temperature. This behavior is a typical convergence pattern for PSR combustion of rich hydrocarbon mixtures. Computed results for several intermediate convergence points and the desired mass flow rate of 1600 g/s are given in table 4.2.

4.2.2 Example Problem 2

This problem is also a rich propane-air PSR combustion ($\varphi = 1.5$) with the same initial temperature and pressure as example problem 1. The reaction mechanism of all global reactions is a modification of that of example problem 1, and several additional reactions have rates controlled by nonparticipating species H₂ and O₂.

The complete data file for this case is shown in table 4.3, where it can be seen that a much larger reactor volume and lower maximum flow rate were used than in example 1. This mechanism was arbitrarily changed from the previous one for illustrative purposes and could be quite unrealistic. Convergence difficulties were encountered in this problem, and the given volume and initial mass flow rate had to be found by trial and error until several successful convergences were obtained. Computed results for some of these conditions are shown in table 4.4. Although a maximum flow rate of 60 g/s was desired, no successful convergence was obtained for a mass flow rate above 25 g/s. The attempted convergence temperature began dropping rapidly, indicating a blowout situation.

4.2.3 Example Problem 3

This problem is the same PSR problem as in example 1, but it uses a reaction mechanism consisting of both global and molecular steps. The latter group of reactions (all reversible) is the hydrogen-oxygen submechanism of the benzene oxidation mechanism used by Bittker (ref. 6). The global reactions are taken from example problem 1.

The data file for this case is shown in table 4.5 and computed results, in table 4.6. Note that the desired flow rate of

2500 g/s was again not reached because a blowout condition was encountered at 450 g/s.

4.2.4 Example Problem 4

The constant-volume static reaction of a rich ($\varphi = 2$) propane-air mixture is illustrated in this example, whose purpose is to show the use of a quasi-global mechanism in an integration problem. The problem also illustrates the calculation of sensitivity coefficients for global reactions in an integration problem. The mechanism contains both molecular and global reactions. The molecular steps are all irreversible and were used by K. Kundu in work at NASA Lewis. Global reactions are taken from example problems 1 and 3. This mechanism is not a realistic one and is used here only for illustrative purposes. It should not be used for modeling any real combustion system.

The problem data file for this case is given in table 4.7. Sensitivity coefficients were computed for most of the dependent variables with respect to the rate constant parameters of both the molecular and global reactions. The sensitivity analysis computation was similar for both reaction types because both global and molecular reactions use the same form for the rate coefficient expression (eq. (2.6)). Only differences in the net rate expressions (eqs. (2.3) to (2.5) and eq. (2.9)) had to be considered. All computed results, and especially values of sensitivity coefficients, were found to be sensitive to the settings of the integration accuracy control parameters EMAX and ATOLSP.

In table 4.8 computed results are shown for several dependent variables and their sensitivity coefficients with respect to the A_i factor for the most controlling reaction, which is (global) reaction 14, the reaction of C₃H₈ with O₂. Results are given for three values of the relative error control variable EMAX. As the table shows, an EMAX value of 10^{-4} computed inaccurate values of temperature and five species mole fractions. EMAX had to be reduced to 10^{-6} or lower to obtain good accuracy. The accuracy of sensitivity coefficients was even more sensitive to the EMAX value used. Brute-force calculations of several sensitivity coefficients were also performed, and all results agreed with the values calculated by GLSENS for EMAX = 10^{-7} . These results for the effect of error control parameters on accuracy are consistent with those reported in chapter 13 of reference 2 for the original LSENS code using a mechanism of molecular reactions only.

4.3 Perfectly Stirred Reactor Sensitivity Calculations

Before example problems are presented, error control for a PSR calculation is briefly discussed to help GLSENS users properly evaluate the accuracy of computed results.

4.3.1 Error Control for PSR Problems

For kinetics problems solved by numerical integration of differential equations, accuracy for both the direct and sensitivity analysis solutions depends on the values of two error control parameters set by the user in each problem data file. This error control has been discussed and illustrated in great detail in parts I and II of the LSENS documentation (refs. 1 and 2). The situation is quite different for PSR calculations. The computation accuracy is controlled by two control numbers built into the code (in subroutine WSR) and used to test for proper convergence of the numerical solution of the nonlinear algebraic equations that describe the reactor. Error control is self-setting, therefore, and cannot be adjusted by the user in the problem data file. In the development of the Newton-Raphson direct solution, optimum values of the two test numbers were obtained. Further reduction of these numbers will not change the answers and may cause numerical difficulties in the convergence process. One additional test number, which affects the computed values of trace species concentrations, is used in subroutine WSR. To avoid numerical problems during the Newton-Raphson iteration procedure, a minimum value that any species mole number can achieve has to be set. The value of this lower limit is given by the variable SMALNO, which is set in a DATA statement, along with the value of its natural logarithm, DLOGSN. Variation of SMALNO in a series of test calculations showed that it had to be set at 1.0×10^{-10} . In many computations for several test cases trace species concentrations near this lower limit sometimes showed unexpected variation.

Sensitivity coefficients were obtained by the exact solution of a set of linear equations whose matrix of coefficients depends on the accuracy of the direct solution. Therefore, the trace species concentrations and their sensitivity coefficients were probably less accurate than values for the other dependent variables.

4.3.2 PSR Sensitivity Analysis Problems and Comparisons With Brute-Force Results

The five example problems presented here illustrate PSR sensitivity analysis computations for several fuel-oxidant combinations. The fuels hydrogen, benzene, and propane react with oxygen alone and in the presence of nitrogen and/or the inert gas argon. Brute-force sensitivity coefficients have been calculated for each test case and compared with results from GLSENS. One of these cases (example problem 7) illustrates a simplified model of a gas turbine combustor.

4.3.2.1 Example problem 5.—This first PSR sensitivity analysis problem is the reaction of a stoichiometric mixture of hydrogen and oxygen alone. The reaction mechanism of all molecular reactions is taken from Brabbs and Musiak (ref. 16). The problem data file for this case, shown in table 4.9, calls for the calculation of sensitivity coefficients of all species

concentration variables and temperature with respect to all reaction preexponential factors and initial temperature. Also, the value of TINY in namelist PROB has been set to 10^{-3} in order to set equal to zero all coefficients with magnitudes smaller than this number. Experience with sensitivity analysis has shown that such small-magnitude coefficients indicate unimportant effects of changing the rate parameter. The values of the variables OUTPUT (= FALSE) and ORDER (= TRUE) have been set in namelist SENRXN to print only the table of sensitivity coefficients indexed by dependent variable.

Sensitivity coefficients with respect to the most important rate coefficients and initial temperature for this problem are shown in tables 4.10(a) and (b). Also listed are sensitivity coefficients calculated by using the brute-force formulas (eqs. (2.55) and (2.57)). Results are tabulated for two stable species, hydrogen and water, as well as for three radical species and temperature. Part (a) shows that, for rate coefficient sensitivities, agreement was generally excellent between GLSENS and the brute-force values for coefficients with magnitudes of at least 0.01 and good for the smaller magnitude coefficients. In this mixture the dominant reactions were two catalytic collisional processes, the dissociation of water and the $H + O_2$ recombination to form the hydroperoxyl radical, although other reactions did affect the overall rate. These controlling reactions can be contrasted to the lower temperature ignition of a hydrogen-oxygen mixture, for which the most sensitive reaction promoting ignition is the $H + O_2$ reaction to form an oxygen atom and the OH radical. This chain-branching reaction is the main propagation step for the free-radical process that ignites the fuel-oxygen mixture. The catalytic collisional processes that control the PSR reaction have little control of the ignition reaction. Sensitivity coefficients with respect to initial temperature are shown in table 4.10(b). Brute-force coefficients were again compared with those calculated by GLSENS, and there was the same excellent agreement between the two methods of computation. The concentrations of oxygen atom and hydroxyl radical were affected most strongly by changing the initial temperature.

4.3.2.2 *Example problem 6.*—This problem uses an abbreviated quasi-global mechanism for the combustion of a propane-air mixture having an equivalence ratio of 1.5. There are 18 molecular and 10 global reactions in the mechanism. The problem is the same as example problem 3 for global reactions, with sensitivity analysis added to the data file, which is shown in table 4.11. The input data call for calculating sensitivity coefficients for six species and temperature with respect to all rate coefficients and initial temperature. Again, only sensitivities with magnitude greater than 0.001 are to have nonzero values.

Sensitivity coefficients calculated by GLSENS and the bruteforce method for this case are presented in table 4.12. Part (a) gives sensitivity coefficients for five species and temperature with respect to the rate coefficients of the seven most important reactions. Of these, six are global steps and the one molecular process is the $H + O_2$ radical branching reaction. As for the previous example, agreement between the GLSENS and bruteforce values was excellent for all sensitivities with magnitude greater than 0.01 and good for all but one of the smaller magnitude coefficients, namely the sensitivity of molecular oxygen concentration to the rate coefficient of reaction 28. This global step converts molecular hydrogen and oxygen to an oxygen atom and water. This reaction is written with OH on both sides because its rate parameters in table 4.11 show that the rate is proportional to the product of OH and oxygen concentrations and is independent of molecular hydrogen concentration. The brute-force value is about 18 percent lower than the GLSENS-computed sensitivity coefficient, 4.08×10^{-3} . The difference was most likely due to an inaccurate brute-force calculation because the sensitivity coefficient magnitude was only a little above the 0.001 cutoff limit. It is also possible that inaccuracies of the numerical procedure in the PSR solution affected the linear equation solution for the sensitivity coefficients. However, for this small a sensitivity coefficient the difference found between the two methods is really not important.

Note that reaction 25, the direct propane-oxygen reaction, appeared to have the strongest control over the entire reaction, with reactions 28 and 24 next in importance. However, it is interesting to observe that six of the seven reactions in the table had a strong effect on the concentration of nitric oxide, one of the significant pollutants in combustion processes.

Table 4.12(b) shows sensitivity coefficients with respect to initial temperature and demonstrates excellent agreement between the GLSENS and brute-force values. An initial temperature change had its greatest effect on the fuel and oxidant concentrations.

4.3.2.3 Example problem 7.—Example problem 7 is also the PSR oxidation of a rich ($\varphi = 1.5$) propane-air mixture at high pressure, but with a lower initial temperature of 614 K. This stirred-reactor problem was used as the first part of example problem 1 in chapter 13 of part II of the original LSENS documentation (ref. 2). That problem showed a simplified model of a gas turbine combustor, which is a PSR reaction of the initial mixture followed by the expansion of the PSR exit gas into a diverging nozzle. In the present example a sensitivity analysis was performed on the stirred-reactor part of the model. A comprehensive 136-step, molecular reaction mechanism was used, instead of the brief global and molecular reaction mechanism of the previous example. The problem data file for this case is given in table 4.13, which shows that sensitivity coefficients are required for nine species variables and temperature. The value of TINY was set to 10^{-3} , as in the other example problems. In namelist SENRXN sensitivities are requested with respect to the rate coefficients of the 13 most important reactions, whose numbers are given in the array RXNUM. The logical variable ORDER was again set equal to TRUE and the variable OUTPUT equal to FALSE to reduce the

number of sensitivity tables printed. A logical variable in the data file also requests sensitivity coefficients with respect to initial temperature.

GLSENS-computed sensitivity coefficients for several of these dependent variables in the PSR problem are shown in table 4.14 and compared with brute-force coefficients. Table 4.14(a) shows sensitivity to the rate coefficients of the four most rate-controlling reactions. The dominating reaction was the collisional decomposition of CH₄ into a methyl radical and a hydrogen atom. Its rate coefficient affected the concentrations of stable species (methane, propane, and ethane) as well as of the methyl and hydroxyl radicals. Also, the last two reactions listed (OH + C₂H₆ and CH₃ + CH₂) significantly controlled the concentrations of CH₄, CH₃, and C₂H₆. These sensitivity analysis results contrast with those for the low-temperature static ignition of a propane-air mixture. A sample calculation for ignition of the same mixture used in this test case showed that the rate-controlling reactions are the following:

$$CH_3 + HO_2 = CH_3O + OH$$
$$C_2H_4 + OH = C_2H_3 + H_2O$$
$$OH + CH_4 = CH_3 + H_2O$$
$$CH_3 + C_3H_8 = CH_4 + C_3H_7$$

None of these reactions was found to be rate controlling for the PSR reaction at higher temperature. Table 4.14(b) shows sensitivity coefficients with respect to initial temperature. Concentrations of the species propane, ethane, and hydroxyl radical were strongly affected by changes in the initial temperature.

Comparing the brute-force and GLSENS sensitivity coefficients in table 4.14 again shows excellent agreement between the two methods. The only small differences occurred for the smallest magnitude coefficients, where discrepancies were evident in the previous problems.

4.3.2.4 *Example problem 8.*—This problem, the first of two benzene-oxygen reactions, is the PSR reaction of an undiluted stoichiometric benzene-oxygen mixture. The reaction mechanism used is a slightly modified version of that given by Bittker in reference 6. The problem data file for this case is shown in table 4.15. In namelist PROB the variable TINY is set equal to 10^{-3} as before, and there is heat loss from the reactor, as defined by the variables WSRHTR, WSRHTO, and WSRHT1 in namelist WSPROB. Sensitivity coefficients for 10 species concentration variables and temperature are requested with respect to all reaction A_i factors and initial temperature.

Sensitivity coefficients calculated by GLSENS and the bruteforce method, for five species concentrations and temperature are shown in table 4.16. The species include the fuel, two intermediate products (benzyl alcohol and carbon monoxide), and two free-radical species (benzoxy and benzyl). Data were omitted if the sensitivity coefficient values were less than 0.001. The coefficients listed are for the most rate-controlling reactions in the mechanism, including pyrolysis reactions of the fuel and benzoxy and benzyl radicals and reactions of C_4H_2 , C_5H_5 , and C_2H_2 . By contrast, none of these reactions was rate controlling in the static ignition of benzene-oxygen mixtures, diluted with argon, at initial temperatures close to 1100 K. Sensitivity analysis for this reaction condition is presented in reference 6. The rate-controlling reactions for ignition are the following:

$$C_{6}H_{6} + O_{2} = C_{6}H_{5}O + OH$$

$$C_{5}H_{6} + O_{2} = C_{5}H_{5}O + OH$$

$$C_{6}H_{5}O = C_{5}H_{5} + CO$$

$$C_{6}H_{5}OH = C_{6}H_{5}O + H$$

$$C_{6}H_{6} + OH = C_{6}H_{5} + H_{2}O$$

Only one of these, the decomposition of C_6H_5O , appears as a rate-controlling reaction in table 4.16. This comparison demonstrates again the different sensitivity analysis results obtained for different temperature regimes in complex chemical reactions. Table 4.16 shows excellent agreement, once more, between the brute-force method and the GLSENS solution for the sensitivity coefficients.

4.3.2.5 *Example problem 9*.—In this final test problem a stoichiometric benzene-oxygen mixture also reacts, but the initial molar concentrations are cut in half by dilution with a mixture of 50 mole percent nitrogen and 50 percent argon. The reaction mechanism adds to that of example problem 8 a set of

nitrogen-oxygen reactions from reference 17. The problem data file for this case is shown in table 4.17. Argon is now listed as an inert species after the list of reactions, and all other data are similar to those for the previous example problem.

Results of the rate coefficient sensitivity analysis are listed in table 4.18. Although several of the same reactions appear here and in table 4.16, there are significant differences in relative sensitivity coefficient values for the two cases. First, the benzene pyrolysis reaction, which was quite rate controlling for the undiluted oxidation, was not important for the highly diluted reaction. Also, the OH radical attack on benzene was a strongly rate-controlling reaction for the diluted reaction but was not for the pure benzene-oxygen reaction. This reaction is also listed in the preceding example as a rate-controlling step in the lower temperature ignition of benzene-oxygen mixtures. Finally, the relative importance of the OH radical reactions with the species C₄H₂ and C₅H₅ was quite different for the two benzene-oxygen cases. As for the other test cases, table 4.18 demonstrates the very good agreement between sensitivity coefficients calculated by the GLSENS and brute-force methods.

Table 4.19 shows sensitivity coefficients with respect to initial temperature for both example problems 8 and 9. The same dependent variables were used as in tables 4.16 and 4.18. The GLSENS-computed values agreed well with those calculated by the brute-force method, as before. One interesting point to note is that the sensitivity coefficient for temperature was much higher for the diluted reaction than for the pure benzene-oxygen reaction.

This example problem, along with the previous four, gives users model problem data files from which most of their desired PSR sensitivity analysis data files can be obtained with simple modifications.

| ELUBAL CC | global= | truec | ronlv | -true &er | ACTIONS, | ; PSR PR | BLEM | | |
|---------------------------------------|----------------------|------------|--------|---------------|----------|----------|-------------|---|-------|
| | | H20 | + | 0 > | H2 | + | 02 | | |
| | 1. | 1. | | 4.90E+10 | .18 | -510. | | | |
| | | CO | + | H2O > | C02 | + | 82 | | |
| | 1. | 1 | | 1.30E+05 | 1.31 | -7000 | | | |
| | | CO2 | + | H2 > | co | + | H20 | | |
| | 1. | 1 | | 4.41E+10 | .19 | 3527 | | | |
| | | N2 | + | 02 >2 | .0 NO | | | | |
| | 1. | 1 | | 4.00E+14 | .03 | 100000. | | | |
| | | | 2.0 | NO > | N2 | + | 02 | | |
| | | 2 | • | 2.00E+11 | Ο. | 38000. | | | |
| | | CN | +2.0 | 0 > | NO | + | со | | |
| | 1. | 1. | | 8.30E+11 | 0. | 0. | | | |
| | | CN | + | NO > | co | + | N2 | | |
| | 1. | 1. | | 1.25E+12 | Ο. | 0. | | | |
| | 2.0 | CH2 | + | N2 >2 | .0 CN | +2.0 | H2 | | |
| | 1. | 1. | | 5.00E+13 | 0. | 54000. | | | |
| | _ | CH2 | + | 02 > | co | + | H 20 | | |
| | 1. | .5 | | 3.50E+07 | 0. | 5000. | | | |
| | | 02 | + | C3H8 >3 | .0 CH2 | +2.0 | OH | | |
| | 1.6 | .1 | | 1.10E+12 | 0. | 41000. | | | |
| | • | H2 , | + | 02 >2 | .U OH | | | | |
| | 1. | | | 1.00E+00 | U. | 49080. | | | |
| | 1 5 | | +2.0 | | H2O | + | СЗНЯ | + | 0 |
| 07 | .15 | H2 1. | | 1.986+06 | 0. | 4000. | ~ | | ~ ~ ~ |
| 1 | Ť. | n 2 | Ŧ | | H20 | + | 0 | + | OH |
| ±. | 0. | 1. | | 0.965+12 | 1 | 1013. | | | |
| AR | | | | | | | | | |
| DISTANCE | AREA | | | С | 388 | | | | |
| &prob w | elstr=.t | true., | | | | | | | |
| conc=.t | rue., a | end | | | | | | | |
| &wsprop | 4-200 | | | | | | | | |
| ae im | Q=200., | uormax= | 1000.1 | ,mpr=2, | | | | | |
| VOLU | .ue=∠ouu. _ 000 - | | sena | | • | | | | |
| astart t | ~ 000.,[h=0 // | 2-3.3, MQ | oc≖ 10 | Ju., eratio=2 | .v, | | | | |
| SUCTO, SC | 11-0, èt | 5110 | | | | | | | |
| FINTS | | | | | | | | | |
| T T T T T T T T T T T T T T T T T T T | | | | | | | | | |

TABLE 4.1.—DATA FILE FOR EXAMPLE PROBLEM 1 (ALL-GLOBAL REACTIONS; PERFECTLY STIRRED REACTOR PROBLEM)

TABLE 4.2.—COMPUTED RESULTS FOR EXAMPLE PROBLEM 1 (PROPANE-AIR COMBUSTION IN PERFECTLY STIRRED REACTOR)

[Initial temperature $T_0 = 800$ K; pressure p = 5.5 atm; equivalence ratio $\varphi = 2.0$; equilibrium temperature, 2020.68 K.]

| Variable | Convergence number | | | | | | |
|---------------------------------|-------------------------|-------------------------|-------------------------|-------------------------|--|--|--|
| | 1 | 2 | 4 | 5 | | | |
| Temperature, T, K | 1938.31 | 1909.97 | 1834.41 | 1779.68 | | | |
| Mass flow rate, \dot{m} , g/s | 800 | 1000 | 1400 | 1600 | | | |
| Residence time, τ , ms | 2.749 | 2.242 | 1.685 | 1.532 | | | |
| Number of iterations | 14 | 3 | 3 | 4 | | | |
| | Species | s mole fractions | | | | | |
| C ₃ H ₈ | 1.3757×10^{-2} | 1.5092×10^{-2} | 1.8565×10^{-2} | 2.1350×10^{-2} | | | |
| H ₂ | 8.6180×10^{-2} | 8.4019×10 ⁻² | 7.9412×10 ⁻² | 7.6161×10^{-2} | | | |
| O ₂ | 1.6866×10^{-2} | 2.0623×10^{-2} | 3.0477×10^{-2} | 3.8108×10^{-2} | | | |
| H ₂ O | 0.11378 | 0.11083 | 0.10326 | 9.7556×10 ⁻² | | | |
| CO | 0.11368 | 0.11067 | 0.10295 | 9.7126×10 ⁻² | | | |
| NO | 4.3981×10 ⁻⁵ | 6.5574×10 ⁻⁵ | 1.2536×10 ⁻⁴ | 1.6608×10^{-4} | | | |
| 0 | 6.6436×10 ⁻⁵ | 9.9362×10 ⁻⁵ | 1.9333×10 ⁻⁴ | 2.6362×10 ⁻⁴ | | | |
| OH | 2.3687×10 ⁻⁴ | 2.8422×10 ⁻⁴ | 3.5924×10^{-4} | 3.7941×10 ⁻⁴ | | | |

TABLE 4.3.—DATA FILE FOR EXAMPLE PROBLEM 2 (ALL GLOBAL REACTIONS)

TAPE

GLOBAL CODE EXAMPLE PROB. 2 ALL GLOBAL RXNS; NON REACTS CONTROL RATES &rtype global=.true.,gronly=.true., &end

| 910201 | | | | | | | |
|--------|--|--|---|--|--|--|--|
| | H2O | + | 0 > | H2 | + 02 | | |
| 1. | 1. | | 4.90E+10 | .18 | -510. | | |
| | со | + | H2O > | • CO2 | + н2 | | |
| 1. | 1. | | 1.30E+05 | 5 1.31 | -7000. | | |
| | CO2 | + | H2 > | • со | + H2O | | |
| 1. | 1 | | 4.41E+10 |) .19 | 3527. | | |
| + | N2 | + | 02 > | 2.0 NO | + H2 | | |
| 1. | 1. | | 4.00E+14 | .03 | 100000. | | |
| 2.0 | NO | + | H2 > | • N2 | + 02 | + | H2 |
| 2. | 0 | | 2.00E+11 | 0. | 38000. | | |
| + | CN | +2.0 | 0 > | • NO | + CO | + | H2 |
| 1. | 1. | | 8.30E+11 | 0. | 0. | | |
| | CN | + | NO > | • со | + N2 | | |
| 1. | 1. | | 1.25E+12 | 2 0. | 0. | | |
| +2.0 | CH2 | + | N2 > | 2.0 CN | +2.0 H2 | + | 02 |
| 1. | 1. | | 5.00E+13 | s 0. | 54000. | | |
| | CH2 | + | 02 > | • со | + H2O | | |
| 1. | .5 | | 3.50E+07 | 0. | 5000. | | |
| | 02 | + | СЗН8 > | 3.0 CH2 | +2.0 OH | + | H2 |
| 1.6 | .1 | | 1.10E+12 | 2 0. | 41000. | | |
| + | H2 | + | 02 > | 2.0 OH | + C3H8 | | |
| 1. | 1. | | 1.00E+00 | 0. | 49080. | | |
| | C3H8 | +2.0 | OH > | • E2O | + C3H8 | + | 0 |
| .15 | 1. | | 1.98E+06 | 50. | 4000. | | |
| + | H2 | + | 02 > | • E20 | + 0 | + | OH |
| 0. | 1. | | 0.96E+12 | 21 | 1013. | | |
| | | | | | | | |
| APEN | | | | C388 | | | |
| | 1. 1. 1. 1. 1. 1. 2.0 2. + 1. 1. 1. +2.0 1. 1. 1. +2.0 1. 1. +2.0 1. 1. +2.0 1. 1. +1. +2.0 1. +1. +2.0 1. +1. +2.0 1. +1. +2.0 1. +1. +2.0 1. +1. +2.0 1. +1. +2.0 1. +1. +2.0 1. +1. +2.0 1. +1. +2.0 1. +1. +2.0 1. +1. +2.0 1. +1. +2.0 1. +2.0 1. +2.0 1. +2.0 1. +2.0 1. +2.0 1. +2.0 1. +2.0 1. +2.0 1. +2.0 1. +2.0 1. +2.0 1. +2.0 1. +2.0 1. +2.0 1. +2.0 1. +2.0 1. +2.0 1. -2. +2.0 1. -2. +2.0 1. -2. -2. +2.0 1. -2. -2. +2.0 1. -2. -2. -2. -2. -2. -2. -2. -2 | H20 1. 1. CO 1. CO 1. CO | H20 + H20 + H2 + | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ |

```
AR

DISTANCE AREA

&prob welstr=.true.,

conc=.true., &end

&wsprob

delmd= 1., dotmax= 60.,mpr=1,

volume=10000.0, &end

&start t= 800.,p=5.5, mdot= 13.0, eratio=1.5,

scc=3, sch=8, &end

END

FINIS
```

TABLE 4.4.—COMPUTED RESULTS FOR EXAMPLE PROBLEM 2 (PROPANE-AIR COMBUSTION IN PERFECTLY STIRRED REACTOR) [Initial temperature $T_0 = 800$ K; pressure p = 5.5 atm; equivalence ratio $\varphi = 1.5$;

equilibrium temperature, 2357.42 K.]

| Variable | | | | | | | |
|---------------------------------|-------------------------|-------------------------|-------------------------|-------------------------|--|--|--|
| | 1 | 5 | 9 | 13 | | | |
| Temperature, T, K | 2016.44 | 1988.99 | 1947.33 | 1856.68 | | | |
| Mass flow rate, \dot{m} , g/s | 13 | 17 | 21 | 25 | | | |
| Residence time, τ , ms | 647.2 | 505.8 | 422.1 | 377.6 | | | |
| Number of iterations | 33 | 3 | 3 | 4 | | | |
| Species mole fractions | | | | | | | |
| C ₃ H ₈ | 1.1787×10^{-3} | 3.2999×10 ⁻³ | 5.9432×10 ⁻³ | 1.0688×10^{-2} | | | |
| H ₂ | 8.8640×10^{-2} | 8.3809×10 ⁻² | 7.8786×10^{-2} | 7.1373×10^{-2} | | | |
| O ₂ | 2.6382×10^{-2} | 3.1050×10^{-2} | 3.7508×10^{-2} | 5.0324×10^{-2} | | | |
| H ₂ O | 0.10713 | 0.10510 | 0.10143 | 9.3019×10 ⁻² | | | |
| CO | 0.11686 | 0.11159 | 0.10537 | 9.4443×10 ⁻² | | | |
| NO | 9.5537×10 ⁻⁷ | 1.1658×10^{-6} | 1.5018×10^{-6} | 2.0366×10 ⁻⁶ | | | |
| 0 | 5.3194×10 ⁻⁷ | 6.9421×10 ⁻⁷ | 9.4276×10 ⁻⁷ | 1.3623×10 ⁻⁶ | | | |
| OH | 1.3385×10^{-6} | 1.4328×10^{-6} | 1.5275×10^{-6} | 1.4894×10^{-6} | | | |

TABLE 4.5.—DATA FILE FOR EXAMPLE PROBLEM 3 (GLOBAL AND MOLECULAR REACTIONS; PERFECTLY STIRRED REACTOR PROBLEM)

| TAPE | | | | | | | | | | |
|-------------------|---|-----------|----------------|-----------|------|-------------|----------|------|----|---------|
| GLOBAL | AND M | OLECULAR | REACT | CIONS; E | XAMP | LE PROBLEM | 1 3 | | | |
| artype | globa | l=.true. | ,gron] | ly=.fals | e., | ≰end | | | | |
| 0 | + | H2O | * | OH | + | OH | 6.8E+13 | Ο. | | 18365. |
| H | + | 02 | = | OH | + | 0 | 1.89E+14 | 0. | | 16400. |
| 0 | + | H2 | = | OH | + | H | 4.20E+14 | 0. | | 13750. |
| H | + | HO2 | = | H2 | + | 02 | 7.28E+13 | Ο. | | 2126. |
| 0 | + | HO2 | Ŧ | OH | + | 02 | 5.0E+13 | 0. | | 1000. |
| HO2 | + | ОН | = | H2O | + | 02 | 8.0E+12 | 0. | | 0. |
| H | + | HO2 | =2.0 | OH | | | 1.34E+14 | Ο. | | 1070. |
| H 2 | + | EO2 | 2 | H2O2 | + | Ħ | 7.91E+13 | 0. | | 25000. |
| OH | + | H2O2 | - | H2O | + | H02 | 6.1E+12 | 0. | | 1430. |
| HO2 | + | HO2 | = | H2O2 | ÷ | 02 | 1.8E+12 | Ο. | | 0. |
| H | + | H2O2 | * | OH | + | H20 | 7.8E+11 | Ο. | | Ο. |
| м | + | H2O2 | =2.0 | DOH | | | 1.44E+17 | Ο. | | 45510. |
| THIRDB | BODY | | | | | | | | | |
| H2 | 2. | 30 02 | | .78 | | H20 | 6.0 H2 | 02 | | 6.6 |
| END | | | | | | | | | | |
| H2 | + | OH | = | H2O | + | H | 4.74E+13 | 0. | | 6098. |
| H | + | 02 | = | H02 | + | M | 1.46E+15 | Ο. | | -1000. |
| THIRDB | YOOR | | | | | | | | | |
| 02 | 1 | 30 N2 | | 1.3 | | H20 | 21.3 82 | | | 3.0 |
| END | | 502 | | | | | | | | ••• |
| M | + | H20 | - | Ħ | + | OB | 1 30E+15 | 0. | | 105140. |
| רים דער מתקדער | 20DY | 120 | | | • | 011 | 1.502/15 | •• | | |
| 20 INIKUD | 1001 | 00 02 | | 15 | | H 20 | 20 0 N2 | | | 15 |
| 52 F)T) | | 00 02 | | 1.5 | | 120 | 20.0 112 | | | 1.0 |
| END | | <u>^</u> | | 07 | | м | 7 18+19 | _1 | | 0 |
| H | + | 0 | * | UH . | Ť | M | 7.15710 | ~1. | | 0.000 |
| M | + | HZ | = | Ħ | + | 8 | 2.26+14 | 0. | | 96000- |
| THIRDE | BODY | | | | | | 15 0 | | | ~ ~ |
| H2 | 4. | 10 02 | | 2.0 | | H20 | 15.0 N2 | | | 2.0 |
| END | | _ | | _ | | _ | | _ | | |
| M | + | 02 | ** | 0 | + | 0 | 1.80E+18 | -1. | | 118020. |
| END | | - | | | | | | | | |
| | | N2 | + | 02 | | >2.0 NO | | | | |
| | 1 | - | 1. | 4.0 | 0E+1 | 4 .03 | 100000. | | | |
| | | | 2. | 0 NO | | > N2 | + 02 | | | |
| | | | 2. | 2.0 | 0E+1 | 1 0. | 38000. | | | |
| | | CN | +2. | 0 0 | | > NO | + CO | | | |
| | 1 | | 1. | 8.3 | 0E+1 | 10. | 0. | | | |
| | | CN | + | NO | | > co | + N2 | | | |
| | 1 | | 1. | 1.2 | 5E+1 | 20. | 0. | | | |
| | 2 | .0 CH2 | + | N2 | | >2.0 CN | +2.0 H2 | | | |
| | 1 | . 1. | | 5.00 |)E+1 | 30. | 54000. | | | |
| | | CH2 | + | 02 | | > со | + H2O | | | |
| | 1 | ! | 5 | 3.5 |)E+0 | 70. | 5000. | | | |
| | | 02 | • + | C3H8 | | >3.0 CH2 | +2.0 OH | | | |
| | 1 | .6 .: | 1 | 1.10 | DE+1 | 2 0. | 41000. | | | |
| | - | H2 | + | 02 | : | >2.0 OH | | | | |
| | 1 | . 1. | | 1.00 |)E+0 | ο ο. | 49080. | | | |
| | | C388 | +2 | 0 OH | | > H2O | + C3E8 | + | 0 | |
| | | 15 1. | | 1.9 | RE+0 | 6 0. | 4000. | | | |
| 0Ħ | + | H2 | + | 02 | | > H20 | + 0 | + | OF | |
| 1 0 | ່າ | | • | <u> </u> | 5E+1 | 2 - 1 | 1013 | • | •4 | |
| 1.0 | v | | | 0.0 | | • • • • | 20201 | | | |
| AP. | | | | | | | | | | |
| DICTANCE | ADEA | | | | | C388 | | | | |
| DIGINACE | nnen -+-lo | | | | - | . Lend | | | | |
| abron w | apron weistle-true, concentrate, admon 500 rord | | | | | | | | | |
| awsprop | - 000 | 0-5 - 51 | ., uu ndot- | 200 0 | | -1_5, VU. | | a 21 | | |
| ascart t | 000 pob- | .,p-J.J,i | | 200., 210 | | - 4 . Jø | | | | |
| 500-3 | , SUII- | acing | | | | | | | | |

END FINIS

| TABLE 4.6.—COMPUTED RESULTS FOR EXAMPLE PROBLEM 3 (PROPANE-AIR |
|--|
| COMBUSTION IN PERFECTLY STIRRED REACTOR) |
| [Leiti-1 to manufacture T 200 K and a second s |

| equilibrium temperature, 202010 / 11.j | | | | | | | | | |
|--|-------------------------|-------------------------|-------------------------|-------------------------|--|--|--|--|--|
| Variable | Convergence number | | | | | | | | |
| | 1 | 2 | 4 | 5 | | | | | |
| Temperature, T, K | 2176.82 | 2142.84 | 2072.33 | 2034.80 | | | | | |
| Mass flow rate, \dot{m} , g/s | 200 | 250 | 350 | 400 | | | | | |
| Residence time, τ , ms | 2.019 | 1.643 | 1.217 | 1.086 | | | | | |
| Number of iterations | 13 | 13 3 3 | | 3 | | | | | |
| Species mole fractions | | | | | | | | | |
| C ₃ H ₈ | 4.1056×10 ⁻³ | 4.5191×10 ⁻³ | 5.5855×10^{-3} | 6.3101×10 ⁻³ | | | | | |
| H ₂ | 9.0557×10^{-4} | 6.1544×10 ⁻⁴ | 1.1805×10^{-4} | 2.6380×10 ⁻⁹ | | | | | |
| 0 ₂ | 1.0693×10^{-2} | 1.3130×10^{-2} | 1.8679×10^{-2} | 2.1946×10^{-2} | | | | | |
| H ₂ O | 0.18363 | 0.18112 | 0.17541 | 0.17205 | | | | | |
| CO | 0.13698 | 0.13476 | 0.12996 | 0.12724 | | | | | |
| NO | 2.8546×10 ⁻⁴ | 3.2885×10 ⁻⁴ | 4.1960×10 ⁻⁴ | 4.6932×10 ⁻⁴ | | | | | |
| 0 | 4.3280×10 ⁻⁴ | 5.0000×10^{-4} | 6.4372×10 ⁻⁴ | 7.2552×10 ⁻⁴ | | | | | |
| OH | 3.7450×10^{-3} | 3.8708×10^{-3} | 4.0143×10^{-3} | 4.0424×10^{-3} | | | | | |

[Initial temperature $T_0 = 800$ K; pressure p = 5.5 atm; equivalence ratio $\varphi = 1.5$; equilibrium temperature, 2320.64 K.]

TABLE 4.7.—DATA FILE FOR EXAMPLE PROBLEM 4 (INTEGRATION CASE FOR MECHANISM WITH GLOBAL AND MOLECULAR REACTIONS)

| TAPE GLOBAL | LSENS C | | APLE P | ROBLEM | 4;] | INTEGRATI | ON CASE | BOTH TY | ES OF | REACTION |
|----------------|---------|----------|----------|-------------|---------|-----------|----------|----------|-------|----------|
| arc3bc | 910202 | | | ~ ~ ~ ~ ~ ~ | | 02 | 4 90 | E + 10 | 18 | -510 |
| H20 | + 0 | 2 | · · | 2 | Ŧ | 02 | 4.50 | E110 | 027 | _1949 |
| | 2.00 | 2 | > 0 | 2 | | | 4.50 | 5711 | .027 | -1049. |
| | C | 2 | >2.00 | | | | 2.18 | 5+10 | 92 | 110954. |
| CO | + 0 |) | > C | 02 | | | 8.43 | E+09 | 001 | 1000. |
| | c | :02 | > C | 0 | + | 0 | 9.08 | E+18 | -1.84 | 130754. |
| CH2 | + 0 |) | > C | 0 | ÷ | H2 | 0.69 | E+11 | 1. | 0. |
| co | + 8 | 12 | > c | H2 | + | 0 | 5.38 | E+10 | 1.44 | 177439. |
| •• | | - | _ | | | | | | | |
| | | N2 | + | 02 | > | 2.0 NO | | | | |
| | 1 | | 1 | - A 0 | 0E+14 | 1 03 | 100000 | L. | | |
| | ÷ • | | | NO 1.0 | | N2 | | ·02 | | |
| | | | ~ 2.0 | NO 0. | | 0 | 20000 | 02 | | |
| | | | <u> </u> | 2.0 | 05413 | L U. | 38000 | | | |
| | | CN | +2.0 | 0 | ~ ~ ~ ~ | > NO | + | 0 | | |
| | 1. | 1 | • | 8.3 | 0E+11 | 0. | U | • | | |
| | | CN | + | NO | > | • C0 | + | N2 | | |
| | 1. | 1 | • | 1.2 | 5E+12 | 20. | 0 | - | | |
| | 2.0 |) CH2 | + | N2 | > | 2.0 CN | +2.0 | H2 | | |
| | 1. | 1. | | 5.0 | 0E+13 | 30. | 54000 | • | | |
| | | CH2 | + | 02 | > | со | + | H2O | | |
| | 1 | 5 | | 3.5 | DE+07 | 0. | 5000 | | | |
| | ֥ | 02 .0 | + | CARR | | 3 0 0 82 | +2 0 | OH | | |
| | 3 6 | : 1 | • | 1 1 | 05+12 | | 41000 | •• | | |
| 0000 | | , | | | 10+12 | | 41000 | | | |
| Сзна | +_ | HZ | Ŧ | 02. | | 2.0 00 | 40000 | C3H6 | | |
| 0.0 | 1. | 1. | | 1.0 | UE+UL | | 49080 | • | | ^ |
| | | C3H8 | +2.0 | OH | 2 | H20 | + | C3H8 | + | 0 |
| | .15 | i 1. | | 1.9 | 8E+06 | 50. | 4000 | • | | |
| | | | | | | | | | | |
| AR | | | | | | | | | | |
| TIME | | | | | | C3E8 | | | | |
| fr dorga | nocon = | .true., | print | = 1.e | -6,] | .e-4, 0. | 2, .3, . | 5, .575, | .580, | |
| . 585. | 5905 | 92 592 | 235 | 925, . | 5927, | .593, | | | | |
| Senca | | ne. ti | 1v. =1. | e-3. & | end | | | | | |
| fstart t | = 850 | | | ratio= | 2.0. | | | | | |
| astart | - Joech | | , . | LUCIO . | , | | | | | |
| SU | | -0, ae | | | | | | | | |
| END | | | | • | | ^ | e | | | |
| & Solver | emax | = 1.e-/, | , ato | rsb ≖ | r.e-1 | 10, | a en u | | | |
| SENSVAR | | | | | | | | | | |
| H2O | C3H8 | OH | | NO | | CO | CO2 | CH2 | | TEMP |
| END | | | | | | | | | | |
| REAC | | | | | | | | | | |
| &senrxn | allrxn | = .true | ., ou | tput = | .fal | lse., ord | er = .tr | ue., | | |
| | sensa | ij = .tr | le., | _ &end | | | | | | |
| FINIS | | - | • | | | | | | | |

TABLE 4.8.—COMPUTED RESULTS FOR EXAMPLE PROBLEM 4 (PROPANE-AIR COMBUSTION AT CONSTANT VOLUME)

| Variable | EMAX value (ATOLSP = 10^{-9} EMAX) | | | | | | | | | |
|-------------------------------|--------------------------------------|--|-------------------------|--|-------------------------|--|--|--|--|--|
| | 10 |)-4 | 1 | 0 ⁻⁶ | 10 ⁻⁷ | | | | | |
| | Value | Sensitivity coefficient with respect to A ₁₄ | Value | Sensitivity coefficient with respect to A ₁₄ | Value | Sensitivity coefficient with respect to A ₁₄ | | | | |
| Temperature, T, K | 1644.28 | 533 | 1419.60 | 173 | 1418.98 | 172 | | | | |
| Mole fraction: | | | | | | | | | | |
| C ₃ H ₈ | 3.8686×10 ⁻² | -1250 | 5.1507×10^{-2} | -215 | 5.1539×10^{-2} | -214 | | | | |
| H ₂ O | 8.8096×10 ⁻² | 1370 | 6.1291×10 ⁻² | 492 | 6.1220×10^{-2} | 490 | | | | |
| CO | 8.7686×10^{-2} | 1380 | 6.0894×10^{-2} | 494 | 6.0823×10^{-2} | 492 | | | | |
| NO | 6.1677×10^{-7} | 3470 | 1.5784×10^{-7} | 1970 | 1.5707×10^{-7} | 1970 | | | | |
| OH | 8.8876×10^{-4} | 3820 | 2.4437×10 ⁻⁴ | 1850 | 2.4325×10 ⁻⁴ | 1840 | | | | |

[Initial temperature $T_0 = 850$ K; initial pressure $p_0 = 5.5$ atm; equivalence ratio $\varphi = 2.0$; reaction time t = 592.5 ms.]
| 110 EE + Drant 1 EE 1 OK ER and EE 1 KODEEN 5 (111 DKOOEN OK 1 OEN 1 5K 5E (5111 111) | TA | BL | Æ | 4.9 | 9.— | -D/ | ATA | FI | LE | F | DR | Εž | KΑ | Μ | PL | Æ | PF | RO |)BI | LE | М | 5 (| (H | ΥI | DR | 0 | GE | ïN | -0 | X | YC | θEΝ | ١I | PSI | R S | SE | NS | SIT | T١ | ſΠ | ΓY | <u>()</u> |
|---|----|----|---|-----|-----|-----|------------|----|----|---|----|----|----|---|----|---|----|----|-----|----|---|-----|----|----|----|---|----|----|----|---|----|-----|----|-----|-----|----|----|-----|----|----|----|-----------|
|---|----|----|---|-----|-----|-----|------------|----|----|---|----|----|----|---|----|---|----|----|-----|----|---|-----|----|----|----|---|----|----|----|---|----|-----|----|-----|-----|----|----|-----|----|----|----|-----------|

| TAF | Έ | | | | | | | | | | | | | |
|-----------------------|---------------------------------|----------------------|--------------------------|-----------------------|--------------------|-----------------|--------------------------|-----------------------------|------------------|------------------------------|------------|--------------|---------|--|
| I | SENS | HYDR | OGEN - | - ox: | GEN | PSR | WITH | SENSI | TIVITY | ANALYSIS | | | | |
| 81 | tvpe | 8 | end | | | | | | | | | | | |
| | 0 | + | H2O | | = | OH | + | OH | | 6.8E+ | 13 | 0. | 18365. | |
| | H | + | 02 | | = | OH | + | 0 | | 1.89E+ | 14 | 0. | 16400. | |
| | 0 | + | H2 | | - | OH | + | Ħ | | 4.20E+ | 14 | Ο. | 13750. | |
| | H | + | HO2 | | = | H2 | ÷ | 02 | | 7.28E+ | 13 | 0. | 2126. | |
| | 0 | + | HO2 | | = | OH | + | 02 | | 5.0E+ | 13 | 0. | 1000. | |
| | HO2 | + | Off | | # | H2O | + | 02 | | 8.0E+ | 12 | 0. | Ο. | |
| | H | + | HO2 | | =2.0 |)OH | | | | 1.34E+ | 14 | 0. | 1070. | |
| | H2 | + | HO2 | | = | H2O2 | + | H | | 7.91E+ | 13 | 0. | 25000. | |
| | OH | + | H2O2 | | = | H2O | + | HO2 | | 6.1E+ | 12 | 0. | 1430. | |
| | 802 | + | HO2 | | - | H2O2 | + | 02 | | 1.8E+ | 12 | 0. | 0. | |
| | 8 | + | H202 | | = | OH | + | H20 | | 7.8E+ | 11 | 0. | 0. | |
| | M | + | H202 | | =2.0 | ЮН | | | | 1.44E+ | 17 | 0. | 45510. | |
| | THIRDRO | י. צחר | | | | | | | | | - | • • | | |
| 82 | 1111000 | 2.2 | 30 | 02 | | | 78 | H20 | | 6.0 | 820 |)2 | 6.6 | |
| NIZ. | ` | - . | | 02 | | | | | | | | - | | |
| 10141 | , 112 | + | OH | | - | H20 | ÷- | Ħ | | 4 74E+ | 13 | 0. | 6098. | |
| | 112 U | , , | 02 | | _ | 802 | | м | | 1 46E+ | 15 | 0 | -1000 | |
| | יי קרומד נויית | ากร | 02 | | | 1102 | • | •• | | 1.702 | | •• | | |
| 02 | THINDO | 1 | 30 | | | | | #20 | | 21 3 | 82 | | 3.0 | |
| DZ ENT | ` | 1. | 50 | | | | | | | 2110 | | | 0.0 | |
| DINT | , | | =20 | | - | F | <u>ـ</u> | OH | | 1 305+ | 15 | n | 105140 | |
| | THIDDR | ד ערור | n20 | | - | 11 | 1 | 01 | | 1.505. | ÷ | •. | 100110. | |
| 82 | THINDO | | ~~ | 02 | | | 1 5 | 820 | | 20.0 | ENT | ` | | |
| <u>n</u> 2 | | . | 00 | 02 | - | <u></u> | · | M | | 7 15+ | 18 - | -1 | 0 | |
| | <u>п</u> | - - | | | _ | 500 | 1 | 11 | | 2 25- | 1 4 | <u>^</u> . | 96000 | |
| | MUTDOD/ | T | 22 | | - | п | т | 4 | | 2.2.4 | 1.1 | •. | | |
| | THIRDBU | 101 | 10 | ~~ | | | 2 0 | 2 20 | | 15.0 | FNI | ` | | |
| πZ | v | . . | 10 | 02 | _ | <u>`</u> | د.u | 0 | | 1 8057 | 19 | | 118020 | |
| | M | + | 02 | | * | 0 | Ŧ | U | | 1.005+ | 10 | - T . | 110020. | |
| TIN Sy Sy Sy | Æ prob we vsprob start | elstr dotm t = | = .ti ax=102 298., | rue., 200., p = | se del = 2.0 | encal .md=20 | = .t: 000., ndot : | rue., t mpr = = 200., | tiny = 1, vol | 1.e-3, & ume= 200 &end | end 0., | &end | | |
| 82 | | ο. | 6667 | | | | | | | | | | | |
| 02 | | ο. | 3333 | | | | | | | | | | | |
| ENI |) | | | | | | | | | | | | | |
| SEN | isvar | | | | | | | | | | | | | |
| 0 | | H2O | | OH | | H | | 02 | | Ħ2 | 802 | | H2O2 | |
| TEN | æ | END | | | | | | | | | | | | |
| INI | T | | | | | | | | | | | | | |
| TEN | æ | END | | | | | | | | | | | | |
| REA | NC | | | | | | | | | | | | | |
| 6.5 | senrxn | sen | saj = | .tri | ıе., | allr | kn = | .true., | order | = .true. | • • | | | |
| - | outi | out = | .fals | se., | | end | | | | | | | | |
| FIR | IIS | • | | | | | | | | | | | | |

| | rature | Brute force | 2.69×10 ⁻² | 1.77×10 ⁻² | 4.35×10 ⁻³ | 1 1 1 1 | 1.42×10 ⁻³ | 2.09×10 ⁻³ | | | 2.12×10 ⁻² |
|--|----------|---------------------------------------|-----------------------------------|--------------------------|------------------------|------------------------|---|---|--|-------------------------------------|------------------------|
| | Tempe | GLSENS | 2.69×10 ⁻² | 1.78×10 ⁻² | 4.35×10 ⁻³ | | 1.38×10 ⁻³ | 2.04×10 ⁻³ | 1 1 1 1 | | 2.11×10 ⁻² |
| |)2 | Brute force | 2.11×10 ⁻² | 0.312 | 3.47×10 ⁻³ | -7.30×10 ⁻³ | -7.87×10 ⁻² | 1.74×10 ⁻³ | -2.89×10 ⁻³ | | 5.86×10 ⁻² |
| | ЭН | GLSENS | 2.11×10 ⁻² | 0.312 | 3.53×10 ⁻³ | -7.31×10 ⁻³ | -7.85×10 ⁻² | 1.65×10 ⁻³ | -2.85×10 ⁻³ | | 5.85×10 ⁻² |
| | Н | Brute force | 6.36×10 ⁻³ | 5.58×10 ⁻³ | 1.03×10 ⁻³ | 5.69×10 ⁻³ | | L | -1.23×10 ⁻³ | | 7.71×10 ⁻² |
| or E _J | 0 | GLSENS | 6.54×10 ⁻³ | 5.48×10 ⁻³ | 1.11×10 ⁻³ | 5.66×10 ⁻³ | 1 | 1 1 1 1 1 1 | -1.33×10 ⁻³ | mperature | 7.70×10 ⁻² |
| respect to A _j , n _j , | 50 | Brute force | 1.04×10 ⁻² | 6.86×10 ⁻³ | 1.69×10 ⁻³ | 1 | | 1 | 1 1 1 1 1 | pect to initial te | -2.92×10 ⁻² |
| cient (S _{IJ}) with I | Ĥ | GLSENS | 1.04×10 ⁻² | 6.88×10 ⁻³ | 1.66×10 ⁻³ | | 1 | 1 | | $\langle S_{l,T_0} angle$ with res | -2.91×10^{-2} |
| ensitivity coeffi | ~ | Brute force | -6.80×10 ⁻² | -4.42×10 ⁻² | -1.11×10 ⁻² | 1.09×10 ⁻² | -3.82×10 ⁻³ | -5.21×10 ⁻³ | 1.78×10 ⁻³ | ivity coefficient | 0.126 |
| (a) S | 0 | GLSENS | -6.79×10 ⁻² | -4.42×10 ⁻² | -1.11×10 ⁻² | 1.09×10 ⁻² | -3.80×10 ⁻³ | -5.24×10 ⁻³ | 1.78×10 ⁻³ | (b) Sensit | 0.126 |
| | [2 | Brute force | -1.77×10 ⁻² | -1.23×10 ⁻² | -2.73×10 ⁻³ | -4.88×10 ⁻³ | 1 | -1.31×10 ⁻³ | -2.38×10 ⁻³ | | 5.17×10 ⁻² |
| | њ4 | GLSENS | -1.77×10 ⁻² | -1.22×10 ⁻² | -2.79×10 ⁻³ | -4.85×10 ⁻³ | | -1.34×10 ⁻³ | -2.40×10 ⁻³ | | 5.18×10 ⁻² |
| | Reaction | · · · · · · · · · · · · · · · · · · · | H ₂ O + M = H + OH + M | $H + O_2 + M = HO_2 + M$ | $H_2 + M = H + H + M$ | $H + O_2 = OH + O$ | H + HO ₂ = H ₂ + O ₂ | M + HO = M + O + H | H ₂ + OH = H ₂ O + H | | |
| | Reaction | | 15 | 14 | 17 | 7 | 4 | 16 | 13 | | 1 |

TABLE 4.10.—COMPARISON OF GLSENS AND BRUTE-FORCE SENSITIVITY COEFFICIENTS FOR EXAMPLE PROBLEM 5 (REACTION OF HYDROGEN AND OXYGEN) [Equivalence ratio $\varphi = 1.0$; mass flow rate $\dot{m} = 10.200$ g/s; temperature T = 2990.9 K.]

TABLE 4.11.—DATA FILE FOR EXAMPLE PROBLEM 6 (PSR SENSITIVITY WITH GLOBAL AND MOLECULAR REACTIONS)

| | E | | | | | | | | | |
|---|--|--|--|--|--|---|---|--|------------------|----------------|
| G | LOBAL | AND M | OLECULAR | REAC | TIONS; | EXAM | PLE PROB. | 6 FOR PSR | | |
| & r | type | globa. | l=.true. | ,gron | ly=.fal | lse., | &end | | | |
| | 0 | + | H2O | æ | OH | + | OH | 6.8E+13 | 30. | 18365. |
| | Ħ | + | 02 | - | ÓН | + | 0 | 1.89E+14 | 10. | 16400. |
| | 0 | + | H2 | = | OH | + | H | 4.20E+14 | 10. | 13750. |
| | H | + | HO2 | = | H2 | + | 02 | 7.28E+1 | 3 0 | 2126 |
| | | + | 802 | = | 08 | + | 02 | 5 0E+11 | | 1000 |
| | 802 | | 08 | | 820 | + | 02 | 8 OF+13 | | 1000. |
| | 102 10 | т 1 | 802 | -2 | 008 | • | 02 | 1 245+1/ | . 0. | 1070 |
| | п по | Ť | H02 | =2. | 008 | | | 1.346714 | ± 0. | 1070. |
| | 82 | + | HOZ | = | HZOZ | + | H | 7.91E+1: | s 0. | 25000. |
| | он | + | H2O2 | - | H2O | + | HOZ | 6.1E+12 | . 0. | 1430. |
| | HOZ | + | HO2 | = | H2O2 | + | 02 | 1.8E+12 | 2 0. | 0. |
| | Ħ | + | H2O2 | 38 | ÓН | + | H20 | 7.8E+11 | . 0. | 0. |
| | М | + | H2O2 | =2. | OOH | | | 1.44E+17 | 0. | 45510. |
| | THIRDE | SODY | | | | | | | | |
| H2 | | 2.1 | 30 02 | 2 | | 78 | H20 | 6.0 | H2O2 | 6.6 |
| END | | | | | | | | | | |
| | H2 | + | OH | - | H2O | + | H | 4.74E+13 | » O. | 6098. |
| | H | + | 02 | = | EO2 | + | м | 1.46E+15 | i 0. | -1000 |
| | THIRDB | ΩDY | | | | | | 20102010 | | 2000. |
| 02 | | 1 . | 20 172 | | 1 | 2 | 820 | 21 3 | u 0 | 3 0 |
| END. | | ÷ | 50 N2 | • | 1. | | 1120 | 21.3 | nz | 5.0 |
| LND | | | | | | | 07 | 1 200.130 | • | 105140 |
| | M | + | H20 | = | п | Ŧ | OH . | 1.30E+15 | 0. | 105140. |
| | THIRDB | ODY | | | | - | | ~~ ~ | | |
| H2 | | 4.0 | 0 02 | | 1. | 5 | H20 | 20.0 | N2 | 1.5 |
| END | | | | | | | | _ | | |
| | E | + | 0 | - | OH | + | M | 7.1E+18 | -1. | 0. |
| - | M | + | 82 | | H | + | H | 2.2E+14 | 0. | 96000. |
| | THIRDB | ODY | | | | | | | | |
| H2 | | 4.3 | 10 02 | | 2. | 0 | H2O | 15.0 | N2 | 2.0 |
| END | | | | | | | | | | |
| | м | + | 02 | = | 0 | + | 0 | 1.80E+18 | -1. | 118020. |
| | END | | •• | | • | | - | | | |
| | | | 112 | + | 02 | | 20.00 | | | |
| | | - | NZ | - T | 02 | 000.11 | 2.0 NO | 100000 | | |
| | | + | • | ±. `` | 4. | OOF+1 | 4 .03 | 100000. | | |
| | | | | 2 | .U NO | | > N2 | + 02 | | |
| | | | | 2. | 2. | 00E+1 | 10. | 38000. | | |
| | | | | | | | | | | |
| | | | CN | +2 | .00 | : | > NO | + co | | |
| | | 1 | CN. | +2 | .00 8. | 30E+1 | > NO L 0. | + co 0. | | |
| | | 1 | CN . CN | +2 1. + | .00 8. NO | 30E+1 | > NO L 0. > CO | + CO 0. + N2 | | |
| | | 1 | CN CN | +2 1. + 1. | .00 8. NO | 30E+1 | > NO L 0. > CO 2 0. | + CO 0. + N2 0. | | |
| | | 1 | CN CN 0 CH2 | +2 1. + 1. + | .00 8. NO 1. | 30E+1 25E+1 | $\begin{array}{c} & \text{NO} \\ 1 & 0 \\ \end{array} \\ \begin{array}{c} & \text{CO} \\ 2 & 0 \\ \end{array} \\ \begin{array}{c} & 2 \\ \end{array} \\ \begin{array}{c} & 0 \\ \end{array} \\ \end{array} \\ \begin{array}{c} & & 0 \\ \end{array} \\ \end{array}$ | + CO 0. + N2 0. +2 0 F2 | | |
| | | 1 | CN CN 0 CH2 | +2 1. + 1. + | .00 8. NO 1. N2 | 30E+1 25E+1 | > NO 1 0. > CO 2 0. >2.0 CN | + CO 0. + N2 0. +2.0 H2 | | |
| | | 1 1 2 1 | CN CN .0 CH2 .1. | +2 1. + 1. + | .00 8. NO 1. N2 5. | 30E+1 25E+1 00E+1 | > NO 1 0. > CO 2 0. >2.0 CN 3 0. | + CO 0. + N2 0. +2.0 H2 54000. | | |
| | | 1. 2. 1. | CN CN 0 CH2 1. CH2 | +2 1. + 1. + + | .0 0 8. NO 1. N2 5. 02 | 30E+1 25E+1 00E+1 | > NO 1 0. 2 0. 2.0 CN 3 0. > CO | + CO 0. + N2 0. +2.0 H2 54000. + H2O | | |
| | | 1 2 1 1 | CN CN 0 CH2 1. CH2 | +2 1. + 1. + 5 | .0 0 8. NO 1. N2 5. 02 3. | 30E+1 25E+1 00E+1 50E+0 | NO 0. CO 2.0 CN 3 0. CO 7 0. | + CO 0. + N2 0. +2.0 H2 54000. + H2O 5000. | | |
| | | 1. 2. 1. 1. | CN CN 0 CH2 1. CH2 02 | +2 1. + 1. + 5 + + | .0 0 8. NO 1. N2 5. O2 3. C3H8 | 30E+1 25E+1 00E+1 50E+0 | > NO 1 0. > CO 2 0. > 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 | + CO 0. + N2 0. +2.0 H2 54000. + H2O 5000. +2.0 OH | | |
| | | 1 . 2 . 1 . 1 . | CN CN 0 CH2 . 1. CH2 . 02 . 6 | +2 1. + 1. + 5 + 1 | .0 0 8. NO 1. N2 5. O2 3. C3H8 1. | 30E+1 25E+1 00E+1 50E+0 10E+1 | > NO 1 0. > CO 2 0. > 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 2 0. | + CO 0. + N2 0. +2.0 H2 54000. + H2O 5000. +2.0 OH 41000. | | |
| | | 1 . 2 . 1 . 1 . | CN CN 0 CH2 1. CH2 02 02 6 H2 | +2 1. + 1. + 5 + 1 + 5 + 1 + | .0 0 8. NO 1. N2 5. 02 3. C3H8 1. 02 | 30E+1 25E+1 00E+1 50E+0 10E+1 | > NO 1 0. > CO 2 0. > 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 2 0. > 2.0 OH | + CO 0. + N2 0. +2.0 H2 54000. + H20 5000. +2.0 OH 41000. | | |
| | | 1 2 1 1 1 1 | CN CN 0 CH2 1. CH2 02 6 H2 | +2 1. + 1. + 5 + 1 + 5 + 1 + | .0 0 8. NO 1. N2 5. 02 3. C3H8 1. 02 1. | 30E+1 25E+1 00E+1 50E+0 10E+1 | > NO 1 0. > CO 2 0. > 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 2 0. > 3.0 CH2 2 0. > 2.0 OH > 0. | + CO 0. + N2 0. +2.0 H2 54000. + H2O 5000. +2.0 OH 41000. 49080. | | |
| | | 1 2 1 1 1 1 1 | CN CN 0 CH2 1. CH2 02 6 H2 1. C3H8 | +2 +2 + + + + + + + + + + + + + | .0 0 8. NO 1. N2 5. 02 3. C3H8 1. 02 1. | 30E+1 25E+1 00E+1 50E+0 10E+1 00E+0 | > NO 1 0. > CO 2 0. > 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 2 0. > 2.0 OH > 0. > 2.0 OH > 0. | + CO 0. + N2 0. +2.0 H2 54000. + H20 5000. +2.0 OH 41000. 49080. + C3H | 8 + | 0 |
| | | 1. 2. 1. 1. 1. | CN CN CN CH2 CH2 CH2 6 H2 C3H8 C3H8 | +2 1. + 1. + + 5 + 1 + +2. | .0 0 8. NO 1. N2 5. 02 3. C3H8 1. 02 1. 0 0 1. | 30E+1 25E+1 00E+1 50E+0 10E+1 00E+0 | > NO 1 0. > CO 2 0. > 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 2 0. > 2.0 OH 0 0. > H2O 5 0. | + CO 0. + N2 0. +2.0 H2 54000. + H2O 5000. +2.0 OH 41000. 49080. + C3H 4000. | 8 + | 0 |
| | OF | 1. 1. 1. 1. 1. | CN CN CH2 CH2 CH2 O2 6 H2 C3H8 5 1 F2 | +2 1. + 1. + + 5 + 1 + +2. + + +2. + + + + + + + + + + + + + | .0 0 8. NO 1. N2 5. 02 3. C3H8 1. 02 1. .0 OH 1. 02 | 30E+1 25E+1 00E+1 50E+0 10E+1 00E+0 98E+0 | > NO 1 0. > CO 2 0. > 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 2 0. > 2.0 OH) 0. > H2O 5 0. | + CO 0. + N2 0. +2.0 H2 54000. + H2O 5000. +2.0 OH 41000. 49080. + C3H 4000. + O | 8 + | 0 |
| 1 | OH | 1. 1. 2. 1. 1. 1. 1. | CN CN CH2 CH2 CH2 O2 H2 C3H8 L5 H2 L5 H2 L5 L5 H2 L5 L5 L5 L5 L5 L5 L5 L5 L5 L5 | +2 1. + 1. + + 5 + 1 + +2 + +2 + +2 + +2 + + + + + + + + | .0 0 NO 1. N2 5. 02 3. C3H8 1. 02 1. 0 OH 1. 02 | 30E+1 25E+1 00E+1 50E+0 10E+1 00E+0 98E+0 | > NO 1 0. > CO 2 0. > 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 2 0. > 2.0 OH 0 0. > H2O 5 0. > H2O | + CO 0. + N2 0. +2.0 H2 54000. + H2O 5000. +2.0 OH 41000. 49080. + C3H 4000. + 0 1013 | 8 + + | о Он |
| 1 | OH . 0 | 1. 2. 1. 1. 1. 1. | CN CN CN CH2 CH2 O2 H2 C3H8 L5 H2 H2 L5 L5 L5 L5 L5 L5 L5 L5 L5 L5 | +2 1. + 1. + 1. + 5 + 1 + +2. + | .0 0 8. NO 1. 25. 02 3. C3H8 1. 02 1. .0 OH 1. 02 0. | 30E+1 25E+1 50E+0 10E+1 00E+0 98E+0 96E+1 | > NO 1 0. > CO 2 0. 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 2 0. > 2.0 OH 0 0. > 2.0 OH 0 0. > H2O 5 0. > H2O 21 | + CO 0. + N2 0. +2.0 H2 54000. + H20 5000. +2.0 OH 41000. 49080. + C3H 4000. + 0 1013. | 8 + + | о ОН |
| 1 | OH . 0 | 1. 1. 1. 1. 1. 1. | CN CN CH2 CH2 CH2 CH2 C3H8 C3H8 L5 H2 H2 L5 L5 L5 L5 L5 L5 L5 L5 L5 L5 L5 L5 L5 | +2 1. + 1. + 1. + + 5 + 1 + +2. + + | .0 0 8. NO 1. N2 5. 02 3. C3H8 1. 02 1. 0 OH 1. 02 0. | 30E+1 25E+1 00E+1 50E+0 10E+1 00E+0 98E+0 98E+0 | > NO 1 0. > CO 2 0. 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 2 0. > 3.0 CH2 2 0. > 2.0 OH 0 0. > H2O 5 0. > H2O 21 | + CO 0. + N2 0. +2.0 H2 54000. + H2O 5000. +2.0 OH 41000. 49080. + C3H 4000. + 0 1013. | 8 + + | О |
| 1 AR | OH . 0 | 1 1 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 | CN CN CH2 CH2 CH2 CH2 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 | +2 1. + 1. + 5 + 1 + + + + + + + | .0 0 8. NO 1. N2 5. 02 3. C3H8 1. 02 1. 0 OH 1. 02 0. | 30E+1 25E+1 00E+1 50E+0 10E+1 00E+0 98E+0 98E+0 96E+12 | > NO 1 0. > CO 2 0. 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 2 0. > 2.0 OH 0 0. > H2O 5 0. > H2O 21 | + CO 0. + N2 0. +2.0 H2 54000. + H2O 5000. +2.0 OH 41000. 49080. + C3H 4000. + 0 1013. | 8 + + | О |
| 1 AR DIS | OH . 0 TANCE | 1. 1. 1. 1. 1. 1. | CN CN CH2 CH2 CH2 O2 H2 L2 C3H8 L5 H2 L2 L2 L2 L2 L2 L2 L2 L2 L2 L | +2 1. + 1. + 5 + 1 + +2. + + | .0 0 NO 1. N2 5. 02 3. C3H8 1. 02 1. 0 OH 1. 02 0. | 30E+1 25E+1 50E+0 10E+1 10E+1 98E+0 98E+0 96E+1 | NO 1 0. 2 0. 2 0. 2 0. 2 0. 2 0. 2 0. 3 0. 2 0. 3 0. 2 0. 3 0. 2 0. 2 0. 2 0. 2 0. 2 0. 2 0. 2 0. 2 | + CO 0. + N2 0. +2.0 H2 54000. + H2O 5000. +2.0 OH 41000. 49080. + C3H 4000. + O 1013. | 8 + + | о Он |
| 1 AR DIS &p | OH .0 TANCE rob w | 1. 1. 2. 1. 1. 1. + 0. AREA elstr- | CN CN CN CH2 CH2 CH2 CH2 CH2 CH2 CH2 CH2 | +2 1. + 1. + 5 + 1 + + 2. + senca | .0 0 NO 1. N2 5. 02 3. C3H8 1. 02 1. 0 OH 1. 02 0. | 30E+1 25E+1 00E+1 50E+0 10E+1 98E+0 98E+0 96E+1 rue., | <pre>> NO 1 0. > CO 2 0. 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 2 0. > 2.0 OH 0 0. > H2O 5 0. > H2O 5 0. > H2O 5 0. > H2O 5 0. > H2O 5 0. > H2O 5 0.</pre> | + CO 0. + N2 0. +2.0 H2 54000. + H20 5000. +2.0 OH 41000. 49080. + C3H 4000. + 0 1013. | 8 + + | о Он |
| 1 AR dis £p c | OH .0 TANCE rob w onc=.t | 1. 1. 1. 1. 1. 1. + 0. AREA elstr= rue., | CN CN CN CH2 CH2 CH2 CH2 C3H8 L5 L5 H2 L5 L5 L5 L5 L5 L5 L5 L5 L5 L5 | +2 1. + 1. + 5 + 1. + 5 + 1. + + 2. + 5 + + 2. + + - - - - - - - - - - - - - | .0 0 NO 1. N2 5. 02 3. C3H8 1. 02 1. 0 OH 1. 02 0. Al = .t | 30E+1 25E+1 00E+1 50E+0 10E+1 98E+0 98E+0 96E+12 rue., | <pre>> NO 1 0. > CO 2 0. > 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 2 0. > 3.0 CH2 2 0. > 2.0 OH 0 0. > H2O 5 0. > H2O 5 0. > H2O 21</pre> | + CO 0. + N2 0. +2.0 H2 54000. + H20 5000. +2.0 OH 41000. 49080. + C3H 4000. + 0 1013. 0e-3, | 8 + + | ОН |
| 1 AR وDIS: دور در | OH .0 TANCE rob w onc=.t sprob | 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. | CN CN CN CH2 CH2 CH2 C3H8 C3H8 C3H8 L5 H2 L5 H2 L5 H2 L5 H2 L5 H2 L5 H2 L5 H2 L5 H2 L5 H2 L5 L5 L5 L5 L5 L5 L5 L5 L5 L5 | +2 1. + 1. + 5 + + 5 + + + + 2. + sence | .0 0 8. NO 1. N2 5. 02 3. C3H8 1. 02 1. 0 OH 1. 02 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. | 30E+1 25E+1 00E+1 50E+0 10E+1 00E+0 98E+0 98E+0 96E+1 rue., | <pre>> NO 1 0. > CO 2 0. >2.0 CN 3 0. > CO 7 0. >3.0 CH2 2 0. >3.0 CH2 2 0. > H2O 5 0. > H2O 5 0. > H2O 5 0. > H2O 5 0. > H2O 5 0. > H2O 5 0.</pre> | + CO 0. + N2 0. +2.0 H2 54000. + H20 5000. +2.0 OH 41000. 49080. + C3H 4000. + 0 1013. 0e-3, | 8 + + | О |
| 1 AR DISS ÉP C | OH .0 TANCE rob w onc=.t sprob delm | 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. | CN CN CN CH2 CH2 O2 H2 L2 H2 L2 H2 L2 L2 L2 L2 CH2 O2 CH2 O2 L2 CH2 O2 L2 CH2 O2 CH2 CH2 O2 CH2 CH2 CH2 CH2 CH2 CH2 CH2 CH | +2 1. + 1. + 5 + + 5 + + + + + senca x= 800 | .0 0 NO 1. N2 5. 02 3. C3H8 1. 02 1. 0 OH 1. 02 0. Al = .t | 30E+1 25E+1 00E+1 50E+0 10E+1 00E+0 98E+00 98E+00 96E+12 rue., 1, | <pre>> NO 1 0. > CO 2 0. >2.0 CN 3 0. > CO 7 0. >3.0 CH2 2 0. >2.0 OH 0 0. > H2O 5 0. > H2O 21 C3H8 tiny = 1.</pre> | + CO 0. + N2 0. +2.0 H2 54000. + H2O 5000. +2.0 OH 41000. 49080. + C3H 4000. + 0 1013. 0e-3, | 8 + + | О |
| 1 AR DIS و و د د پ | OH .0 TANCE rob w onc=.t sprob delm volu | 1. 1. 1. 1. 1. 1. 1. 1. AREA elstr= rue., d= 500. me=500 | CN CN CN CH2 CH2 CH2 CH2 CH2 CH2 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 CH2 CH2 CH2 CH2 CH2 CH2 CH2 CH2 | +2 1. + 1. + 5 + 1 + + 2. + senca x= 80(\$end | .0 0 NO 1. N2 5. 02 3. C3H8 1. 02 1. 0 OH 1. 02 0. al = .t | 30E+1 25E+1 50E+0 10E+1 10E+1 98E+0 98E+0 96E+1 rue., 1, | <pre>> NO 1 0. 2 0. 2 0. 2 0. 2 0. 3 0. 3 0. 3 0. 2 0. 3 0. 2 0. 2 0. 2 0. 2 0. 2 0. 2 0. 2 0. 2</pre> | + CO 0. + N2 0. +2.0 H2 54000. + H2O 5000. +2.0 OH 41000. 49080. + C3H 4000. + O 1013. 0e-3, | 8 + + | ОН |
| 1 AR DIS قوب د د قرب | OH .0 TANCE rob w onc=.t sprob delm volu | 1. 1. 2. 1. 1. 1. 1. 1. 4. 0. AREA elstr= rue., d= 50. me=500 = 800 | CN CN CN CH2 CH2 CH2 CH2 C3H8 L5 H2 L5 H2 1. C3H8 L5 L5 L5 L5 L5 L5 L5 L5 L5 L5 | +2 1. + 1. + 5 + 1 + + 2. + \$ \$ \$ \$ \$ \$ \$ \$ \$ \$ \$ \$ \$ | .0 0 NO 1. N2 5. 02 3. C3H8 1. 02 1. 0 OH 1. 02 0. All = .t | 30E+1 25E+1 50E+0 10E+1 10E+1 98E+0 98E+0 96E+1 rue., 1, eratic | <pre>> NO 1 0. > CO 2 0. > 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 2 0. > 2.0 OH 0 0. > H2O 5 0. > H2O 5 0. > H2O 5 0. > C3H8 tiny = 1.</pre> | + CO 0. + N2 0. +2.0 H2 54000. + H20 5000. +2.0 OH 41000. 49080. + C3H 4000. + 0 1013. 0e-3, | 8 + + | о Он |
| l AR DISS Ép C Éw | OH .0 TANCE rob w onc≃.t sprob delm volu tart t | 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. | CN CN CN CH2 CH2 CH2 CH2 1. C3H8 15 H2 1. H2 1. c3H8 c3H8 c3H8 c3H8 c3H8 c3H8 c3H8 c3H8 c3H8 c42 c42 c42 c42 c42 c42 c42 c42 | +2 1. + 1. + 1. + 5 + 1 + + 2. + sence x= 800 &end mdot= | .0 0 8. NO 1. 25. 02 3. C3H8 1. 02 1. 0 OH 1. 02 0. Al = .t | 30E+1 25E+1 50E+0 10E+1 98E+0 98E+0 96E+12 rue., 1, eratic | <pre>> NO 1 0. > CO 2 0. > 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 2 0. > 3.0 CH2 2 0. > 2.0 OH 0 0. > H2O 5 0. > H2O 5 0. > H2O 21 C3H8 tiny = 1.</pre> | + CO 0. + N2 0. +2.0 H2 54000. + H20 5000. +2.0 OH 41000. 49080. + C3H 4000. + 0 1013. 0e-3, | 8 + + | О |
| 1 AR DIS Ép C Ew Es Sc | OH .0 TANCE rob w onc=.t sprob delm volu tart t c=3,sc | 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. | CN CN CN CH2 CH2 CH2 CH2 1. C3H8 15 1. H2 1. C3H8 1. C3H8 1. C3H8 1. C3H8 1. CH2 | +2 1. + 1. + 5 + 1. + 5 + + 2. + senca x= 800 &end mdot= | .0 0 8. NO 1. N2 5. 02 3. C3H8 1. 02 1. 02 1. 02 0. al = .t | 30E+1 25E+1 00E+1 50E+0 10E+1 00E+0 98E+0 98E+0 98E+0 96E+1 1, rue., 1, eratio | <pre>> NO 1 0. > CO 2 0. > 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 2 0. > 3.0 CH2 2 0. > 2.0 OH 0 0. > H2O 5 0. H2O 5 0. H2</pre> | + CO 0. + N2 0. +2.0 H2 54000. + H2O 5000. +2.0 OH 41000. 49080. + C3H 4000. + 0 1013. 0e-3, | 8 + + | О |
| 1 AR DIS Ép C Éw És Sc END | OH .0 TANCE rob w onc=.t sprob delm volu tart t c=3, sc | 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. | CN CN CN CH2 CH2 CH2 CH2 CH2 CH2 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 CH2 CH2 CH2 CH2 CH2 CH2 CH2 CH2 | +2 1. + 1. + 5 + 1 + + 2. + 1 + + 2. x= 800 &end mdot= | .0 0 NO 1. N2 5. 02 3. C3H8 1. 02 1. 0 OH 1. 02 0. al = .t | 30E+1 25E+1 50E+0 10E+1 10E+1 98E+0 98E+0 96E+1 rue., 1, eratio | <pre>> NO 1 0. 2 0. 2 0. 2 0. 2 0. 3 0. 3 0. 3 0. 2 0. 3 0. 2 0. 2 0. 2 0. 2 0. 2 0. 2 0. 2 0. 2</pre> | + CO 0. + N2 0. +2.0 H2 54000. + H2O 5000. +2.0 OH 41000. 49080. + C3H 4000. + 0 1013. 0e-3, | 8 + + | о Он |
| 1 AR DIS ÉP C S S C S C S C | OH .0 TANCE rob w onc=.t sprob delm volu tart t c=3, sc SVAR | 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. | CN CN CN CH2 CH2 CH2 CH2 CH2 C3H8 1. C3H8 1. C3H8 1. C3H8 1. C3H8 1. C3H8 1. CH2 | +2 1. + 1. + 5 + 1 + + 2. + x= 800 &end mdot= | .0 0 NO NO 1. N2 5. 02 3. C3H8 1. 02 1. 0 OH 1. 02 0. All = .t 0., mpr= 200., | 30E+1 25E+1 50E+0 10E+1 10E+1 98E+0 98E+0 96E+12 rue., 1, eratio | <pre>> NO 1 0. 2 CO 2 0. 2.0 CN 3 0. 2.0 CN 3 0. 2.0 CN 3.0 CH2 2 0. 2.0 OH 0 0. 420 CH2 2 0. 2.0 OH 0 0. 420 CH2 2 0. 2.0 CH2 2.0 CH2 2</pre> | + CO 0. + N2 0. +2.0 H2 54000. + H20 5000. +2.0 OH 41000. 49080. + C3H 4000. + 0 1013. 0e-3, | 8 + + | О |
| 1 AR & DIS & D. & W. & S. S. S. S. C.3F | OH .0 TANCE rob w onc=.t sprob delm volu tart t c=3, sc SVAR 8 | 1. 1. 2. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1 | CN CN CN CH2 CH2 CH2 CH2 C3H8 L5 L5 L5 L5 L5 L5 L5 L5 L5 L5 | +2 1. + 1. + 5 + 1 + 5 + 1 + + 2. \$ enca \$ end \$ mdot= 2 | .0 0 NO NO 1. N2 5. 02 3. C3H8 1. 02 1. 0 OH 1. 02 0. Al = .t 200., OH | 30E+1 25E+1 00E+1 50E+0 10E+1 98E+0 98E+0 96E+1 rue., 1, eratio | <pre>> NO 1 0. > CO 2 0. > 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 2 0. > 2.0 OH 0 0. > H2O 5 0. > H2O 21 C3H8 tiny = 1.</pre> | + CO 0. + N2 0. +2.0 H2 54000. + H20 5000. +2.0 OH 41000. 49080. + C3H 4000. + 0 1013. 0e-3, | 8 + + TEMP | 0 OH END |
| 1 AR DIS Ép C S S C S S C S S C S S C S C S N T T | OE .0 TANCE rob w onc=.t sprob delm volu tart t c=3, sc SVAR 8 T | 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. | CN CN CN CH2 CH2 CH2 CH2 1. C3H8 15 H2 1. C3H8 1. C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 CH2 CH2 CH2 CH2 CH2 CH2 CH2 CH2 | +2 +2 + + + + + + + + + + + + + | .0 0 8. NO 1. N2 5. 02 3. C3H8 1. 02 1. 02 1. 02 0. 81 = .t | 30E+1 25E+1 00E+1 50E+0 10E+1 00E+0 98E+0 98E+0 98E+0 96E+1 1, rue., 1, eratio | <pre>> NO 1 0. > CO 2 0. > 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 2 0. > 3.0 CH2 2 0. > 2.0 OH 0 0. > H2O 5 0. > H2O 21 C3E8 tiny = 1.</pre> | + CO 0. + N2 0. +2.0 H2 54000. + H2O 5000. +2.0 OH 41000. 49080. + C3H 4000. + 0 1013. 0e-3, | 8 + + TEMP | O OH END |
| 1 AR DIS Ép C. Éw SEND SEND SEND INITEN | OE .0 TANCE rob w onc=.t sprob delm volu tart t c=3, sc SVAR 8 T P | 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. | CN CN CN CH2 CH2 CH2 CH2 CH2 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C42 CH2 CH2 CH2 CH2 CH2 CH2 CH2 CH | +2 1. + 1. + 1. + 5 + 1 + + 2 x= 800 &end mdot= | .0 0 NO 1. N2 5. 02 3. C3H8 1. 02 1. 0 OH 1. 02 0. mpr= 200., OH | 30E+1 25E+1 50E+0 10E+1 10E+1 98E+0 98E+0 96E+1 1, eratic | <pre>> NO 1 0. > CO 2 0. > 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 2 0. > 2.0 OH 0 0. > H2O 5 0. H2O C3H8 tiny = 1.</pre> | + CO 0. + N2 0. +2.0 H2 54000. + H2O 5000. +2.0 OH 41000. 49080. + C3H 4000. + 0 1013. 0e-3, | 8 + + TEMP | O OH END |
| 1 AR DIS Ép. C. ÉW SSD SEND SENN INI TEM | OH .0 TANCE rob w onc=.t sprob delm volu tart t c=3, sc SVAR 8 T P C | 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. | CN CN CN CH2 CH2 CH2 CH2 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C12 CH2 CH2 CH2 CH2 CH2 CH2 CH2 CH | +2 1. + 1. + 5 + 1 + + 2. * * * * * * * * * * * * * | .0 0 NO NO 1. N2 5. 02 3. C3H8 1. 02 1. 0 OH 1. 02 0. All = .t 0., mpr= 200., OH | 30E+1 25E+1 50E+0 10E+1 10E+1 98E+0 98E+0 96E+1 1, eratio | <pre>> NO 1 0. 2 0. 2.0 CN 3 0. 2.0 CN 3 0. 2.0 CN 3 0. 2.0 CH 2 0. 2.0 OH 0 0. 420 5 0. 420 5 0. 420 5 0. 5</pre> | + CO 0. + N2 0. +2.0 H2 54000. + H20 5000. +2.0 OH 41000. 49080. + C3H 4000. + 0 1013. 0e-3, | 8 + + TEMP | O OH END |
| 1 AR DISS ÉP CC END CSH INI TEM REA | OH .0 TANCE rob w onc=.t sprob delm volu tart t c=3, sc SVAR 8 T P C C | 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. | CN CN CN CH2 CH2 CH2 CH2 C3H8 1. C3H8 1. C3H8 1. C3H8 1. C3H8 1. C3H8 1. CH2 CH2 CH2 | +2 +2 + + + + + + + + + + + + + + + + + | .0 0 NO NO 1. N2 5. 02 3. C3H8 1. 02 1. 0 OH 1. 02 0. All = .t 200., OH | 30E+1 25E+1 50E+0 10E+1 10E+1 98E+0 98E+0 96E+1 1, eratio | <pre>> NO 1 0. > CO 2 0. > 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 2 0. > 2.0 OH 0 . > 2.0 OH 0 . > H2O 5 0. > H2O 21 C3H8 tiny = 1.</pre> | + CO 0. + N2 0. +2.0 H2 54000. + H20 5000. +2.0 OH 41000. 49080. + C3H 4000. + 0 1013. 0e-3, NO | 8 + + TEMP | O OH END |
| 1 AR dISS &p. c. &w. ≻ SEND SEND INI TEM. REA &s | OH .0 TANCE rob w onc=.t sprob delm volu tart t c=3, sc SVAR 8 T P C cenrxn | 1. 1. 2. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1 | CN CN CN CH2 CH2 CH2 CH2 C3H8 L5 H2 L5 H2 L5 L5 L5 L5 L5 L5 L5 L5 L5 L5 | +2 +2 + + + + + + + + + + + + + * * * * | .0 0 8. NO 1. N2 5. 02 3. C3H8 1. 02 0. 0 1. 02 0. 0. 01 = .t 200., 0H 0rder fend | 30E+1 25E+1 00E+1 50E+0 10E+1 98E+0 98E+0 96E+1 rue., 1, eratio | <pre>> NO 1 0. > CO 2 0. > 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 2 0. > 2.0 OH 0 0. > H2O 5 0. > H2O 21 C3H8 tiny = 1. c3H8 tiny = 1.</pre> | + CO 0. + N2 0. +2.0 H2 54000. + H20 5000. +2.0 OH 41000. 49080. + C3H 4000. + 0 1013. 0e-3, NO | 8 + + TEMP | 0 OH END |
| 1 AR DIS Ép C END SEN SEN SEN INI TEM REA ES | OE .0 TANCE rob w onc=.t sprob delm volu tart t c=3, sc SVAR 8 T P .C .enrxn out | 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. | CN CN CN CH2 CH2 CH2 CH2 CH2 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C3H8 C42 CH2 CH2 CH2 CH2 CH2 CH2 CH2 CH | +2 1. + 1. + 1. + 5 + 1 + + 2. cue., | .0 0 NO NO 1. N2 5. 02 3. C3H8 1. 02 1. 0 OH 1. 02 0. Al = .t 200., OH order &end | 30E+1 25E+1 00E+1 50E+0 10E+1 00E+0 98E+0 98E+0 98E+0 96E+12 rue., 1, eratio | <pre>> NO 1 0. > CO 2 0. > 2.0 CN 3 0. > CO 7 0. > 3.0 CH2 2 0. > 3.0 CH2 2 0. > H2O 5 0. > H2O 5 0. > H2O 21 C3E8 tiny = 1. > =1.5, H2O cue., allr</pre> | + CO 0. + N2 0. +2.0 H2 54000. + H2O 5000. +2.0 OH 41000. 49080. + C3H 4000. + 0 1013. 0e-3, NO xn = .true. | 8 + + TEMP | O OH END |

| | erature | Brute force | -2.90×10 ⁻³ | 4.58×10 ⁻² | 4.92×10 ⁻² | 1.81×10 ⁻² | 1.93×10 ⁻³ | 5.79×10 ⁻³ | 4.10×10 ⁻³ | | 0.495 |
|------------------------------------|----------------|-------------|---|---|------------------------------------|--|--------------------------------|------------------------|-----------------------------|--------------------------------------|--------|
| | Temp | GLSENS | -3.01×10 ⁻³ | 4.61×10 ⁻² | 4.92×10 ⁻² | 1.81×10 ⁻² | 1.78×10 ⁻³ | 5.80×10 ⁻³ | 4.21×10^{-3} | | 0.496 |
| | 0 | Brute force | 0.643 | -0.449 | -0.114 | -4.86×10 ⁻² | -0.982 | 0.963 | -0.625 | | -0.796 |
| | Z | GLSENS | 0.643 | -0.449 | -0.112 | -4.88×10 ⁻² | -0.981 | 0.963 | -0.625 | | -0.798 |
| | 0 | Brute force | -8.33×10 ⁻³ | 9.42×10 ⁻² | 2.46×10 ⁻² | 1.21×10 ⁻² | 2.08×10 ⁻³ | | 1.04×10 ⁻² | | 0.263 |
| n _j , or E _j | H | GLSENS | -8.58×10 ⁻³ | 9.45×10 ⁻² | 2.48×10 ⁻² | 1.20×10 ⁻² | 2.04×10 ⁻³ | | 1.07×10 ⁻² | nperature | 0.265 |
| ith respect to A _j , | H | Brute force | 0.302 | -6.56×10 ⁻² | 6.93×10 ⁻² | 1.47×10 ⁻² | 5.01×10 ⁻³ | 2.31×10 ⁻³ | -0.316 | pect to initial ter | 0.817 |
| efficient (S _{IJ}) w | 0 | GLSENS | 0.302 | -6.54×10 ⁻² | 6.76×10 ⁻² | 1.48×10 ⁻² | 5.00×10 ⁻³ | 2.23×10 ⁻³ | -0.316 | $\langle S_{i,T_0} \rangle$ with res | 0.819 |
| a) Sensitivity co | 22 | Brute force | 3.30×10 ⁻³ | -0.730 | -0.261 | -9.85×10 ⁻² | -6.61×10 ⁻³ | -3.11×10 ⁻² | -1.10×10 ⁻² | tivity coefficient | -2.23 |
|) | 0 | GLSENS | 4.08×10 ⁻³ | -0.731 | -0.262 | -9.86×10 ⁻² | -6.63×10 ⁻³ | -3.11×10 ⁻² | -1.13×10 ⁻² | (b) Sensi | -2.23 |
| | H ₈ | Brute force | 7.68×10 ⁻² | -0.865 | 5.25×10 ⁻² | 3.35×10 ⁻² | -1.68×10 ⁻² | 7.91×10 ⁻³ | -7.09×10 ⁻² | | -2.13 |
| | ບົ | GLSENS | 7.60×10 ⁻² | -0.863 | 5.30×10 ⁻² | 3.37×10 ⁻² | -1.68×10 ⁻² | 7.95×10 ⁻³ | -7.07×10 ⁻² | | -2.12 |
| | Reaction | | $\begin{array}{c} 0H + H_2 + 0_2 \rightarrow \\ H_2 O + O + O + OH \end{array}$ | $0_2 + C_3 H_8 \rightarrow 3CH_2 + 2OH$ | $CH_2 + 0_2 \rightarrow CO + H_2O$ | $\begin{array}{c} 2CH_2 + N_2 \rightarrow \\ 2CN + 2H_2 \end{array}$ | $CN + NO \rightarrow CO + N_2$ | CN + 20 → N0 + C0 | H + O ₂ = OH + O | | |
| | Reaction | | 28 | 25 | 24 | 23 | 22 | 21 | 7 | | |

TABLE 4.12.—COMPARISON OF GLSENS AND BRUTE-FORCE SENSITIVITY COEFFICIENTS FOR EXAMPLE PROBLEM 6 (REACTION OF PROPANE AND AIR WITH GLOBAL REACTIONS) [Equivalence ratio $\varphi = 1.5$; mass flow rate $\dot{m} = 350$ g/s; temperature T = 2072.23 K.]

| TABLE 4.13.—DATA | FILE FOR EXAMPLE PROBLEM 7 | (PROPANE-AIR PSR) |
|------------------|----------------------------|-------------------|
| | | (|

| TAPE | | | | | | | | | |
|-----------|--------|----------|----------|------------|----------|------------|-----------------------------|------------|-------------|
| LSENS | PROI | PANE - | AIR WEI | LL-STIR | RED RE | ACTOR | WITH SENSITIVIT | Ϋ́Υ | |
| frtybe | ė | C3H8 | - | C2H5 | + | CH3 | 5 0E+15 | ٥ | 83500 |
| CH3 | + | C3H8 | | CH4 | + | C3H7 | 3.55E+12 | 0. | 10300. |
| 0115 | | C3H7 | = | C2H4 | + | CH3 | 3.0E+14 | 0. | 33200. |
| м | + | CH4 | = | CH3 | + | H | 2.0E+17 | 0. | 88000. |
| E | + | CH4 | | СНЗ | + | H2 | 1.26E+14 | Ο. | 11900. |
| CH4 | + | 02 | - | CH3 | + | HO2 | 7.94E+13 | 0. | 56000. |
| 0 | + | CH4 | = | CH3 | + | OH | 1.9E+14 | Ο. | 11720. |
| OB | + | CH4 | * | CH3 | + | H2O | 2.5E+13 | 0. | 5010. |
| CH3 | + | 02 | = | CH30 | + | 0 | 2.4E+13 | 0. | 28680. |
| CH3 | + | OH | = | CH30 | + | H | 6.3E+12 | 0. | 0. |
| м | + | CH30 | * | CH2O | + | H | 5.0E+13 | 0. | 21000. |
| CH3 | + | CH3 | = | C2H6 | | | 2.4E+14 | 4 | 0. |
| H | + | C2E6 | - | C2H5 | + | H2 | 1.326+14 | 0. | 9700. |
| 0 | + | C2H6 | * | C2H5 | +, | UH | 1.135+14 | 0. | 7850. |
| OH M | + | C2H0 | - | C2H3 | - - | n20 H | 8.7 <u>E</u> +13 1 0E+17 | 0. | 31000 |
| M CORE | + _ | 0205 | - | C284 | + + | н но2 | 2 05+12 | 0. | 5000. |
| | - - | C2#5 | _ | C2H4 | + | H2 | 4 8E+13 | 0. | 0 |
| CB3 | + | CH2 | - | C2H4 | + | H | 2 0E+13 | 0. | 0. 0 |
| н | | C2H4 | = | H2 | + | - С2H3 | 1.5E+14 | 0. | 10200 |
| M | + | C2H4 | = | C2H2 | + | H2 | 2.6E+17 | 0. | 79300. |
| C2H4 | + | OB | = | C2H3 | + | H2O | 4.8E+12 | Ο. | 1230. |
| C2H4 | + | OH | 22 | CH3 | + | CH2O | 2.0E+12 | Ο. | 960. |
| C2H4 | + | 0 | # | CH3 | + | HCO | 3.3E+12 | Ο. | 1130. |
| C2H4 | + | 0 | = | CH2O | + | CH2 | 2.5E+13 | Ο. | 5000. |
| М | + | C2H3 | = | C2H2 | + | H | 3.0E+15 | 0. | 32000. |
| C2H3 | + | 02 | - | CH2O | + | HCO | 3.98E+12 | 0. | -250. |
| C2H3 | + | H | | C2H2 | + | E2 | 6.0E+12 | 0. | 0. |
| C2H3 | + | 0 | = | C2H2O | + | H | 3.3E+13 | 0. | 0. |
| C2H3 | + | OH | | C2H2 | + | H2O | 5.0E+12 | 0. | υ. |
| C2H3 | + | CH2 | | C2H2 | + | CH3 | 3.0E+13 | <u> </u> | 0. |
| C2H3 | + | C2H | =2. | C2# | - | 13 | 3.UET13 4 2E115 | 0. | 0. |
| M C2E2 | + | 0 | - | C2A C#2 | + | п СО | 4.25T10 1 6F+14 | U | 10/000. |
| C2H2 | + + | ñ | _ | C280 | + | ਸ | 4 0E+14 | 0.0 | 10660 |
| C2H2 | + | OH OH | = | C2H | + | 820 | 6.3E+12 | 0.0 | 7000 |
| C2H2 | + | 0E | = | C2820 | + | H | 3.2E+11 | 0.0 | 200. |
| C2H | + | 02 | Ŧ | C2HO | + | 0 | 5.00E+13 | 0. | 1500. |
| C2H | + | 0H | - | C2EO | + | H | 2.0E+13 | 0. | 0. |
| C2HO | + | 02 | =2. | 000 | + | OН | 1.46E+12 | 0. | 2500. |
| C2BO | + | 0 | =2. | 0C0 | + | Ħ | 1.202E+12 | Ο. | Ο. |
| C2HO | + | OH | =2. | 0BCO | | | 1.0E+13 | Ο. | 0. |
| C2HO | + | H | 1 | 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. | OC2HO | * | C2H2 | +2. | 000 | 1.0E+13 | 0. | 0. |
| C2H2O | + | OH | = | CH2O | + | HCO H2O | 2.85+13 | 0. | 2000 |
| C2H20 | + | UH UH | - | CZRU | + | E20 | 1.3ET12 1.12E±12 | <u>,</u> . | 3000. |
| C2H2O | + | п 17 | | | ∓ | EO 22 | 1.13ET13 7 5F113 | 0. | 3420. |
| C2B20 | + | n 0 | - | C2EO | | 08 | 5 OF+13 | 0 | 8000. |
| C2B20 | + | õ | - | CH20 | + | 00 | 2 0E+13 | 0. | 0000. |
| M | ÷ | C2820 | - | CB2 | + | co | 2.0E+16 | <u>0</u> . | 60000. |
| C28 | + | 0 | | co | + | CH | 5.0E+13 | ō. | 0. |
| CESO | + | 02 | - | CH2O | + | HO2 | 1.0E+13 | 0. | 7170. |
| CH3O | + | Ħ | = | CH2O | + | H2 | 2.0E+13 | ο. | 0. |
| м | + | CH2O | = | ECO | + | Ħ | 5.0E+16 | 0. | 81000. |
| CH2O | + | OH | = | HCO | + | E20 | 3.0E+13 | 0. | 1200. |
| CH20 | + | E | - | HCO | + | H2 | 2.5E+13 | 0. | 3990. |
| CH2O | + | 0 | = | HCO | + | OH | 3.5E+13 | 0. | 3510. |
| CH3 | + | CH2O | = | CH4 | + | HCO | 1.0E+10 | 0.5 | 6000. |
| CH3 | + | HCO | = | CH4 | + | C0 | 3.0E+11 | .5 | 0. |
| СНЗ | + | HOZ | - | CHO | + | UR B | 2.0E+13 | U. | U. 01600 |
| M | + + | CH3 | | CE2 H2 | 7 1 | CH2 | 1.335+10 9 7F+13 | 67 | 25700 |
| 0 | + + | CH3 | - | OH OH | + | CH2 | 1.9E+11 | . 68 | 25700 |
| ~ | • | | | . | | | | | |

| TABLE 4 | .13.— | Continued |
|---------|-------|-----------|
|---------|-------|-----------|

| | | | TABLE | 4.13 | -Continued. | | | |
|--|---|------------|---|--------|---|---|---|--|
| OH + CH + CH2 + HC0 + HC0 + HC0 + CO + CO + CO + O + H + O + H + O + H + OH + HO2 + H + M + THIRDBODY + H2 2.3 | CH3 CO2 O2 O2 OC OH H CH2 CH2 CH2 O2 OC OH HC0 O2 OH HC0 O2 OH HC2 HC2 HC2 HC2 HC2 HC2 HC2 HC2 HC2 HC | | TABLE H2O HCO CH2O CH2O CH C2H3 C2H2 CO CO CO CO CO CO CO CO CO CO CO CO CO | 4.13. | Continued. CH2 CO O O O H H20 H2 EO2 OH H20 H2 CO M O H OH OH OH OH OH OH OH OH | 2.7E+11 3.7E+12 1.0E+13 5.0E+11 2.0E+11 5.0E+11 5.0E+13 3.0E+13 3.0E+13 3.0E+13 2.0E+13 2.0E+13 2.0E+13 2.0E+13 2.0E+13 2.0E+13 2.0E+14 2.4E+15 2.5E+12 4.17E+11 5.75E+13 6.8E+13 1.89E+14 7.28E+13 5.0E+13 8.0E+12 1.34E+14 7.91E+13 6.1E+12 7.8E+11 1.44E+17 6.0 B | .67 0. 0.5 .7 .5 0.7 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. | 25700. 0. 6960. 25800. 5900. 4970. 0. 0. 0. 0. 15570. 4100. 15570. 4100. 22930. 18365. 16400. 13750. 2126. 1000. 0. 1070. 25000. 1430. 0. 45510. 6.6 |
| END E2 + | ОН | = 1 | H 20 | + | н | 4.74E+13 | 0. | 6098. |
| H + THIRDBODY | 02 | a [| HO2 | + | М | 1.46E+15 | 0. | -1000. |
| 02 1.3 END | 0 N2 | | 1.3 | | H20 | 21.3 C | :02 | 7.0 |
| M + THIRDBODY | H20 | =] | Ħ | ÷ | OH | 1.30E+15 | 0. | 105140. |
| H2 4.0 CO2 4.0 | 0 02 END | | 1.5 | | H2O | 20.0 N | 2 | 1.5 |
| H + M + | 0 #2 | = (=) | OH H | + + | M H | 7.1E+18 2.2E+14 | -1. 0. | 0. 96000. |
| THIRDBODY | 0 02 | | 2.0 | | 820 | 15.0 N | 2 | 2.0 |
| END | 02 | _ / | 0 | + | 0 | 1 80E+18 | -1 | 118020 |
| | N2 | - (| ECN | + | Ň | 1.0E+11 | 0. | 19000 |
| | 82 | = 1 | HCN | + | Ħ | 6.0E+13 | 0 . | 5300. |
| 0 + | HCN | | OH | + | CN | 1.4E+11 | . 68 | 16900. |
| | BCN | | ENCO | ÷ | R | 4.0E+11 | 0. | 2800. |
| | 0 | | | ÷ | N | 1 2E + 13 | 0. | 0. |
| | 0" | | | _ | 8 | 25E+14 | 0. | 6000 |
| | NCO | _ 1 | | + | я | 1 0E+14 | 0. | 9000 |
| | RCO R | | 11100 | ÷ | ro CO | 1 0E+14 | 0 | 8500. |
| | | - 1 | NCO | + | 0 | 3 28413 | 0. | 1000 |
| | 02 | | | т 1 | čo | 3 75+12 | 0 | 0 |
| | 202 | _ ! | | г - | <u>co</u> | 2 NF+13 | 0 | 0 |
| 0 + | NCO | = ; | NO | т L | 0 | 1 05+13 | 0. | ő. |
| N + | NCO | = : | NZ NU | т ⊥ | <u> </u> | 2 05+13 | 0 | 0 |
| | NO | - | N N | + | HCO | 1.6E+13 | 0. | 9940 |
| | NO | | <u>^</u> | + | HCN | 2.0E+12 | 0. | Ο. |
| | 08 | 32 | Ň | + | H20 | 5.0E+11 | 0.5 | 2000. |
| HO2 + | NO | - | NO2 | + | OH | 2.09E+12 | 0. | -477. |
| 0 + | NO2 | - | NO | + | 02 | 1.0E+13 | Ο. | 596. |
| NO + | 0 | * | NO2 | + | M | 5.62E+15 | Ο. | -1160. |
| NO2 + | H | 75 | NO | ÷ | ОН | 3.47E+14 | Ο. | 1470. |
| | - | | | | | | | |

| NO | + | H | | = | N | + | OH | 2.63E+ | 14 | 0. | | 50410. |
|---|--|---|-------------------------|------------------|--|----------------------------|-----------------------------|--------------------------------|------|---------|----------|--------|
| NO | + | 0 | | - | N | + | 02 | 3.8E | ;+9 | 1. | | 41370. |
| 0 | + | N2 | | = | NO | + | N | 1.80E+ | -14 | 0. | | 76250. |
| N | + | NO2 | | =2. | ONO | | | 4.0E+ | ·12 | 0. | | 0. |
| м | + | N20 | | = | N2 | + | 0 | 6.92E+ | 23 | -2.5 | | 65000. |
| 0 | + | N20 | | = | N2 | + | 02 | 1.0E+ | 14 | 0. | | 28020. |
| ò | + | N20 | | =2. | ONO | | | 6.92E+ | 13 | 0. | | 26630. |
| N20 | + | Ħ | | - | N2 | + | OH | 7.59E+ | ·13 | 0. | | 15100. |
| NO2 | + | H2 | | = | HNO2 | + | H | 2.4E+ | ·13 | 0. | | 29000. |
| OH | + | NO2 | | = | ENO3 | + | M | 3.0E+ | ·15 | Ο. | | -3800. |
| THIRDE | BODY | | | | | | | | | | | |
| 02 | 0. | 70 | H2 | | 1. | 4 | END | | | | | |
| 0H | + | NO | | * | HNO2 | + | м | 5.6E+ | ·15 | 0. | | -1700. |
| HNO | + | H | | = | H2 | + | NO | 5.0E+ | ·12 | 0. | | 0. |
| H | + | NO | | × | HNO | + | М | 5.4E+ | 15 | Ο. | | -600. |
| HNO | + | OH | | = | H20 | + | NO | 3.6E+ | ·13 | Ο. | | 0. |
| &prob v tir &wsprob &start C3H8 N2 O2 AR CO2 END | <pre>weistra hy = 1 dotm r=.tru t=614 0.08 0.68 0.21 0.01 0.00</pre> | .e-3, ax=16 e., w .0, p 73262 92887 1232 1737 04162 | 00.0, srht: =5.0, | de L=0. md | L=.1415 &en 1md=800 05, wsr .ot=10.0 | d .0, ht0=- , mo: | volum -42.88, lef=.fa | e=300.0, &end lse., &end | | | | |
| INIT TEMP SENSVAR | END | | | | | | | | | | | _ |
| C3H8 | CH4 | | СНЗ | | H2 | | OH | H20 | C: | 282 | C2H | 6 |
| CO REAC | TEMP | | END | | | | | | | | . | |
| <pre>&senrxn 35.</pre> | sens., 37., | aj ≖ 49., | .tru 64 | ≥., ., 8 | order = 3., 86. | .tru | ie., rx: &end | num =1.,4.,5. | ,11, | , 13.,1 | 5.,19 | • • |
| FINIS | | | | | | | | | | | | |

TABLE 4.13.—Concluded.

(a) $\langle S_{ij} \rangle$ for reaction rate coefficients

| | | | The line of | ant nomana | | | | | |
|----------|-------------------------------------|-----------------------------------|---------------------------------|-----------------------|-----------------------|--------------------|-------------|-----------------------|-----------------------|
| Reaction | Reaction | C ₃ H ₈ con | centration | CH ₄ con | centration | CH ₃ co | ncentration | H ₂ conce | ntration |
| number | | GLSENS | Brute force | GLSENS | Brute force | GLSENS | Brute force | GLSENS | Brute force |
| 1 | $C_3H_8 = C_2H_5 + CH_3$ | -0.996 | -0.996 | 1.56×10^{-3} | 1.60×10^{-3} | | | 1.63×10^{-3} | 1.63×10^{-3} |
| 4 | $CH_4 + M \approx CH_3 + H + M$ | -0.208 | -0.208 | 0.859 | 0.859 | 0.217 | 0.217 | -0.162 | -0.162 |
| 15 | $OH + C_2 H_6 \neq C_2 H_5 + H_2 O$ | 3.74×10^{-2} | 3.74×10^{-2} | -0.223 | -0.223 | -0.191 | -0.191 | 3.53×10^{-2} | 3.53×10^{-2} |
| 19 | $CH_3 + CH_2 = C_2H_4 + H$ | 4.85×10^{-2} | 4.86×10^{-2} | -0.308 | -0.308 | -0.249 | -0.249 | 5.20×10^{-2} | 5.20×10^{-2} |
| | * | • | (b) $\langle S_{i,T_0} \rangle$ | for initial tem | perature | | • | | |
| | | -3.96 | -3.96 | 3.83×10^{-2} | 3.81×10^{-2} | 0.979 | 0.979 | 8.67×10^{-2} | 8.69×10^{-2} |

| | crature | Brute force | | 1.07×10^{-2} | -2.09×10 ⁻³ | -2.56×10 ⁻³ | | 0.214 |
|---------------|-----------------------------------|-------------|-----------------------------|---------------------------|----------------------------------|----------------------------|--------------|------------------------|
| | Tempe | GLSENS | | 1.07×10^{-2} | -1.91×10^{-3} | -2.48×10 ⁻³ | | 0.214 |
| | ncentration | Brute force | 2.45×10 ⁻³ | 0.322 | -0.428 | -0.472 | | -2.08 |
| | C ₂ H ₆ coi | GLSENS | 2.38×10 ⁻³ | 0.322 | -0.428 | -0.472 | | -2.08 |
| | entration | Brute force | | -6.25×10 ⁻² | 1.59×10 ⁻² | 1.45×10 ⁻² | | 9.16×10 ⁻² |
| | CO conc | GLSENS | | -6.25×10 ⁻² | 1.58×10 ⁻² | 1.42×10 ⁻² | | 9.16×10 ⁻² |
| (a) Concluded | centration | Brute force | | 3.12×10 ⁻² | -3.95×10 ⁻³ | -7.89×10 ⁻³ |) Concluded. | -3.18×10 ⁻² |
| (a) | H ₂ O conc | GLSENS | 1 | 3.14×10 ⁻² | -4.01×10 ⁻³ | -7.94×10 ⁻³ | Ð | -3.12×10 ⁻² |
| | entration | Brute force | -2.37×10^{-3} | -0.458 | 5.52×10 ⁻² | 9.70×10 ⁻² | | 1.27 |
| | OH conc | GLSENS | -2.21×10^{-3} | -0.458 | 5.51×10 ⁻² | 9.71×10 ⁻² | | 1.27 |
| | Reaction | | $C_3H_8 \neq C_2H_5 + CH_3$ | $CH_4 + M = CH_3 + H + M$ | $OH + C_2 H_6 = C_2 H_5 + H_2 O$ | $CH_3 + CH_2 = C_2H_4 + H$ | | |
| | Reaction | uniliper | 1 | 4 | 15 | 61 | | 1 |

| -0 |
|----------|
| ٥. |
| ÷ |
| ÷. |
| |
| |
| F |
| • |
| C |
| T |
| i (|
| - 5- |
| 4 |
| - |
| |
| V |
| LT) |
| |
| |
| μa μ |
| ~ |
| 2 |
| 5 |
| |

| TABLE 4.15.—DATA FILE FOR EXAMPLE PROBLEM 8 (BEN | VZENE-OXYGEN PSR) |
|--|-------------------|
|--|-------------------|

| TAPE | | | | | | | | | | |
|--------------|------------|---------------|------|---------|----------|-------------------|-------|-----------|------------|---------|
| C6H6 OXYGE | N | NO ARGON | PSR | SENSITI | VITY | TEST | CASE; | MECHANISM | K-72 | |
| &rtype | | & end | | | | | | | | |
| C6H6 | + | 02 | = | C6H5O | + | OH | | 4.0E+13 | 0. | 34000. |
| C6H6 | + | C6H5 | * | C12H10 | + | H | | 4.0E+11 | 0. | 4000. |
| | | C6H6 | | C6H5 | ÷ | H | | 5.0E+15 | 0. | 108000. |
| C646 | ъ | 80000 | - | C685 | + | H2 | | 2.5E+14 | 0. | 16000. |
| Cono | 1 | 0 | - | C6850 | _ | 8 | | 2 783F+13 | 0 | 4910 |
| Cono | Ť | 0 | _ | CONJO | | | | 2 1225112 | 0. | 4590 |
| Сбно | + | OH | - | Cons | Ŧ | <u>n</u> 20 | | 2.1326+13 | 0. | 4300. |
| M | + | C4H3 | ÷ | C4H2 | + | H | | 1.0E+16 | 0.0 | 60000. |
| | | C6850 | = | C585 | + | CO | | 2.51E+11 | 0. | 43900. |
| C6H5 | + | 02 | - | C6H50 | + | 0 | | 2.1E+12 | 0. | 7470. |
| C6H5 | + | HO2 | Ŧ | C6850 | + | OH | | 2.0E+13 | 0. | 1000. |
| | | C6H5 | = | C4H3 | + | C2B2 | | 4.50E+13 | 0. | 72530. |
| | | C6H5OH | × | C6850 | + | Н | | 2.00E+16 | 0. | 88000. |
| C68508 | + | H | = | Сбнб | + | OF | | 2.20E+13 | 0. | 7910. |
| CEUSOU | 1 | IJ | - | C6450 | ÷ | 82 | | 1.15E+14 | 0 | 12400 |
| Conjon | - - | n 0 (11507 | _ | CONSO | ; | C596 | | 2 675114 | 0. | 25227 |
| COHS | + | Consun | | COHSU | T | CJE0 | | 2.0/5714 | | 70600 |
| _ | | C5H6 | = | CSH5 | + | <u>н</u> | | 8.135+24 | -2.981 | 70002. |
| C5H6 | + | 02 | - | C5H5O | + | ОН | | 1.UE+13 | υ. | 20/10. |
| C6H5OH | + | OH | = | C6H50 | + | H20 | | 3.0E+13 | 0. | 0. |
| C6H5OH | + | HO2 | = | C6H5O | ÷ | H2O2 | | 3.0E+13 | 0. | 1500. |
| | | C5H5O | = | C4H5 | + | со | | 3.0E+16 | 0. | 15000. |
| C5H5 | + | 0 | = | C5850 | | | | 1.0E+13 | Ο. | 0. |
| C585 | + | ОН. | = | C58408 | + | H | | 1.0E+13 | Ο. | 0. |
| 0040 | | C58408 | = | C4H4 | + | HCO | | 1.0E+15 | Ο. | 22000. |
| 0595 | Ŧ | 802 | ~ | C5850 | + | 08 | | 2 0E+13 | 0 | 0. |
| CJHJ OSRC | Ţ | 102 | _ | C5#50 | , 1 | E20 | | 5 05+13 | 0 | 0 |
| Cono | т <u>,</u> | 102 | _ | 012010 | т | 1120 | | 2 15+12 | 0. | 0 |
| | 2 | .00685 | = | CIZHIU | | 0000 | | 3.16712 | 0. | 22000 |
| | | C4H5 | * | C2H3 | + | CZHZ | | 1.4E+13 | 0. | 32900. |
| C4H2 | + | 0 | = | C2HO | + | C2H | | 1.0E+13 | Ο. | 0. |
| C4H2 | + | OH | - | HCO | + | C3H2 | | 3.0E+13 | 0. | 0. |
| C4H2 | + | 0 | F | co | + | C3H2 | | 1.2E+12 | 0. | 0. |
| м | + | C2H4 | - | C282 | + | 82 | | 9.33E+16 | 0. | 77200. |
| C2H4 | + | OH | - | C2E3 | + | H20 | | 4.786E+12 | 0. | 1230. |
| C284 | + | 0 | - | CH3 | + | HCO | | 3.311E+12 | 0. | 1130. |
| C2H4 | + | 0 | - | CH2O | + | CH2 | | 2.512E+13 | 0. | 5000. |
| C2H4 | | 0F | = | CH3 | + | CH2O | | 1.995E+12 | 0. | 960. |
| NF | | C2#3 | _ | C2H2 | | 9 | | 3 05+15 | 0 | 32000 |
| M | - T | 0203 | | 0202 | | <u>ч</u> со | | 3 00F+12 | <u>.</u> | -250 |
| C2H3 | + | 02 | - | CH20 | + ' | ncu no | | 5.905+12 | <u> </u> | 2.50. |
| C2H3 | + | H | * | CZHZ | + | <u><u>n</u>20</u> | | 0.0ET12 | v. | · · · |
| C2H3 | + | OH | = | C2H2 | + | H2O | | 5.012E+12 | 0. | v. |
| C2H3 | ÷ | CH2 | = | C2H2 | + | CH3 | | 3.020E+13 | 0. | 0. |
| C2B3 | + | C2H | =2.(| DC2H2 | | | | 3.020E+13 | 0. | 0. |
| C2H3 | + | 0 | * | C2H2O | ÷ | H | | 3.3E+13 | 0. | Ο. |
| CH2 | + | CH2 | # | C2H2 | + | H 2 | | 4.0E+13 | 0. | 0. |
| CH2 | + | CH2 | - | C2H3 | ÷ | H | | 5.012E+12 | 0. | Ο. |
| CH2 | + | OF | æ | CH | + | H2O | | 2.51E+11 | .67 | 25700. |
| CH2 | ÷ | õ | = | CH | ÷ | OH | | 2.0E+11 | 68 | 25000. |
| CH2 | | 02 | _ | CO2 | 12 0 | | | 1 59F+12 | 0 | 1000 |
| | Ť | 02 | - | 02 | 12.1 | - | | 4 1602416 | 0. | 107000 |
| M | + | | - | C28 | - - | а 7 | | 9.1095710 | 0. | 107000. |
| C2H2 | + | C2H2 | # | C4H3 | ÷ | н | | 2.0E+12 | 0. | 45900. |
| C2H2 | + | 0 | = | CH2 | + | co | | 1.6E+14 | 0.0 | 9890. |
| C2H2 | + | 0 | # | C280 | + | Ħ | | 4.0E+14 | 0.0 | 10660. |
| C2H2 | + | OH | = | C2H | + | H 2O | | 6.310E+12 | 0. | 7000. |
| C2H2 | + | OH | = | C2E2O | + | H | | 3.2E+11 | 0. | 200. |
| C2H2 | + | C2H | = | C4H2 | + | н | | 3.0E+13 | 0. | 0. |
| C2H2O | + | OF | - | CH20 | + | ECO | | 2.8E+13 | 0. | 0. |
| C2820 | + | OF | = | C2HO | + | H20 | | 7.5E+12 | 0_ | 3000 |
| C2820 | + | ч н | - | CH3 | + | 00 | | 1 13E+13 | 0. | 3428 |
| C2820 | т - | и и | - | C280 | ÷ | H2 | | 7 55+12 | 0 | 8000 |
| 02020 | + | n 0 | - | C200 | т 1 | 08 | | 1.JUTIJ | <u>,</u> | 9000. |
| C2H2O | + | 0 | - | CZHO | + | 00 | | 2.05+13 | <u>, .</u> | 0000. |
| C2H2O | + | 0 | = | CH2O | + | 00 | | 2.0E+13 | 0. | U. |
| M | + | C2H2O | = | CH2 | ÷ | co | | 2.0E+16 | υ. | 60000. |

| C2HC |) + | 02 | | =2. | 0CO | | + | OH | 1.46E+ | -12 | Ο. | 2500. |
|---|---|------------------------------------|-----|----------|-------------|----------|----------|---------------|------------------------|----------------|------------|--------------|
| C2H |) + | 0 | | =2. | 000 | | + | Ħ | 1.202E+ | -12 | 0. | 0. |
| C2H | ` | 0H | | =2 | 0400 | | | | 1 054 | .13 | <u>^``</u> | 0 |
| 0210 | · · | | | -2. | 0000 | | | ~~ | 1.05 | 1.5 | •: | 0. |
| C2H |) + | H | | - | CH2 | | + | CO | 5.0E4 | -13 | Ο. | σ. |
| C2HC |) + | CH2 | | = | C2H | 3 | + | co | 3.0E4 | -13 | Ο. | 0. |
| C2H(| + ר | CH2 | | - | CH2 | 0 | + | C2H | 1 054 | .13 | Ω | 2000 |
| ~~~~~ | · `. | 00000 | | | 000 | š | | ~~~~ | 1.05 | | <u> </u> | 2000. |
| | 2 | .0C2HO | | = | C2H | 2 | +2. | 000 | 1.0E4 | -13 | 0. | υ. |
| C2H | + | OH | | - | C2H | 0 | + | Ħ | 2.0E+ | -13 | 0. | 0. |
| C28 | + | 02 | | = | C2H | ò | + | 0 | 5 0054 | .13 | 0 | 1500 |
| C211 | т | 02 | | _ | | 0 | 1 | | 5.0024 | 1.5 | | 1500. |
| C2H | + | 0 | | = | CO | | + | СН | 5.012E+ | -13 | 0. | 0. |
| м | + | CH4 | | - | CH3 | | + | Ħ | 2.0E+ | -17 | 0. | 88000. |
| CRA | - | 02 | | - | 003 | | т. | PO2 | 7 94354 | 12 | ۰. ۱ | 56000 |
| 014 | т | 02 | | - | Chu | | T | 102 | 7.94367 | 13 | v . | 50000. |
| CH4 | + | Ξ | | * | CH3 | | + | 82 | 1.26E+ | -14 | Ο. | 11900. |
| OH | + | CH4 | | Ŧ | CH3 | | + | H20 | 2.5E+ | 13 | ٥. | 5010. |
| ~ | | 0124 | | _ | 022 | | · | 01 | 1 05 | 1 4 | ×. | 11720 |
| 0 | Ŧ | 024 | | - | Спо | | Ŧ | UH I | 1.551 | .т.а | υ. | 11/20. |
| CH3 | + | 02 | | - | CH3 | 0 | + | 0 | 4.786E+ | ·13 | 0. | 29000. |
| CH3 | + | OH | | = | CH3 | 0 | + | H | 6.3E+ | 12 | 0 | 0 |
| | | 000 | | | 000 | ž | | | 5.02 | 10 | ÷. | |
| M | + | CH30 | | # | CHZ | 0 | + | п | 5.UE+ | -13 | υ. | 21000. |
| CH3C |) + | 02 | | = | CH2 | 0 | + | HO2 | 1.0E+ | 12 | Ο. | 6000. |
| 0830 | · · | | | - | 002 | <u>^</u> | ÷ | #2 | 2 054 | 12 | ō. | 0 |
| | , , | n | | - | | | T | 112 | 2.064 | 15 | | . |
| CH3 | + | CH3 | | | C2H | 4 | + | HZ | 1.0E+ | 16 | 0. | 32000. |
| CH3 | + | 0 | | = | CH2 | 0 | + | H | 1.288E+ | 14 | 0 | 2000 |
| ~~~ | | ~~~~~ | | _ | ~~~ | - | | | | 10 | × - | |
| CH3 | + | CH20 | | = | CH4 | | + | HCO | 1.0E+ | τŬ | 0.5 | 6000. |
| CH3 | + | HCO | | = | CH4 | | + | co | 3.020E+ | 11 | . 5 | 0. |
| 0112 | | 200 | | | 0112 | ^ | | 04 | 2 005 | 12 | ~ | |
| CES | + | nO2 | | | Cno | 0 | Ŧ | Оn | 2.005+ | 13 | υ. | υ. |
| M | + | CH2O | | = | HCO | | + | H | 5.0E+ | 16 | 0. | 81000. |
| CH20 | ` | 0B | | = | 900 | | + | 820 | 3 05+ | 13 | Δ | 1200 |
| CHEC | | | | | 400 | | | | 5.01 | 10 | | 1200. |
| CH2C |) + | н | | = | HCO | | + | HZ | 2.5E+ | 13 | 0. | 3990. |
| CB20 |) + | 0 | | - | HCO | | + | OH | 3.5E+ | 13 | 0. | 3510. |
| 800 | | <u>-</u> <u>-</u> <u>-</u> | | _ | 000 | ^ | | 02 | 1 051 | 7.4 | ~ | 2000 |
| HCU | Ŧ | nųz | | 36 | CH2 | 0 | Ŧ | 02 | 1.05+ | 14 | υ. | 3000. |
| M | + | HCO | | * | Ħ | | + | co | 2.94E+ | 14 | 0. | 15569. |
| RCO | + | 02 | | = | co | | + | 802 | 3 311E+ | 12 | 0 | 7000 |
| | , | 00 | | _ | ~~ | | | | 0.0110 | ~~ | · · · | ,,,,,, |
| HCO | + | он | | = | CO | | + | H20 | 1.0E+ | 14 | υ. | 0. |
| HCO | + | B | | = | co | | + | 82 | 1.995E+ | 14 | 0. | 0. |
| 800 | + | 0 | | - | co. | | 1 | OF | 1 054 | 1.4 | 0 | 0 |
| ACO | т | | | | | | Ŧ | 04 | 1.02+ | 7.4 | v . | 0. |
| CH | + | 02 | | - | ECO | | + | 0 | 1.0E+ | 13 | Ο. | 0. |
| 0 | + | 0 | | * | CO2 | | + | м | 5 9E+ | 15 | n | 4100 |
| ~~~~ | , | š | | | 000 | | | ~ | 0.52 | | <u>.</u> . | 1100. |
| CO | + | 02 | | - | C02 | | + | 0 | 2.56+ | 12 | 0. | 4/690. |
| co | + | OH | | - | CO2 | | + | Ħ | 4.17E+ | 11 | 0. | 1000. |
| <u></u> | + | 802 | | - | CO2 | | + | OH | 5 7584 | 12 | 0 | 22930 |
| | 1 | 102 | | | 002 | | : | 011 | 5.7551 | 10 | · · · | 22330. |
| 0 | + | H2O | | = | OH | | + | OH | 6.8E+ | 13 | Ο. | 18365. |
| Ħ | + | 02 | | = | OH | | + | 0 | 1.89E+ | 14 | 0. | 16400. |
| ~ | | 80 | | _ | 07 | | | | 4 205+ | 1 / | 0 | 12750 |
| 0 | Ŧ | <u>n</u> 2 | | - | 0n | | Ŧ | n | 4.2057 | 14 | υ. | 13750. |
| H | + | HO2 | | 228 | Ħ2 | | + | 02 | 7.28E+ | 13 | 0. | 2126. |
| 0 | + | HO2 | | = | OH | | + | 02 | 5 02+ | 13 | 0 | 1000 |
| | | | | | | | | 00 | 5.02 | | ۷. | 1000. |
| HOZ | + | OH | | <u>ن</u> | <u>H</u> 20 | | + | 02 | 8.05+ | 12 | | Ο. |
| H | + | HO2 | | =2. | BOB | | | | 1.34E+ | 14 | 0. | 1070. |
| F 2 | _ | 802 | | - | 8203 | 2 | + | Ħ | 7 915- | 12 | 0 | 25000 |
| 112 | | 102 | | - | 4204 | - | | | 1.510 | | 0. | 25000. |
| OH | + | H202 | | - | m20 | | Ŧ | HU2 | 6.1E+ | 12 | υ. | 1430. |
| HO2 | + | HO2 | | = | H202 | 2 | + | 02 | 1.8E+ | 12 | 0. | 0. |
| 1 | ـ | 8202 | | - | OF | | + | 820 | 7 251 | 11 | 0 | n. |
| | T . | 1202 | | - | 01 | | | 120 | 1.051 | | | 0. |
| M | + | 8202 | | - | BO | | + | OH | 1.44E+ | 17 | 0. | 45510. |
| THIR | DBODY | | | | | | | | | | | |
| | | 20 | ~~ | | | 70 | | 820 | C O | | 00 | 6.6 |
| 04 | ۷. | 30 | 02 | | | . / 0 | | <u>п</u> 20 | 0.0 | n2 | .04 | 0.0 |
| END | | | | | | | | | | | | |
| 82 | + | 0H | | = | 820 | | + | H | 4 74E+ | 13 | 0 | 6098 |
| | | 00 | | | 200 | | | | | | ×. | |
| н | + | 02 | | = | HO2 | | Ŧ | M | 1.46E+ | 12 | U. | -1000. |
| THIR | DBODY | | | | | | | | | | | |
| ~~~~~ | | 20 | 000 | | | 7 0 | | #20 | 01 0 | U 2 | | 2 0 |
| 02 | ±. | .30 | UU2 | | | 1.0 | | n20 | 21.3 | <u>م</u> 2 | | 3.0 |
| C6H6 | 20 |).0 | CH4 | | | 5.0 | | END | | | | |
| м | + | 820 | | - | Ħ | | + | OH | 1 308+ | 15 | 0 | 105140 |
| L.T. | | 620 | | - | | | т | <u>UU</u> | T.JOET. | | ۷. | 100140. |
| | DBODY | | | | | | | | | | | |
| THIR | | | 02 | | | 1.5 | | H2 O | 20.0 | C6 | H6 | 20.0 |
| THIR H2 | 4 | .00 | | | | | | | 20.0 | 00 | | ~~.~ |
| THIR H2 | 4. | .00 | | | | | | | | | | |
| THIR E2 CO2 | 4. 4. | 00 | END | | | | | | | | | |
| THIR H2 CO2 H | 4. 4. + | .00 .00 .00 | END | Ŧ | OН | | + | м | 7.1E+: | 18 | -1. | 0. |
| THIR H2 CO2 H | 4. 4. + | 00 00 0 82 | END | - | OB H | | + + | M H | 7.1E+: 2 2F+: | 18 | -1. 0 | 0. |
| THIR H2 CO2 H M | 4. 4. + + | 00 00 0 H2 | END | - | OH H | | + + | M H | 7.1E+: 2.2E+: | 18 14 | -1. 0. | 0. 96000. |
| THIR H2 CO2 H M THIR | 4. 4. + DBODY | 00 00 0 H2 | END | - | OH H | | + + | M H | 7.1E+ 2.2E+ | 18 14 | -1. 0. | 0. 96000. |
| THIR H2 CO2 H M THIR H2 | 4. 4. + DBODY 4. | 00 00 0 H2 | END | 2 2 | OH H | 2.0 | + + | м н н20 | 7.1E+ 2.2E+ 15.0 | 18 14 EN | -1. 0. | 0. 96000. |
| THIR H2 CO2 H THIR H2 | 4. 4. * * * * * * * * * * * * * * * | 00 00 H2 10 | END | - | OH H | 2.0 | + + | м н н20 | 7.1E+ 2.2E+ 15.0 | 18 14 EN | -1. 0. | 0. 96000. |

TABLE 4.15.—Concluded.

DISTANCE AREA .11765 C6H6 .88235 02 END INIT TEMP END SENSVAR со C6H5OH C2H2 C6H6 C6H50 DЯ C685 H20 C585 TEMP END CH2O REAC sensaj=.true., order =.true., output =.false., allrxn=.true., &end FINIS

| | | | [Equivale | nce ratio q | 0 = 1.0; mass | flow rate m : | = 6000 g/s; tei | mperature $T = \frac{1}{2}$ | 3168.7 K.] | | | ŧ | |
|---|---------------------------------|-----------|----------------|---------------|-------------------------------|-----------------------|-----------------------|-----------------------------|--|-----------------------|-----------------------|------------------------|------------------------|
| Reaction | ථ - | <u>اب</u> | H ₆ | U I | ₆ H ₅ 0 | ບັ | 5H5 | C ₆ H | l ₅ OH | | 0 | Tempe | rature |
| CLSENS Bru | GLSENS Bru | Bru | te force | GLSENS | Brute force | GLSENS | Brute force | GLSENS | Brute force | GLSENS | Brute force | GLSENS | Brute force |
| | | | | | | Sensitivit | y coefficient (S | ()) with respect | to A _j , n _j , or E _j | | | | |
| $C_4H_2 + OH = HCO + C_3H_2$ 0.876 0. | 0.876 0. | 0 | 876 | 00.1 | 1.00 | 0.563 | 0.563 | 1.12 | 1.12 | -0.707 | -0.707 | -6.64×10 ⁻² | -6.64×10 ⁻² |
| C ₆ H ₆ = C ₆ H ₅ + H -0.843 -0.84 | -0.843 -0.84 | -0.8 | 6 | -0.790 | -0.790 | 4.60×10 ⁻² | 4.60×10 ² | -0.787 | -0.787 | 4.49×10 ⁻² | 4.50×10 ⁻² | 3.27×10 ⁻³ | 3,24×10 ⁻³ |
| C ₆ H ₅ O = C ₅ H ₅ + CO | | 1 | 1 | -0.996 | -0.996 | | | -0.923 | -0.924 | | | 1 | |
| $C_2H_2 + C_2H = C_4H_2 + H$ -0.570 -0.570 | -0.570 -0.570 | -0.570 | | -0.652 | -0.652 | -0.367 | -0.367 | -0.731 | -0.731 | 0.460 | 0.460 | 4.32×10 ⁻² | 4.32×10 ⁻² |
| $C_4H_2 + O = C_2HO + C_2H = -0.342 -0.342$ | -0.342 -0.342 | -0.342 | | -0.391 | -0.392 | -0.220 | -0.220 | -0.438 | -0.438 | 0.276 | 0.276 | 2.59×10 ⁻² | 2.59×10 ⁻² |
| $C_2H_2 + C_2H_2 = C_4H_3 + H$ -0.207 -0.207 | -0.207 -0.207 | -0.207 | | -0.238 | -0.238 | -0.133 | -0.133 | -0.269 | -0.269 | 0.165 | 0.165 | 1.57×10 ⁻² | 1.57×10 ⁻² |
| C ₅ H ₅ + OH = C ₅ H ₄ OH + H 0.116 0.116 | 0.116 0.116 | 0.116 | | 0.135 | 0.136 | 7.38×10 ⁻² | 7.41×10 ⁻² | 0.147 | 0.148 | 9.86×10 ⁻² | 9.89×10 ⁻² | -8.91×10 ⁻³ | -8.92×10 ⁻³ |
| $C_6H_5 = C_4H_3 + C_2H_2$ -3.39×10 ⁻² -3.38×10 | -3.39×10 ⁻² -3.38×10 | -3.38×10 | r-2 | -0.104 | -0.104 | -0.994 | -0.995 | -9.87×10 ⁻² | -9.87×10 ⁻² | 9.79×10 ⁻² | 9.82×10 ⁻² | 8.85×10 ⁻³ | 8.92×10 ⁻³ |

| (REACTION OF BENZENE AND OXYGEN) | |
|--|--|
| Y COEFFICIENTS FOR EXAMPLE PROBLEM 8 | |
| TABLE 4.16.—COMPARISON OF GLSENS AND BRUTE-FORCE SENSITIVITY | |

TABLE 4.17.—DATA FILE FOR EXAMPLE PROBLEM 9 (BENZENE-OXYGEN-NITROGEN-ARGON PSR)

TAPE C6H6-0

| 6H6-02-N2 | PLUS | ARGON | PSR | CASE | WITH | SENSITIVITY | MECHANISM | K-72 | |
|-----------|------|-------|-----|------|------|-------------|---------------|------|--|

| Ertype | | fend | | | | | | | |
|--------|--------|----------|-----|-------------|----------|------------|----------------------------|------------------|------------|
| Сене | + | 02 | - | C6850 | + | OH | 4.0E+13 | ٥. | 34000. |
| C686 | 1 | C645 | = | C12H10 | + | H | 4.0E+11 | 0 | 4000 |
| COLO | т | Cons | _ | CEUS | | 11 17 | 5 05+15 | 0. 0 | 108000 |
| o cric | | Cono | _ | COND | Ť | п по | 2 58414 | 0. | 16000 |
| COHO | + | н | æ | Cons | Ţ | <u>n</u> 2 | 2.36714 | v. | 10000. |
| C6H6 | + | o | | C6H50 | + | H | 2.783E+13 | 0. | 4910. |
| C6H6 | + | OH | | C6H5 | + | H20 | 2.132E+13 | 0. | 4580. |
| M | + | C4H3 | = | C4H2 | + | H | 1.0E+16 | 0.0 | 60000. |
| | | C6H50 | 72 | C5H5 | ŧ | CO | 2.51E+11 | Ο. | 43900. |
| C6H5 | + | 02 | = | C6H5O | + | 0 | 2.1E+12 | Ο. | 7470. |
| C685 | ÷ | 802 | | C6850 | + | ŎН. | 2.0E+13 | 0. | 1000. |
| 00110 | • | C695 | | C483 | | C2H2 | 4 50E+13 | 0 | 72530 |
| | | 060500 | _ | C4115 | • | 0 | 2 008+16 | 0 | 99000 |
| | | Conson | - | Consu | т , | л ОТ | 2.002+10 | 0. | 7010 |
| Сбн5он | + | H | = | CORD | + | OH | 2.202+13 | 0. | /910. |
| C6H5OH | + | H | | C6H50 | + | H2 | 1.15E+14 | 0. | 12400. |
| C5H5 | + | С6Н5ОН | = | C6H5O | + | C5H6 | 2.67 E+14 | 0. | 25227. |
| | | C5H6 | = | C5H5 | + | H | 8.13E+24 | -2.981 | 78682. |
| C5H6 | + | 02 | # | C5850 | + | OH | 1.0E+13 | 0. | 20716. |
| C6H5OH | + | OE | = | C6H5O | + | H20 | 3.0E+13 | 0. | 0. |
| C68508 | + | HO2 | = | C6850 | + | 8202 | 3.0E+13 | 0. | 1500. |
| conson | • | 05 WEA | _ | CAN5 | | 0 | 3 05+16 | 0 | 15000 |
| 0595 | | Compo | | | т | 0 | 3.0E+10 | <u>.</u> | 13000. |
| C5H5 | + | 0 | = | 05850 | | | 1.02+13 | 0. | 0 . |
| C5H5 | + | ОН | = | C5H4OH | + | Ħ | 1.0E+13 | 0. | U. |
| | | С5н4он | = | C4H4 | + | HCO | 1.0E+15 | 0. | 22000. |
| C585 | + | HO2 | # | C5850 | + | OH | 2.0E+13 | 0. | 0. |
| C5H6 | + | HO2 | - | C5850 | + | H20 | 5.0E+13 | 0. | 0. |
| | 2. | OC685 | = | C12H10 | | | 3.1E+12 | Ο. | 0. |
| | | C485 | | C283 | + | C282 | 1.4E+13 | 0. | 32900. |
| C492 | + | 0 | | C2HO | + | C2H | 1 0E+13 | 0 | 0 |
| 0402 | | 0" | _ | 800 | | C282 | 2 05+13 | 0 | ۰°. |
| C4n2 | + | 0H | - | HCU RC | Ţ | 0382 | 3.02+13 | 0. | 0. |
| C482 | + | 0 | = | 0 | + | C382 | 1.26+12 | 0. | 0. |
| M | + | C2H4 | = | C282 | + | 82 | 9.33E+16 | 0. | 77200. |
| C2H4 | + | OH | - | C2H3 | + | H20 | 4.786E+12 | 0. | 1230. |
| C2H4 | + | 0 | - | CH3 | + | HCO | 3.311E+12 | 0. | 1130. |
| C284 | + | 0 | | CH2O | + | CH2 | 2.512E+13 | Ο. | 5000. |
| C2H4 | + | OH | 30 | CH3 | + | CH2O | 1.995E+12 | 0. | 960. |
| м | + | C2H3 | - | C2H2 | + | H | 3.0E+15 | ο. | 32000. |
| C283 | + | 02 | - | CH20 | + | HCO | 3.98E+12 | 0. | -250 |
| C283 | , , | 52 | | C2#2 | | #2 | 5 0F+12 | n [°] . | |
| C2H3 | - - | <u>п</u> | - | C2H2 | - | 112 | E 0102:12 | <u>.</u> | ~ · · |
| CZH3 | + | OH | × | C282 | Ŧ | H20 | 5.012E+12 | U . | 0. |
| C2H3 | + | CH2 | - | C2H2 | + | CH3 | 3.020E+13 | 0. | υ. |
| C2H3 | + | C2H | =2. | 0C2H2 | | | 3.020E+13 | 0. | 0. |
| C2H3 | + | 0 | - | C2820 | + | H | 3.3E+13 | 0. | 0. |
| CH2 | + | CB2 | * | C2H2 | + | 82 | 4.0E+13 | Ο. | 0. |
| CH2 | + | CH2 | - | C2H3 | + | H | 5.012E+12 | 0. | 0. |
| CH2 | + | OH | | CH | + | H2O | 2.51E+11 | . 67 | 25700 |
| CH2 | ÷. | 0 | - | CH | + | OH | 2 0E+11 | 68 | 25000 |
| CH2 | ÷ | 02 | - | <u>co</u> 2 | 12 | 04 | 1 59F±12 | 0 | 1000 |
| | - - | 02 | - | 002 | · · · | | 4 1602:16 | <u>.</u> | 107000 |
| M | + | | = | C2H | Ŧ | | 4.1096+10 | 0. | 107000. |
| C2H2 | + | C2H2 | * | C4H3 | + | н | 2.0E+12 | 0. | 45900. |
| C2H2 | + | 0 | # | CH2 | + | co | 1.6E+14 | 0.0 | 9890. |
| C2H2 | + | 0 | = | C2HO | + | Ħ | 4.0E+14 | 0.0 | 10660. |
| C2H2 | + | OH | = | C2H | + | H20 | 6.310E+12 | 0. | 7000. |
| C2H2 | + | OH | - | C2H2O | + | Ħ | 3.2E+11 | 0. | 200. |
| C2H2 | + | C28 | - | C482 | + | Ħ | 3.0E+13 | 0. | 0. |
| C2820 | | 08 | - | 0300 | ÷ | HCO | 2 0 0 1 1 2 2 0 0 1 1 2 | n | 0 |
| C2#20 | | 01 | - | C120 | T T | 820 | 4.00TLJ 7 50119 | 0. | 3000 |
| 02820 | 7 | | - | | T | 00 | 1.35712 | <u>,</u> . | 2400. |
| C2H2O | + | <u>п</u> | = | CHJ | + | | 1.135+13 | U. | 3428. |
| C2H2O | + | H | = | CZHO | + | HZ | 7.5E+13 | υ. | 8000. |
| C2H2O | + | 0 | = | C2HO | + | OH | 5.0E+13 | 0. | 8000. |
| C282O | + | 0 | * | CH2O | + | co | 2.0E+13 | 0. | Ο. |
| м | + | C2H2O | = | CH2 | + | co | 2.0E+16 | 0. | 60000. |

| 6380 | | ~ ~ | | 2 000 | | 011 | 1 465+13 0 | 2500 |
|------------|--------|-------------|------|------------|-------------|---|--------------|---------|
| CZHO | + | 02 | Ŧ | 2.000 | + | OH | 1.40E+12 U. | 2500. |
| C2HO | + | 0 | = | 2.000 | + | Е | 1.202E+12 0. | 0. |
| C2HO | + | ОН | = | 2.0HCO | | | 1.0E+13 0. | 0. |
| C2HO | + | H | = | CH2 | + | co | 5.0E+13 0. | 0. |
| C2HO | + | CH2 | = | C2H3 | 3 + | со | 3.0E+13 0. | 0. |
| C2H0 | + | CH2 | - | CH2C |) + | C2H | 1.0E+13 0 | 2000 |
| 02110 | ່າ | 00200 | _ | C282 | , . , _, | 2 000 | 1 05+13 0 | 2000. |
| | . 2 | . 00200 | - | C2112 | . т. | 2.000 | 1.0E+13 0. | 0. |
| Ç2H | + | OH | = | C2HC |) + | Ħ | 2.0E+13 U. | υ. |
| C2H | + | 02 | = | C2HC | > + | 0 | 5.00E+13 0. | 1500. |
| C2H | + | 0 | | со | + | CH | 5.012E+13 0. | Ο. |
| м | + | CH4 | = | CH3 | + | H | 2.0E+17 0. | 88000. |
| CH4 | + | 02 | = | CH3 | + | HO2 | 7.943E+13 0. | 56000. |
| CH4 | + | н Н | Ŧ | CH3 | + | 82 | 1.26E+14 0 | 11900 |
| | | CUA | _ | CH3 | | 820 | 2 58413 0 | 5010 |
| | т | | _ | | - T | 120 | 1 00+14 0 | 11720 |
| 0 | - | CH4 | = | CH3 | . T | Un | | 11/20. |
| СНЗ | + | 02 | = | CH3C |) + | 0 | 4./86E+13 U. | 29000. |
| CH3 | + | OH | = | CH3C |) + | н | 6.3E+12 0. | 0. |
| м | + | CH30 | = | CH2C |) + | H | 5.0E+13 0. | 21000. |
| CH3O | + | 02 | * | CH2C |) + | HO2 | 1.0E+12 0. | 6000. |
| CH30 | + | 8 | - | CH2C |) + | H2 | 2.0E+13 0 | 0 |
| CES | | <u></u> | - | C2H4 | | 82 | 1 05+16 0 | 32000 |
| | Ť | | | 02114 | : T | 12 | 1 2805-14 0 | 32000. |
| CH3 | + | 0 | Ŧ | CH20 | , + | H | 1.2882+14 0. | 2000. |
| CH3 | + | CH20 | - | CH4 | + | HCO | 1.0E+10 0.5 | 6000. |
| CH3 | + | HCO | = | CE4 | + | co | 3.020E+11 .5 | Ο. |
| CH3 | + | HO2 | = | CH3O |) + | OH | 2.00E+13 0. | 0. |
| M | + | CH20 | | HCO | + | н | 5.0E+16 0. | 81000 |
| CH20 | ÷ | 01120 | # | RCO | + | H20 | 3 0E+13 0 | 1200 |
| 0120 | | | _ | n00 | | 120 | 2 55+12 0 | 2000 |
| CH20 | Ť | n | ж. | nco | | п <u>г</u> | 2.56+13 0. | 3990. |
| CH2O | + | 0 | = | HCO | + | OH | 3.5E+13 0. | 3510. |
| HCO | + | HO2 | = | CH2O |) + | 02 | 1.0E+14 0. | 3000. |
| M | + | HCO | * | H | + | co | 2.94E+14 0. | 15569. |
| BCO | + | 02 | # | co | + | HO2 | 3.311E+12 0. | 7000. |
| HCO | + | OH | = | со | + | H2O | 1.0E+14 0. | 0. |
| HCO | + | Ħ | = | co | + | H 2 | 1.995E+14 0. | 0 |
| 800 | | ā | = | cõ | | 08 | 1 0F+14 0 | 0 |
| | Ŧ. | ~~~ | _ | | - T | 01 | 1.05+14 0. | 0. |
| CH | + | 02 | | HCO | + | 0 | 1.0E+13 U. | 0. |
| CO | + | 0 | = | CO2 | + | м | 5.9E+15 0. | 4100. |
| CO | + | 02 | = | CO2 | + | 0 | 2.5E+12 0. | 47690. |
| CO | + | OE | = | CO2 | + | H | 4.17E+11 0. | 1000. |
| co | + | HO2 | = | CO2 | + | OH | 5.75E+13 0. | 22930. |
| 0 | ÷ | H20 | = | OH | + | OH | 6.8E+13 0. | 18365. |
| - - | ÷ | 02 | - | 0E | + | 0 | 1 89E+14 0 | 16400 |
| | | 22 | - | 08 | | ц ц | 4 205+14 0 | 12750 |
| 0 | | 82 | _ | UH TO | | л 02 | 4.20D+12 0. | 13750. |
| н | + | HOZ | | HZ | + | 02 | 7.286+13 0. | 2120. |
| 0 | + | 802 | = | OH | + | 02 | 5.0E+13 0. | 1000. |
| HO2 | + | OH | ** | H2O | + | 02 | 8.0E+12 0. | 0. |
| B | + | HO2 | =; | 2.00H | | | 1.34E+14 0. | 1070. |
| H2 | + | HO2 | = | H2O2 | + | B | 7.91E+13 0. | 25000. |
| OH | + | H2O2 | - | H2O | + | EO2 | 6.1E+12 0. | 1430. |
| 802 | + | HO2 | = | 8202 | + | 02 | 1.8E+12 0. | 0. |
| 102 | , T | 8202 | _ | 02 | | #20 | 7 95+11 0 | 0. |
| <u>н</u> | | 8202 | _ | | | 08 | 1 AAE+17 0 | 45510 |
| M | + | H202 | - | OH | Ŧ | 0H | 1.44671/ 0. | 43510. |
| THIRDBO | DY | | | | | | | |
| H 2 | 2. | .30 | 02 | | .78 | H 2O | 6.0 H2O2 | 6.6 |
| END | | | | | | | | |
| H2 | + | OH | | H2O | + | H | 4.74E+13 0. | 6098. |
| Ħ | + | 02 | = | HO2 | + | M | 1.46E+15 0. | -1000. |
| THIRDBO | DY | | | | | | | |
| ^2 | 1 | 30 | N2 | | 1 3 | 820 | 21 3 CO2 | 7 0 |
| 02 | | | 004 | | <u> </u> | = | | / |
| 000 | 24 | | CH4 | | 5.0 | 82 | 3.0 END | 105140 |
| M | + | HZQ | = | н | + | OH | 1.30E+15 U. | 105140. |
| THIRDBO | DY | | | | | | | |
| H2 | 4. | .00 | 02 | | 1.5 | H2O | 20.0 N2 | 1.5 |
| CO2 | 4. | .00 | C686 | 2 | 0.0 | END | | |
| H | + | 0 | * | OH | + | M | 7.1E+18 -1. | ٥. |
| м | + | H2 | - | Ħ | + | Ħ | 2.2E+14 0. | 96000. |
| TUTODO. | 0 P V | | | | | | | |
| TELKDB | UUI . | 1 10 | ~~ | | ~ ^ | 220 | 15.0 15.0 | 2 0 |
| HZ | 4 | 1.10 | 02 | | 2.0 | n20 | 13.0 NZ | 2.0 |
| END | | | | | | | | |

TABLE 4.17.—Continued.

TABLE 4.17.—Concluded.

| | м | + | 02 | | = | 0 | + | 0 | 1.80E+18 | -1. | 118020. |
|----|----------|-----|-----|----|--------------|------|----|-----|----------|------|---------|
| | 802 | + | NO | | = | NO2 | + | OH | 2.09E+12 | 0. | -477. |
| | 0 | + | NO2 | | = | NO | + | 02 | 1.0E+13 | Ο. | 596. |
| | NO | + | 0 | | Ŧ | NO2 | + | м | 5.62E+15 | Ο. | -1160. |
| | NO2 | + | Ĥ | | = | NO | + | OH | 3.47E+14 | 0. | 1470. |
| | NO | + | 0 | | = | N | + | 02 | 3.8E+9 | 1. | 41370. |
| | 0 | + | N2 | | = | NO | + | N | 1.8E+14 | 0. | 76250. |
| | NO | + | Ħ | | - | N | + | OH | 2.63E+14 | 0. | 50410. |
| | M | + | N20 | | = | N2 | + | 0 | 6.92E+23 | -2.5 | 65000. |
| | 0 | + | N20 | | - | N2 | + | 02 | 1.0E+14 | 0. | 28020. |
| | õ | + | N20 | | ≠2 .0 | ONO | | | 6.92E+13 | 0. | 26630. |
| | N | + | NO2 | | =2.0 | ONO | | | 4.0E+12 | 0. | 0. |
| | N20 | + | Ħ | | = | N2 | + | OH | 7.59E+13 | 0. | 15100. |
| | NO2 | + | H2 | | = | HNO2 | + | H | 2.4E+13 | 0. | 29000. |
| | OH | + | NO2 | | = | HNO3 | + | м | 3.0E+15 | 0. | -3800. |
| | THIRDBOD | Ŷ | | | | | | | | | |
| 02 | | 0.1 | 70 | H2 | | 1 | .4 | END | | | |
| | OH | + | NO | | æ | HNO2 | + | м | 5.6E+15 | 0. | -1700. |
| | HNO | + | H | | = | H2 | + | NO | 5.0E+12 | 0. | 0. |
| | H | | NO | | = | HNO | + | М | 5.4E+15 | Ο. | -600. |
| | HNO | + | OH | | = | H20 | + | NO | 3.6E+13 | Ο. | 0. |

AR

| DISTANCE | AREA | | | | | | |
|----------|------------|---------------|------------|---------------|------------|-------------|-----------|
| &prob w | elstr=.tru | e., send | al = .true | ., tiny = 1 | e-3, & | end | |
| &wsprob | dotmax= 6 | 000., del | md= 1000., | mpr= 1, v | rolume = 3 | 200., | |
| - | wsrhtr =.t | rue., wsr | ht1= .05, | wsrht0 = -4 | 2.88, | ≨end | |
| €start | t= 614., p | <i>≈</i> 5.0, | mdot= 150 | 0., | &end | | |
| C686 | .058825 | | | | | | |
| 02 | .441175 | | | | | | |
| N2 | .2500 | | | | | | |
| AR | .2500 | | | | | | |
| END | | | | | | | |
| SENSVAR | | | | | | | |
| C6E6 | C6H5O | C6H5 | H20 | С6Н5ОН | C2H2 | C5H6 | CH2O |
| OH | CO | NO | TEMP | END | | | |
| INIT | | | | | | | |
| TEMP | END | | | | | | |
| REAC | | | | | | | |
| &senrxn | sensaj=. | true., or | der =.true | ., output = | false., | allrxn =.t: | rue.,&end |
| FINIS | | | | | | | |
| | | | | | | | |

| | | | [Equival | ence ratio | φ = 1.0; mass | : flow rate m๋ | = 6000 g/s; tei | mperature T : | = 2586.1 K.] | | | | |
|----------|--|------------------------|------------------------|---------------|---------------|------------------------|------------------------------|------------------|--|------------------------|------------------------|------------------------|------------------------|
| Reaction | Reaction | 0 | 6H6 | U | 6H5O | ບ້ | 5H5 | C ₆ I | H ₅ OH | 0 | 0 | Tempe | rature |
| number | | GLSENS | Brute force | CLSENS | Brute force | GLSENS | Brute force | GLSENS | Brute force | CLSENS | Brute force | GLSENS | Brute force |
| | | | | | | Sensitivit | ty coefficient $\langle S_i$ | y) with respect | to A _j , n _j , or E _j | | | | |
| 22 | C ₅ H ₅ + OH <i>±</i> C ₅ H ₄ OH + H | 0.418 | 0.418 | 0.760 | 0.760 | 0.513 | 0.513 | 1.38 | 1.38 | -0.298 | -0.298 | -5.99×10 ⁻² | -5.99×10 ⁻² |
| 21 | $C_5H_5 + O = C_5H_5O$ | -0.417 | -0.417 | -0.759 | -0.759 | -0.512 | -0.512 | -1.38 | -1.38 | 0.298 | 0.298 | 5.97×10 ⁻² | 5.97×10 ⁻² |
| 9 | $C_6H_6 + OH = C_6H_5 + H_2O$ | -0.351 | -0.351 | -0.400 | -0.400 | 0.119 | 0.119 | -0.535 | -0.535 | 4.20×10 ⁻² | 4.20×10 ⁻² | 1.04×10 ⁻² | 1.04×10 ⁻² |
| × | C ₆ H ₅ O = C ₅ H ₅ + CO | -9.22×10 ⁻³ | -9.13×10 ⁻³ | -0.986 | -0.986 | -8.71×10 ⁻³ | -8.68×10 ⁻³ | -0.937 | -0.937 | 7.94×10 ⁻³ | 7.92×10 ⁻³ | 1 1 1 1 | |
| 29 | $C_4H_2 + OH = HCO + C_3H_2$ | 0.293 | 0.292 | 0.514 | 0.514 | 0.360 | 0.360 | 0.944 | 0.944 | -0.197 | -0.198 | -4.10×10 ⁻² | -4,10×10 ⁻² |
| 49 | $C_2H_2 + C_2H_2 = C_4H_3 + H$ | -0.240 | -0.240 | -0.442 | -0.442 | -0.301 | -0.301 | -0.836 | -0.836 | 0.155 | 0.155 | 3.47×10 ⁻² | 3.47×10 ⁻² |
| ŝ | $C_6H_6 + O = C_6H_5O + H$ | -0.200 | -0.200 | 0.601 | 0.602 | -0.179 | -0.179 | 0.713 | 0.714 | -8.72×10 ⁻² | -8.72×10 ⁻² | -1.56×10 ⁻² | -1.56×10 ⁻² |
| 28 | $C_4H_2 + 0 = C_2H0 + C_2H$ | -0.152 | -0.152 | -0.267 | -0.267 | -0.187 | -0.187 | -0.489 | -0.489 | 0.104 | 0.103 | 2.13×10 ⁻² | 2.13×10 ⁻² |
| = | $C_6H_5 = C_4H_3 + C_2H_2$ | -0.141 | -0.141 | -0.224 | -0.224 | -0.940 | -0.940 | -0.264 | -0.264 | 3.97×10 ⁻² | 3.97×10 ⁻² | 6.31×10 ⁻³ | 6.28×10 ⁻³ |

| Variable | Example | e problem 8 ^a | Exampl | e problem 9 ^b |
|----------------------------------|-----------------------|--|-------------------------|--------------------------|
| | GLSENS | Brute force | GLSENS | Brute force |
| | Sensitivity c | oefficients (S _{i,} temper | $_{T_0}$ with restature | spect to initial |
| C ₆ H ₆ | -0.775 | -0.776 | -0.876 | -0.876 |
| C ₆ H ₅ O | -0.812 | -0.812 | -1.42 | -1.42 |
| C_6H_5 | -0.503 | -0.503 | -1.08 | -1.08 |
| C ₆ H ₅ OH | -1.00 | -1.00 | -2.84 | -2.84 |
| СО | 0.438 | 0.438 | 0.297 | 0.297 |
| Temperature | 5.79×10^{-2} | 5.81×10 ⁻² | 0.118 | 0.118 |

TABLE 4.19.—COMPARISON OF BRUTE-FORCE AND GLSENS SENSITIVITY COEFFICIENTS WITH RESPECT TO INITIAL TEMPERATURE FOR EXAMPLE PROBLEMS 8 AND 9

^aC₆H₆-O₂; initial temperature $T_0 = 614$ K; mass flow rate $\dot{m} = 6000$ g/s; temperature T = 3168.7 K. ^bC₆H₆-O₂-N₂-Ar; initial temperature $T_0 = 614$ K; mass flow rate $\dot{m} = 6000$ g/s; temperature T = 2586.1 K.

Chapter 5 Concluding Remarks

This reference publication describes a generalized version of the Lewis chemical kinetics and sensitivity analysis code, LSENS. The new code, GLSENS, allows the user to put global reactions into a chemical mechanism along with molecular steps. The rate expression for a global process does not obey the law of mass action. It is determined empirically by leastsquares fitting of actual measurements of temperature and composition over a range of experimental conditions. Any combination of molecular and global steps can be used for all the chemical models and in the sensitivity coefficient computations for a static chemical reaction. The new code also incorporates the ability to perform sensitivity analysis calculations for a perfectly stirred reactor modeling computation. The sensitivity calculations are performed rapidly and conveniently at the same time that the main kinetics calculations are being done.

The GLSENS code has been extensively tested and found to be accurate and efficient. All computed sensitivity coefficients were compared with values obtained by the direct-variation, or brute force, technique. Results of the two methods agreed well in all comparisons.

Nine example problems are described in detail to illustrate the abilities of the new generalized code. Several of the cases show computation of PSR sensitivity coefficients and excellent agreement with brute-force-computed coefficients.

This report is to be used in conjunction with the threevolume documentation of the LSENS code (refs. 1 to 3) as the complete documentation of the new GLSENS code.

Lewis Research Center National Aeronautics and Space Administration April 5, 1995

Appendix—Multiple-Case File Setup Showing Changing and Adding of Global and Molecular Reactions

To illustrate the setup of multiple-case files using molecular and global reactions, a problem data file of seven cases has been prepared. It is presented in table A.1 and shows several examples of setting all the logical variables in namelist RTYPE. Each case is discussed here, and partial results from the execution of each case are presented. The computational results give the user insight into performing PSR problems with GLSENS and also explain some of the messages printed by the code when the computations run into certain problem situations.

Case 1

The first case is a perfectly stirred reactor combustion of hydrogen and oxygen using a partial molecular reaction mechanism that contains no third-body steps; it is being used for illustrative purposes only. There are no nonreacting (inert) species in the mixture. There are no global reactions, so no variables have to be set in namelist RTYPE because the default values of the variables GLOBAL and GRONLY are FALSE. Therefore, only a dummy line is needed. Because there is no integration or assigned variable for a PSR problem, the word TIME is written on the integration and assigned variable, units, and fuel name line, just to identify it. In namelist WSPROB mass flow rate is assigned with a desired final value (DOTMAX) of 1000 g/s to be reached by increments of 100 g/s (DELMD).

Computed results are shown in table A.2. The initial conditions for a successful first convergence are usually obtained by varying the initial mass flow rate for an assigned-mass-flowrate problem. Typical initial values range from 10 to 200 g/s, but for this case MDOT had to be lowered to 0.1 g/s in namelist START because an incomplete mechanism is being used for demonstration purposes. The first successful convergence was easily accomplished (in 10 iterations) to a reaction temperature of 1102 K, which is considerably lower than the equilibrium temperature of 3104 K. This is not a typical situation and was caused, in part, by the use of an unrealistic chemical mechanism. As shown in the other test cases, the first converged temperature is usually within a few hundred degrees of the equilibrium value used as the first estimate. The PSR calculation subroutine is programmed to test for the occurrence of false solutions to the set of nonlinear algebraic equations. One common example is convergence to a temperature higher than the previous converged temperature (or the equilibrium temperature on the first convergence). The calculation will be aborted or restarted with a higher mass flow rate if the first convergence and the first two increments of mass flow rate do not give monotonically decreasing temperatures that are all lower than the equilibrium temperature. In the present case the temperature decrements are very small as the mass flow rate is incremented to its final value of 1000 g/s and a final reactor temperature of just under 1098 K.

Case 2

Case 2 is a propane-air PSR combustion problem and the mechanism is constructed by, first, changing the rate coefficient of the last reaction in case 1 and then adding the molecular third-body reactions of the hydrogen-oxygen mechanism, including many third-body ratios different from 1. A global propane oxidation mechanism, similar to the one used in the example problems of chapter 4 is then added. In namelist RTYPE the variable GLOBAL now is set equal to TRUE; and GRONLY, to FALSE. In addition the variables MRCHNG, MRADD, and GLADD are set equal to TRUE to tell GLSENS that a rate coefficient change is being made and both types of reaction are being added. Note that this namelist is preceded by the CHANGE action line and followed by the reaction line with its changed rate coefficient. The list is ended by a blank line, which is followed by an ADD action line. The new molecular reactions (and any third-body efficiencies different from 1) are then given. This list is ended by the word END written in the first reactant field after the last reaction. The new global reactions follow, two lines per reaction, using the formats given in table 3.3. This list terminates with the word END written in the first species field after the last global reaction. The next line of the file contains the name AR in the first two columns and introduces the inert gas argon as part of the reacting mixture of this case. It is followed by the integration and assigned variable, units, and fuel name line, which contains the program name C3H8 for the fuel propane starting in column 41. This name is needed because the simplified equivalence ratio method is used in namelist START below to specify the initial mixture mole fractions. As in case 1 the namelist WSPROB sets all the variables for the assigned-mass-flow-rate PSR problem. Note that the namelist PROB contains no variables because all settings from case 1 are saved and no new variables are set. The same PROB may be used for any case using the CHANGE, ADD, or REPEAT options when the previous variables do not have to be changed and no new ones are needed.

Table A.3 shows some of the computed results. The initial mass flow rate was set at 140 g/s. However, the messages printed after the initial estimates show that the code had to increase this value to 560 g/s in order to achieve a converged temperature lower than the equilibrium temperature. The first converged temperature was about 28 K lower than the equilibrium value and the calculation then proceeded smoothly. However, the desired final mass flow rate of 4000 g/s was not reached. The messages printed after the last convergence at a flow rate of 1610 g/s indicated a blowout condition in the reactor. First, the iteration procedure had a problem at the next attempted convergence. The code then restarted the iteration after doubling the last converged flow rate. Convergence was easily obtained in 13 iterations, but the temperature was the same as the inlet temperature, indicating that blowout had occurred.

Case 3

Case 3 is essentially the same as case 2. The only change, other than initial conditions, is the addition of two more molecular reactions to the mechanism of case 2. The action variable ADD, therefore, follows the title line. In namelist RTYPE all seven variables are set for illustrative purposes, even though some have their default values. GLOBAL and GRONLY are set to the same values they had in case 2. The variables GLADD, GLCHNG, and MRCHNG must now have the (default) value FALSE, and MRPREV must also be set to FALSE because the previous case used both molecular and global reactions. Finally, MRADD must be set to TRUE again because it is initialized to FALSE. Note that, after the list of two added reactions, there is a blank line ending the list and a second one which indicates that no new inert species are being added to the mixture.

As shown in table A.4, the initial mass flow rate was set at 450 g/s but the converged temperature was about 2 K higher than the equilibrium temperature. The code then doubled the

initial mass flow rate, and convergence was obtained at a temperature about 130 K below the equilibrium temperature. Computed results were very close to those for case 2, including the reaching of a blowout condition at a mass flow rate greater than 1600 g/s.

Case 4

Case 4 is a propane-air, constant-volume combustion reaction with the same mechanism used in case 3. The ACTION line, therefore, contains the word REPEAT. The following namelist RTYPE has only to reset the variables GLOBAL and MRPREV to their nondefault values of TRUE and FALSE, respectively. The next line is the integration and assigned variable, units, and fuel name line, which contains the word TIME starting in column 1 (indicating time integration) and the fuel name C3H8 starting in column 41. Namelist PROB, which follows, sets the logical variable RHOCON equal to TRUE and lists the reaction times at which output is to be printed in the array PRINT. It is important to notice that PROB must also reset the variable WELSTR to the value FALSE because an integration problem is being solved. The remainder of the data for this case consists of namelist START followed by the initial mole fractions and namelist SOLVER, which is now added to set the integration accuracy-control parameters.

The computed results for this problem are shown in table A.5. The rapid reaction consumed the hydrogen much faster than the propane, and the results show a negative concentration at the final print station time of 5 μ s. Carbon monoxide (CO) was formed at first but then was rapidly destroyed, so that its concentration also went negative. These negative concentrations indicate an incomplete mechanism. Note that GLSENS prints any negative concentrations in an integration problem and prints a message indicating which species concentrations have become negative.

Case 5

Case 5 is a propane-air PSR combustion reaction, but a new all-global reaction mechanism is used so that this problem has the action option NEW and all variables are reset to their default values. In namelist RTYPE both the variables GLOBAL and GRONLY are set equal to TRUE. No other variables have to be set. The remaining data for this assigned-mass-flow-rate problem are given as in the previous cases, except the initial-mixture composition, which is listed as individual species mole fractions after namelist START.

Table A.6 shows that the iteration procedure converged smoothly for the initial mass flow rate of 100 g/s to a temperature about 140 K below the equilibrium temperature. The calculation did not reach the desired final flow rate of 1600 g/s. Convergence problems were experienced at a flow rate above 140 g/s, and restarting at higher flow rates did not help the situation. The reactor was probably approaching

blowout condition, even though the calculation did not show a convergence temperature the same as the initial-mixture temperature, as happened in cases 2 and 3.

Case 6

Case 6 is similar to case 5 but changes one reaction rate coefficient and adds one new global reaction. The CHANGE option is written on the action line, and namelist RTYPE sets the variables GLCHNG and GLADD as well as GLOBAL and GRONLY equal to TRUE. The variable MRPREV must be set to FALSE as in the previous case. The changed and added global reactions follow namelist RTYPE as in the previous cases.

Computed results for this case are shown in table A.7. This PSR case is similar to case 5 and uses an all-global mechanism modified from that case. The initial flow rate of 100 g/s had to be increased by GLSENS to 800 g/s in order to get proper convergence to a temperature about 100 K less than the equilibrium temperature. The calculation then proceeded smoothly to the required final mass flow rate of 1500 g/s.

Case 7

The last case is a different propane-air PSR problem using a mechanism that adds several molecular reactions to the allglobal mechanism of the previous case. Namelist RTYPE sets the variables GLOBAL and MRADD equal to TRUE and the variables GRONLY and MRPREV equal to FALSE. The other three variables are reset by the code to their default values of FALSE. The list of added molecular reactions follows this namelist and is in turn followed by a blank line (indicating the absence of any new inert species) and the remainder of the case data.

The results shown in table A.8 indicate that the initial mass flow rate of 140 g/s had to be increased to 560 g/s to get a successful convergence to a temperature only 7 K less than the equilibrium temperature. The calculation ended normally at the required final flow rate of 1160 g/s.

This set of cases illustrates many of the typical situations that would be encountered in the task of developing a combined molecular and global reaction mechanism. See table 3.2 for a summary of the required values of the variables in namelist RTYPE for these problems and several other possible mechanism change situations.

| TAPE | | | | | | | | | | | |
|--------------------------|-------|------------------------------------|----------------|---------------------|------------------------|-------------|-----------|-----------|------------|----------|------------|
| GLOBAL | CODE | TEST CASE | : MOI | LECULAR | REAC | TIONS | ONLY | AND NO | INERT | S CAS | 5E 1 |
| &rtype | | &en | d | | | | | | | | |
| 0 | + | H20 | - | OH | + | OB | | 6.8 | E+13 | 0. | 1836 |
| Ħ | + | 02 | × | OH | + | 0 | | 1.89 | E+14 | Ο. | 1640 |
| 0 | + | H2 | | OH . | + | R | | 4.20 | E+14 | 0. | 1379 |
| ů. | | 802 | - | u2 | | 02 | | 7 28 | 5-13 | 0 | 2124 |
| п О | | 102 | - | 82 07 | Ţ | 02 | | 7.20 | E-13 | 0. | 2120 |
| 0 | + | HO2 | | OH | + | 02 | | 5.0 | E+13 | 0. | 1000 |
| HO2 | + | OH | - | H2O | + | 02 | | 8.0 | E+12 | 0. | 0. |
| H | + | HO2 | =2. | . 00H | | | | 1.34 | E+14 | ο. | 1070 |
| 82 | + | HO2 | = | H2O2 | + | н | | 7.91 | E+13 | 0. | 2500 |
| OH | + | H2O2 | = | H2O | + | H02 | | 6.1 | E+12 | 0. | 1430 |
| HO2 | + | HO2 | = | H2O2 | + | 02 | | 1.8 | E+12 | 0. | 0. |
| R | + | H202 | - | OH | + | H20 | | 5.0 | E+11 | 0. | 0. |
| - | | | | | | - | | | | | |
| TIME &prob &wsprob | wels | tr=.true., delmd= 00 .p=5 5. | 100. | , dotm | &end ax= 1(&end | 000., | mpi | r=2, volu | ume= : | 2000., 5 | end |
| 02 | | 193301 | | | | | | | | | |
| W2 | • | 193301 | | | | | | | | | |
| 82 | • | 806699 | | | | | | | | | |
| END | | | | | | | | | | | |
| FINIS | | | | | | | | | | | |
| GLOBAL | TEST | CASE: CHA | NGE A | AND ADD | GLOBA | L ANI | MOLI | ECULAR RI | EACTI | ONS CAS | E 2 |
| CHANGE | | | | | | | | | | | |
| &rtype | glob | al=.true., | gronl | ly≃.fal: | se., | | | | | | |
| mrch | ing=. | true., mr | add = | .true | ., gla | ıdd = | .true | e., &end | | | |
| н | -+ | H2O2 | = | OH | ÷ | H 20 | | 7.81 | E+11 | Ο. | 0. |
| - | | - | | | | | | | | | |
| ADD | | | | | | | | | | | |
| м | + | H202 | =2 | BOD | | | | 1.44 | E+17 | 0. | 4551 |
| 1978797 | BODY | | | | | | | | | | |
| | | AF | | | 70 | 820 | | £ ^ | | 202 | c c |
| <u>a</u> 2 | | 2.30 02 | | • | /0 | d20 | | 0.0 | HZ | .04 | 0.0 |
| END | | | | | | | | | | | |
| H2 | + | OH | - | H2O | + | H | | 4.741 | 5+13 | 0. | 6098 |
| Ħ | + | 02 | = | EO2 | + | м | | 1.46 | E+15 | 0. | -100 |
| THIRD | BODY | | | | | | | | | | |
| 02 | | 1.30 N2 | | 1 | . 3 | H20 | | 21.3 | 3 82 | 2 | 3.0 |
| END | | | | - | | | | | | | |
| M | , | 820 | | | т | ۸¤ | | 1 307 | | ٥ | 1461 |
| PD | + | n 20 | - | 4 | - | UA. | | 1.30 | | υ. | 1021 |
| THIRD | BODY | | | - | ~ | | | | | | |
| E2 | | 4.00 02 | | 1 | .5 | E20 | | 20.0 |) N2 | 2 | 1.5 |
| END | | | | | | | | | | | |
| Ħ | + | 0 | - | OH | + | м | | 7.1E | 2+18 | -1. | ο. |
| м | + | 82 | - | H | + | H | | 2.23 | 3+14 | 0. | 960 |
| TRIBL | BODY | | | | | | | | | | |
| 82 | | 4 10 02 | | 2 | .0 | 820 | | 15.0 | א (| , | 2.0 |
| | | 4.10 02 | | - | | | | | | • | 2.0 |
| END | | ~ | _ | ~ | | ~ | | 1 007 | 0110 | • | 1100 |
| M | + | 02 | - | 0 | - | 0 | | 1.001 | 5418 | -1. | 1180 |
| co | + | 0 | > | C02 | | | | 8.43 | 5+09 | 001 | 1000 |
| | | CO2 | > | со | + | 0 | | 9.08E | E+18 | -1.84 | 1307 |
| END | | | | | | | | | | | |
| | | E20 | + | 0 | | > | H2 | + | 02 | | |
| | | 1. | 1. | 4 | .90E+1 | .0 | 18 | -510 | | | |
| | | | | 820 | | > . | CO2 | + | E 2 | | |
| | | 1 | 1 | | 305+0 | 5 1 | 31 | -7000 | | | |
| | | ±. | . | | | | <u>co</u> | | 820 | | |
| | | 1 002 | ، ۲ | | 41 | 2 | 10 | 7 2507 | | | |
| | | 1. | 1. | 4 | .415+1 | | 13 | 3527. | • | | |
| | | N2 | . + | 02 | | >2.0 | NO | | | | |
| | | 1. | 1. | 4. | .00E+1 | .4. | 03 | 100000. | | | |
| | | | 2 | .0 NO | | > | N2 | + | 02 | | |
| | | | 2. | 2. | .00E+1 | 1 | 0. | 38000. | · | | |
| | | CN | +2 | .00 | | > | NO | + | со | | |
| | | 1. | 1. | 8 | .30E+1 | 1 0 |). | 0 | | | |
| | | CN | + | NO | | > | со | + | N2 | | |
| | | 1. | 1. | 1 | .25E+1 | 2 | Ο. | 0 | | | |
| | | 2.0 CH2 | + | N2 | | >2.0 | CN | +2.0 | H2 | | |
| | | 1 1 | • | | 005+1 | 3.0 | 1 | 54000 | | | |
| | | ±. ±. | | ~ ~ ~ | | | | 54000 | | | |
| | | CH2 | - + | 02 | c | | | + | n20 | | |
| | | 1. | . 5 | 3 | .50E+C |)/(| · . | 5000 | • | | |
| | | 02 | + | C3H | 8 | >3.0 | CH2 | +2.0 | OH | | |
| | | 1.6 | .1 | 1 | .10E+1 | 12 (|). | 41000 | | | |
| | | н2 | + | 02 | | >2.0 | ОН | | | | |
| | | 1 1 | | 1 | 005+0 | 10 | 1 | 49080 | | | |
| | | ··· ··· | . ~ | • • •= ⁺ | | ~ ` | 820 | | | ـ | 0 |
| | | C388 | +4 | | 00 | ć. | 0.212.0 | 4000 | CORd | Ŧ | 0 |
| | | .15 1. | | 1 | . 98E+C | 10 (| - | 4000 | • | | <u></u> |
| ОН | | + H2 | + | 02 | | > | H20 | + | U | + | OH |
| 1. | | 0. 1. | | 0 | .96E+1 | - 12 | 1 | 1013 | • | | |
| | | E20 | + | 0 | | > | H2 | + | 02 | | |
| | | 1. | 1. | 4 | .90E+1 | .0 | 18 | -510 | | | |
| END | | | | • | | | - | | | | |
| 1.1 | | | | | | | | | | | |

END

TABLE A.1.—Continued.

AR TIME C388 &prob \$end &wsprob delmd= 50., dotmax= 4000.,mpr=2, volume= 500., 4end &START T= 800.,P=5.5,MDOT= 140.0, eratio =1.5, scc = 3.0, sch = 8.0, &END END FINIS GLOBAL TEST CASE; ADD MOLECULAR REACTIONS TO PREV. CASE CASE 3 ADD frtype global=.true.,gronly=.false., gladd = .false., glchng = .false.,

 mrprev = .false., mrchng = .false., mradd=.true., & end

 + 02 = OH + OH 1.7E+13

 + H202 = OH + H02

 82 47780. ٥. 0 8.0E+13 0. 1000. END TIME C388 SPROB WELSTR=.TRUE., \$END &WSPROB DELMD= 50., DOTMAX= 1800., MPR=2, VOLUME= 500., &END &start t= 800.,p=5.5, mdot= 450., eratio = 1.5, scc = 3.0, sch = 8.0, &end END FINIS GLOBAL TEST CASE; INTEGRATION CASE WITH PREVIOUS MECHANISM; CASE 4 REPEAT &rtype global=.true., mrprev = .false., TIME H2 N2 .720502 CO2 .0002768 02 .193301 C3H8 .02 .0085997 AR END £solver emax = 1.e-6, atolsp = 1.e-15, &end FINIS GLOBAL CODE TEST CASE: ALL GLOBAL REACTIONS; NEW CASE CASE 5 NEW &rtype global=.true.,gronly=.true., &end 1. 0 **B2O** H2 > + 02 4.90E+10 1. .18 -510. со 820 > CO2 82 + 1.30E+05 1.31 -7000. 1. 1. C02 H2 > CO + H2O + 3527. 4.41E+10 1. 1. .19 N2 + 02 >2.0 NO 3.00E+14 .03 100000. 1. 1. 2.0 NO > N2 02 + 2.00E+11 38000. 2. Ο. +2.0 0 CN NO + 0. co > 8.30E+11 1. 1. ٥. CN + NO co + N2 > 1. 1. 1.25E+12 0. ο. 2.0 CH2 N2 >2.0 CN +2.0 H2 5.00E+13 0. 2 > CC 3.50E+07 0. 1. 1. 54000. CH2 02 со + **H2O** 1. . 5 5000. 02 C3H8 >3.0 CH2 +2.0 OH 1.6 . 1 1.10E+12 0. 41000. 02 H2 + >2.0 OH 1. 1. 1.00E+00 0. 49080. C3H8 +2.0 OH 820 > + C3H8 + 0 1.98E+06 0. 4000. .15 1. OH + H2 + 02 > 820 0 OH + + 0.96E+12 -.1 1. 1. ٥. 1013. AR TIME C388 &probwelstr=.true.,&end&wsprobdelmd=10.,&start t=800.,p=5.5,mdot=100.,&end mpr=1, volume= 200., &end 02 .193301 N2 .720502 C388 .0773205 .0088765 AR END FINIS

TABLE A.1.—Concluded.

ALL GLOBAL REACTIONS - CHANGE AND ADD ONE GLOBAL REACTION CASE 6 CHANGE global=.true.,gronly=.true., glchng=.true., *&rtype* gladd = .true., mrprev = .false., &end N2 + 02 >2.0 NO + 1. 4.00E+14 .03 100000. 1. ADD H20 > ₩2 02 0 ÷ + 4.90E+10 .18 -510. 1. 1. END AR TIME C3H8 &prob &end &wsprob delmd= 200., dotmax= 1500.,mpr=2, volume=2500., &end &start t= 800.,p=5.5,mdot= 100., &end .193301 02 .720502 N2 .0773205 C3E8 .0088765 AR END FINIS GLOBAL AND MOLECULAR REACTIONS; MOLECULAR REACTIONS ADDED CASE 7 ADD &rtype global=.true.,gronly=.false., mrprev = .false., mradd=.true., &end 18365. 0 + 820 = ΒO + OĦ 6.8E+13 0. -+ н + 02 OH 0 1.89E+14 0. 16400. 4.20E+14 0 + H2 × OH + Ħ 0. 13750. * 02 7.28E+13 H ÷ HO2 H2 + ٥. 2126. = OH 02 5.0E+13 ٥. 1000. 0 + HO2 + 802 OH . H20 + 02 8.0E+12 Ο. Ο. + 1.34E+14 1070. HO2 =2.00H 0. H + HO2 -H2O2 + H 7.91E+13 ٥. 25000. H2 + H202 -H20 + HO2 6.1E+12 Ο. 1430. + OR æ H2O2 02 1.8E+12 Ο. 0. HO2 + HO2 + H2O2 * OH + H2O 7.8E+11 ٥. ٥. Ħ + H202 =2.00H 1.44E+17 Ο. 45510. М THIRDBODY 6.0 H2O2 H2 2.30 02 .78 H20 6.6 END 4.74E+13 Ο. 6098. **E**2 + OH -820 H + 1.46E+15 0. + -HO2 + м -1000. Ħ 02 THIRDBODY N2 820 21.3 Н2 3.0 1.30 1.3 02 END OH 1.30E+15 ο. 105140. + **H2O** = ₽ + м THIRDBODY 4.00 02 1.5 H20 20.0 N2 1.5 H2 END 0 OH М 7.1E+18 -1. 0. ÷ + Ħ *** H2 -E + н 2.2E+14 0. 96000. М + THIRDBODY 15.0 N2 4.10 02 2.0 H20 2.0 **H**2 END 1.80E+18 02 = 0 + 0 -1. 118020. М + -.001 8.43E+09 co 0 > CO2 1000 + 9.08E+18 -1.84 0 C02 130754. > CO + END СЗЯ8 TIME &PROB WELSTR=.TRUE., &END &WSPROB DELMD= 100., DOTMAX= 1160., MPR=1, VOLUME= 500., & END \$START T= 800., P=5.5, MDOT= 140.0, eratio =1.5, scc = 3.0, sch = 8.0, & END

END FINIS TABLE A.2.—COMPUTED RESULTS FOR TEST CASE 1 (HYDROGEN-OXYGEN PSR PROBLEM USING ALL MOLECULAR REACTIONS)



ACTIVATION ENERGY 18365.00 16400.00 13750.00

2126.00 1000.00 0.00 1070.00

25000.00

.0000

1430.00 0.00 0.00

0

۵

0

0

0

0.000002+00

XX

TABLE A.2.—Continued.

CHEMICAL PROPERTIES

| SPECIES 0 H20 0H H2 H2 H02 H202 | CONCENTRATION (MOLES/CM**3) 0.0000E+00 0.0000E+00 0.0000E+00 1.61956E-05 6.75887E-05 0.0000E+00 0.0000E+00 | MOLE FRACTION 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 1.9330IE-01 8.06699E-01 0.00000E+00 0.00000E+00 | NET SPECIES PRODUCTION RATE (MOLE/CHXX3/SEC) 0.00000E+00 0.00000E+00 2.25347E-10 -2.25347E-10 2.25347E-10 2.25347E-10 0.00000E+00 | REACTION NUMBER 1 2 3 4 5 6 7 7 8 9 10 11 | RATE CONST CGS UNITS 6.2545E+09 7.3608E+10 1.9113E+13 2.6655E+13 8.0000E+12 6.8359E+13 1.1708E+07 2.4813E+12 1.800E+12 5.0000E+11 | NET REACTION CONV R((MOLE-CM*x5/G*x2/SEC 0.0000E+00 0.0000E+00 -5.26082E-04 0.00000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 | ATE NET RATE/POSI- TIVE DE RODO 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 |
|--|--|--|---|--|--|---|--|
| MIXTURE | MOLECULAR WEIGH | T 7.81154 | TOTAL ENERGY EXCHANG (Cal-cm**3/g**2/s) | E RATE (EC) | 2.76731E+01 | MASS FRACTION SUM | 1.00000000 |
| | | | COD INTITALIZATION OF | ISENS = | N. 433333 S | | |
| | | | **EQUILIBRIUM | CONDITION | S XX | | |
| | TIME 0.00 | 000E+00 SEC | AREA 0.0000 | OE+OD SQ | CM | AXIAL POSITION 0. | 00000E+00 CM |
| | | NPERTIES | | | INTEGRATION | INDICATORS | |
| | PRESS | IRF | 5.50000 | | STEPS FRO | M LAST PRINT | C |
| | CATM | | 0.00 | | AVERAGE S | TEP SIZE | 0.00000E+00 |
| | (CM/ | ŚĘĆ) | 99835F-04 | | METHOD OR | DER | 0 |
| | | MXX3) PATHRE | 3183.95 | | | | |
| | (DEG | | 000005-01 | | TOTAL NUM | IBFR OF STEPS | 0 |
| | (G/S | EC) | £ 0265 | | FUNCT EVA | HATTONS | C |
| | (CAL | /G/DEG K) | 0.0245 | | JACOBTAN | EVALUATIONS | 0 |
| | CANNA | ROUBER | 1 2384 | | ••••••• | | - |
| | FNTHA | | 54525F+82 | | | | |
| | (CAL | | 16667F+08 | | | | |
| | (CAL | /G/DEG K) | 140012.00 | | | | |
| | | | CHEMICAL P | ROPERTIES | | | |
| | | MOLE ERACTION | | PEACTION | | NET PEACTION CONV P | ATE NET PATE/POSI- |
| SPECIES | (MOLES/CMXX3) | NULE FRACTION | RATE (MOLE/CMXX3/SEC) | NUMBER | CGS UNITS | (MOLE-CMXX3/GXX2/SE | C) TIVE DIR RATE |
| H20 | 9.37412E-06 | 4.34104E-01 | 4.15227E-07 | ź | 1.3235E+13 | -1.93939E+00 -1.85043E+01 | 0.00000 |
| H | 1.36271E-06 | 6.31051E-02 | -6.76196E-07 | 4 | 5.1575E+13 | 1.41732E-01 2.95487E-03 | 0.00000 |
| HZ | 1.03544E-05 | 4.79498E-01 | 7.45053E-07 | 6 | 8.0000E+12 | 9.19158E-03 2.14840E-01 | 0.00000 |
| H02 H202 | 1.02949E-11 | 4.76743E-07 | -4.69738E-10 | 8 | 1.3738E+12 | -1.10281E-02 | 0.00000 |
| | | | | 10 | 1.8000E+12 | 1.45917E-07 | 0.00000 |
| | | T 0.05417 | TOTAL ENERGY EVOLUANC | IL E DATE - | 3.0000ET11 | MASS EPACTION SIM | 1 10000001 |
| MIXTURI | E MULECULAR WEIGH | 11 9.25415 | CAL-CMXX3/GXX2/S | EC) | 2.301305403 | PASS PRACTION SOM | 1.00000011 |
| | | | | | | | |
| | | COMPUT No. OF | ATIONAL WORK REQUIRED F TTERATIONS = 8 | CPU TIME | = 1.666665E-0 | 2 S | |
| | | | | | | | |
| - | | | | | | | |
| 0 | INITIAL ESTIMATES 1.78863F-06 | S (SIGMAS) AT TO | PERATURE - 5105.55 K | | | | |
| H20 DH | 4.69092E-02 2.27336E-03 | | | | | | |
| H 02 | 6.81913E-D3 6.44778E-D5 | | | | | | |
| H2 H02 | 5.18145E-02 3.26786E-07 | | | | | | |
| H202 | 5.15168E-08 | | | | | | |
| WELLSTI | RRED REACTOR CALC | JULAIIUN GLO | DAL CUDE TEST CASE: MOLE | CULAR REAC | TIONS ONLY AND | NU INERTS CASE 1 | |
| DDFAAUES | | INITIAL ST | IAIE FIN | IAL STATE | FINALZ | INITIAL RATIO | |
| TEMP | ATM DEG K | 5.50000 800.000 | 5 | 102.07 | | L. UUDOO L. 37758 | |
| DENSITY | GM/CMXX3 | 5.02109 6.54484E | -04 4.7 | 5096E-04 | i | 1.09689 0.72591 | |
| ENTHALPY SP. HEAT | CAL/GM (CP) CAL/GM/K | 456.525 9.30602E- | -01 9.6 | 56.525 2486E-01 | | L.00000 L.03426 | |
| MOL. HT. Gamma | OF MIXT | 7.811 | 2 | 7.8115 1.3593 | | | |

| | SPECIES | | | MOLE FRACT | MASS FRACT | NOLE FRACT | MASS FRACT | |
|--------|--|------------------------------|--|--|--|--|--|--------|
| | 0 H20 DH H 02 H2 H22 H222 | | | 0.00000E+00 0.0000E+00 0.0000E+00 1.93301E-01 8.06699E-01 0.00000E+00 0.00000E+00 | 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 7.91%28E-01 2.0%172E-01 0.0000E+00 0.0000E+00 | 4.12446E-D3 3.73312E-D1 2.61348E-D3 3.69187E-D1 3.27611E-D3 2.47487E-D1 7.81154E-10 7.81154E-10 | 8.44761E-03 8.60942E-01 5.69007E-03 4.76385E-02 1.34201E-02 6.38649E-02 3.30067E-09 3.40146E-09 | |
| | VOLUME | 2000.00 | CMXX | 3 MASS FL | 0 0.100000 G | M/SEC | | |
| | MDOTZVOL | IIMF = | 0.80885 | RESTRENCE TIME | = 9501.925 | MSEC ITERATIONS = | 10 | |
| | MELIST | TODER DE | ACTOP CALC | HATTON GLOBAL | CODE TEST CASE | MOLECHLAR REACTIONS | INLY AND NO INERTS | CASE 1 |
| | ALLUI | IARLD RU | ACTOR CALC | THITTAL CTA | re | ETNAL STATE | ETNALZINITIAL PATTO | |
| | | | | INITIAL JIA | | FINAL SIAIL | | |
| | PRESSUR TEMP. ENTROPY DENSITY ENTHALP SP. HEA MOL. NT GAMMA | E Y T (CP) . Of MIX | ATM DEG K CAL/GM/K GM/CM××3 CAL/GM CAL/GM/K T | 5.5000 800.000 5.02109 6.54484E-0 456.525 9.30602E-0 7.8115 1.3762 | 4 1 | 5.50000 1098.26 5.50748 4.76743E-04 456.525 9.61760E-01 7.8115 1.3596 | 1.0000 1.37282 1.09687 0.72843 1.00000 1.03348 | |
| | SPECIES | | | MOLE FRACT | MASS FRACT | MOLE FRACT | MASS FRACT | |
| | 0 H20 OH H2 H22 H02 H22 H222 | | | 0.00000E+00 0.0000E+00 0.0000E+00 1.93301E-01 8.06699E-01 0.00000E+00 0.00000E+00 | 0.00000E+00 0.00000E+00 0.00000E+00 7.91828E-01 2.08172E-01 0.00000E+00 0.00000E+00 | 4.66892E-03 3.69883E-01 3.01596E-03 3.65214E-01 4.51704E-03 2.52701E-01 7.81154E-10 7.81154E-10 | 9.56277E-03 8.53035E-01 6.56636E-03 4.71258E-02 1.85034E-02 6.52105E-02 3.30067E-09 3.40146E-09 | |
| | VOLUME | 2000.00 | CMXX | 3 . MASS FL | 0 900.100 G | M/SEC | | |
| | MDOTZVOL | UMF = | 0.45005 | RESIDENCE TIME | = 1.059 | MSEC ITERATIONS = | 2 | |
| | MELLST | TPPED O | ACTOR CAL | IN ATTON GLORA | CODE TEST CASE | MOLECULAR REACTIONS | DNLY AND NO INERTS | CASE 1 |
| | necto, | | NOTON ONCE | TNITTA: CTA | TE | ETNAL CTATE | ETHAL/TNTTTAL PATTO | |
| | | _ | | INTIAL SIM | | FIRE STATE | 1 INAL/ INITIAL KATIO | |
| | PRESSUR TEMP. ENTROPY DENSITY ENTHALP SP. HEA MOL. WT GAMMA | Y T (CP) . OF MI | ATM DEG K CAL/GM/K GM/CM**3 CAL/GM CAL/GM/K (T | 5.50000 800.000 5.02109 6.54484E-0 456.525 9.30602E-0 7.8115 1.3762 | 4 1 | 5.50000 1097.88 5.50746 4.76907E-04 456.525 9.61689E-01 7.8115 1.3597 | 1.0000 1.37235 1.09687 0.72868 1.00000 1.03341 | |
| | SPECIES | | | MOLE FRACT | MASS FRACT | MOLE FRACT | MASS FRACT | |
| | 0 H20 OH H 02 H2 H02 H222 | | | 0.00000E+00 0.00000E+00 0.00000E+00 1.93301E-01 8.06699E-01 0.0000E+00 0.00000E+00 | 0.00000E+00 0.0000E+00 0.0000E+00 7.91828E-01 2.08172E-01 0.0000E+00 0.0000E+00 | 4.71882E-03 3.69536E-01 3.05414E-03 3.64817E-01 4.64676E-03 2.53228E-01 7.81154E-10 7.81154E-10 | 9.66496E-03 8.52233E-01 6.64948E-03 4.70745E-02 1.90347E-02 6.53465E-02 3.30067E-09 3.40146E-09 | |
| | VOLUME | 2000.0 | n CMBB | 3 MASS FL | 0 1000.00 0 | W/SEC | | |
| | MDOT /VOI | | 0 5000 | | = 0.056 | MSEC ITERATIONS = | 2 | |
| | FIDO I / TOL | . UML - | 0.50000 | V RESIDENCE TIME | 0.754 | HOLO ITERATIONS | - | |
| | | | | COMPUTATION No. of iteratio | AL WORK REQUIRED F NS = 30 CPU | FOR PSR CALCULATION: U TIME = 3.6666667E-0 | 1 S | |
| | S) END | OF THIS | CASE | | | | | |
| . LULA | | | | | | | | |
| | | | | TOTAL CPU TIME (I | NCLUDING I/O) REQU | JIRED = 0.833333 | S | |
| | | | | | | | | |

TABLE A.2.—Concluded.

_(LSENS) READ DATA FOR NEXT CASE

** DATA LINES **

GLOBAL TEST CASE: CHANGE AND ADD GLOBAL AND MOLECULAR REACTIONS CASE 2 CHANGE

| årtype gl | obal | =.tru | e.,g | ronly | /=.f | als | 8., | | | | | | | | |
|------------------|------------|----------|----------------|------------|------------|--------------|---------------------|----------------|--------|----------------|------------------|----------|----------|----|------------------|
| mrchng H | =.tr + | H2Ó2 | nra: | dd = = | .tr OH | ue., | , gla + BIAN | dd = . H20 | true. | , &e 7 | nd .8E+ | 11 | 0. | | 0. |
| ADD | | | | | | | <i>JE444</i> | K LANE | - | | | | | | |
| M | * • | H202 | | =2.0 | DOH | | | | | 1. | 44E+ | 17 | Ο. | | 45510. |
| H2 FND | "z. | 30 | 82 | | | .71 | 3 | H20 | | 6 | . 0 | H2 | 02 | | 6.6 |
| H2 H | + | 0H 02 | | = | H20 H02 | | + + | H M | | 4. 1. | 74E+ 46E+ | 13 15 | 0. 0. | | 6098. -1000. |
| THIRDBO | DY 1. | 30 | N2 | | | 1.3 | 3 | H20 | | 2 | 1.3 | HZ | | | 3.0 |
| M | + | H20 | | = | н | | + | OH | | 1. | 30E+ | 15 | 0. | | 105140. |
| THIRDBO H2 | DY 4. | 00 | 02 | | | 1.5 | 5 | H20 | | 2 | 0.0 | N2 | | | 1.5 |
| END | | n | | - | 014 | | | м | | 7 | 164 | 18 | -1 | | 0 |
| M | + | H2 | | = | H | | ÷ | H | | ź | .2E+ | 14 | 0. | | 96000. |
| H2 END | 4 . | 10 | 02 | | | 2. | 0 | H20 | | 1 | 5.0 | N2 | | | 2.0 |
| M | + | 02 | | - | 0 | | ÷ | 0 | | 1. | 80E+ | 18 | -1. | | 118020. |
| C0 | + | 0 | | > | C02 | | + | Ô | | 8. 9. | 43E+ 08E+ | 09 18 | 001 | | 1000. 130754. |
| END | | | _ | · . | | | - | | | | | | •••• | | |
| | 1 | HZ | 0 | , + | 0 | 6 | 90F+1 | א < ה ח | 12 | -5 | 30 | 2 | | | |
| | • | • co | | ••• | н | 20 | | 5 6 | 02 | + | ШH | 2 | | | |
| | 1 | • | ~ | 1. | | _1 | 30E+0 | 51. | 31 | -70 | 00. | | | | |
| | 1 | | 2 | 1.* | n | 4.4 | 41E+1 | ó.1 | 9 | 35 | 27." | 20 | | | |
| | - | N2 | | + | 0 | 2 | | 2.0 | 10 | | | | | | |
| | I | • | | 1. , | n N | <u>م</u> ٩.۱ | 00E+1 | 9.U | 13 | 1000 | υ α. Π | 2 | | | |
| | | | : | z. ້ | | Ž2.1 | 00E+1 | í | j. | 380 | 00.Ŭ | - | | | |
| | | CN | | +2 | .0 0 | • | | ۹ ج | 10 | + | ູເ | 0 | | | |
| | 1 | CM | T | • + | N | ດົ່ | 30541 | > 0 | 0 | + | И | 2 | | | |
| | 1 | •••••• | _ 1 | • . | |]1. : | 25E+1 | 2 0 |). | | 0. | _ | | | |
| | 2 | .0 CH | 2 ₁ | + | N | 251 | 00E+1 | >2.UC 3 N | SM | - +2 - 54 A | .0 H 0n | Z | | | |
| | * | . СН | 2 | + | 0 | 2ີ່ | 002.1 | , °č | 0 | + | Ъ | 20 | | | |
| | 1 | • •• | • | 5 | _ | 3.1 | 50E+0 | 7 0. | | 50 | 00. | | | | |
| | 1 | .6 02 | | , + | C | 3118 | 10E+1 | >3.0C 2 fl. | inz. | 410 | .0 U 80. | n | | | |
| | • | т, нз | • | • + | 0 | 2 | | >2.0 C | ы | | ••• | | | | |
| | 1 | • | 1. | | • • | _1 .4 | 00E+0 | Q 0. | 200 | 498 | 80. | 7110 | | | |
| | | 15 | по 1. | 72 | | " 1.9 | 98E+0 | 6 0 | 120 | 40 | 00. | JNO | . • | U | |
| OH | + | H2 | | + | 0 | 2 | | > 1 | 120 | + | 0 | | + | OH | |
| 1. | 0 | H2 | <u>1.</u> | + | n | 0.9 | 96E+1 | 2 - | 1 | 10 | 13. | 2 | | | |
| | 1 | | | 1. | | 4. | 90E+1 | é. i | เลื | -5 | 10. | - | | | |
| END | | | | | | | | | | | | | | | |
| TIME | | | | | | | | C3H8 | | | | | | | |
| &prob | | | | åen: | d | | | | | | | | | | |
| āwsprob deīmd | = 50 | da | tmav | = 60 | 80 | mpr | =2. | | | | | | | | |
| volum | e= 5 | ŏó., | | &en | ď | | | | _ | | | | | | |
| ASTART T= | 800 | .,P=5 | .5,M | DOT= | 140 | .0, | erat | io =1. | .5, sc | c = | 3.0, | sch | = 8.0, | &E | END |
| FINIS | | | | | | | | | | | | | | | |

.

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

GLOBAL TEST CASE: CHANGE AND ADD GLOBAL AND MOLECULAR REACTIONS CASE 2

| REACTION | | | | REACTI | ON | | | REACTION RAT | E VARIABLES | ACTIVATION |
|----------|---------|-----|-------------|--------|-----------|---|---------|---------------|-------------|------------|
| NUMBER | | | | | | | | A | a | ENERGY |
| 1 | 1×0 | + | 1×H20 | = | 2X0H | | | 6.80000E+13 | 0.0000 | 18365.00 |
| 2 | 1 X H | + | 1×02 | = | 1 XOH | + | 1×0 | 1.89000E+14 | 0.0000 | 16400.00 |
| 3 | 1 80 | + | 1×H2 | = | 1 XOH | + | 1 XH | 4.20000E+14 | 0.0000 | 13758.00 |
| č | 1 1 1 | + | 1 \$802 | = | 1 1 1 1 2 | + | 1×02 | 7.28000F+13 | 0.0000 | 2126.00 |
| ÷. | 1¥0 | ÷ | 1#802 | Ŧ | 1 808 | ÷ | 1 102 | 5.00000F+13 | 0.0000 | 1000.00 |
| ž | 11102 | ÷ . | 1 100 | = | 1 ¥H20 | + | 1 1 1 2 | 8.00000F+12 | 0.0000 | 0.00 |
| ž | 144 | ÷ | 18402 | Ξ | 2408 | • | | 1 34000F+14 | 0 0000 | 1070 00 |
| é | 1882 | ÷ | 1 #102 | 3 | 184202 | + | 1 ¥H | 7 91000F+13 | 0.0000 | 25000 00 |
| ă | 1 204 | | 184202 | = | 14420 | ÷ | 1 + 402 | 6 10000E+12 | 0 0000 | 1630 00 |
| 10 | 1.000 | • | 28402 | - | 128202 | ÷ | 1 202 | 1 80000F+12 | 0.0000 | 0.00 |
| 11 | 1 × 4 | | 1202 | - | 1 ×08 | | 1 8820 | 7 800005+11 | 8 0000 | 0.00 |
| 11 | 101 | | 1 1 1 2 0 2 | - | 1400 | • | 141120 |) 66000E+17 | 0.0000 | 45510 00 |
| 12 | 1 2 4 2 | | 1200 | | 1200 | | 1 ×4 | 1.9400000717 | 0.0000 | 43310.00 |
| 13 | 1×12 | | 1×00 | - | 1×020 | | 120 | 4./4000ETIJ | 0.0000 | -1000 00 |
| | 1×1 | | 1202 | - | IXNUZ | | | 1.45000000115 | 0.0000 | -1000.00 |
| 15 | | | 17020 | - | 120 | | 1201 | 1.300002713 | 0.0000 | 105140.00 |
| 16 | 170 | • | 120 | = | TXON | + | m. | /.100002+18 | ~1.0000 | 0.00 |
| 17 | M | + | IXHZ | = | 2*# | | | 2.200002+14 | 0.0000 | 96000.00 |
| 18 | M | + | 1¥02 | - | 2¥0 | | | 1.80000E+18 | -1.0000 | 118020.00 |
| 19 | 1×C0 | + | 1*0 | > | 1×C02 | _ | | 8.43000E+09 | -0.0810 | 1000.00 |
| 20 | | | 1¥C02 | > | 1¥C0 | + | 1×0 | 9.08000E+18 | -1.8400 | 130754.00 |

TABLE A.3.—Continued.

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

| M(H2 , M(O2 , M(H2 , M(H2 , | $\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$ | 30000 30000 00000 10000 | M(02 , M(N2 , M(02 , M(02 , | 12) = 0.78000 14) = 1.30000 15) = 1.50000 17) = 2.00000 | MCH20 MCH20 MCH20 MCH20 | , 12) , 14) , 15) , 17) | = 6.00000 = 21.30000 = 20.00000 = 15.00000 | MCH202 MCH2 MCN2 MCN2 MCN2 | (12) = 6.60000 (14) = 3.00000 (15) = 1.50000 (17) = 2.00000 |
|--|--|---|--|--|---|----------------------------------|--|--|--|
| | | | XXX GLOB | AL REACTIONS × | ×× | | | | |
| NUMBER | | | | REACTION | | | | | |
| 21 22 23 25 26 27 28 29 30 31 32 33 31 32 33 34 | ×OH | 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1 | 0×H20 + 0×C0 + 0×C02 + 0×CN + 0×CN + 0×CN + 0×C12 + 0×C12 + 0×12 + 0×12 + 0×12 + 0×12 + 0×12 + 0×12 + 0×12 + 0×12 + 0×12 + | 1.0%0 1.0%H2 1.0%H2 2.0%N0 2.0%N0 1.0%N0 1.0%N2 1.0%N2 1.0%C3H8 1.0%C2 2.0%0H 1.0%02 1.0%02 1.0%0 | > 1.0%H2 > 1.0%C02 > 1.0%C0 > 2.0%N0 > 1.0%N2 > 1.0%N2 > 1.0%N0 > 1.0%C0 > 2.0%CN > 2.0%CH2 > 2.0%OH > 1.0%H20 > 1.0%H20 > 1.0%H20 | | + 1.0×02 + 1.0×H2 + 1.0×H20 + 1.0×C0 + 1.0×C0 + 1.0×H2 + 2.0×H2 + 2.0×H2 + 2.0×H4 + 1.0×H20 + 2.0×H8 + 1.0×C3H8 + 1.0×0 | + 1.0×0 + 1.0×0 | н |
| REACTION | | RE | ACTANT EXPONEN | TS BEYR I | | | REAC | TION RATE V | ARIABLES |
| NUMBER 21 22 23 24 25 26 27 28 28 29 30 31 32 33 33 34 | | REAF 1 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 | 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.600 1.600 0.150 0.000 1.000 | 1.000 1.000 1.000 2.000 1.000 1.000 1.000 0.500 0.500 0.100 1.000 1.000 1.000 | | | <pre>4.90000E+10 1.30000E+05 4.41000E+10 4.00800E+14 2.00000E+11 1.25000E+11 1.25000E+12 5.00000E+11 3.50000E+10 1.00000E+10 1.00000E+10 1.98000E+06 9.60000E+10 4.90000E+10</pre> | 0.180 1.310 0.190 0.030 0.0000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000000 | $\begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} $ |
| | XX <u>Nem</u> I | INPUT DATA | GIVEN IN CGS | UNITS XX | | XX OUTF | PUT REQUIRED IN | CGS UNITS | XX |

** ASSIGNED VARIABLE PROFILE **

WELL - STIRRED REACTOR CASE

VOLUME OF REACTOR = 5.00000E+02 CM¥¥3 Mass flow rate to start iteration = 1.40000E+02 g/s

ASSIGNED MASS FLOW RATE PROBLEM: MASS FLOW RATE INCREMENT = 5.00000E+01 G/S Maximum Mass flow Rate = 4.00000E+03 G/S

FUEL-AIR REACTION, FUEL-AIR EQUIVALENCE RATIO = 1.5000 OXYGEN FRACTION IN AIR = 0.2095

NUMBER OF REACTING SPECIES: 15 NUMBER OF INERT SPECIES: 1 ** INITIAL CONDITIONS **

| TIME | 0.00000E+00 | SEC | A | REA | 0.00000E+00 | SQ CM | AXIAL POSITION | 0.000008+00 | CM |
|------|-------------------------------|-----|-------------|-----|-------------|-------|------------------------|-------------|----|
| Fi | LOW PROPERTIES | | | | | | INTEGRATION INDICATORS | | |
| | PRESSURE | | 5.50000 | | | | STEPS FROM LAST PRINT | 0 | |
| | (ATM) VELOCITY (CM/SEC) | | 0.00 | | | | AVERAGE STEP SIZE | 0.00000E+0 | 0 |
| | DENSITY (G/CMXX3) | | 2.50173E-03 | | | | METHOD ORDER | 0 | |
| | TEMPERATURE | | 800.00 | | | | | | |
| | MASS FLOW RAT | E | 1.40000E+02 | | | | TOTAL NUMBER OF STEPS | 0 | |
| | ENTROPY | 、 | 1.8011 | | | | FUNCT EVALUATIONS | 0 | |
| | MACH NUMBER | , | 0.0000 | | | | JACOBIAN EVALUATIONS | 8 | |
| | GAMMA | | 1.2701 | | | | | | |
| | ENTHALPY | | 9.23468E+01 | | | | | | |
| | SP. HEAT (CP) (CAL/G/DEG K |) | 3.12948E-01 | | | | | | |

TABLE A.3.—Continued.

CHEMICAL PROPERTIES

| SPECIES 0 H20 0H H20 02 H22 H02 H02 C0 C02 N2 N0 CN CN CN CH2 C3H8 AR | CONCENTRATION (MOLES/CMXX3) 0.80008E+00 0.00008E+00 0.00008E+00 0.00008E+00 0.00008E+00 0.00008E+00 0.00008E+00 0.00008E+00 0.00008E+00 0.00008E+00 0.00008E+00 0.00008E+00 0.00008E+00 0.00008E+00 0.00008E+00 7.34696E-07 | MOLE FRACTION 0.0000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.282264E-04 7.34704E-01 0.00000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0. | NET SPECIES PRODUCTION RATE (MOLE/CMXX3/SEC) 3.57038E-26 0.00000E+00 9.11685E-08 0.00000E+00 0.00000E+00 0.00000E+00 1.86163E-30 -2.38549E-22 0.00000E+00 1.36753E-07 -4.55842E-08 0.00000E+00 | REACTION NUMBER 2 3 4 5 6 7 8 9 10 11 13 15 16 17 8 9 10 11 13 15 15 16 17 8 9 20 22 24 24 | <pre>RATE CONST COS UNITS 6.5377E+08 6.2545E+09 7.3668E+10 1.9113E+13 2.6655E+13 8.0000E+12 6.8359E+13 1.1708E+07 2.44813E+12 1.8000E+12 7.8000E+12 7.8000E+12 2.7387E+15 2.4666E-14 8.8750E+15 2.4666E-14 8.8750E+15 1.3075E-12 1.2901E+10 7.8718E-23 2.2465E+11 6.7502E+10 2.3465E+11 2.507E+10 8.9027E+100 3.9081E-14 1.5922F+11 2.2605E+11 2.2605E+11</pre> | NET REACTION CONV RATE (MOLE-CMXX3/GXZ/SEC) 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0000E+00 | E NET RATE/POSI- TIVE DIR RATE 0.000000 |
|---|--|--|---|--|---|--|---|
| MIXTURE | MOLECULAR WEIGHT | r 29.85916 | TOTAL ENERGY EXCHANGE | RATE | 3.39759E-16 | MASS FRACTION SUM | 1.00000000 |

CPU TIME FOR INITIALIZATION OF LSENS = 0.616667 S **EQUILIBRIUM CONDITIONS **

| TIME | 0.00000E+00 | SEC | AREA | 0.0000E+00 | SQ CM | AXIA: POSITION | 0.00000E+00 CM |
|------|-------------------------------|-----|-------------|------------|-------|------------------------|----------------|
| | FLOW PROPERTIES | 5 | | | | INTEGRATION INDICATORS | |
| | PRESSURE | | 5.50000 | | | STEPS FROM LAST PRINT | 0 |
| | VELOCITY | | 0.00 | | | AVERAGE STEP SIZE | 0.00000E+00 |
| | DENSITY (G/CMXX3) | | 7.34828E-04 | | | METHOD ORDER | 0 |
| | TEMPERATURE | | 2350.31 | | | | |
| | MASS FLOW RAT | Ξ | 1.40000E+02 | | | TOTAL NUMBER OF STEPS | 0 |
| | ENTROPY | ~ | 2.3604 | | | FUNCT EVALUATIONS | 0 |
| | MACH NUMBER | 0 | 0.0000 | | | JACOBIAN EVALUATIONS | 0 |
| | GAMMA | | 1.2641 | | | | |
| | ENTHALPY | | 9.23468E+01 | | | | |
| | SP. HEAT (CP) (CAL/G/DEG) | 0 | 3.69088E-01 | | | | |

CHEMICAL PROPERTIES

| SPECIES | CONCENTRATION | MOLE FRACTION | NET SPECIES PRODUCTION RATE (MOLE/CMTT3/SEC) | REACTION | RATE CONST | NET REACTION CONV RATE | NET RATE/POSI- |
|---------|---------------|---------------|---|----------|-------------|----------------------------|----------------|
| n | 2 17893F-10 | 7.64039E+06 | -2.50908E-04 | 1 | 1.3329E+12 | -7.60162E-04 | 0.00000 |
| H28 | 4.05534F-06 | 1.42200E-01 | 8.69456E-03 | ž | 5.6424E+12 | -2.68460E-05 | 0.00000 |
| OH | 1.53281E-88 | 5.37479E-04 | -3.22697E-04 | 3 | 2.2114E+13 | -6.59110E-04 | 0.00000 |
| H | 3.72907E-08 | 1.30759E-03 | 2.13187E-07 | 4 | 4.6178E+13 | 1.43082E-06 | 0.00000 |
| 02 | 2.11927E-10 | 7.43118E-06 | 3.89433E-04 | 5 | 4.0363E+13 | 7.03729E-09 | 0.00000 |
| HZ | 1.73940E-06 | 6.09920E-02 | -8.55659E-03 | 6 | 8.0000E+12 | 1.29043E-07 | 0.00000 |
| H02 | 3.90703E-13 | 1.37000E-08 | -1.11365E-07 | 7 | 1.0656E+14 | 2.24499E~06 | 0.00000 |
| H202 | 7.34828E-14 | 2.57667E-09 | 2.33318E-05 | 8 | 3.7453E+11 | 1.99374E-01 | 0.42297 |
| C0 | 3.10378E-06 | 1.08834E-01 | 8.94626E-03 | . 9 | 4.4911E+12 | -6.86707E-03 | 0.42297 |
| C02 | 1.26895E-06 | 4.44958E-02 | -8.94626E-03 | 10 | 1.8000E+12 | 2.15231E-07 | 0.42297 |
| N2 | 1.80796E-05 | 6.33959E-01 | -9.51429E-10 | 11 | 7.8000E+11 | -2.90148E-03 | 0.42297 |
| NO | 2.64686E-09 | 9.28118E-05 | 8.94424E-10 | 12 | 8.4429E+12 | -4.30001E+01 | 0.42297 |
| CN | 7.34828E-14 | 2.57667E-09 | 1.00844E-09 | 13 | 1.2845E+13 | 1.94110E-01 | 0.00000 |
| CH2 | 7.34828E-14 | 2.57667E-09 | 6.93592E-09 | 14 | 1.8086E+15 | 3.66684E-06 | 0.00000 |
| C3H8 | 7.34828E-14 | 2.57667E-09 | -2.73787E-09 | 15 | 2.1/38E+05 | -5.108332-04 | 0.00000 |
| AR | 2.15801E-07 | 7.56703E-03 | 0.00008E+00 | 16 | 3.0209E+15 | 2.9333/E-06 | 0.00000 |
| | | | | 17 | 2.6038E+05 | -2.102966-04 | 0.00000 |
| | | | | 18 | 8.12342+03 | -2.3529/6-10 | 0.00000 |
| | | | | 19 | 0./J20ETUY | 8.45/3UETUU D.28601E+00 | 1.00000 |
| | | | | 21 | 3.73102700 | 7.204712700 | 1.00000 |
| | | | | 22 | 1 51725+10 | J.010//ETU2 7 57/575105 | 1.00000 |
| | | | | 22 | 8 85785410 | 3.330332705 | 1 00000 |
| | | | | 24 | 2 53745405 | 1 \$0066F-03 | 1 00000 |
| | | | | 25 | 5 \$566F+07 | 7 596055-04 | 1 00000 |
| | | | | 24 | * 3000E411 | 2 661165-05 | 1.00000 |
| | | | | 20 | 1 25005412 | 2.40114E-03 6 60252E-06 | 1.00000 |
| | | | | 28 | 4 7603F+R# | 1 171225-04 | 1 00000 |
| | | | | 20 | 1 10005400 | 2 X7784F-05 | 1 00000 |
| | | | | 30 | 1 40705402 | 5 07030F-03 | 1 00000 |
| | | | | | 1,07375700 | 3.U/UJ7E-UJ | 1.00000 |

| | | | TABLE A.3.—Conti | nued. | | |
|---|---|---|---|---|--|----------------------|
| | | | 31 32 | 2.7300E-05 8.4084E+05 | 1.86371E-14 2.55717E+02 | 1.00000 1.00000 |
| | | | 33 34 | 3.5560E+11 2.2102E+11 | 2.13927E+00 3.61677E+02 | 1.00000 1.00000 |
| MIXTURE MOLECU | LAR WEIGHT 25 | 5.766666 TOTAL ENE (CAL-C | RGY EXCHANGE RATE M**3/G**2/SEC) | -2.09583E+06 | MASS FRACTION SUM | 1.0000010 |
| | | COMPUTATIONAL HORK No. of Iterations | REQUIRED FOR ÉQUI = 12 CPU TI | LIBRIUM CALCULATION NE = 4.999995E-02 | 1: S | |
| INITIAL | ESTIMATES (SIGMAS |) AT TEMPERATURE * | 2350.31 K: | | | |
| | 0 H2D DH H B2 H2D H2D2 H2D2 C0 C02 C02 C02 C02 C02 C02 C02 C02 C02 | 2.96523E-07 5.51876E-03 2.08595E-05 5.07475E-05 2.88403E-07 2.36709E-03 5.31693E-10 1.00000E-10 4.22382E-03 2.46038E-02 3.60201E-06 1.00000E-10 1.00000E-10 1.00000E-10 2.93675E-04 | | | | |
| (NSR) XXX FOR MASS FLO | CONV. NO. 1, C N RATE = 1.40000 | ONVERGED TEMP. (AFTE E+82 G/S, TEMPER | R 13 ITERATIONS) Ature = 2.43751E+ | IS GREATER THAN DR D3 K, PREVIOUS | EQUAL TO THE PREVIOUS TEMPERATURE = 2.3503 | TEMP. *** 1e+03 k |
| (NSR) XX REST/ | ART: MASS FLOW RA | TE = 2.80000E+02 G/ | S, TEMPERATURE | = 2.35031E+03 K > | 3 | |
| | | | | | | |
| (NSR) XXX FOR Mass fldi | CONV. NO. 1, C N RATE = 2.80000 | ONVERGED TEMP. (AFTE E+02 G/S, TEMPER | R 13 ITERATIONS) ATURE ≢ 2.39895E+ | LS GREATER THAN OR D3 K, PREVIOUS | EQUAL TO THE PREVIOUS Temperature = 2.3503 | TEMP. XXX 1e+03 k |
| (WSR) XX REST | ART: MASS FLOW RA | TE = 5.60000E+02 8/ | S, TEMPERATURE | = 2.35031E+03 K 3 | (¥ | |
| WELLST | IRRED REACTOR CA | LCULATION GLOBAL Initial State | TEST CASE: CHANGE | AND ADD GLOBAL AND Inal state | MOLECULAR REACTIONS FINAL/INITIAL RATIO | CASE 2 |
| PRESSUR TEMP: ENTROPY DENSTY ENTHALP SP. HALP NOL. WT GAMMA | E ATM DEB K Câl/Gm/K Gm/Cm/xx3 Y Cal/Gm T (CP) Cal/Gm/k . OF MIXT | 5 56000 800.800 1.80111 2.501735-03 92.3468 3.129485-01 29.8592 1.2701 | 3 | 5.50000 2322.08 2.25758 .08713E-04 92.3468 .75502E-91 28.0169 1.2329 | 1.00000 2.90260 1.25344 0.32326 1.00000 4.19989 | |
| SPECIES | | MOLE FRACT | MASS FRACT | MOLE FRACT | MASS FRACT | |
| 8 H20 0H H 02 H02 H02 C0 C0 C0 C0 C0 C0 C0 C0 C0 C0 C0 C0 C0 | 508.09¢ CM | 0.00000E+00 0.0000E+00 0.0000E+00 1.97112E-01 0.0000E+00 0.0000E+00 0.00000E+00 2.82264E-04 7.34744E-01 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 3.7349E-02 8.7369E-03 8.7689E-03 8.7689E-03 | 6.00000E+00 0.0000E+00 2.11236E-01 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 4.16032E-04 6.89288E-01 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 8.0000E+00 1.17317E-02 560.000 GH | 6.87192E-04 1.43809E-01 4.89021E-03 1.11930E-03 5.94161E-03 8.82955E-06 4.21885E-07 2.50038E-02 8.69366E-02 6.87537E-01 4.51698E-04 3.22787E-03 8.69793E-03 1.56204E-02 8.22787E-03 | 3.92430E-04 9.24711E-02 2.96854E-05 1.35318E-02 4.27496E-04 1.04021E-05 5.1220E-07 2.29985E-02 1.36563E-01 6.87452E-01 4.83769E-04 2.99047E-03 3.35335E-03 2.45852E-02 1.17317E+02 | |
| MDOT/YOL | UNE = 1.120 | DO RESIDENCE TIME = | 0.722 1 | SEC ITERATIONS = | 14 | |
| HELLST | IRRED REACTOR CA | LCULATION GLOBAL INITTAL STATE | TEST CASE: CHANGE | AND ADD GLOBAL AND Thal statf | NOLECULAR REACTIONS | CASE 2 |
| PRESSUR TEMP. ENTROPY DENSITY ENTHALP SP. HEA MOL. WT GARMA | E ATM DEG K CAL/GM/K GM/CH*X3 Y CAL/GM/K T (CP) CAL/GM/K . OF MIXT | 5.50000 800.000 1.80111 2.50173E-03 92.3468 3.12948E-01 29.8592 1.2701 | | 5,5000 1955.97 2,18426 ,72001E-04 92,3468 ,69334E-01 28,3646 1,2341 | 1.00000 2.44496 1.21273 0.38853 1.00000 1.18018 | |

| TABLE A.3.—Co | oncluded |
|---------------|----------|
|---------------|----------|

| SPECIES | NOLE FRACT | MASS FRACT | MOLE FRACT | MASS FRACT |
|----------------|--------------------------|----------------|--------------|-------------|
| 0 | 0.00000E+00 | 0.0000E+00 | 1.13807E-03 | 6.41940E-04 |
| H20 | 0.00080E+00 | 0.00000E+00 | 1.15773E-01 | 7.35311E-02 |
| OH | 0.00000E+00 | 8.0000E+00 | 3.95050E-03 | 2.36870E-03 |
| н | 0.80000E+80 | 0.00000E+00 | 4.24100E-04 | 1.50709E-05 |
| 02 | 1.97112E-01 | 2.11236E-01 | 4.598555-02 | 5.18773E-02 |
| H2 | 0.00000E+00 | 9.00000E+00 | 1.20109E-03 | 8.53581E-05 |
| HOZ | 0.00000E+00 | 0.00000E+00 | 3.05287E-05 | 3.55250E-05 |
| H202 | 0.00000E+00 | Q.00800E+D0 | 2.20101E-06 | 2.63944E-06 |
| CO | 0.00000E+00 | 0.00000E+D0 | 7.41554E-03 | 7.32294E-03 |
| C02 | 2.82264E-04 | 4.16032E-04 | 7.70176E-02 | 1.19499E-01 |
| N2 | 7.34704E-01 | 6.89288E~01 | 6.97275E-01 | 6.88642E-01 |
| NO | 0.00000E+00 | 0.00000E+00 | 6.77813E-04 | 7.17039E-04 |
| CN | 0.00000E+00 | 0.00000E+00 | 6.29312E-04 | 5.77242E-04 |
| CH2 | 0.00000E+00 | 0.00000E+00 | 1.83603E-02 | 9.07948E-03 |
| C3H8 | 5.91335E-82 | 8.73286E-02 | 2.17887E-02 | 3.38732E-02 |
| AR | 8.76890E-03 | 1.17317E-02 | 8.32998E-03 | 1.17317E-02 |
| VOLUME 500.000 | CMXX3 MASS FLO | 1518.00 GM/SEC | | |
| MDOT/VOLUME = | 3.02000 RESIDENCE TIME = | 0.322 MSEC | ITERATIONS = | 3 |

(WSR)

CONV. NO. = 21 NO. ITERATIONS = 3 MASS FLOW RATE = 1.56000E+03 G/S TEMPERATURE = 1.92269E+03 K RESIDENCE TIME = 3.17559E-04 S Nellstirred reactor calculation... Global test case: change and add global and molecular reactions case 2

| | | | INITIAL STATE | | FINAL STATE | FINAL/INITIAL RATIO |
|-------|---|---|--|--|--|---|
| | PRESSURE TEMP. ENTROPY DENSITY ENTHALPY SP. HEAT MOL. WT. 1 GAMMA | ATM DEG K CAL/GM/K GM/CMXX3 CAL/GM CP) CAL/GM/K DF MIXT | 5.50000 800.000 1.80111 2.50173E-03 92.3468 3.12948E-01 29.8592 1.2701 | | 5.50000 1478.52 2.16364 1.01711E-03 92.3468 3.67837E-01 28.5056 1.2338 | 1.00000 2.34815 1.20128 0.40656 1.00000 1.17539 |
| | SPECIES | | NOLE FRACT | MASS FRACT | MOLE FRACT | MASS FRACT |
| | 0 H20 OH H2 H2 H202 CD CD CD CD CD CD CD CD CD CD CD CD CA NC CA SH8 AR | | C.00000E+00 0.00000E+00 0.00000E+00 1.97112E-01 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 2.82264E-04 7.34704E-01 0.00000E+00 0.0000E+000E+ | $\begin{array}{c} 0.00000E+00\\ 0.00000E+00\\ 0.00000E+00\\ 0.00000E+00\\ 2.11236E-01\\ 0.00000E+00\\ 0.00000E+00\\ 0.00000E+00\\ 0.00000E+00\\ 4.16032E-04\\ 6.89283E-01\\ 0.00000E+00\\ 0.0000E+00\\ 0.0000E+0\\ 0.$ | 1.18240E-03 1.07409E-01 3.47916E-03 5.66938E-02 6.34489E-04 3.34605E-05 2.93797E-06 5.47125E-03 7.26205E-02 7.00907E-01 6.48177E-04 3.354835E-04 1.72462E-02 2.46516E-02 8.37140E-03 | 6.63646E-D4 6.78813E-02 2.07577E-03 1.10465E-05 6.36412E-02 4.486846-05 3.87439E-05 3.87439E-05 3.50576E-06 5.37620E-03 1.2119E-01 6.82804E-01 6.82296E-04 3.06203E-04 3.8634E-02 3.81342E-02 1.17317E-02 |
| | VOLUME 5 | 0.000 CM | EX3 MASS FLO | 1610.00 | GM/ SEC | |
| | MDOT/VOLUNI | ≣ = 3.2200 | 0 RESIDENCE TIME = | 0.316 | MSEC ITERATIONS | = 4 |
| (NSR) | XXX 75 I | ERATIONS DID N | NDT SATISFY CONVERGEN | CE REQUIREMENTS DE+03 G/S TE | XXX MPERATURE = 1.8543 | 8E+03 K |
| | PSR : | OLUTION ABANDO | NED | | | |

ITERATION NUMBER: 75 CURRENT TEMPERATURE = 1854.38 K CURRENT MDOT = 1.66000E+03 G/S I WCID TZ(1) -0.18179E-02 0.75625E-02 -0.29014E-02 0.81588E-02 -0.88945E-03 -0.10227E-01 -0.29400E-04 -0.16762E-02 0.18781E-01 -0.25667E-02 0.81832E-02 -0.14576E-01 12345

| | 0.142/05 01 | -0.00745 |
|---|--------------|----------|
| 6 | -D.10196E-01 | -0.10227 |
| 7 | -0.25369E-04 | -0.29400 |
| | | |

TABLE A.4.—COMPUTED RESULTS FOR TEST CASE 3 (PROPANE-AIR PSR PROBLEM OF CASE 2 WITH ADDED MOLECULAR REACTIONS IN MECHANISM)

** DATA LINES **

GLOBAL TEST CASE; ADD MOLECULAR REACTIONS TO PREV. CASE CASE 3 ADD &rtype global=.true.,gronly=.false., gladd = .false., glchng = .false., mrprev = .false., mrchng = .false., mradd=.true., & end H2 + 02 = 0H + 0H 1.7E+13 0. 47780. 0 + H202 = 0H + H02 8.0E+13 0. 1000. END - BLANK LINE -C3H8 AMSPROB DELMD= 50., DOTMAX= 1800.,MPR=2, VOLUME= 500., aEND &start t= 800.,p=5.5, mdot= 450., eratio = 1.5, scc = 3.0, sch = 8.0, & end FINIS

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

GLOBAL TEST CASE; ADD MOLECULAR REACTIONS TO PREV. CASE CASE 3

| REACTION | | | | REACTI | ON | | | REACTION RAT | E VARIABLES | |
|------------|-------|---|-----------|--------|--------|---|--------|--------------|-------------|------------|
| NUMBER | | | | | | | | A | N | ACTIVATION |
| 1 | 1×0 | + | 1×H20 | = | 2×0H | | | 6.80000E+13 | 0.0000 | 18365.00 |
| 2 | 1×H | + | 1×02 | = | IXOH | + | 1×0 | 1.8900DE+14 | 0.0000 | 16400.00 |
| 3 | 1×0 | + | 1×H2 | ¥ | 1 808 | + | 188 | 4.2000DE+14 | 0.0080 | 13750.00 |
| 4 | 1×H | + | 1×H02 | = | 1×H2 | + | 1×02 | 7.28000E+13 | 0.0000 | 2126.00 |
| 5 | 1¥9 | + | 1×H02 | 2 | 1 808 | + | 1#02 | 5.00000F+13 | 0.0000 | 1000.00 |
| 6 | 1×H02 | ÷ | 1 × 0 H | = | 1 ¥H20 | + | 1 #02 | 8.00000F+12 | 0.0000 | 0.00 |
| 7 | 1×H | + | 1*802 | = | 2308 | | | 1.34800E+14 | 0.0000 | 1070.00 |
| 8 | 1×H2 | + | 1×H02 | = | 1×H202 | + | 188 | 7.91000E+13 | 0.0000 | 25008.00 |
| 9 | 1×0H | + | 1×H202 | = | 13820 | + | 18802 | 6.10000E+12 | 0.0000 | 1430.00 |
| 10 | | | 2×H02 | Ŧ | 1×H202 | + | 1802 | 1.80000E+12 | 0.0000 | 0.00 |
| <u>ī</u> 1 | 1×H | + | 1×H202 | = | 1 XOH | + | 13820 | 7.80000F+1) | 0.0000 | 0.00 |
| 12 | - H | + | 1×H202 | = | 2408 | | 2-7120 | 1 66000F+17 | 0.0000 | 45510.00 |
| 13 | 1×H2 | ÷ | 1×0H | × | 11120 | + | 138 | 4.74808F+13 | 0.0000 | 6098.00 |
| 14 | 188 | + | 1+02 | = | 1¥H02 | + | M | 1.46000E+15 | 0.0000 | -1008.00 |
| 15 | M | ÷ | 1 8 8 2 0 | = | 1 88 | ÷ | าะกิห | 1.30000F+15 | 0,0000 | 105140.00 |
| 16 | 1×H | + | 1×0 | = | 1308 | ÷ | M | 7.10000F+18 | -1.0000 | 0.00 |
| 17 | M | + | 1×H2 | = | 281 | | | 2.20000E+14 | 0.0000 | 96000.00 |
| 18 | M | + | 1×02 | = | 230 | | | 1.80000E+18 | -1.0000 | 118020.00 |
| 19 | 1×0 | + | 180 | > | 1*C02 | | | 8.43000F+09 | -0.0010 | 1000.00 |
| 20 | | | 1*002 | > | 1¥C0 | + | 180 | 9.08000F+18 | -1.8400 | 130754.00 |
| 21 | 1 XH2 | + | 1802 | 2 | 2408 | | | 1 70000F+13 | 0.0000 | 47780.00 |
| 22 | 1×0 | + | 1×H202 | Ξ | 1×0H | + | 1×H02 | 8.00000E+13 | 0.0000 | 1000.00 |

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

| MCH2 | , 12) = 2.30000 | M(02 | , 12) = 0.78000 | MCH20 | , 12) = 6.00000 | M(H202 | , 12) = 6.60000 |
|------|-----------------|------|-----------------|-------|------------------|--------|-----------------|
| M(02 | , 14) = 1.30000 | MCN2 | , 14) = 1.30000 | MCH20 | , 14) = 21.30000 | M(H2 | , 14) = 3.00000 |
| M(H2 | , 15) = 4.00000 | M(02 | , 15) = 1.50000 | MCH20 | , 15) = 20.00000 | M(N2 | , 15) = 1.50000 |
| M(H2 | , 17) = 4.10000 | M(02 | , 17) = 2.00000 | M(H2O | , 17) = 15.00000 | M(N2 | , 17) = 2.00000 |

| XXX | GLOBAL | REACTIONS | XXX |
|-----|--------|-----------|-----|
|-----|--------|-----------|-----|

| NUMBER | | | | | RE | ACTION | | | | | | | | |
|---|--------|-----------|--|--------------|---|--|---|-------------------------|----------------|---|--------|--|----|---|
| 23 24 25 27 28 27 28 31 33 34 33 34 33 34 33 34 5 36 | 1.0×0H | ÷ | 1.0%H20 1.0%C02 1.0%C02 1.0%N2 1.0%N2 1.0%CH 2.0%CH2 1.0%CH2 1.0%CH2 1.0%CH2 1.0%H2 1.0%H2 1.0%H2 1.0%H20 | ÷+++ +++++++ | 1.0×0 1.0×H20 1.0×H2 2.0×H2 1.0×02 2.0×N0 1.0×N2 1.0×N2 1.0×02 1.0×02 2.0×0H 1.0×02 1.0×02 1.0×0 | >>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>> | 1.0×H2 1.0×C02 1.0×C0 2.0×N0 1.0×N2 1.0×N2 1.0×C0 2.0×CN 1.0×C0 2.0×CN 1.0×C0 2.0×CH 2.0×CH 1.0×H20 1.0×H20 | | *** ***** *** | 1.0*02 1.0*H2 1.0*H20 1.0*C0 1.0*C0 1.0*N2 2.0*H2 1.0*H2 1.0*H2 1.0*H2 1.0*C3 1.0*C4 1.0*C3 1.0*C4 1.0*C4 1.0*C0 | + + | 1.0×0 1.0×0H | | |
| REACTION | | | REACTANT EXPONENTS | | | | | REACTION RATE VARIABLES | | | | ES | | |
| 23 25 26 27 28 29 31 32 31 32 34 35 35 | | | 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 0.150 0.000 1.000 | | 1.000 1.000 1.000 2.000 1.000 1.000 1.000 0.500 0.500 0.100 1.000 1.000 | • | | | 41442815311194 | 90000E+10 30000E+05 41000E+05 0000E+14 30000E+11 30000E+11 25000E+12 0000E+12 0000E+07 10000E+12 0000E+06 60000E+10 | | 8.1800 1.3100 0.1900 0.0300 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.1800 | ĩ | ENERGY -510.00 -7000.00 3527.00 10000.00 38000.00 0.00 54000.00 41000.00 4000.00 4000.00 1013.00 |
| | XX | NEW INPUT | DATA GIVEN I | N CO | S UNITS | XX | | ¥X | OUTPL | IT REQUIRED | IN CG | S UNITS | жx | |

TABLE A.4.—Continued.

** ASSIGNED VARIABLE PROFILE **

WELL - STIRRED REACTOR CASE

VOLUME OF REACTOR = 5.00000E+02 CMXX3 MASS FLOW RATE TO START ITERATION = 4.50000E+02 G/S

ASSIGNED MASS FLOW RATE PROBLEM: MASS FLOW RATE INCREMENT = 5.00000E+01 G/S Maximum Mass Flow Rate = 1.80000E+03 G/S

FUEL-AIR REACTION, FUEL-AIR EQUIVALENCE RATIO = 1.5000 OXYGEN FRACTION IN AIR = 0.2095

NUMBER OF REACTING SPECIES: 15 NUMBER OF INERT SPECIES: 1 ** INITIAL CONDITIONS **

| TIME | 0.00000E+00 | SEC | AREA | 0.00000E+00 | SQ CM | AXIAL POSITION | 8.00000E+00 CM |
|------|-------------------------------|------------------|------|-------------|-------|------------------------|----------------|
| FL | OW PROPERTIES | | | | | INTEGRATION INDICATORS | |
| | PRESSURE | 5.5000 | 0 | | | STEPS FROM LAST PRINT | 0 |
| | VELOCITY | 0.00 | | | | AVERAGE STEP SIZE | 0.00000E+00 |
| | DENSITY (G/CMXX3) | 2.50173E-03 | | | | METHOD ORDER | 0 |
| | TEMPERATURE (DEG K) | 800.00 | | | | | |
| | MASS FLOW RAT | E 4.50000E+02 | | | | TOTAL NUMBER OF STEPS | 0 |
| | ENTROPY | 1.8011 | | | | FUNCT EVALUATIONS | 0 |
| | MACH NUMBER | 0.0000 | | | | JACOBIAN EVALUATIONS | 0 |
| | GAMMA | 1.2701 | | | | | |
| | ENTHALPY | 9.23468E+01 | | | | | |
| | SP. HEAT (CP) (CAL/G/DEG K | 3.12948E-01) | | | | | |

CHEMICAL PROPERTIES

| SPECIES | CONCENTRATION (MOLES/CM**3) | MOLE FRACTION | NET SPECIES PRODUCTION RATE (MOLE/CMXX3/SEC) | REACTION NUMBER | RATE CONST CGS UNITS | NET REACTION CONV RATE (MOLE-CMXX3/GXX2/SEC) | NET RATE/POSI- TIVE DIR RATE |
|---------|--------------------------------|---------------|---|--------------------|--------------------------|---|---------------------------------|
| 0 | 0.00000E+80 | 0.00000E+00 | 3.57838E-26 | 1 | 6.5377E+08 | 0.0000E+00 | 0.0000 |
| H20 | D.00000E+00 | 0.00000E+00 | 0.0000E+00 | 2 | 6.2545E+09 | 0.00000E+00 | 0.00000 |
| OH | 0.00000E+00 | 0.00000E+00 | 9.11685E-08 | 3 | 7.3608E+10 | D.00000E+00 | 0.00000 |
| H | 8.00000E+00 | 0.00000E+00 | 0.0000E+00 | 4 | 1.9113E+13 | 0.000002+00 | 0.00000 |
| 02 | 1.65148E-05 | 1.97112E-01 | -4.55842E~08 | 5 | 2.6655E+13 | 0.000B0E+00 | 0.00000 |
| H2 | 0.00000E+00 | 0.0000CE+00 | 0.00000E+00 | 6 | 8.0000E+12 | 0.0000E+00 | 0.00000 |
| HO2 | 8.0000E+00 | 0.00000E+00 | 0.00000E+00 | <u> </u> | 6.83592+13 | D.UUUUUE+00 | 0.00000 |
| H202 | 0.00000E+00 | 0.00000E+00 | 0.000002+00 | õ | 1.1/082+0/ | 0.000000000 | 0.00000 |
| CB | 0.000002+00 | 0.80080E+00 | 1.861635-30 | | 2.48135+12 | 0.000002+00 | 0.00000 |
| COZ | 2.369935-08 | 2.822646-04 | -1.861632-30 | 10 | 1.800000412 | 0.0000000000 | 0.00000 |
| NZ | 6.13366E-U3 | 7.34/046-01 | ~2.365492-22 | 11 | 7.0000ETII E 71/7E+0/ | 0.0000000000 | 0.00000 |
| | 0.0000000000 | 0.00000000000 | 4.770776-22 | 12 | 1 02205412 | B 00000E+00 | 0.00000 |
| CHA | 0.000002700 | 0.00000000000 | 1 367635-07 | 10 | 2 73976416 | 0 00000000000 | 5.00000 |
| C749 | 6 05665E-06 | 5 01335E-02 | -6 552625-02 | 12 | 2 6606E-16 | 0 00000E+00 | 0.00000 |
| | 4.93443E~00 7 36606E-87 | \$ 76\$90E-03 | 8 80008F+00 | 16 | \$ \$750F+15 | 8 888885+68 | 1 10000 |
| AK | 1.340706-01 | 0.700902-03 | 0.000002+00 | 17 | 1 3075F-12 | 0 0000000000 | 2 00000 |
| | | | | 18 | 1,2901F-17 | 2.85221F-21 | 1,00000 |
| | | | | iğ | 6 6661F+09 | A. 00000E+00 | 0.0000 |
| | | | | 20 | 7.8718F-23 | 2.97450F-25 | 1.00000 |
| | | | | 21 | 1.5051E+00 | 0.000008+00 | 0.00000 |
| | | | | 22 | 4.2648E+13 | 0.00008E+00 | 0.00000 |
| | | | | 23 | 2.2495E+11 | 0.00000E+00 | 0.00000 |
| | | | | 24 | 6.7500E+10 | 0.00000E+00 | 0.00000 |
| | | | | 25 | 1.7080E+10 | 0.00000E+00 | 0.00000 |
| | | | | 26 | 2.3465E-13 | 3.81152E-17 | 1.00000 |
| | | | | 27 | 8.3160E+00 | 0.00000E+00 | 0.00000 |
| | | | | 28 | 8.3000E+11 | 0.0000E+00 | 0.0000 |
| | | | | 29 | 1.2500E+12 | 0.0000E+00 | 0.00000 |
| | | | | 30 | 8.8483E-02 | 0.00000E+00 | 0.0000 |
| | | | | 31 | 1.5071E+06 | 8.00000E+00 | 0.00000 |
| | | | | 32 | 6.9297E+80 | 7.28341E-03 | 1.00000 |
| | | | | 33 | 3.9081E-14 | 0.0000E+00 | 0.0000 |
| | | | | 34 | 1.5992E+05 | 0.0C0C0E+00 | 0.0000 |
| | | | | 35 | 2.6015E+11 | 0.0000E+00 | 0.0000 |
| | | | | 36 | 2.2495E+11 | 0.00000E+00 | 0.00000 |
| MIXTUR | E MOLECULAR WEIGH | T 29.85916 | TOTAL ENERGY EXCHANGE (CAL-CM**3/G**2/SE | E RATE EC) | 3.39759E-16 | MASS FRACTION SUM | 1.0000000 |

TABLE A.4.—Continued.

CPU TIME FOR INITIALIZATION OF LSENS = 0.216667 S **EQUILIBRIUM CONDITIONS **

| TIME | 0.00000E+00 | SEC | AREA | 0.00000E+00 | SQ CM | AXIAL POSITION | 8.08000E+00 CM |
|------|--------------------------------|----------|-----------|-------------|-------|------------------------|----------------|
| F | LOW PROPERTIES | | | | | INTEGRATION INDICATORS | |
| | PRESSURE | | 5.50000 | | | STEPS FROM LAST PRINT | 0 |
| | VELOCITY | | . 0.00 | | | AVERAGE STEP SIZE | 0.00000E+00 |
| | DENSITY (G/CMXX3) | 7.3 | 34828E-04 | | | METHOD ORDER | 0 |
| | TEMPERATURE | | 2350.31 | | | | |
| | MASS FLOW RATE | E 4.! | 50008E+82 | | | TOTAL NUMBER OF STEPS | 0 |
| | ENTROPY | 、 | 2.3604 | | | FUNCT EVALUATIONS | 0 |
| | MACH NUMBER | , | 0.0000 | | | JACOBIAN EVALUATIONS | 0 |
| | GAMMA | | 1.2641 | | | | |
| | ENTHALPY (CAL/G) | 9.2 | 23468E+01 | | | | |
| | SP. HEAT (CP) (CAL/G/DEG K) | 3.6 | 59088E-01 | | | | |

CHEMICAL PROPERTIES

| NIXTUR | E MOLECULAR WEIGH | T 25.76666 | TOTAL ENERGY EXCHANGE (CAL-CMXX3/GXX2/SE | E RATE C) | -2.09583E+06 | MASS FRACTION SUM | 1.00000010 |
|--|--|--|---|--|--|---|---|
| MIXTUR | E MOLECULAR HEIGH | T 25.76666 | TOTAL ENERGY EXCHANGE (Cal-cmxx3/gxx2/56 | 26 27 28 29 30 31 32 33 34 35 35 36 RATE | 2.5376±405 5.8546±407 8.3000±411 1.2500±412 4.7603±408 1.1999±407 1.6939±408 2.7300±-05 8.4084±405 3.5560±411 2.2102±411 -2.09583±406 | 1.600442-03 7.596055-04 2.46114E-05 4.50252E-04 1.17122E-03 2.37704E-05 5.07039E-03 1.86371E-14 2.55717E+02 2.13927E+00 3.61677E+02 MASS FRACTION SUM | 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.000000 1.0000000000 |
| | | | | 17 18 19 20 21 22 23 24 25 | 2.6038E405 8.1234E403 6.7526E+09 3.9510E400 6.1305E408 6.4581E+13 2.2102E+11 1.5172E+10 9.0570E+10 | -2.10296E-04 -2.35297E-10 8.45730E+00 9.28491E+00 -1.53826E-07 -1.40369E-03 3.61677E+02 3.53653E+05 3.70220E+05 | 0.00000 0.00000 1.00000 0.00000 0.00000 0.42297 1.00000 1.00000 1.00000 |
| OH H 22 H 22 H 22 C 22 C 22 C 22 C 22 N 20 C 23 N 20 C 3 H 2 C 3 C 3 C 3 C 3 C 3 C 3 C 3 C 3 C 3 C 3 | 1.53281E-08 3.72907E-08 2.11927E-10 1.73940E-06 3.90703E-13 7.348228E-14 3.10378E-06 1.80796E-05 2.64686E-09 7.34828E-14 7.34828E-14 7.34828E-14 2.15801E-07 | 5.37679E-04 1.30759E-03 7.43118E-06 6.09920E-02 1.37000E-08 2.57667E-09 1.08834E-01 4.44958E-02 6.33959E-01 9.28118E-05 2.57667E-09 2.57667E-09 2.57667E-09 7.56703E-03 | -3.22698E-04 2.13187E-07 3.89433E-04 -8.55659E-03 -1.12123E-07 2.33325E-05 8.96626E-03 -9.51429E-10 1.00844E-09 6.93592E-09 -2.73787E-09 0.00000E+00 | 3456789 1011234516 | 2.21146+15 4.0178E+13 8.0000E+12 1.0656E+14 3.7453E+14 1.6000E+12 7.8000E+11 8.4429E+12 1.2845E+13 1.8086E+15 2.1738E+05 3.0209E+15 | -6.59110E-04 1.43082E-06 7.03729E-09 1.29043E-07 2.24499E-06 1.99374E-01 -6.86707E-03 2.15231E-07 -2.90148E-03 -4.30001E+01 1.94110E-01 3.66684E-06 -5.10833E-04 2.93337E-06 | 0.0000 0.0000 0.0000 0.0000 0.0000 0.42297 0.42297 0.42297 0.42297 0.42297 0.42297 0.0000 0.00000 0.00000 0.00000 |
| SPECIES 0 H20 | CONCENTRATION (MOLES/CM**3) 2.17893E-10 4.05534E-06 | MOLE FRACTION 7.64039E-06 1.42200E-01 | NET SPECIES PRODUCTION RATE (MOLE/CMXX3/SEC) -2.50907E-04 8.69456E-03 | REACTIO NUMBER 1 2 | N RATE CONST CGS UNITS 1.3329E+12 5.6424E+12 | NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC) -7.60162E-04 -2.68460E-05 | NET RATE/POSI- TIVE DIR RATE 0.00000 0.00000 |

COMPUTATIONAL NORK REQUIRED FOR EQUILIBRIUM CALCULATION, NO. OF ITERATIONS = 12 CPU TIME = 3.333378E-02 S

INITIAL ESTIMATES (SIGMAS) AT TEMPERATURE = 2350.31 K:

| 0 | 2 965235-07 |
|------|-------------|
| ม้วถ | 5 51874F-A3 |
| 01 | 2 08505F-05 |
| 201 | E 076755-05 |
| n | 3.0/4/35-03 |
| 02 | 2.884032~07 |
| H2 | 2.36709E-03 |
| H02 | 5.31693E-10 |
| H202 | 1.00000E-10 |
| CO. | 4 22382F-03 |
| čůz | 1 726875-03 |
| 002 | 2 660745-03 |
| NZ | 2.460365-02 |
| NG | 3.60201E-06 |
| CN | 1.00000E-10 |
| CH2 | 1.000002-10 |
| C3H8 | 1.00000F-10 |
| AD | 2 03475E-04 |
| AK | 2.330736-04 |
TABLE A.4.—Continued.

| (WSR) | XXX FOR CONV. Mass flow rate | NO. 1, CONVE = 4.50000E+02 | RGED TEMP. (AFTE G/S, TEMPER | R 14 ITERATION ATURE = 2.3527 | (S) IS GREATER THAN (4E+03 K, PREVIO | OR EQUAL TO THE PRE DUS TEMPERATURE = 2 | VIOUS TEMP. *** 2.35031E+03 K |
|-------|---|--|--|--|--|--|----------------------------------|
| (WSR) | XX RESTART: M | IASS FLOW RATE = | 9.00000E+02 G/ | S, TEMPERAT | TURE = 2.35031E+03 | К жж | |
| | NELLSTIRRED RE | EACTOR CALCULATI | ONGLOBAL TE | ST CASE; ADD MO | LECULAR REACTIONS TO | PREV. CASE CAS | E 3 |
| | | | INITIAL STATE | | FINAL STATE | FINAL/INITIAL RAT | TIO |
| | PRESSURE TEMP. ENTROPY DENSITY ENTHALPY SP. HEAT (CP) MOL. WT. OF MI) GAMMA | ATM DEG K CAL/GM/K GM/CMXX3 CAL/GM CAL/GM/K (T | 5.50000 800.000 1.80111 2.50173E-03 92.3468 3.12948E-01 29.8592 1.2701 | | 5.50000 2217.39 2.23959 8.49004E-04 92.3468 3.73920E-01 28.0866 1.2334 | 1.00000 2.77173 1.24345 0.33937 1.00000 1.19483 | |
| | SPECIES | MOLE | FRACT | MASS FRACT | MOLE FRACT | MASS FRACT | |
| | 0 H20 OH H2 H2 H22 H202 CD CD CD CD CD CD CD CD CD CD CD CD CD | 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0 | 000E+00 000E+00 000E+00 112E-01 000E+00 000E+00 000E+00 000E+00 000E+00 000E+00 000E+00 000E+00 000E+00 000E+00 335E-02 890E-03 | 0.00000E+00 0.00000E+00 0.00000E+00 2.11236E-01 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 6.89288E-01 6.89288E-01 0.00000E+00 0.00000E+00 8.73286E-02 1.17317E-02 | 8.92493E-04 1.37250E-01 5.01543E-03 9.33721E-04 1.93856E-02 4.09560E-03 1.48347E-05 7.46335E-07 1.70515E-02 8.58796E-02 6.89512E-01 5.80529E-04 2.57135E-03 1.20367E-02 1.65318E-02 8.24834E-03 | 5.08405E-04 8.80343E-02 3.03700E-03 3.35094E-05 2.20858E-02 2.93945E-04 1.74334E-05 9.03859E-07 1.70052E-02 1.34568E-01 6.87716E-01 6.87716E-01 6.87716E-01 6.8194E-03 6.01129E-03 2.59551E-02 1.17317E-02 | |
| ١ | OLUME 500.000 | CM¥¥3 | MASS FLO | 900.000 G | M/ SEC | | |
| | MDOT/VOLUME = | 1.80000 RE | SIDENCE TIME = | 0.472 | MSEC ITERATIONS | = 13 'n PREV CASE - CAS | F 3 |
| | RELESITRED R | CACIOR GALCULAI | INITIAL STATE | | FINAL STATE | FINAL/INITIAL RA | TIO |
| | PRESSURE TEMP. ENTROPY DENSITY ENTHALPY SP. HEAT (CP) MOL. HT. OF MI GAMMA | ATM DEG K CAL/GM/K GM/CMXX3 CAL/GM CAL/GM/K XT | 5.50000 800.000 1.80111 2.50173E-03 92.3468 3.12948E-01 29.8592 1.2701 | | 5.50000 1991.29 2.19287 9.52978E-04 92.3468 3.69995E-01 28.3117 1.2341 | 1.00000 2.48912 1.21751 0.38093 1.00000 1.18229 | |
| | SPECIES | MOL | E FRACT | MASS FRACT | MDLE FRACT | MASS FRACT | |
| | 0 H20 OH H22 H22 H22 H202 C0 C02 N2 N2 N0 CH CH2 C3H8 AR | 9.0 9.0 9.0 9.0 9.0 0.0 0.0 0.0 0.0 0.0 | 0000E+00 0000E+00 0000E+00 0000E+00 0000E+00 0000E+00 0000E+00 0000E+00 0000E+00 2264E-04 4704E-01 0000E+00 0000E+00 0000E+00 0000E+00 1335E-02 6690E-03 | 0.00000E+00 0.00000E+00 0.00000E+00 2.11236E-01 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 4.16032E-04 6.89288E-01 0.00000E+00 0.00000E+00 0.00000E+00 8.73286E-02 1.17317E-02 | 1.10597E-03 1.19266E-01 4.13083E-03 4.74856E-04 4.15614E-02 1.47633E-03 2.92002E-05 1.85824E-06 8.30454E-03 7.88301E-02 6.95879E-01 6.75110E-04 8.20074E-04 1.84359E-02 2.06945E-02 8.31444E-03 | 6.25001E-04 7.58908E-02 2.48146E-02 1.69061E-05 4.69740E-02 1.05115E-04 3.40426E-05 2.23256E-06 8.21617E-03 1.22539E-01 6.88548E-01 7.15515E-04 9.13391E-03 3.22322E-02 1.17317E-02 | |
| | VOLUME 500.00 | 0 CMXX3 | MASS FLO | 1450.00 | SM/ SEC | | |
| | MDOT/VOLUME = | 2.90000 R | ESIDENCE TIME = | 0.329 | MSEC ITERATIONS | = 3 | |
| (HSR) | CONV. NO. = Mass flow rate Wellstirred r | 13 NO. ITER = 1.50000E+03 Eactor Calculat | ATIONS = 3 G/S TEMPERJ IONGLOBAL TE INITIAL STATE | ATURE = 1.9636 EST CASE; ADD MO | 5E+03 K RESIDENC Diecular reactions T Final State | CE TIME = 3.22616E O PREV. CASE CAS FINAL/INITIAL RA | -04 S Se 3 Atio |
| | PRESSURE TEMP. ENTROPY DENSITY ENTHALPY SP. HEAT (CP) MOL. HT. OF MI GAMMA | ATM DEG K CAL/GM/K GM/CM**3 CAL/GM CAL/GM/K XT | 5.50000 800.000 1.80111 2.50173E-03 92.3468 3.12948E-01 29.8592 1.2701 | | 5.50000 1932.21 2.17798 9.85460E-04 92.3468 3.68893E-01 28.4080 1.2340 | 1.00000 2.41526 1.20924 0.39391 1.00000 1.17877 | |

| SURE OPY ITY HALPY HEAT (CP WT. OF | ATM DEG K CAL/GM/K GM/CMXX3 CAL/GM) CAL/GM/K MIXT | 5.5000 800.000 1.80111 2.50173E-03 92.3468 3.12948E-01 29.8592 1.2701 | 5.50000 1932.21 2.17798 9.85460E-04 92.3468 3.68893E-01 28.4080 1.2340 | 1.80000 2.41526 1.20924 0.39391 1.00000 1.17877 |
|---|--|--|---|--|
| IA | | 1.2701 | 1.2340 | |

63

| SPECIES | MOLE FRACT | MASS FRACT | MOLE FRACT | MASS FRACT |
|---|---|--|---|--|
| 0 H20 DH H2 H02 H02 H02 C0 C02 N2 N2 N0 CH2 C3H8 AR | 0.00000E+00 0.0000E+00 0.0000E+00 1.97112E-01 0.00000E+00 0.0000E+00 0.0000E+00 2.82264E-04 7.34704E-01 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.00000E+00 5.91335E-02 8.76890E-03 | C.00000E+00 O.0000E+00 O.0000E+00 O.1236E-01 O.0000E+00 O.000E+00 O.000E+00 O.000E+00 O.000E+00 O. | 1.14023E-03 1.13272E-03 3.78700E-03 3.78700E-04 4.91890E-02 9.33964E-04 3.23518E-05 6.65623E-03 6.65623E-03 6.85928E-01 6.66088E-04 5.29466E-04 1.81714E-02 2.26247E-02 8.34272E-03 | 6.42178E-04 7.18329E-02 2.26702E-03 1.34370E-05 5.54067E-02 7.05307E-05 3.75890E-05 2.74093E-06 6.56308E-03 1.17454E-01 6.8698E-01 7.03560E-04 8.97238E-03 3.51192E-02 1.17317E-02 |
| VOLUME 500.000 | CMXX3 MASS FLD | 1550.00 GM/SEC | | |
| MDOT/VOLUME = | 3.10000 RESIDENCE TIME = | 0.318 MSEC | ITERATIONS = | 3 |
| (WSR) CONV. NO. = 15 MASS FLOW RATE = | NO. ITERATIONS = 4 1.60000E+03 G/S TEMPERAT | TURE = 1.89288E+03 # | RESIDENCE T | IME = 3.15163E-D4 S |

(WSR) *** 75 ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREMENTS *** MDOT = 1.65000E+03 G/S TEMPERATURE = 1.81754E+03 K PSR SOLUTION ABANDONED

| ITERATION NUMBER: | 75 | CURRENT | TEMPERATURE = | = 1817.54 K | CURRENT MDOT = | 1.65000E+03 G/S |
|-------------------|----|---------|---------------|-----------------|----------------|-----------------|
| | | I | NCD | TZ(1) | | |
| | | 1 | -0.36271E-0 | 02 -0.37634E-02 | | |

XX DATA LINES XX

1 2 3 4 5 6 7 8 CC 12345678901234567890123456789012345678901234567890123456789012345678901234567890

GLOBAL TEST CASE; INTEGRATION CASE WITH PREVIOUS MECHANISM; CASE 4 REPEAT Server global=.true., mrprev = .false., &end TIME C3H8 #prob rhocon = .true., print = 1.e-6, 2.0e-6, 3.0e-6, 3.5e-6, 4.0e-6, 5.e-6, weistr = .false., &end H2 .0573205 N2 .720502 C02 .0002768 02 .193301 C3H8 .02 AR .0085997 END &solver emax = 1.e-6, atolsp = 1.e-15, &end FINIS

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM

NASA LEWIS RESEARCH CENTER

GLOBAL TEST CASE; INTEGRATION CASE WITH PREVIOUS MECHANISM; CASE 4

| REACTION | | | | REACTI | ON | | | REACTION RAT | E VARIABLES | |
|----------|----------|----|--------|--------|---------|-----|-------|---------------|-------------|-----------|
| NUMPER | | | | | | | | A | n | ENERGY |
| 1 | 1×0 | + | 1×H20 | = | 2×0H | | | 6.80000E+13 | 0.0000 | 18365.08 |
| 2 | 1 XH | + | 1×02 | = | 1.808 | + | 180 | 1.89000F+14 | 0.0000 | 16400.00 |
| 3 | 1.80 | + | 1882 | = | TXOH | + | 1 8 1 | 4.20000F+14 | 0.0000 | 13750 00 |
| Ğ | 1 ## | ÷ | 1+102 | = | 1 # 1 2 | ÷ | 1102 | 7 280005+13 | 0 0000 | 2126 00 |
| 5 | 1*0 | ÷. | 14402 | = | าะกษ | ÷ | 1+02 | 5 000005+13 | 0.0000 | 1000 00 |
| ź | 18402 | ÷ | 1 100 | - | 1+120 | ÷ - | 1+02 | \$ 00000E+12 | 0 0000 | 1000.00 |
| ž | 120 | ÷ | 12402 | - | 2204 | • | 1-06 | 3 360005-16 | 0.0000 | 1070.00 |
| ź | 1+12 | ÷ | 18802 | = | 149202 | + | 1 24 | 7 010005414 | 0.0000 | 25000 00 |
| ă | 1 201 | | 124202 | _ | 1×120 | | 12402 | 6 30000E113 | 0.0000 | 1670 00 |
| 10 | 1.000 | • | 22102 | - | 120202 | - | 1×02 | 1 800005112 | 0.0000 | 1430.00 |
| 10 | 1 944 | | 1202 | - | 1×0202 | | 1802 | 1.00000000000 | 0.0000 | 0.00 |
| 11 | 170 | | 1×0202 | - | 1×00 | Ŧ | 1×120 | 7.000002+11 | 0.0000 | 0.00 |
| 12 | 1 | | 120202 | = | 2808 | - | | 1.44000E+1/ | 0.0000 | 45510.00 |
| 13 | TANS | + | 1404 | = | IXH2U | + | 171 | 4.74000E+13 | 0.0000 | 6098.00 |
| 14 | 188 | ÷ | 1×02 | z | 1XH02 | + | M | 1.46000E+15 | 0.0000 | -1000.00 |
| 15 | м | + | 1×H20 | = | 1×H | + | 1×0H | 1.30000E+15 | 0.0000 | 105140.00 |
| 16 | 1×H | + | 1×0 | = | 1×0H | + | M | 7.10000E+18 | -1.0000 | 0.00 |
| 17 | M | + | 1×H2 | * | 2×H | | | 2.20000E+14 | 0.0000 | 96000.00 |
| 18 | M | + | 1×02 | = | 2¥0 | | | 1.80000E+18 | -1.0000 | 118020.00 |
| 19 | 1×C0 | + | 1×0 | · > | 1×C02 | | | 8.43000E+89 | -0.0010 | 1000.00 |
| 20 | | | 1×C02 | > | 1¥CD | + | 1*0 | 9.08000E+18 | -1.8400 | 130754.00 |
| 21 | 1×H2 | + | 1×02 | = | 2×0H | | | 1.70000E+13 | 0.0000 | 47780.00 |
| 22 | 1×0 | + | 1×H202 | = | 1×0H | + | 1×H02 | 8.00000E+13 | 0.0000 | 1000.00 |

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

| MCH2 | , 12) = 2.30000 | MCOZ | , 12) = 0.78000 | MCH20 | , 12) = 6.00000 | M(H202 | , 12) = 6.60000 |
|------|------------------|------|-----------------|-------|------------------|--------|-----------------|
| M(02 | , 14) = 1.30000 | MCN2 | , 14) = 1.30000 | MCH2O | , 14) = 21.30000 | M(H2 | , 14) = 3.00000 |
| M(H2 | , 15) = 4.00000 | MC02 | , 15) = 1.50000 | M(H20 | , 15) = 20.00000 | M(N2 | , 15) = 1.50000 |
| M(H2 | ·, 17) = 4.10000 | MC02 | , 17) = 2.00000 | M(H2O | , 17) = 15.00000 | MCN2 | , 17) = 2.00000 |

XXX GLOBAL REACTIONS XXX

| NUMBER | | | | | REACT | ION | | | | | | |
|---|--------|--------|--|-----------------|--|--|---|---|--|-------|-----------------|----------------------|
| 23 25 26 28 29 31 32 33 34 5 36 | 1.0¥0H | ÷ | 1.0%H20 1.0%C0 1.0%C02 1.0%K02 2.0%CN 2.0%CH2 1.0%CH2 1.0%CH2 1.0%CH2 1.0%C2 1.0%C3H8 1.0%H20 | ++++ ++++ +++++ | 1.0×0 1.0×H20 1.0×H2 2.0×H2 2.0×H0 2.0×H0 1.0×H2 1.0×02 1.0×C3H8 1.0×C3H8 1.0×C2 2.0×0 1.0×0 | >>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>> | 1.0%H2 1.0%C02 2.0%N0 1.0%N0 1.0%N0 1.0%N0 1.0%C0 2.0%CN 1.0%C0 3.0%CH2 2.0%CH 1.0%H20 1.0%H20 1.0%H20 | + + + + + + + + + + + + + | 1.0×02 1.0×H2 1.0×H20 1.0×C0 1.0×C0 1.0×C2 2.0×H2 1.0×H2 2.0×H2 2.0×H2 1.0×H20 2.0×H4 1.0×C3H8 1.0×C3H8 1.0×C3 | + + | 1.0×0 1.0×0H | |
| REACTION | | | REACTANT EXP | ONEI | NTS | | | | REA | CTION | RATE VARIA | BLES |
| NUMBER | | REXP 1 | REXP 2 | | REXP 3 | | | | A | | N | ACTIVATION ENERGY |
| 23 | | 0.080 | 1.000 | | 1.000 | | | 4 | .90800E+10 | | 0.1800 | -518.00 |
| 24 | | 0.000 | 1.000 | | 1.000 | | | 1 | . 300000E+05 | | 1.3100 | -/000.00 |
| 25 | | 8.080 | 1.808 | | 1.000 | | | 4 | .00000E+14 | | 0.0300 | 100000.00 |
| 27 | | 0.000 | 0.000 | | 2.000 | | | 2 | .00000E+11 | | 0.0000 | 38000.00 |
| 28 | | 0.000 | 1.000 | | 1.000 | | | 8 | .30000E+11 | | 0.0000 | 0.00 |
| 29 | | 0.000 | 1.000 | | 1.000 | | | 1 | .25000E+12 | | 0.0000 | 0.00 |
| 30 | | 0.000 | 1.000 | | 1.000 | | | 2 | 5000002+13 | | 0.0000 | 54000.00 |
| 31 | | 0.000 | 1.600 | | 0.100 | | | 1 | 10000F+12 | | 0.0000 | 41000.00 |
| 33 | | 0.000 | 1.000 | | 1.000 | | | ī | .00000E+00 | | 0.0000 | 49080.00 |
| 34 | | 0.000 | 0.150 | | 1.000 | | | ī | .98000E+06 | | 0.0000 | 4000.00 |
| 35 | | 1.000 | 0.000 | | 1.000 | | | 9 | .60000E+11 | | -0.1000 | 1013.00 |
| 36 | | 0.000 | 1.000 | | 1.000 | | | 4 | .900082+10 | | 0.1200 | -510.00 |

TABLE A.5.—Continued.

** <u>New</u> Input data given in CGS Units **

XX OUTPUT REQUIRED IN CGS UNITS XX

** ASSIGNED VARIABLE PROFILE ** This is a constant density problem - an assigned variable is not required

> NUMBER OF REACTING SPECIES: 15 NUMBER OF INERT SPECIES: 1

NUMBER OF SPECIES ODE'S REQUIRED FOR THIS CASE: 15 TOTAL NUMBER OF ODE'S REQUIRED FOR THIS CASE: 16

INTEGRATION CONTROLS

INTEGRATION METHOD (MF): 21 MAXIMUM RELATIVE ERROR: 1.00000E-06 SPECIES ABSOLUTE ERROR: 1.00000E-15

MAXIMUM NUMBER OF STEPS ALLOWED FOR THE COMPLETE PROBLEM: 2000

** OUTPUT REQUIRED AT FOLLOWING 6 PRINT STATIONS **

| STATIO | N | TIME (SEC) |
|----------------------------------|---------|---|
| 1 2 3 4 5 6 ** | INITIAL | 1.00000E-06 2.00000E-06 3.00000E-06 3.50000E-06 4.00000E-06 5.00000E-06 CONDITIONS ** |

TIME 0.00000E+00 SEC

| FLOW PROPERTIES | | INTEGRATION INDICATORS | |
|--------------------------------|-------------|------------------------|-------------|
| PRESSURE | 5.50000 | STEPS FROM LAST PRINT | 0 |
| VELOCITY (CM/SEC) | 0.00 | AVERAGE STEP SIZE | 0.00000E+00 |
| DENSITY (G/CMXX3) | 1.16135E-03 | METHOD ORDER | 0 |
| TEMPERATURE (DEG K) | 1600.00 | | |
| MASS FLOW RATE (G/SEC) | 0.0000E+00 | TOTAL NUMBER OF STEPS | 0 |
| ENTROPY (CAL/G/DEG K) | 2.0791 | FUNCT EVALUATIONS | 0 |
| MACH NUMBER | 0.0900 | JACOBIAN EVALUATIONS | 0 |
| GAMMA | 1.2740 | | |
| ENTHALPY (CAL/G) | 3.72713E+02 | | |
| SP. HEAT (CP) (CAL/G/DEG K) | 3.33274E-01 | | |

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

CHEMICAL PROPERTIES

| SPECIES 0 H20 H2 H22 H02 H02 H02 C0 C02 N2 N2 C0 C02 N2 C0 C02 N2 C0 C02 N2 C0 C02 N2 C0 C02 N2 C0 C02 N2 C0 C02 N2 C0 C02 N2 C0 C02 N2 C0 C02 C02 C02 C02 C02 C02 C02 C02 C02 | CONCENTRATION (MOLES/CMXX3) 0.0000E+00 0.0000E+00 0.0000E+00 8.09779E-06 2.40128E-06 0.0000E+00 0.00000E+00 0.00000E+00 1.15957E-08 3.01834E-05 0.00000E+00 0.00000E+00 0.00000E+00 3.60260E-07 | MOLE FRACTION 0.0000E+00 0.0000E+00 0.00000E+00 1.93301E=01 5.73205E=02 0.00000E+00 0.00000E+00 0.00000E+00 2.76840E=04 7.20502E=01 0.00000E+00 0.00000E+00 0.00000E+00 2.00000E+00 3.59970E=03 | NET SPECIES PRODUCTION RATE (MOLE/CM*X3/SEC) -9.83591E-05 1.56676E-03 9.91942E-03 1.31087E-04 -4.99243E-03 -1.77620E-03 1.31080E-04 0.00000E+00 1.66512E-03 -2.67274E-09 5.34547E-09 0.00000E+00 1.45841E-02 -4.86135E-03 0.00000E+00 | REACTION NUMBER 2 3 4 5 6 7 8 9 10 11 12 12 12 12 12 12 14 15 16 15 16 17 18 20 21 22 23 | RATE CONST CGS UNITS 2.1085f+11 1.0872E+12 3.7302E+13 3.6507E+13 8.0000E+12 9.5708E+13 3.0432E+10 3.0432E+10 3.0432E+10 3.0432E+11 8.7496E+11 8.7496E+11 1.9996E+15 1.6960E+01 8.5187E-02 6.1098E+09 1.5933E+05 5.0583E+06 6.8411E+13 2.1707E+11 8.1707E+11 1.977E+12 1.977E+12 1.977E+12 1.977E+13 1.977E+13 1.977E+13 1.977E+14 1.977E+14 1.977E+14 1.977E+14 1.977E+14 1.977E+14 1.977E+14 1.977E+14 1.977E+14 1.977E+14 1.977E+14 1.977E+14 1.977E+14 1.977E+14 1.977E+14 1.977E+15 | NET REACTION CONV RATE (MOLE-CMXX3/GXX2/SEC) 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 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 2.64572E-03 2.14264E-05 0.00000E+00 1.36999E-07 7.29275E+01 0.00000E+00 0.00000E+00 | NET RATE/POSI- TIVE DIR RATE 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 1.00000 0.00000 1.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 |
|--|--|--|---|--|--|--|--|
| | | | | 23 24 | 2.1707E+11 1.8514E+10 | 0.00000E+00 0.00000E+00 | 0.00000 |

TABLE A.5.—Continued.

| | | 26 1.0 27 1.2 28 8.3 29 1.2 30 2.1 31 7.2 32 2.7 33 1.6 34 5.6 35 3.3 36 2.1 | 1935E+01 1.98168E-01 2897E+06 0.0000E+01 1000E+11 0.0000E+01 500E+12 0.0000E+01 034E+06 0.00000E+01 629FE+06 3.60441E+02 769E+06 3.60441E+02 1272E+05 0.0000E+01 380E+11 0.0000E+01 1707E+11 0.0000E+01 | 3 1.00000 0 0.00000 0 0.00000 0 0.00000 0 0.00000 0 0.00000 0 0.00000 0 0.00000 3 1.00000 0 0.00000 0 0.00000 0 0.00000 0 0.00000 |
|--|--|---|--|---|
| DERIVATIVES (CGS UNITS): T | -5.04396E+06 RH0 | 0.00000E+00 | | |
| MIXTURE MOLECULAR WEIGHT | 27.72230 TOTAL ENERGY EXCH (CAL-CM**3/G** | ANGE RATE 5.11257 2/SEC) | E+06 MASS FRACTION S | SUM 1.00000000 |
| TIME 1.0000DE-0 | CPU TIME FOR INITIALIZATION 06 SEC AREA 0.00 | OF LSENS = 0.833 1000E+00 SQ CM | 333 S Axial Position | 0.00000E+00 CM |
| FLOW PROPERTI | IES | INT | EGRATION INDICATORS | |
| PRESSURE | 5.58525 | s. | FEPS FROM LAST PRINT | 107 |
| (ATM) VELOCITY | 0.00 | A | VERAGE STEP SIZE | 0.94404E-08 |
| (CM/SEC) DENSITY | 1.16135E-03 | М | ETHOD ORDER | 5 |
| TEMPERATURE | E 1627.92 | | | |
| MASS FLOW F | RATE 0.00000E+00 | Ti | JTAL NUMBER OF STEPS | 107 |
| ENTROPY | 2.0928 | FI | JNCT EVALUATIONS | 128 |
| MACH NUMBER | R 0.0000 | ji | COBIAN EVALUATIONS | 13 |
| GAMMA | 1.2726 | | | |
| ENTHALPY (CAL/G) | 3.74490E+02 | | | |
| SP. HEAT (C (CAL/G/DEC | CP) 3.33980E-01 G K) | | | |
| | CHEMICAL | PROPERTIES | | |
| IPECIES CONCENTRATION (MOLES/CMXX3) NOLE 0 3.19217E-07 7.63 120 8.98284E-07 2.14 0H 3.16661E-07 9.45 02 7.32362E-06 1.75 H20 6.9396E-07 9.45 02 7.32362E-06 1.77 H21 1.14721E-06 2.77 H22 6.59396E-07 1.63 C0 5.46803E-10 1.33 C02 1.11953E-08 2.67 H202 3.01834E-05 7.21 H0 3.49233E-14 8.35 CN 9.2669F-13 2.22 CN2 1.42817E-03 3.41 CSH8 8.35033E-07 1.95 AR 3.60260E-07 8.61 | FRACTION NET SPECIES PRODUCTI RATE (MOLE/CMXXX/SE 3461E-03 3461E-03 1.53419E+00 34620-02 3.60541E+00 7348E-03 1.02544E+00 9446E-03 1.02544E+00 95156E-01 -3.09190E+00 4374E-02 -4.61715E+00 9149E-05 2.43739E-03 9149E-05 2.4372E-02 1.08272E-04 1.08272E-02 9234E-03 2.18022E-06 9234E-02 -5.16088E-03 1621E-03 0.00000E+00 | ON REACTION RATE ICO NUMBER COS 1 2.32 1.11 3 5.91 4.3.7 5 3.6 6 8.01 7 9.63 3.94 9.92 10 1.84 1.91 1.11 11 7.81 12 1.11 12 1.11 1.3 7.12 14 1.99 1.15 9.91 15 9.92 1.6 5.5 22 5.6 6.00 24 1.65 2.21 2.4 20 3.12 2.11 2.4 21 2.6 1.65 2.25 6.00 26 1.8 3.52 3.24 3.54 23 2.25 6.00 2.81 3.1 7.46 32 3.1 7.46 3.2 3.44 3.2 3.57 34 5.77 3.54 5.77 3.55 | CONST NET REACTION CONV UNITS (MOLE-CM**3/G**2/) 180E+11 -2.67982E405 178E+12 1.63230E406 182E+12 1.17971E406 192E+13 7.31763E404 100E+12 1.23849E404 102E+12 1.88417E405 126E+13 -6.22012E403 100E+12 5.65545E401 100E+12 1.23849E404 100E+12 5.65545E401 100E+11 1.43173E+02 100E+11 1.43173E+02 100E+12 1.2522E+03 100E+11 1.43173E+02 184E+15 1.71340E404 164E+15 1.71340E+04 165E401 -8.12522E+03 1282E+00 -4.2463E404+02 128E400 -8.12522E+03 128E401 -1.66840E+02 128E401 -1.73509E+02 128E401 -1.73509E+02 128E405 3.67170E+01 15E+11 4.61673E+04 15E+11 3.005956= 108 | RATE NET RATE/POSI- SEC) TIVE DIR RATE 0.84410 0.63751 0.72556 0.99979 0.99997 0.99997 0.99997 0.99997 0.99979 0.99979 0.99979 0.99979 0.99979 0.99979 0.99979 0.99979 0.99979 0.99979 0.99979 0.99972 0.99972 0.99963 1.00000 |

27.77552 TDTAL ENERGY EXCHANGE RATE -4.19411E+1B (CAL-CM**3/G**2/SEC) MIXTURE MOLECULAR WEIGHT MASS FRACTION SUM 1.00000003

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 8.666668E-01 S UP TO THIS TIME - 8.666668E-01 S Negative concentration for species co

| FLOW PROPERIES INTEGRATION INDICATORS VESSURE (SSURE (CGVSEC) DESITY (CGVSEC) DESI |
|---|
| PRESSURE (NPT) VECONET) 6.07310 STEPS PRON LAST PRINT 5 VECONET) 0.00 AVERAGE STEP SIZE 0.10023E-06 DENSITY (COCONENT) 1.6013E-05 METHOD ORDER 5 VECONETY (COCONENT) 1.803.71 TOTAL NUMBER OF STEPS 206 MASS FLOM RATE 0.0000E+00 TOTAL NUMBER OF STEPS 206 ENTROPY (CAL/GO/DEG K) 2.1179 FUNCTIONS 225 GAMMA 1.2609 20000E+00 JACOBIAN EVALUATIONS 25 SPECIES CONCENTRATION NOLE FRACTION NOT (CAL/GO/DEG K) 3.40096E-01 20000E+00 10000E+00 JPECIES CONCENTRATION NOLE FRACTION NOT (CAL/GO/DEG K) 10100E/DEAS/CONCONT NET REACTION CONV, RATE |
| VELOCITY 0.00 AVERAGE STEP SIZE 0.10023E-06 (CATTOR) 1.16135E-03 METADO ORDER 5 (CATTOR) 1.16135E-03 METADO ORDER 5 (CATTOR) 1.16135E-03 METADO ORDER 5 (DEC TTOR) 1.16135E-03 METADO ORDER 5 (CAL/CD/DEC K) 0.000 JACOBIAN EVALUATIONS 246 (CAL/CD/DEC K) 0.000 JACOBIAN EVALUATIONS 25 MACH WOMBER 0.0000 JACOBIAN EVALUATIONS 25 (CAL/CD/DEC K) 0.000 JACOBIAN EVALUATIONS 25 (CAL/CD/DEC K) 0.000 METADO ORDER 5 (CAL/CD/DEC K) 0.000 METADO ORDER 5 (CAL/CD/DEC K) 0.000 JACOBIAN EVALUATIONS 25 (CAL/CD/DEC K) 0.000 METADO ORDER 5 SP. HEAT (CP) 3.40096E-01 (CAL/CD/DEC K) 0.0005 SP. HEAT (CP) 3.40096E-01 (CAL/CD/DEC K) 0.1201E-02 S 1.01261E-02 S 1.01261E MET RATE/ 0 4.1205E-07 1.01201E-02 S 1.01261E-02 S 1.0156E-03 ORDER 5 (MOLES/CMMAS) 0.0075E-02 S 1.01261E-02 S 1.0156E-03 ORDER 5 (MOLES/CMMAS) 0.0075E-03 S 1.01261E-02 S 1.0156E-03 ORDER 5 (MOLES/CMMAS) 0.0075E-03 S 1.01261E-03 ORDER 5 (MOLES/CMMAS) 0.0077E-03 S 1.0075EE-03 S 1.0075EE-03 S 0.0077EF-03 S 0.0077EF |
| DERSITY 1.16135E-05 METHOD ORDER 5 TOPECHAR3D 1889.71 10000 7000000000000000000000000000000000000 |
| TEMPERATURE 1889.71 MGDETON RATE 0.00000E+00 TOTAL NUMBER OF STEPS 206 GAMMA 1.2609 JACOBIAN EVALUATIONS 245 GAMMA 1.2609 JACOBIAN EVALUATIONS 25 GAMMA 1.2609 CAL/G-DEG K) CAL/G-DEG K) 25 GAMMA 1.2609 S.P. NEAT (CP) 3.40096E-01 CAL/G-DEG K) CHEMICAL PROPERTIES CHEMICAL PROPERTIES SPECIES CONCENTRATION NET SPECIES PRODUCTION REACTION COST UNITS (MELE-CHARS/GRAZ/SEC) NET REACTION CONV RATE (MELE/POSI- CAL/G-DEG K) NET REACTION REACTION REACTION REACTION CONV RATE (MELE/POSI- CAL/G-DEG K) NET REACTION COST UNITS (MELE-CHARS/GRAZ/SEC) NET REACTION CONV RATE (MELE/POSI- CAL/G-DEG K) NET REACTION COST UNITS (MELE-CHARS/GRAZ/SEC) NET REACTION CONV RATE (MELE/POSI- CAL/G-DEG K) NET REA |
| MSS FLOW RATE 0.00000E+00 TOTAL NUMBER OF SIEPS 206 PENTROPY 2.1179 FUNCT EVALUATIONS 248 ICAL/GO/DEG K) 0.0000 JACOBIAN EVALUATIONS 25 GAMMA 1.2609 ENTRALPY 3.910236402 SF, HEAT (CP) 3.40096E-01 CAL/GO/DEG K) 1.2609 CAL/GO/DEG K) NET SPECIES FROME NET REACTION NET REACTION VCLL/GO/DEG K) NET SPECIES PRODUCTION REACTION NET REACTION NET REACTION 0 4.66265E-07 1.01201E-02 -1.01451E-01 5.1155411 -1.404547640 0.20440 120 2.2228E-67 1.01201E-02 -2.34735E-02 4.1337640 0.20440 120 2.2228E-68 1.61356-03 4.1337640 0.20440 0.20840 120 2.2328E-69 1.6335E-03 1.84437E-02 2 3.8310E+13 4.1831E+04 0.99775 120 2.6323E-67 1.6335E-03 1.1346412 -7.43359E+02 0.99775 120 3.63265E-03 1.1346472 |
| COLL CLLTY FUNCT EVALUATIONS 246 MACH NUMBER 0.0000 JACOBIAN EVALUATIONS 25 OMMA 1.2609 ENTHALPY 3.91023E+02 5 SF. HEAT (CP) 3.40096E=01 CALCO SF. HEAT (CP) 3.40096E=01 CONCENTRATION MOLE FRACTION NET SPECIES PRODUCTION REACTION REACTION CONV. RATE NET RATE/POSI- 0 (162635C) 1.01201E=02 8.82441E=02 2 2.3973E+12 -2.30375E+03 0.203540 12 2.63224E=06 5.47339E=02 -3.3816E=02 3 1.0137E+13 4.3831E+04 0.203540 12 2.63224E=06 3.6300E=01 -3.3816E=02 3 1.0137E+13 4.3831E+04 0.99775 12 6.382390E=02 6 8.000E+12 -2.03493E+03 0.99775 12 6.38338E=01 -3.43165E=03 7 1.0173E+14 2.343640E+04 0.99775 12 6.38308E=03 -5.47249E=04 7 1.0173E+14 2.3435E+04 0.99775 12 7.63046E=03 |
| DRCH NUMBER 0.0000 JACUBIAN EFALUATIONS 23 OAHHA 1.2609 ENTHALPY 3.90235:402 (CAL70) (CAL70) (CAL70) S.40096E-01 SPECIES CONCENTRATION MOLE FRACTION HET SPECIES PRODUCTION REACTION RATE CONST NET REACTION CONV RATE NET REACTION CONV RATE NET REACTION NET REACTION 0 4.162655-07 1.01201E-02 1.01451E-01 1 5.1115E-11 7.40456E+04 0.20840 12 2.23224E-05 3.6379E-02 6.24241E-02 2 2.3017E+03 0.20840 14 2.26224E-05 1.01201E-02 1.01201E-02 2 2.3017E+03 0.20840 0.20840 14 2.25224E-05 3.6390E-04 -2.34635E-02 3 1.3297E+13 -8.6749E+04 0.99712 12 5.5038E-07 1.01264E-03 -5.47248E-04 1.0078E+14 2.05648E+04 0.99717 12 3.6390E-04 -2.34895E-02 6 8.1000E+12 6.05255E+03 0.99717 120 3.50381E-05 -5.47248E+04 |
| Difference Difference <thdifference< th=""> Difference Differen</thdifference<> |
| Intervention of the second sec |
| CHEMICAL PROPERTIES CHEMICAL PROPERTIES SPECIES CONCENTRATION NOLE FRACTION NET RATE CNOLE CONST NET REACTION CONV RATE NET RATE CNOLE CONST O A.16201E-02 2 2.3375E-12 CONCENTRATION NET RATE CNOLE CONST NET REACTION CONV RATE NET RATE/POSI- O A.16201E-02 2 2.3375E-12 CONCENTRATION NET RATE/POSI- NET RATE NET RATE/POSI- A.16305E-07 1.01201E-02 2 2.3375E-12 C.30157E-10 C.20840 A.160305E-01 - A.160305E-02 6 8.0007612 C.30157E-10 C.2000E-12 C.70295E-10 C.2000E-12 C.70295E-103 0 A.16076E-10 A.2000E-12 C.2000E-12 C.2000E-12 C.2000E-12 C.2000E-1 |
| CHEMICAL PROPERTIES SPECIES CONCENTRATION MOLE FRACTION NET SPECIES PRODUCTION REACTION RATE CMOLE/CHMAXJ/SEC/ NET REACTION NET REACTION NET SPECIES PRODUCTION REACTION NET REACTION <t< td=""></t<> |
| SPECIES CONCENTRATION MOLE FRACTION RET SPECIES PRODUCTION NUMBER RATE (MOLE/CNEX/SEC) RATE CONST NUMBER RATE CONST SUBSTREE NET REACTION CONV RATE NET RATE/POST NUMBER 0 4.16265E-07 1.01201E-02 -1.01451E-01 1 5.1115E+11 7.40454E+046 0.20324 0H 2.85226E-06 5.47555E-02 -3.33176E-02 3 1.0790E+13 -2.30157E+06 0.61815 0L 7.60826E-08 3.6390E-01 -3.78355E-02 4 4.1325E+13 8.36789E+03 0.99775 12 4.9662E-08 3.6390E-01 -2.34695E-02 6 8.0000E+12 6.05258E+03 0.99775 142 1.46637E-05 -5.47249E-04 7 1.0078E+14 2.05640E+04 0.99775 142 1.9662E-08 -8.6190E-05 8 1.01596+11 -7.4839E+02 0 9.99775 142 1.9664E-08 1.21596E+12 2.70299E+02 0.99775 0.99775 0.99775 0.99775 142 1.9666E-08 1.610272E-03 7.6206E+03 10 1.0078E+14 |
| 0H 2.88228E-07 7.00729E-03 -3.33176E-02 3 1.0790E+13 -8.06954E+04 0.41815 H 7.69813E-08 1.87154E-03 -3.78435E-02 4 4.1329E+13 4.18851E+04 0.99775 H2 1.49642E-08 3.63900E-04 -2.54895E-02 6 8.000E+12 6.05258E+03 0.99716 H22 3.5038E-09 8.63153E-05 -5.47249E-04 7 1.0078E+14 2.03640E+04 0.99717 H202 3.0885E-10 7.59948E-06 -6.4815E-05 8 1.0159E+11 -7.48349E+02 0.98240 C0 -3.59652E-08 -8.74372E-04 -4.33519E-03 9 4.1682E+12 2.70299E+02 0.98240 C0 -3.59652E-08 1.24837E-03 7.62006E-03 10 1.800E+12 1.40042E+01 0.83840 N2 3.01833E-05 7.33803E-01 -1.16996E-04 11 7.8090E+11 1.37509E+01 0.99995 N0 4.47375E-11 1.08764E-06 1.6505108E-05 12 7.8524E+11 -6.73256E+03 0.42348 CN 1.61437E-10 3.92479E-06 1.77681E-04 13 9.3439E+12 -6.89726E+04 0.69773 CH2 1.36053E-07 3.3076E-03 7.19063E-02 14 1.9055E+15 6.95112E+04 0.69773 CH2 1.36053E-07 3.3076E-03 7.19063E-02 15 8.99935E+02 -5.36371E+03 0.99997 AR 3.60260E-07 8.75849E-03 0.0000E+00 16 3.7772E+15 3.67714E+03 0.999997 22 5.72285E+10 -2.243455E+02 0.999997 19 6.4186E+00 -7.11586E+01 1.00000 20 6.4185E-07 -3.4738E+04 1.00000 20 6.4185E+02 -2.43455E+02 0.999997 22 5.72285E+10 4.1192547E-02 0.99999 23 2.1824E+11 1.51702E+05 1.0000 20 6.4185E+07 -8.47581E+00 0.69576 23 2.1824E+11 1.51702E+05 1.0000 20 6.4185E+07 -8.47581E+00 0.69576 22 6.1277E+13 5.7621E+04 1.00000 20 6.4185E+02 -2.43455E+02 0.999997 20 6.4185E+03 -2.43455E+02 0.999997 20 6.4185E+03 -2.43455E+02 0.999997 20 6.4185E+03 -2.43455E+01 1.00000 20 6.4185E+03 -2.43455E+03 0.99997 20 7.2285E+04 1.1957E+01 1.00000 20 6.4185E+03 -2.01346E+03 1.00000 20 6.4185E+03 -2.01346E+03 1.00000 20 7.8242E+01 4.00000E+00 0.00000 20 7.2382E+01 4.11957E+01 1.00000 20 6.425E+07 -8.4758E+03 1.00000 20 6.425E+07 -8.4758E+03 1.00000 2 |
| U2 b.39377E-06 1.60305E-01 1.68437E-02 5 3.8330E+13 4.18831E+14 0.797716 H22 3.55038E-09 8.63153E-05 -5.47249E-04 7 1.0078E+14 2.03640E+04 0.99716 H22 3.08835E-10 7.53948E-06 -6.48815E-05 8 1.0159E+11 -7.48349E+02 0.98240 C0 -3.59652E-08 -8.74372E-04 -4.33519E-03 9 4.1682E+12 2.70299E+02 0.98240 N2 3.01833E-05 7.33803E-01 -1.16996E-04 11 7.8000E+12 1.41042E+01 0.83840 N2 3.01833E-05 7.33803E-01 -1.16996E-04 11 7.8000E+11 -6.3236E+03 0.99998 N0 4.4637E-10 3.92479E-06 1.77681E-04 13 9.3439E+12 -6.89926E+04 0.69773 CN 1.61437E-10 3.92479E-06 1.77681E-04 13 9.3439E+12 -6.89926E+04 0.69773 CK2 1.36633E-07 1.92367E-02 -2.51229E-02 15 8.9935E+02 -5.36371E+03 0.99998 AR 3.60260E-07 8.75349E-05 0.00000E+00 16 3.7572E+15 3.67176E+03 0.99998 19 6.4186E+09 -7.11586E+01 1.00000 20 6.4186E+09 -7.11586E+01 1.00000 21 5.0648E+07 -8.4738E+02 0.99998 19 6.4186E+09 -7.11586E+01 1.00000 22 6.1237E+13 5.76218E+13 0.99998 19 6.4186E+09 -7.11586E+01 1.00000 23 2.1397E+01 -2.37434E+02 0.99998 19 6.4186E+09 -7.11586E+01 1.00000 20 6.4189E+03 2.44378E+04 1.00000 20 6.4186E+09 -7.11586E+01 1.00000 20 6.4186E+09 -7.11586E+01 1.00000 21 5.0648E+07 -8.47581E+00 0.69576 23 2.1237E+01 1.51702E+05 1.00000 24 1.9576E+01 1.9576E+03 1.00000 25 7.2235E+10 4.11927E+01 1.00000 26 1.3648E+03 2.01396E+01 1.00000 27 8.0530E+07 -8.65307E+01 1.00000 28 8.3000E+10 4.135702E+15 1.00000 29 1.2500E+12 6.69365E+03 1.00000 20 1.6432E+03 2.01396E+01 1.00000 20 2.8426E+07 8.65307E+01 1.00000 20 1.2500E+12 6.69365E+03 1.00000 20 1.2500E+12 6.69365E+03 1.00000 27 8.0530E+06 1.1927E+03 1.00000 28 8.3000E+11 4.13550E+01 1.00000 30 2.8426E+07 1.86272E+04 1.00000 31 9.2428E+06 2.3947F+03 1.00000 32 1.9936E+07 1.86272E+04 1.00000 33 2.1073E-06 1.54220E+13 1.00000 34 6.6422E+07 1.86272E+04 1.00000 35 2.1073E-06 1.54220E+13 1.00000 35 4.6422E+07 1.86272E+04 1.00000 35 4.6422E+07 1.86272E+04 1.00000 35 4.6422E+07 1.86272E+04 1.00000 35 4.6422E+05 1.777229E+049 1.00000 35 4.6422E+05 1.777229E+049 1.00000 35 4.6422E+05 1.777229 |
| H202 3.08835E-107 0.50134E-03 -2.747851E-03 7 10135E+11 -7.48339E+02 0.98420 C0 -3.59632E-08 -8.74372E-04 -4.33519E-03 9 4.1682E+12 2.70299E+02 0.98240 C02 5.13486E-08 1.24837E-03 7.62006E-03 10 1.8000E+12 1.41042E+01 0.83840 N2 3.01833E-05 7.33803E-01 -1.16996E-04 11 7.8000E+11 1.37509E+01 0.99995 N0 4.47375E-11 1.08764E-06 5.63108E-05 12 7.8524E+11 -6.73236E+03 0.42348 CN 1.61437E-10 3.92479E-06 1.77681E-04 13 9.3439E+12 -6.89926E+04 0.69773 CH2 1.36035E-07 1.92347E-02 -2.51229E-02 15 8.9993E+02 -5.36371E+03 0.99997 AR 3.60260E-07 8.75849E-03 0.0000E+00 17 1.7368E+03 -2.43455E+02 0.99999 18 2.1357E+01 -2.37434E+02 0.999999 18 2.1357E+01 -2.37434E+02 0.999999 19 6.4106E+09 -7.11586E+01 1.00000 20 6.4185E+05 2.44578E+04 1.00000 21 5.0648E+07 -2.44578E+04 1.00000 22 6.13648E+03 2.01457E+04 1.00000 23 2.1824E+11 1.51702E+05 1.0000E+00 0.00900E 23 2.1824E+11 4.13550E+01 1.00000 24 1.6428E+10 0.0000E+00 0.0000E+00 17 25 7.2285E+10 4.11927E+01 1.00000 26 1.3648E+03 2.01396E-01 1.00000 27 8.0500E+01 4.13550E+01 1.00000 26 1.3648E+03 2.01396E-01 1.00000 27 8.0500E+01 4.13550E+01 1.00000 26 1.3648E+03 2.01396E-01 1.00000 27 8.0500E+01 4.13550E+01 1.00000 28 8.3000E+12 4.6453E+03 0.98607 31 9.2428E+06 2.0395E+01 1.00000 31 9.2428E+06 2.3963E+03 1.00000 32 1.9936E+07 4.6452E+05 1.14725E+05 1.100000 33 2.1075E+06 1.54220E+05 1.100000 34 6.4222E+05 1.1775E+05 1.540220E+03 1.00000 35 2.1075E+05 1.54220E+05 1.1775E+05 1.00000 36 6.4224E+05 2.1775E+06 1.54220E+03 1.00000 37 8.0500E+00 31 9.2428E+00 2.0395E+07 4.65507E+01 1.00000 36 6.4224E+05 2.1775E+06 1.54220E+03 1.00000 37 9.2428E+06 2.39617E+03 1.00000 38 9.2428E+07 4.65507E+01 1.00000 39 1.9232E+057 1.86272E+04 1.00000 30 2.84226E+07 8.65507E+01 1.00000 31 9.2428E+05 2.1775E+06 1.54220E+03 1.00000 32 1.9936E+07 1.86272E+04 1.00000 33 2.1075E+05 1.5722E+05 1.17725E+05 |
| CO2 5.13482E=08 1.24857E=03 7.22062E=03 10 1.8050E+15 1.4052E+61 0.53860 N2 3.01833E=05 7.33803E=01 -1.16996E=04 11 7.8000E+11 1.37509E+01 0.99995 N0 4.47372E=11 1.08764E=06 5.63108E=05 12 7.8524E+11 -6.73236E+03 0.42348 CN 1.61437E=10 3.92479E=06 1.77681E=04 13 9.3439E+12 -6.89926E+04 0.98992 C3H8 7.91175E=07 1.92347E=02 -2.51229E=02 15 8.9993E+02 -5.36371E+03 0.99998 AR 3.60260E=07 8.75849E=03 0.00000E+00 16 3.7572E+15 3.6774E+03 0.99998 17 1.7368E+03 -2.43455E+02 0.999998 18 2.1357E+01 -2.37434E+02 0.999998 19 6.4106E+09 -7.11586E+01 1.00000 21 5.0648E+07 -8.47581E+00 0.69576 22 6.1297E+13 5.76218E+03 0.98676 22 6.1297E+13 5.76218E+03 0.98676 22 6.1297E+13 5.76218E+03 0.98676 24 1.6428E+10 0.0000E+00 0.09807 25 7.2285E+10 4.13550E+01 1.00000 26 1.3648E+03 2.01396E=01 1.00000 27 8.0580E+06 1.1976E=08 1.00000 28 8.3000E+11 4.13550E+01 1.00000 29 1.2500E+12 6.65507E+01 1.00000 29 1.2500E+12 6.65507E+01 1.00000 20 30 2.8426E+07 8.65507E+01 1.00000 20 31 9.2428E+07 1.86272E+04 1.00000 31 9.2428E+07 1.86272E+04 1.00000 33 2.1075E=06 1.59272E+03 1.00000 33 2.1075E=06 1.59272E+03 1.00000 34 9.936E+07 1.86272E+04 1.00000 35 2.1075E=06 1.59272E+05 1.000000 35 4.6428E+07 1.86272E+05 1.000000 35 4.000000000000000000000000000000000000 |
| N0 4.47375E-11 1.08764E-06 5.63108E-05 12 7.8524E+11 -6.75236E+03 0.42348 CN 1.61437E-10 3.92479E-06 1.77681E-04 13 9.3439E+12 -6.89926E+04 0.69773 CH2 1.36053E-07 3.03766E-03 7.19063E-02 14 1.9055E+15 6.95112E+04 0.98992 C3H8 7.91175E-07 1.92347E-02 -2.51229E-02 15 8.9993E+02 -5.36371E+03 0.99998 AR 3.60260E-07 8.75849E-03 0.0000E+00 16 3.7572E+15 3.61747E+03 0.99998 18 2.1357E+01 -2.37434E+02 0.99998 19 6.4189E-03 2.44355E+01 1.00000 20 6.4189E-03 2.443578E-04 1.00000 0.00000E 21 5.0648E+07 -8.43578E-04 1.00000 21 5.0648E+07 -8.43578E-01 1.00000 0.00000E 22 6.1297E+13 5.76218E+00 0.69576 22 6.1297E+13 5.76218E+01 0.00000 0.00000 24 1.6422E+11 1.51702E+05 1.00000 23 2.1824E+11 1. |
| CH2 1.36053E-07 3.30766E-03 7.19063E-02 14 1.9055E+15 6.95112E+04 0.98992 C3H8 7.9175E-07 1.92547E-02 -2.51229E-02 15 8.7993E+02 -5.36371E+03 0.99999 AR 3.60260E-07 8.75849E-05 0.0000E+00 16 3.7572E+15 3.67174E+03 0.99999 17 1.7368E+03 -2.43455E+02 0.99999 18 2.1357E+01 -2.37434E+02 0.99999 18 2.1357E+01 -2.37434E+02 0.99998 18 2.1357E+01 -2.37434E+02 0.99998 19 6.4185E+03 2.87581E+00 0.69576 22 6.1397E+15 5.75218E+03 0.98607 21 5.0648E+07 -8.47581E+03 0.98607 23 2.1824E+11 1.51702E+05 1.00000 23 2.1824E+11 1.51702E+01 1.00000 25 7.2285E+10 4.11927E+01 1.00000 24 1.6428E+03 2.01396E-03 1.00000 27 8.0580E+06 1.19276E+01 1.00000 25 7.2285E+10 4.11927E+01 1.00000 28 8.3000E+11 |
| AR 3.60260E-07 8.75849E-03 0.0000E+00 16 3.7572E+15 3.67174E+03 0.99998 17 1.7586E+01 -2.37434E+02 0.99999 18 2.1357E+01 -2.37434E+02 0.99999 18 2.1357E+01 -2.37434E+02 0.99999 18 2.1357E+01 -2.37434E+02 0.99999 19 6.4106E+09 -7.11586E+01 1.00000 20 6.4189E-03 2.44378E-04 1.00000 20 6.4189E-03 2.44378E-04 0.69576 22 6.1297E+13 5.76218E+03 0.98607 21 5.0648E+07 -8.47581E+00 0.00000 0.00000 24 1.6428E+11 1.51702E+05 1.00000 23 2.1824E+11 1.51702E+05 1.00000 25 7.2285E+10 4.11927E+01 1.00000 26 1.3648E+03 2.01396E-01 1.00000 29 1.2500E+11 4.13550E+01 1.00000 27 8.0580E+06 1.1927E+03 1.00000 29 1.2500E+12 6.69363E-03 1.00000 |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$ |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ |
| 20 1.3640E+02 2.04376E-08 1.00000 27 8.0580E+03 1.0576E-08 1.00000 28 8.3000E+11 4.13550E+01 1.00000 29 1.2500E+12 6.63550E+03 1.00000 30 2.8426E+07 8.65507E+01 1.00000 31 9.2428E+06 2.39417E+03 1.00000 32 1.9936E+07 1.86272E+04 1.00000 33 2.1075E-06 1.54220E-13 1.00000 34 6.8242E+02 1.772257E+04 1.00000 |
| 29 1.2500E+12 6.69363E-03 1.00000 30 2.8426E+07 8.65507E+01 1.00000 31 9.2428E+06 2.39417E+03 1.00000 32 1.9936E+07 1.86272E+04 1.00000 33 2.1075E-06 1.54220E+13 1.00000 34 6.8242E+05 1.77259E+104 1.00000 |
| 31 9.2428E+06 2.39417E+03 1.00000 32 1.9936E+07 1.86272E+04 1.00000 33 2.1075E-06 1.54220E-13 1.00000 34 6.8242E+05 1.77259E+04 1.00000 |
| 33 2.1075E-06 1.54220E-13 1.00000 34 6.8242E+05 1.77259E+04 1.00000 |
| |
| 35 3.44/3E+11 4.85/61E+05 1.00000 36 2.1824E+11 1.51702E+05 1.00000 |
| DERIVATIVES (CGS UNITS): T 2.23588E+07 RH0 0.00000E+00 |
| MIXTURE MOLECULAR WEIGHT 28.23417 TOTAL ENERGY EXCHANGE RATE -1.04075E+10 MASS FRACTION SUM 1.00000002 (Cal-cm**3/0**2/SEC) |
| |
| |
| |
| COMPUTER TIME (CPU) REQUIRED; FOR THIS STEP - 3.333282E-02 S UP TO THIS TIME ~ 1.700000E+00 S Negative concentration for species H2 |
| NEGATIVE CONCENTRATION FOR SPECIES CO |
| TIME 5.00000E-06 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM |
| FLOW PROPERTIES INTEGRATION INDICATORS |
| PRESSURE 6.42873 STEPS FROM LAST PRINT 32 (ATM) |
| VELOCITY 0.00 AVERAGE STEP SIZE 0.30449E-07 (CM/SEC) |
| DENSITY 1.16135E-03 METHOD ORDER 4 _(G/CM**3)_ |
| TEMPERATURE 1905.03 (DEG K) |
| MASS FLOW RATE 0.00000E+00 TOTAL NUMBER OF STEPS 243 (G/SEC) |
| CNIKUPT 2.1205 FUNCT EVALUATIONS 305 (CAL/G/DEG K) |
| CANNA 1.2408 |
| UM/WIA 1, CD VO |
| ENTHALPY 3 92070E+02 |

TABLE A.5.—Continued.

TABLE A.5.—Concluded.

CHEMICAL PROPERTIES

| SPECIES | CONCENTRATION (MOLES/CM**3) 3 D*932E-07 | MOLE FRACTION | NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC) -4.98532E+02 | REACTION NUMBER 1 | RATE CONST CGS UNITS 5.3165E+11 | NET REACTION CONV RATE (MDLE-CM**3/G**2/SEC) 8.05900E+04 | NET RATE/POSI- TIVE DIR RATE 0.28005 |
|---------|---|---------------|---|-------------------------|---------------------------------------|--|--|
| H20 | 2.36307E-06 | 5.74598E-02 | 6.36814E-02 | 2 | 2.4832E+12 | -2.10116E+05 | 0.29133 |
| OH | 2.46937E-07 | 6.00444E-03 | -2.19949E-02 | 3 | 1.1113E+13 | -8.80663E+04 | 0.59358 |
| H | 4.20261E-08 | 1.02189E-03 | -1.39248E-02 | 9 | 9.15186+15 | 5.7654UE+U3 | 0.99826 |
| 02 | 6.60548E~06 | 1.606172-01 | -8./51/4E-V4 -1 17168E-02 | 2 | 3.8393E+13 8 0000F+12 | 6 23605E+03 | 0.99506 |
| HZ | 2 004415-00 | 7 047145-05 | -3 36603 F-86 | 7 | 1.0101F+14 | 9.10169E+03 | 0.99499 |
| 102 | 2.900412-09 | 5 \$35375-86 | -3.12076F-05 | ź | 1.0718E+11 | -3.24528E+02 | 0.99283 |
| 68 | -3.75646E-08 | -9.13411E-04 | 1.70741E-03 | ğ | 4.1810E+12 | 1.79205E+02 | 0.97551 |
| čů2 | 5.99783E-08 | 1.45842E-03 | 4.39934E-03 | 10 | 1.8000E+12 | 9.00204E+00 | 0.79850 |
| N2 | 3.01830E-05 | 7.33921E-01 | -2.39490E-04 | 11 | 7.8000E+11 | 5.83201E+00 | 0.99988 |
| NO | 1.90745E-10 | 4.63810E-06 | 1.42181E-04 | 12 | 8.6564E+11 | -3.79455E+03 | 0.32368 |
| CN | 5.52384E-10 | 1.34316E-05 | 3.36799E-04 | 13 | 9.466/E+12 | -/.655362+04 | 0.70740 |
| CH2 | 2.48428E-07 | 6.04071E-03 | 7.565091-02 | 12 | 1.90146413 | -2 68217F±03 | 0,7031/ n 99992 |
| CSH8 | 7.51243E-07 | 1.826/05-02 | -2./36465-02 | 15 | 3 72705+15 | 1 67538F+03 | 0.99994 |
| AK | 3.602602-07 | 8./399/E-US | 0.000002+00 | 17 | 2.1333E+03 | -7.22141E+01 | 0.99998 |
| | | | | is | 2.7278E+01 | -1.29656E+02 | 0.99996 |
| | | | | 19 | 6.4243E+09 | -5.52770E+01. | 1.00000 |
| | | | | 20 | 8.3682E-03 | 3.72139E-04 | 1.00000 |
| | | | | 21 | 5.6105E+07 | -1.22859E+01 | 0.71198 |
| | | | | 22 | 6.1428E+13 | 3.31713E+03 | 0.98237 |
| | | | | 23 | 2.18322+11 | 1.181692+05 | 1.00000 |
| | | | | 24 | 1.03302710 | 0.000000000 | 0.00000 |
| | | | | 25 | 1 6912F+03 | 2 50003E-01 | 1.00000 |
| | | | | 27 | 8 7412F+86 | 2.35807E-07 | 1.00000 |
| | | | | 28 | 8.3000E+11 | 1.05017E+02 | 1.00000 |
| | | | | 29 | 1.2500E+12 | 9.76520E-02 | 1.00000 |
| | | | | 30 | 3.1912E+07 | 1.77416E+02 | 1.00000 |
| | | | | 31 | 9.3423E+06 | 4.42268E+03 | 1.00000 |
| | | | | 32 | 2.1765E+07 | 2.02894E+04 | 1.00000 |
| | | | | 22 | 2.34115-06 | U.UUUUUE+UU 1 F108(E+06 | 1 49000 |
| | | | | 34 | 8.003UETUJ 1.6520E113 | 1.31900CTU4 6 17678E±05 | 1 40800 |
| | | | | 36 | 2.1832E+11 | 1.18169E+05 | 1.00000 |
| DERIVA | TIVES (CGS UNITS |); T | 2.08524E+06 RHO | 0.000 | 00E+00 | | |
| MIXTUR | RE MOLECULAR WEIG | HT 28.23896 | TOTAL ENERGY EXCHANGE (CAL-CM**3/G**2/SE | RATE - C) | -5.92238E+09 | MASS FRACTION SUM | 1.0000001 |
| | | | | | | | |

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 3.999996E-01 S UP TO THIS TIME - 2.133333E+00 S (LSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

| TOTAL | NO. | OF STEPS - | | 243 |
|-------|-----|---------------------------|------|--------|
| TOTAL | NO. | OF DERIVATIVE EVALUATIONS | - | 305 |
| TOTAL | NO. | OF JACOBIAN EVALUATIONS - | | 37 |
| TOTAL | CPU | TIME - | 2.13 | 3333 S |

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 3.433333 S

(LSENS) READ DATA FOR NEXT CASE



*** GLOBAL REACTIONS ***

| NUMBER | | | | | REA | CTION | | | | | | | | | |
|--|--------|--|--|------|--|--|-------------|--|----|---|------|-------|---|-------------|---|
| 1 2 3 4 5 6 7 8 9 10 11 2 | | | 1.0xH20 1.0xC0 1.0xC02 1.0xN2 1.0xCN 1.0xCN 2.0xCH2 1.0xCH2 1.0xCH2 1.0xC2 1.0xH2 1.0xH2 | ++++ | 1.0×0 1.0×H20 1.0×H2 1.0×02 2.0×N0 2.0×N0 1.0×N2 1.0×N2 1.0×C3H8 1.0×C3H8 1.0×C3H8 | >>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>> | 11121121321 | .0×H2 .0×C0 .0×C0 .0×N0 .0×N2 .0×C0 .0×C0 .0×C0 .0×C0 .0×C0 .0×C12 .0×0H 0×H20 | | + 1.0×02 + 1.0×H2 + 1.0×H20 + 1.0×02 + 1.0×C0 + 1.0×C0 + 2.0×H2 + 2.0×H2 + 2.0×H2 + 2.0×H2 | | | 1 020 | | |
| 13 | 1.0×0H | + | 1.0×H2 | ÷ | 1.0×02 | > | i | . 0×H20 | | + 1.0×0 | | ÷ | 1.0×0H | | |
| REACTION NUMBER 1 2 3 4 5 6 7 7 8 9 10 11 12 13 | ×× | REXP 1 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 | REACTANT EXP(REXP 2 1.000 1.000 0.000 0.000 1.000 1.000 1.000 1.600 0.150 0.150 0.000 DATA GIVEN I | NEN | TS REXP 3 1.000 1.000 1.000 2.000 1.000 1.000 1.000 0.100 1.00 | ş XX | | | ×× | A 4.90000E+10 1.30000E+10 4.41000E+10 3.00000E+14 2.00000E+11 1.25000E+12 5.00000E+12 3.50000E+12 1.00000E+10 1.98000E+10 9.6000E+11 1.98000E+10 9.6000E+11 1.98000E+10 9.6000E+11 0UTPUT REQUIRE | EACT | ION I | RATE VAR: N 0.1300 0.1900 0.0300 0.00000 0.00000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 | IABLE ** | S ACTIVATION ENERGY -510.00 -7000.00 3527.00 38000.00 38000.00 54000.00 54000.00 41000.00 4000.00 1013.00 |

** ASSIGNED VARIABLE PROFILE **

WELL - STIRRED REACTOR CASE

VOLUME OF REACTOR = 2.00000E+02 CMXX3 MASS FLOW RATE TO START ITERATION = 1.00000E+02 G/S

TABLE A.6.—Continued.

ASSIGNED MASS FLOW RATE PROBLEM: MASS FLOW RATE INCREMENT = 1.00000E+01 G/S Maximum Mass Flow Rate = 1.60000E+03 G/S

NUMBER OF REACTING SPECIES: 12 NUMBER OF INERT SPECIES: 1 ** INITIAL CONDITIONS **

| TIME | 0.0000DE+00 | SEC | AREA | 0.0000E+00 | SQ CM | AXIAL POSITION | 0.00000E+00 CM |
|------|-------------------------------|-----|-------------|------------|-------|------------------------|----------------|
| F | LOW PROPERTIES | | | | | INTEGRATION INDICATORS | |
| | PRESSURE | | 5.50000 | | | STEPS FROM LAST PRINT | 0 |
| | VELOCITY | | 0.00 | | | AVERAGE STEP SIZE | 0.0000E+00 |
| | DENSITY | | 2.52469E~03 | | | METHOD ORDER | 0 |
| | TEMPERATURE | | 800.00 | | | | |
| | MASS FLOW RAT | E | 1.00000E+02 | | | TOTAL NUMBER OF STEPS | 0 |
| | ENTROPY | 、 | 1.8096 | | | FUNCT EVALUATIONS | 0 |
| | MACH NUMBER | , | 0.0000 | | | JACOBIAN EVALUATIONS | 0 |
| | GAMMA | | 1.2519 | | | | |
| | ENTHALPY | | 8.37665E+01 | | | | |
| | SP. HEAT (CP) (CAL/G/DEG K |) | 3.27783E-01 | | | | |

CHEMICAL PROPERTIES

| SPECIES | CONCENTRATION (MOLES/CNXX3) | MOLE FRACTION | NET SPECIES PRODUCTION RATE (MOLE/CMXX3/SEC) | REACTION | RATE CONST | NET REACTION CONV RATE (MOLE-CMXX3/GXX2/SEC) | NET RATE/POSI- TIVE DIR RATE |
|---------|--------------------------------|---------------|---|------------|-------------|---|---------------------------------|
| H20 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 1 | 2.2495E+11 | 0.00000E+00 | 0.00000 |
| 0 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 2 | 6.7500E+10 | 0.0000E+00 | 0.00000 |
| 82 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 3 | 1.7080E+10 | 0.00000E+00 | 0.00000 |
| 02 | 1.61956E-05 | 1.93301E-01 | -4.53833E-08 | 4 | 1.7599E-13 | 2.69941E-17 | 1.00000 |
| CO | 0.00000E+00 | 0.00000E+00 | 0.0000E+00 | 5 | 8.3160E+00 | 0.0000CE+00 | 0.00000 |
| C92 | 0.00000E+00 | 0.00000E+00 | 0.0000E+00 | 6 | 8.3000E+11 | 0.00000E+00 | 0.0000 |
| NZ | .6.03667E-05 | 7.20502E-01 | -1.72062E-22 | 7 | 1.2500E+12 | 0.0000E+00 | 0.0000 |
| NO | 0.0000E+00 | 0.00000E+00 | 3.44124E-22 | 8 | 8.8483E-02 | 0.0000E+00 | 0.00000 |
| CN | D.0000E+00 | 0.00000E+00 | 0.00000E+00 | 9 | 1.5071E+06 | 0.0000CE+00 | 0.00000 |
| CH2 | 8.0000E+00 | 0.00000E+00 | 1.36150E-07 | 10 | 6.9297E+00 | 7.11999E-03 | 1.00000 |
| C3H8 | 6.47824E-06 | 7.73205E-02 | -4.53833E-08 | 11 | 3.9081E-14 | 0.00000E+00 | 0.00000 |
| он | 0.0000E+00 | 0.00000E+00 | 9.07666E-08 | 12 | 1.5992E+05 | 0.00000E+00 | 0.00000 |
| AR | 7.43711E-07 | 8.87650E-03 | 0.0000E+00 | 13 | 2.6015E+11 | 0.0000E+00 | 0.00000 |
| MIXTUR | E MOLECULAR WEIGHT | 30.13325 | TOTAL ENERGY EXCHANGE (CAL-CM**3/G**2/SE | RATE C) | 0.90000E+00 | MASS FRACTION SUM | 1.00000000 |

CPU TIME FOR INITIALIZATION OF LSENS = 0.500000 S **EQUILIBRIUM CONDITIONS **

| TIME | 0.00000E+00 | SEC | AREA | 0.00000E+00 | SQ CM | AXIAL POSITION | 0.00000E+00 CM |
|------|-------------------------------|-----|-------------|-------------|-------|------------------------|----------------|
| F | LOW PROPERTIES | | | | | INTEGRATION INDICATORS | |
| | PRESSURE | | 5.50000 | | | STEPS FROM LAST PRINT | 0 |
| | VELOCITY | | 0.00 | | | AVERAGE STEP SIZE | 0.00000E+00 |
| | DENSITY (G/CMXX3) | | 7.86509E-04 | | | METHOD ORDER | 0 |
| | TEMPERATURE (DEG K) | | 2021.03 | | | | |
| | MASS FLOW RAT | E | 1.00000E+02 | | | TOTAL NUMBER OF STEPS | 0 |
| | ENTROPY | • | 2.4443 | | | FUNCT EVALUATIONS | C |
| | MACH NUMBER | | 0.0000 | | | JACOBIAN EVALUATIONS | C |
| | GAMMA | | 1.2820 | | | | |
| | ENTHALPY (CAL/G) | | 8.37664E+01 | | | | |
| | SP. HEAT (CP) (CAL/G/DEG K |) | 3.80893E-01 | | | | |

CHEMICAL PROPERTIES

| SPECIES | CONCENTRATION (MOLES/CM**3) | MOLE FRACTION | NET SPECIES PRODUCTION RATE (MOLE/CMXX3/SEC) | REACTION NUMBER | RATE CONST CGS UNITS | NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC) | NET RATE/POSI- TIVE DIR RATE |
|---------|--------------------------------|---------------|---|--------------------|-------------------------|---|---------------------------------|
| H20 | 3.26171E-06 | 9.83480E-02 | 1.59430E-02 | 1 | 2.1895E+11 | 1.23633E+00 | 1.00000 |
| 0 | 1.07090E-12 | 3.22900E-08 | 4.95289E-06 | 2 | 1.5893E+10 | 4.42519E+05 | 1.00000 |
| H2 | 4.81052E-06 | 1.45048E~01 | -1.59373E-02 | 3 | 7.7821E+10 | 4.68284E+05 | 1.00000 |
| 02 | 7.86509E-14 | 2.37151E-09 | 7.64769E-07 | 4 | 5.7878E+03 | 1.38388E~08 | 1.00000 |
| C0 | 5.28064E-06 | 1.59223E-01 | 1.59381E-02 | 5 | 1.5552E+07 | 5.88118E-08 | 1.00000 |
| C02 | 7.73802E-07 | 2.33319E-02 | ~1.59381E-02 | 6 | 8.3000E+11 | 1.13011E-07 | 1.00000 |
| N2 | 188058E-05 | 5.67039E-01 | -1.02252E-10 | 7 | 1.2500E+12 | 7.68680E-06 | 1.00000 |
| NO | 4.83659E-11 | 1.45834E-06 | -4.74076E-12 | 8 | 7.2365E+07 | 1.73029E-04 | 1.00000 |
| CN | 7.86509E-14 | 2.37151E-09 | 2.09245E-10 | 9 | 1.0078E+07 | 3.59358E-07 | 1.00000 |

| | | | TABLE A.6. | -Continued. | | |
|--|---|--|---|---|---|--|
| CH2 C3H 8 Oh Ar | 7.86509E-14 7.86509E-14 7.22352E-10 2.31686E-07 | 2.37151E-09 2.37151E-09 2.17806E-05 6.98587E-03 | -2.14286E-10 -2.14013E-15 -1.14353E-05 0.00000E+00 | 10 4. 11 4. 12 7. 13 3. | 0527E+07 3.4596 9272E-06 3.0136 3133E+05 9.2429 4847E+11 3.20048 | 5E-09 1.00000 0E-18 1.00000 5E+00 1.00000 8E-05 1.00000 |
| MIXTURE | MOLECULAR WEIGHT | 23.71507 | TOTAL ENERGY EXCHANG (CAL-CMXX3/GXX2/S | E RATE 0.0000 EC) | 0E+00 MASS FRACTI | ION SUM 1.00000009 |
| | | COMPUTAT | TANAL LIABY DEALITER E | | ALCINATION. | |
| I | NITIAL ESTIMATES | NO. OF I (SIGMAS) AT TEMPE | TERATIONS = 12 RATURE = 2021.03 K: | CPU TIME = 1.6 | 66737E-02 S | |
| | H20 0 H2 02 02 02 02 N2 N0 CN CH2 C3H 04 04 AR | 4.14707 E- 1.36158E- 6.11629E- 9.83843E- 2.39105E- 6.14944E- 1.00000E- 1.00000E- 9.18427E- 9.19427E- 9.1947E- 9.1947E- 9.1947E- 9.1947E- 9.1947E- 9.1947E- 9.1947E- 9.1947E- 9.1947E | 03 09 03 10 03 04 02 08 10 10 10 10 10 07 04 00 04 00 04 00 04 00 04 00 05 05 05 05 05 05 05 05 05 05 05 05 | EE. ALL CLOBAL P | TACTIONS - NEW CASE | CASE 5 |
| M | VELLSTIKKED REACT | INIT | IAL STATE | FINAL STATE | FINAL/INITIAL | RATIO |
| PR TE EN DE SP MO GA | RESSURE ATM EMP. DEG ITROPY CAL. ENSITY GM/(ITHALPY CAL. 2. HEAT (CP) CAL. 21. WT. OF MIXT IMMA | 5.5 K 800 GM/K 1.8 MXX3 2.5 GM 83. GM/K 3.2 3 | 0000 .000 0955 2469E-03 7665 7783E-01 0.1332 1.2519 | 5.50000 1866.72 2.32614 9.22862E-04 83.7665 3.82594E-01 25.7019 1.2534 | 1.00000 2.33340 1.28548 0.36553 1.00000 1.16661 | |
| SPE | ECIES | MOLE FRAC | T MASS FRACT | MOLE I | FRACT MASS FRA | CT |
| H2 D H22 C0 C0 C0 C0 C0 C0 C0 C0 C0 C0 C0 C0 C0 | 20 22 20 22 20 20 20 20 20 20 20 20 20 2 | 0.000000 0.00000 1.93301 0.00000 0.000000 0.000000 7.20502 0.000000 0.000000 0.00000 0.000000 7.73205 0.00000 0.000000 8.876500 8.876500 | 00 0.0000E+00 00 0.0000E+00 00 0.00000E+00 01 2.05268E-00 00 0.00000E+00 01 2.05268E-00 00 0.00000E+00 01 6.69815E-00 00 0.00000E+00 00 0.0000E+00 00 0.0000E+00 00 0.0000E+00 00 0.0000E+00 00 0.0000E+00 00 0.0000E+00 00 0.0000E+00 | 1.06379 1.52770 8.14100 2.62291 1.06123 3.20964 6.14407 1.00021 8.36060 7.630221 1.705221 3.3551372 | VE-01 7.45646E- VE-02 6.38507E- VE-02 3.26560E- VE-02 3.26560E- VE-02 5.49597E- VE-01 1.15661E- VE-02 5.49597E- VE-01 6.69305E- VE-04 1.16771E- VE-03 4.46336E- VE-04 8.46336E- VE-02 2.92570E- VE-04 2.1765E- VE-04 2.1765E- | 02 05 03 02 01 02 01 04 04 04 04 04 04 04 04 04 04 02 02 |
| VOLUM | ME 200.000 | CMXX3 | MASS FLD 100.000 | GM/SEC | | |
| MDC H | DT/VOLUME = (VELLSTIRRED REACTO | D.50000 RESIDEN DR CALCULATION | CE TIME = 1.4 . GLOBAL CODE TEST CAS | 846 MSEC ITERA Se: All global Ri | ATIONS = 16 EACTIONS; NEW CASE | CASE 5 |
| | | INIT | IAL STATE | FINAL STATE | FINAL/INITIAL | RATIO |
| PR TE EN DE SF MC GA | RESSURE ATM EMP. DEG NTROPY CAL/ ENSITY GM/ THALPY CAL 2. HEAT (CP) CAL/ DL. NT. OF MIXT IMMA | К 800 /GM/К 1.8 /M¥¥3 2.5 /GM 83. /GM/К 3.2 3 | 0000 .000 2955 26695-03 7783E-03 7783E-01 0.1332 1.2519 | 5.50000 1840.61 2.31665 9.39340E-04 83.7665 3.81967E-01 25.7948 1.2526 | 1.0000 2.30077 1.28023 0.37206 1.00000 1.16530 | |
| SPE | ECIES | MOLE FRAC | T MASS FRACT | MOLE | FRACT MASS FRA | ICT |
| H2 0 H2 02 02 02 02 02 02 04 04 04 04 04 04 04 | 20 2 2 2 2 2 2 2 2 3 4 2 3 4 8 4 8 4 8 8 | 0.00000E+ 0.00000E+ 1.93301E- 0.0000E+ 7.20502E- 0.0000E+ 0.00000E+ 0.00000E+ 7.73205E- 0.00000E+ 7.73205E- 0.00000E+ 8.87650E- | 00 0.0000E+00 00 0.0000E+00 00 0.0000E+00 01 2.05268E-00 00 0.0000E+00 02 1.31495-00 00 0.0000E+00 03 1.17677E-03 | 1 1.03750 1.86021 7.98761 2.96772 1.03453 1.03453 1.61641 1.20870 5.82633 7.8454 1.82743 1.82743 2.7.59853 | 5E-01 7.24638E- DE-04 1.15380E- FE-02 6.24216E- DE-01 1.12336E- LE-01 1.12336E- SE-02 5.43640E- SE-01 6.09433E- SE-04 1.40607E- SE-04 5.87670E- SE-03 4.26621E- SE-04 2.34588E- SE-04 2.42588E- SE-03 1.17677E- | 02 04 03 02 01 02 01 04 04 03 02 04 04 03 02 02 |
| VOLUM | ME 200.000 | CMXX3 | MASS FLO 110.000 | GM/SEC | · | |
| MDC MDC | VOLUME = (VELLSTIRRED REACT(| D.55000 RESIDEN DR CALCULATION | CE TIME = 1.3 . GLOBAL CODE TEST CAS | VUS MSEC ITERA Se: All global Ri | ATIONS = 3 EACTIONS; NEW CASE | CASE 5 |
| PR | RESSURE ATM | INIT | IAL STATE 0000 | FINAL STATE 5,50000 | FINAL/INITIAL 1.00000 | RATIO |
| TEN EN SP GA | EMP. DEG VIROPY CAL ENSITY GM/(VIHALPY CAL 2. HEAT (CP) CAL DL. WT. OF MIXT MMMA | K 800 GM/K 1.8 M##5 2.5 GM 83. GM/K 3.2 3 | .000 0955 2449E-03 7665 7783E-01 0.1332 1.2519 | 1810.12 2.30522 9.59338E-04 83.7665 3.81447E-01 25.9076 1.2517 | 2.26265 1.27392 0.37998 1.00000 1.16372 | |

| TABLE A.6.— | Continued. |
|-------------|------------|
|-------------|------------|

| | SPECIES | MOLE | FRACT | MASS FRACT | MOLE FRACT | MASS FRACT |
|-------|---|--|--|---|--|---|
| | H20 0 H2 02 C0 C02 N2 N0 CN CN CH2 C3H8 DH AR | 0.000 0.000 1.933 0.000 7.205 0.000 0.000 0.000 0.000 7.732 0.000 8.876 | 00E+00 00E+00 10E-01 10E-01 00E+00 00E+00 12E-01 10E+00 10E+00 10E+00 10E+00 10E+00 10E+00 55E-02 00E+00 | 0.00000E+00 0.00000E+00 2.05268E-01 0.00000E+00 0.00000E+00 6.69815E-01 0.00000E+00 0.00000E+00 0.00000E+00 1.3149E-01 0.00000E+00 1.13149E-01 | 1.00629E-01 2.25408E-02 3.38253E-02 1.00260E-01 3.15536E-02 6.19200E-01 1.44619E-04 3.84734E-04 7.91299E-03 1.97741E-02 3.71866E-04 7.63173E-03 | 6.99736E-02 1.39202E-04 6.07572E-03 4.17780E-02 1.08397E-01 5.3608E-02 6.69529E-01 1.67497E-04 3.86369E-04 4.28422E-03 3.36566E-02 2.44115E-04 1.17677E-02 |
| | VOLUME 200.000 | CMXX3 | MASS FLO | 120.000 0 | MAZEC TIERLINE - | - |
| | NELLSTIRRED RE | ACTOR CALCULATION | I GLOBAL C | DDE TEST CASE: | ALL GLOBAL REACTIONS; | NEW CASE CASE 5 |
| | | I | INITIAL STATE | | FINAL STATE | FINAL/INITIAL RATIO |
| | PRESSURE TEMP. ENTROPY DENSITY ENTHALPY SP. HEAT (CP) MOL. WT. OF MIX GAMMA | ATM DEG K CAL/GM/K GM/CM¥¥3 CAL/GM CAL/GM/K T | 5.50000 800.000 1.80955 2.52469E-03 83.7665 3.27783E-01 30.1332 1.2519 | | 5.50000 1771.71 2.29023 9.85816E-04 83.7665 5.80763E-01 26.0577 1.2504 | 1.00000 2.21464 1.26564 0.39047 1.00000 1.16163 |
| | SPECIES | MOLE I | RACT | MASS FRACT | MOLE FRACT | MASS FRACT |
| | H20 H2 D2 C0 C02 N2 N0 CN CH2 C3H8 OH AR | 0.000 0.000 0.000 1.933 0.000 7.000 7.205 0.000 0.000 0.000 7.732 0.000 0.000 8.876 | 00E+00 10E+00 00E+00 01E-01 00E+00 00E+00 12E-01 10E+00 10E+00 00E+00 00E+00 00E+00 00E+00 00E+00 00E+00 00E+00 00E+00 00E+00 00E+00 | 0.00000E+00 0.00000E+00 2.05268E-01 0.00000E+00 0.00000E+00 0.00000E+00 6.69815E-01 0.00000E+00 0.00000E+00 1.13149E-01 0.00000E+00 1.13149E-01 0.00000E+00 | 9.65660E-02 2.74493E-04 7.57757E-02 9.61201E-02 6.22854E-01 1.71843E-04 2.29289E-04 7.76221E-03 2.17894E-02 3.80663E-04 7.67596E-03 | 6.67616E-02 1.68538E-04 5.86193E-03 4.82499E-02 1.03323E-01 5.25411E-02 6.69600E-01 1.97881E-04 4.17838E-04 4.17838E-03 3.68731E-02 2.48450E-04 1.17677E-02 |
| | VOLUME 200.000 | CM××3 | MASS FLO | 130.000 | IM/SEC | |
| | MDOT/VOLUME = Wellstirred Re | 0.65000 RESI Actor Calculation | DENCE TIME = N GLOBAL C | 1.517 DDE TEST CASE: | MSEC ITERATIONS = All global reactions; | 4 NEW CASE CASE 5 |
| | | . : | INITIAL STATE | | FINAL STATE | FINAL/INITIAL RATIO |
| | PRESSURE TEMP. ENTROPY DENSITY ENTHALPY SP. HEAT (CP) MOL. WT. OF MIX GAMMA | ATM DEG K CAL/GM/K GM/CM**3 CAL/GM CAL/GM/K T | 5.50000 800.000 1.80955 2.52469E-03 83.7665 3.27783E-01 30.1332 1.2519 | | 5.50000 1705.10 2.26265 1.03540E-03 83.7665 3.79479E-01 26.3395 1.2481 | 1.00000 2.13138 1.25039 0.41011 1.00000 1.15771 |
| | SPECIES | MOLE | RACT | MASS FRACT | MOLE FRACT | MASS FRACT |
| | H20 0 H2 02 C0 C02 N2 N2 CH CH CH CH2 C3H8 CH CH2 C3H8 CH CH2 C3H8 CH CH2 C3H8 CH2 CH2 C3H8 CH2 CH2 CH2 CH2 CH2 CH2 CH2 CH2 CH2 CH2 | 0.000 0.000 1.933 0.000 7.205 0.000 0.000 0.000 7.732 0.000 7.732 0.000 8.876 | 00E+00 00E+00 01E-01 01E-01 00E+00 00E+00 02E+00 00E+00 00E+00 00E+00 00E+00 00E+00 00E+00 00E+00 00E+00 | 0.00000E+00 0.00000E+00 2.05268E-01 0.0000E+00 0.00000E+00 0.00000E+00 6.69815E-01 0.00000E+00 0.00000E+00 1.13149E-01 1.00000E+00 1.17677E-02 | 8.91865E-02 3.51692E-04 7.15417E-02 8.9307E-02 8.86313E-02 3.02031E-02 6.29643E-01 2.03736E-04 9.40160E-05 7.02425E-03 2.56018E-02 3.68789E-04 7.75897E-03 | 6.10001E-02 2.13628E-04 5.47518E-03 6.00026E-02 9.42537E-02 6.69657E-01 2.32097E-04 9.28673E-05 3.74068E-03 4.28611E-02 2.38125E-04 1.17677E-02 |
| | VOLUME 200.000 | CMXX3 | MASS FLO | 140.000 6 | M/SEC | |
| | MDOT/VOLUME = | 0.70000 RESI | IDENCE TIME = | 1.479 | MSEC ITERATIONS = | 5 |
| (WSR) | *** IN COMPUTI | NG CONV. NO. 6, Temperature | MASS FRACTION = 1.12164E+03 | N SUM = 1.3800 3 K, MASS F | 3E+OD ON ITERATION NO Low Rate = 1.50000E+ | . 17 *** 02 g/s |
| (WSR) | ** RESTART: MA | SS FLOW RATE = 2 | 2.80000E+02 G/: | S, TEMPERAT | URE = 1.70510E+03 K | XX |
| (WSR) | *** IN COMPUTI | NG CONV. ND. 6, Temperature | MASS FRACTION = 1.24041E+03 | N SUM = 1.2380 5 K, Mass F | 1E+00 ON ITERATION NO Low Rate = 2.80000E+ | . 1 *** 02 G/S |

| (WSR) | ** RESTART: MASS FLOW | RATE = 5.60000E+02 G/S, | TEMPERATURE = 1.70510E+03 K ** |
|----------------|---|---|--|
| (WSR) .ksr) | XXX IN COMPUTING CONV Tei XX RESTART: MASS FLOM | . NO. 6, MASS FRACTION SUM MPERATURE = 1.15180E+03 K, RATE = 1.12000E+03 G/S, | = 1.40184E+00 ON ITERATION NO. 1 *** MASS FLOW RATE = 5.60000E+02 G/S TEMPERATURE = 1.70510E+03 K ** |
| WSR) | *** IN COMPUTING CONV. Ten | ND. 6, MASS FRACTION SUM IPERATURE = 1.14817E+03 K, | = 1.40026E+00 ON ITERATION NO. 1 *** Mass flow rate = 1.12000E+03 G/S |
| (HSR) | *** ABOVE PROBLEM ENCO PSR Solution Abani | UNTERED 4 TIMES *** Ioned | |
| LSENS) | A FATAL ERROR HAS OC | CURRED - CASE TERMINATED | |

TABLE A.6.—Concluded.

TABLE A.7.—COMPUTED RESULTS FOR TEST CASE 6 (PROPANE-AIR PSR CASE WITH GLOBAL REACTION MECHANISM MODIFIED FROM CASE 5)



XXX GLOBAL REACTIONS XXX

| NUMBER | | | | | RE | ACTION | | | | | | | | | |
|---|--------|---|--|-------------|---|--------|--|----|----------------------|--|-------|-------|---|------|--|
| 1 3 4 5 6 7 8 9 10 11 12 13 14 | 1.0×0H | ÷ | 1.0%H20 1.0%C0 1.0%C02 1.0%N2 2.0%CH2 2.0%CH2 1.0%CH2 1.0%CH2 1.0%CH2 1.0%H2 1.0%H2 1.0%H20 | **** ****** | 1.0×0 1.0×H20 1.0×H2 1.0×02 2.0×0 1.0×N0 1.0×N2 1.0×N2 1.0×02 1.0×02 2.0×0H 1.0×02 1.0×02 1.0×02 | * | 1.0%H2 1.0%C0 2.0%N0 1.0%N0 1.0%N0 2.0%C0 2.0%CN 1.0%C0 3.0%CH2 2.0%CH 1.0%H20 1.0%H20 1.0%H20 1.0%H2 | | +++ +,++++ +++ | 1.0×02 1.0×H2 1.0×H2 1.0×02 1.0×02 1.0×02 2.0×H2 1.0×H2 1.0×H2 2.0×H2 1.0×H2 1.0×H2 1.0×H2 1.0×D | i | + + | 1.0×0 1.0×0H | | |
| REACTION NUMBER | | REXP 1 | REACTANT EXP | ONEN | ITS REXP | 3 | | | | A | EACI | ION I | RATE VAR N | IABL | ES ACTIVATION |
| 1 2 3 4 5 6 7 8 9 10 11 12 13 14 | | D.000 C.000 C.000 D.000 C.000 C.000 C.000 C.000 C.000 C.000 C.000 D.000 L.000 D.000 L.000 D.000 L.000 | 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 0.155 0.000 | | 1.000 1.000 2.000 1.000 1.000 1.000 0.500 0.500 0.500 1.000 1.000 1.000 | | | | 414428155311 1994 | 90000E+10 30000E+105 41000E+10 00000E+14 00000E+11 30000E+11 30000E+12 00000E+13 50000E+12 00000E+12 00000E+12 90000E+100 98000E+100 90000E+11 90000E+11 | | | $\begin{array}{c} 0.1800\\ 1.3100\\ 0.1900\\ 0.0300\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.1000\\ 0.1800\\$ | | ENERGY -510.00 -700.00 3527.00 100000.00 38000.00 54000.00 54000.00 49080.00 49080.00 1013.00 -510.00 |
| | XX | <u>NEW</u> INPUT | DATA GIVEN | EN CO | 35 UNITS | ¥X | | Χ¥ | OUTP | UT REQUIRE | ED II | A CGS | UNITS | Ж¥ | |

** ASSIGNED VARIABLE PROFILE **

WELL - STIRRED REACTOR CASE

VOLUME OF REACTOR = 2.50000E+03 CM**3 MASS FLOW RATE TO START ITERATION = 1.00000E+02 G/S

ASSIGNED MASS FLOW RATE PROBLEM: MASS FLOW RATE INCREMENT = 2.00000E+02 G/S Maximum Mass Flow Rate = 1.50000E+03 G/S

NUMBER OF REACTING SPECIES: 12 NUMBER OF INERT SPECIES: 1 ** INITIAL CONDITIONS **

| TIME 0.00000E+00 SEC | AREA 0.00000E+0 | D SQ CM A | XIAL POSITION O | .00000E+00 CM |
|--|---|--------------------------------|----------------------------|-----------------------------|
| FLOW PROPERTIES | | INTEGRATION I | NDICATORS | |
| PRESSURE | 5.50000 | STEPS FROM | LAST PRINT | 0 |
| VELOCITY | 0.00 | AVERAGE STE | P SIZE | 0.00000E+00 |
| (CM/SEC) DENSITY | 2.52469E-03 | METHOD ORDE | R | 0 |
| (G/CM**3) TEMPERATURE | 800.00 | | | |
| (DEG K) Mass Floh Rate | 1.00000E+02 | TOTAL NUMBE | R OF STEPS | 0 |
| (G/SEC) ENTROPY | 1.8096 | FUNCT EVALU | ATIONS | 0 |
| (CAL/G/DEG K) Mach Number | 0.0000 | JACOBIAN EV | ALUATIONS | 0 |
| GAMMA | 1.2519 | | | |
| ENTHALPY | 8.37665E+01 | | | |
| (CAL/G) SP. HEAT (CP) (CAL/G/DEG K) | 3.27783E-01 | | | |
| | CHEMICAL PROPE | RTIES | | |
| SPECIES CONCENTRATION MOLE FRACTION | NET SPECIES PRODUCTION RE | ACTION RATE CONST N | ET REACTION CONV | RATE NET RATE/POSI- |
| H20 0.00000E+00 0.00000E+00 | KAIE (MULE/CM225/SEC) N 0.00000E+00 | 1 2.2495E+11 | 0.00000E+00 | CJ TIVE DIR RATE 0.00000 |
| H2 0.00000E+00 0.00000E+00 H2 0.00000E+00 0.00000E+00 | 0.0000E+00 0.0000E+00 | 3 1.7080E+10 | 0.00000E+00 0.00000E+00 | 0.00000 |
| CO 0.00000E+00 0.00000E+00 | -4.33833E-06 D.0000E+00 | 5 8.3160E+00 | 0.00000E+00 | 0.00000 |
| N2 6.03667E-05 7.20502E-01 | -2.29416E-22 | 7 1.2500E+12 | 0.00000E+00 | 0.00000 |
| NO 0.00000E+00 0.0000E+00 CN 0.00000E+00 0.00000E+00 | 4.36632E-22 0.00000E+00 | 9 1.5071E+06 | 0.00000E+00 7.11988E-03 | 0.00000 |
| C3H8 6.47824E-06 7.73205E-02 | -4.53833E-07 | 10 8.9297E+00 11 3.9081E-14 | 0.00000000000 | 0.00000 |
| AR 7.43711E-07 8.87650E-03 | 0.00000E+00 | 13 2.6015E+11 14 2.2495E+11 | 0.00000E+00 0.00000E+00 | 6.00000 0.00000 |
| MIXTURE MOLECULAR NEIGHT 30.1332 | 5 TOTAL ENERGY EXCHANGE RA (CAL-CM**3/G**2/SEC) | TE 0.00000E+00 | MASS FRACTION SU | M 1.0000000 |
| CPU TJ | IME FOR INITIALIZATION OF LSEN **Equilibrium Con | IS = 0.150000 S Iditions ## | | |
| TIME 0.00000E+00 SEC | AREA 0.00000E+0 | IO SQICM A | XIAL POSITION O | .00000E+00 CM |
| FLOW PROPERTIES | | INTEGRATION I | NDICATORS | |
| PRESSURE | 5.50000 | STEPS FROM | LAST PRINT | 0 |
| VELOCITY | 8.00 | AVERAGE STE | P SIZE | 0.00000E+00 |
| (CM/SEC) DENSITY | 7.86509E-04 | METHOD ORDE | R | 0 |
| (G/CMXX3) TEMPERATURE | 2021.03 | | | |
| (DEG K) MASS_FLOH RATE | 1.00000E+02 | TOTAL NUMBE | R OF STEPS | 0 |
| (G/SEC) Entropy | 2.4443 | FUNCT EVALU | ATIONS | 0 |
| (CAL/G/DEG K) Mach Number | 0.0000 | JACOBIAN EV | ALUATIONS | 0 |

TABLE A.7.—Continued.

| JACOBIAN | EVALUATIONS | |
|----------|-------------|--|
| | | |
| | | |

CHEMICAL PROPERTIES

1.2820

8.37664E+01 3.80893E-01

GAMMA

ENTHALPY (CAL/G) SP. HEAT (CP) (CAL/G/DEG K)

| SPECIES | CONCENTRATION | MOLE FRACTION | NET SPECIES PRODUCTION | REACTION | N RATE CONST | NET REACTION CONV RAT | E NET RATE/POSI- |
|-----------|-------------------|---------------|---|----------|--------------|-----------------------|------------------|
| | (MOLES/CM××3) | | RATE (MOLE/CMXX3/SEC) | NUMBER | CGS UNITS | (MOLE-CM**3/G**2/SEC) | TIVE DIR RATE |
| H20 | 3.26171E-06 | 9.83480E-02 | 1.59423E-02 | 1 | 2.1895E+11 | 1.23633E+00 | 1.00000 |
| 0 | 1.07090E-12 | 3.22900E-08 | 4.18810E-06 | ž | 1.5893E+10 | 4.42519E+05 | 1.00000 |
| H2 | 4.81052E-06 | 1.45048E-01 | -1.59365E-02 | 3 | 7.7821E+10 | 4.68284E+05 | 1,00000 |
| 02 | 7.86509E-14 | 2.37151E-09 | 1.52956E-D6 | Ä | 7.7170E+03 | 1.84517E-08 | 1.00000 |
| 00 | 5.28064F-06 | 1.59223E-01 | 1.59381F-02 | Ś | 1 5552E+07 | 5 88118F-08 | 1 00000 |
| Č02 | 7.73802E-07 | 2.33319E-02 | -1.59381E-02 | 6 | 8.3000F+11 | 1.13011F-07 | 1.00000 |
| N2 | 1.88058E-05 | 5.67039E-01 | -1.02255E-10 | 7 | 1.2500F+12 | 7 68680F-06 | 1 00000 |
| NO | 4.83659F-11 | 1.45834E-06 | -4 73505F-12 | ż | 7 2365F+07 | 1 73029F-04 | 1 00000 |
| ĊŇ | 7.86509F-14 | 2 37151F-09 | 2 R9245E-10 | ă | 1 00786+07 | 3 60358F-07 | 1 00000 |
| CH2 | 7 86509F-16 | 2 37151F-09 | -2 162865-10 | 10 | 6 0527F+87 | 3 45045E-09 | 1 00000 |
| C3H8 | 7 86509F-14 | 2 37151F-09 | -2 16013E-15 | ŧĭ | 4 9272E-04 | 3 013405-18 | 1 00000 |
| NH | 7 223526-10 | 2 178065-05 | -1 163536-05 | 12 | 7 31336+05 | 0 26205E+00 | 1 00000 |
| AP | 2 316865-07 | 4 02527E-03 | 0 000005400 | 12 | 3 68675111 | 3 20068E-05 | 1 00000 |
| | E:31000E-07 | 0.303072-03 | 0.000002000 | 14 | 2 12055411 | 1 234335400 | 1.00000 |
| | | | | 14 | 2.10992+11 | 1.230332+00 | 1.00000 |
| MIXTUR | E MOLECULAR WEIGH | IT 23.71507 | TOTAL ENERGY EXCHANGE (CAL-CMXX3/GXX2/SE | E RATE | 0.00000E+00 | MASS FRACTION SUM | 1.0000009 |

SP

TABLE A.7.—Continued.

| | INITIAL ESTIMAT | 'ES (SIGMAS) | COMPUTATIONAL WORK NO. OF ITERATIONS = AT TEMPERATURE = | REQUIRED FOR EQUI = 12 CPU TI 2021.03 K: | LIBRIUM CALCULATI ME = 1.666641E-0 | 0N1 2 S | |
|----------------|--|--|--|--|--|---|---------------------------------------|
| | | H20 4 D 1 H2 6 O2 1 C0 6 C02 5 N2 2 N0 6 CN 1 CH2 1 CH2 1 CH2 1 CH2 1 CH2 1 CH2 1 CH2 1 CH2 2 CH8 1 CH2 2 CH8 2 CH 2 CH8 2 CH2 2 CH2 2 CH2 2 CH2 2 CH2 2 CH2 2 CH2 CH2 CH2 CH2 CH2 CH2 CH2 CH2 CH2 CH2 | 4.14707E-03 .36158E-09 .11629E-03 .00000E-10 .71402E-03 .83843E-04 .39105E-02 .14944E-08 .00000E-10 .00000E-10 .00000E-10 .18427E-07 .94575E-04 | | | | |
| | WELLSTIRRED R | EACTOR CALCU | TNITIAL STATE | AL REACTIONS - CHA FT | NGE AND ADD UNE G Nai state | FINAL REACTION C | ASE 6 |
| | PRESSURE TEMP. ENTROPY DENSITY ENTHALPY SP. HEAT (CP) MOL. WT. OF MI) GAMMA | ATM DEG K CAL/GM/K GM/CM**3 CAL/GM CAL/GM/K (T | 5.50000 800.000 1.80955 2.52469E-03 83.7665 5.27783E-01 30.1332 1.2519 | 8. 3. | 5.50000 1934.60 2.38309 59087E-04 83.7665 81218E-01 24.7956 1.2662 | 1.00000 2.41824 1.31695 0.34027 1.00000 1.16302 | |
| | SPECIES | , | IOLE FRACT | MASS FRACT | MOLE FRACT | MASS FRACT | |
| | H20 0 H2 C0 C0 C02 N2 N0 CN CH2 C3H8 OH AR | | 0.00000E+00 0.0000E+00 1.93301E+01 0.0000E+00 0.000E+00 0.0000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+0 | 0.00000E+00 0.0000E+00 2.05268E-01 0.0000E+00 0.0000E+00 0.0000E+00 0.669815E-01 0.00000E+00 0.00000E+00 1.13149E-01 1.17677E-02 | $\begin{array}{c} 1.22126E-01\\ 1.84123E-06\\ 1.02900E-01\\ 5.22441E-03\\ 1.22134E-01\\ 3.16861E-02\\ 5.85567E-01\\ 1.22333E-06\\ 1.46165E-02\\ 1.38415E-03\\ 7.01732E-03\\ 3.69903E-05\\ 7.30416E-03\\ \end{array}$ | 8.87304E-02 1.18805E-06 8.36359E-03 6.74211E-03 1.37969E-01 5.62397E-02 6.61558E-01 1.48040E-06 1.53369E-02 7.83007E-04 1.24795E-02 2.53717E-05 1.17677E-02 | |
| | VOLUME 2500.0 | D CMXX3 | MASS FLO | 100.000 GM/S | EC | | |
| | MDDT/VOLUME # | 0.04000 | RESIDENCE TIME = | 21.477 MS | SEC ITERATIONS = | 14 | |
| (HSR) | *** FOR CONV. Mass flow rate | NO. 2, CO = 3.00000E | NVERGED TEMP. (AFTE +02 G/S, TEMPER | R 5 ITERATIONS) ATURE ≈ 1.94931E4 | IS GREATER THAN D 03 K, PREVIOU | R EQUAL TO THE PREVIC Is temperature ≠ 1.93 | 0US TEMP. *** 6460E+03 K |
| (WSR) | ¥¥ RESTART: M | ASS FLOW RAT | E = 2.00000E+02 G/ | S, TEMPERATURE | E = 2.02103E+03 K | (* * | |
| (NSR) | *** FOR CONV. Mass flow rate | ND. 1, CO = 2.00000E | NVERGED TEMP. (AFTE +02 g/S, TEMPER | R 13 ITERATIONS) Ature = 1.94694E4 | IS GREATER THAN C 03 K, PREVIOU | R EQUAL TO THE PREVIO S TEMPERATURE = 1.93 | UUS TEMP. XXX 460E+03 K |
| (WSR) | ** RESTART: M | ASS FLOW RAT | E = 4.00000E+02 G/ | S, TEMPERATURE | E = 2.02103E+03 K | (* * | |
| (NSR) (NSR) | *** FOR CONV. Mass Flom Rate ** Restart: M Wellstirred R | NO. 1, CO = 4.00000E ASS FLOW RAT Eactor Calcu | NVERGED TEMP. (AFTE +02 G/S, TEMPER E = 8.00000E+02 G/ Lation All glob. | R 13 ITERATIONS) ATURE = 1.94721E4 S, TEMPERATURI AL REACTIONS - CHA | IS GREATER THAN C 103 K, PREVIOU E = 2.02103E+03 N NGE AND ADD ONE G | DR EQUAL TO THE PREVIO Is temperature ≈ 1.93 (¥¥ Flobal reaction c | DUS TEMP. *** 5460e+03 k :Ase 6 |
| | | | INITIAL STATE | FI | NAL STATE | FINAL/INITIAL RATIO |) |
| | PRESSURE TEMP. ENTROPY DENSITY ENTHALPY SP. HEAT (CP) MOL. WT. OF MI GAMMA | ATM DEG K CAL/GM/K GM/CM¥¥3 CAL/GM CAL/GM/K KT | 5.50000 800.000 1.80955 2.52469E-03 83.7665 3.27783E-01 30.1332 1.2519 | 8. 3. | 5.5000 1916.92 2.34918 88948E-04 83.7665 82830E-01 25.4231 1.2566 | 2.39616 1.29821 0.35210 1.00000 1.16794 | |
| | SPECIES | 1 | MOLE FRACT | MASS FRACT | MOLE FRACT | MASS FRACT | |
| | H20 0 H2 C0 C0 C02 N2 N0 CN CN CN CN CN C3H8 DH AR | | 0.00000E+00 0.00000E+00 1.93301E+01 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 0.00000E+00 | 0.00000E+00 0.00000E+00 2.05268E-01 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 1.13149E-01 0.00000E+00 1.17677E-02 | 1.12731E-01 3.61974E-05 8.72016E-02 1.79598E-02 1.12675E-01 3.22747E-02 6.06071E-01 2.39898E-05 3.59355E-03 5.97986E-03 1.37268E-02 2.36778E-04 7.48901E-03 | 7.98830E-02 2.27799E-05 6.91422E-03 2.26050E-02 1.24142E-01 5.58705E-02 6.67822E-01 2.83144E-05 3.67759E-03 3.29930E-03 2.38090E-03 1.58398E-04 1.17677E-02 | |

| VOLUME | 2500. | 00 | CM××3 | MAS | S FLO | 800.000 | GM/SEC | | | | |
|---|---|--|---|---|---|---|---|---|-----------------------------|--|---|
| MDOT/VOLU Wellsti | JME = IRRED | 0. Reactor | 32000 CALCUI | RESIDENCE | TIME = ALL GLOB | 2. NAL REACTION | 778 MSEC S – Changi | ITERATION AND AND ON | S = 15 E G loba l | REACTION | CASE 6 |
| | | | | INITIA | . STATE | | FINA | STATE | FIN | AL/INITIAL | RATIO |
| PRESSURE TEMP. ENTROPY DENSITY ENTHALPY SP. HEAT MOL. WT. GAMMA | E T (CP) . OF # | ATM DEG I CAL/G GM/CP CAL/G CAL/G IIXT | ()M/K)X×3 ;M ;M/K | 5.500 800.0 1.809 2.524 83.76 3.277 30.1 1.1 | 10 55 59E-03 53E-01 1332 2519 | | 5. 18 2. 9.48 3.81 25 1 | 50000 5555 51250 5455-04 7665 22E-01 8208 2526 | | 1.00000 2.28194 1.27794 0.37551 1.00000 1.16425 | |
| SPECIES | | | 1 | IOLE FRACT | | MASS FRACT | | MOLE FRACT | | MASS FRAG | т |
| H20 D H2 C0 C02 N2 N0 CH2 C3H8 OH AR | | | | 0.00000E+00 0.0000E+00 0.93301E-01 0.0000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.73205E-02 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 | | 0.00000E+0 0.0000E+0 2.05268E-0 0.0000E+0 0.0000E+0 6.69815E-0 0.00000E+0 0.00000E+0 0.00000E+0 1.13149E-0 0.0000E+0 1.17677E-0 | 0 0 1 0 0 1 0 0 0 0 0 0 0 0 2 2 | 1.82509E-01 9.95728E-05 7.97738E-02 1.02345E-01 3.13087E-02 1.02345E-01 6.16403E-02 6.16901E-01 6.52160E-05 9.13988E-04 7.78644E-03 1.86930E-02 5.57854E-04 7.60617E-03 | | 7.15205E- 6.16984E- 6.22784E- 3.87997E- 1.11024E- 6.69284E- 7.57868E- 9.209284E- 9.209284E- 4.22987E- 3.19235E- 2.35706E- 1.17677E- | 02 05 02 02 01 02 01 02 04 04 02 04 02 04 |
| VOLUME | 2500. | .00 | CM××3 | MA | SS FLO | 1400.00 | GM/SEC | | | | |
| MDOT/VOLU | UME = | 0. | 56000 | RESIDENCE | TIME = | 1. | 693 MSEC | ITERATION | S = 3 | DEACTION | CASE 6 |
| NELLSTI | IRRED | REACTOR | CALCU | LATION | ALL GLOI | BAL REACTION | S – CHANG | E AND ADD ON | C GLUDAL | REACTION | 0455 0 |
| NELLSTI | IRRED | REACTOR | CALCU | LATION | ALL GLOI L STATE | BAL REACTION | S - CHANG Fina | E AND ADD ON L state | FIN | AL/INITIAL | RATIO |
| NELLSTI PRESSURE TEMP. ENTROPY DENSITY ENTHALPY SP. HEAT MOL. MT. GAMMA | IRRED E Y T (CP) . OF P | ATM DEG I Cal/C GM/CP Cal/C Cal/C 11XT | CALCU SM/K SM/K IXX3 SM SM/K | LATION INITIA 5.500 800.0 1.809 2.524 83.76 3.277 30. 1.1 | ALL GLOB 55 59 59 59 59 59 59 59 59 59 59 59 59 | MAL REACTION | S - CHANG FINA 5. 18 2. 9.63 83 3.81 25 1 | E AND ADD ON STATE 50000 12.65 50347 525E-04 .7665 246E-01 .9133 .2518 | FIN | AL/INITIAL 1.00000 2.25332 1.27295 0.38164 1.00000 1.16310 | RATIO |
| NELLSTI PRESSURE TEMP. ENTROPY DENSITY ENTHALPY SP. HEAT MOL. WT. GAMMA SPECIES | IRRED E Y T (CP) | ATM DEG I Cal/(GM/Cr Cal/(Cal/(11XT | CALCUI SM/K SM/K SM/K | LATION (INITIA) 5.500 800.0 1.809 2.524 83.76 3.277 30. 1. 1. MOLE FRACT | ALL GLOB STATE 00 55 59E-03 55 53E-01 1332 2519 | MASS FRACT | S - CHANG FINA 5. 18 2. 9.63 83 3.81 25 1 | E AND ADD ON STATE 50000 12.65 30347 525E-04 .7665 246E-01 .9133 .2518 MOLE FRACT | FIN | AL/INITIAL 1.00000 2.25332 1.27295 0.38164 1.00000 1.16310 MASS FRA | RATIO |
| NELLSTI PRESSURE ENTROPY DENSITY ENTHAPY SP. HEAT GAMMA SPECIES H20 0 H2 C0 C0 C0 C0 C0 C0 C0 C0 C0 C0 C0 C0 C0 | IRRED E T (CP) . OF P | REACTOF ATM DEG L CAL/C GM/CC CAL/C 11XT | CALCUI | LATION INITIA 5.500 800.0 1.809 2.524 83.76 3.277 30. 1.1 MOLE FRACT 0.00000E+00 0.0000E+00 0.000E+00 0.0000E+00 0.0 | ALL GLOB STATE DO DD S5 S5 S5 S5 S5 S5 S5 S5 S5 S5 S5 S5 S5 | MASS FRACT 0.00000E+0 0.00000E+0 0.00000E+0 0.00000E+0 0.00000E+0 0.00000E+0 0.00000E+0 0.00000E+0 0.00000E+0 0.00000E+0 0.00000E+0 1.13149E-0 1.00000E+0 1.17677E-0 | S - CHANG FINA 5. 2. 9.63 3.81 25 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 | E AND ADD ON STATE 50000 12.65 50347 525E-04 .7665 246E-01 .9133 .2518 MOLE FRACT 1.05036E-01 1.15475-01 1.154774E-02 3.46098E-02 3.13991E-02 3.99102E-03 1.99102E-04 7.83380E-03 1.99102E-04 7.63341E-03 | FIN | AL-/INITIAL 1.00000 0.25332 1.27295 0.38164 1.00000 1.16310 MASS FRA MASS FRA MASS FRA 6.95461E- 7.12606E- 6.08890E- 4.27376E- 8.70153E- 6.69647E- 8.70153E- 6.24304E- 1.26308E- 1.17677E- | CT RATIO CT 02 05 03 02 01 02 01 02 01 02 01 02 01 02 01 02 04 02 04 02 |
| NELLSTI PRESSURE TEMP: ENTROPY DENSITY SP. HEAT SP. HEAT GAMMA SPECIES H20 0 H2 02 CD CD CD CD CD CD CD CD CD CD CD CD CD | IRRED E Y (CP) . OF) 2500. | REACTOF ATM DEG F CAL/C GM/CL CAL/C 11XT | CMLCUI | LATION INITIA 5.500 800.0 1.809 2.524 83.76 3.277 30. 1.1 MOLE FRACT 0.00000E+00 0.0000E+00 0.000E+00 0.000E+00 0.0 | ALL GLOB STATE State | MASS FRACT 0.00000E+0 0.00000E+0 0.00000E+0 0.00000E+0 0.00000E+0 0.00000E+0 0.00000E+0 0.00000E+0 0.00000E+0 0.00000E+0 1.13149E-0 0.00000E+0 1.17677E-0 1.500.00 | S - CHANG FINA 5. 2. 9.63 3.81 25 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 | E AND ADD ON STATE S0000 22.65 50347 525E-04 7665 246E-01 9133 .2518 MOLE FRACT 1.00036E-01 1.15417E-04 7.82734E-02 3.46098E-02 3.13991E-02 3.46098E-02 3.13991E-02 3.46098E-02 3.13991E-02 3.46098E-04 7.5345E-05 .66980E-04 7.5345E-05 .66980E-04 7.63341E-03 .00056E-04 7.63341E-03 .00056E-04 | FIN | AL-/INITIAL 1.00000 2.25332 1.27295 0.38164 1.00000 1.16310 MASS FRA MASS FRA 6.95461E 7.12606E 6.08490E 4.27376E 1.07927E- 5.33265E- 8.70153E- 8.6647E- 4.2647E- 3.3880E- 1.17677E- | CT RATIO CT 02 05 03 02 01 02 01 02 01 02 04 03 04 02 04 02 02 |
| NELLSTI PRESSURE ENTROPY DENSITY ENTHALPY SP. HEAT MOL. WT. GAMMA SPECIES H20 0 H2 02 C0 C02 N2 N0 C02 N2 N0 C12 C3H8 DH AR VOLUME MDOT/VOLU | 2500. UME = | REACTOF ATM DEG F GM/Ch GM/Ch CAL/C 11XT | CALCUI S. M/K M/K M/K M/K | LATION INITIA 5.500 800.0 1.809. 2.524. 83.76. 30. 1.1 MOLE FRACT 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.00 | ALL GLOB STATE S5 S5 S5 S5 S5 S5 S5 S5 S5 S5 S5 S5 S5 | MASS FRACTION 0.00000E+0 0.0000E+0 0.0000E+ | S - CHANG FINA 5. 2. 9.63 2. 9.63 3.81 25 1 25 1 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 | E AND ADD ON STATE STATE S0000 22.65 30347 265 246E-01 .9133 .2518 MOLE FRACT 1.00036E-01 1.15417E-04 7.82734E-02 3.13991E-02 6.6980E-04 7.51465E-05 6.66980E-04 7.5341E-03 3.13991E-02 6.3341E-03 1.99102E-02 3.70383E-03 ITERATION | S = 3 | MASS FRA MASS FRA MASS FRA MASS FRA 6.95461E- 7.12606E- 1.07927E- 5.33265E- 6.08890E- 4.27376E- 1.07927E- 5.33265E- 6.08418E- 1.07927E- 5.33265E- 6.08418- 1.07927E- 5.33265E- 6.08418- 1.07927E- 5.33265E- 6.08418- 1.07927E- 5.33265E- 6.08418- 1.07927E- 5.33265E- 6.08418- 1.07927E- 5.33265E- 6.08418- 1.07927E- 5.33265E- 6.08418- 1.07927E- 5.33265E- 6.08418- 1.07927E- 5.33265E- 6.08418- 1.07927E- 5.33265E- 6.08418- 1.07927E- 5.33265E- 6.08418- 1.07927E- 5.33265E- 6.08418- 1.07927E- 5.33265E- 6.24418- 1.07927E- 5.33265E- 6.24418- 1.07927E- 5.33265E- 6.24418- 1.07927E- 5.33265E- 6.24418- 1.07927E- 5.33265E- 6.24418- 1.07927E- 5.33265E- 6.24418- 1.07927E- 5.338809E- 2.43088E- 1.17677E- | CT RATIO CT 02 05 02 01 02 02 01 02 02 02 02 04 02 02 04 02 02 04 02 |

TABLE A.7.—Concluded.

(LSENS) END OF THIS CASE

(LSENS) READ DATA FOR NEXT CASE

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 1.050000 S

** DATA LINES **

| GLOBAL AN | ID MOL | ECULA | R RE | ACTI | ONS; | MOLI | ECU | LAR REAC | TIONS | AD | DED | | CASE 7 | |
|----------------------|---------|---------|-------------|------------|------|-------|----------|------------|-------|-----|---------|-----|------------|------------|
| ADD | | | | | | | | | - 4. | ٠ | | | | |
| Artype g | LECOIL | Tru | 8.,9 8.m | ronı A | y 11 | 126 | • • | mrprev · | та | 126 | • • | | | |
| 0 | 4 | H20 | aen | " <u> </u> | 0H | | + | OH | | 6 | .8E+ | 13 | 0. | 18365. |
| ň | + | 02 | | = | ŌН | | + | 0 | | 1.4 | 59Ë+ | 14 | 0. | 16400. |
| ö | ÷ | HŽ | | z | ÕН | | ÷ | Ĥ | | 4. | 20Ē+ | 14 | ō. | 13750. |
| Ĥ | + | H02 | | = | HZ | | + | 02 | | 7.3 | 28E+ | 13 | 0 . | 2126. |
| 0 | + | HD2 | | = | OH | | + | 02 | | 5 | .0E+ | 13 | 0. | 1000. |
| H02 | + | OH | | = | H20 | | + | 02 | | 8 | .0E+ | 12 | 0. | 0. |
| H | + | H02 | | =2. | OOH | | | | | 1. | 34E+ | 14 | 0. | 1070. |
| HZ | + | HOZ | | = | H202 | 2 | + | H | | 7. | 91E+ | 13 | 0 . | 25000. |
| UH | ÷. | HZUZ | | = | HZU | | * | HUZ | | 6 | .15+ | 12 | ų. | 1450. |
| HUZ | | 102 | | Ξ | 1204 | 2 | ÷. | UZ | | 4 | . OCT | 12 | <u>u</u> . | U . |
| | . I. | H202 | | | 00 | | T | N2U | | - 1 | . O C T | 14 | ų. | 45570 |
| THTPN | UDA VUU | 1202 | | -2. | oon | | | | | 1., | 44 C T | 71 | υ. | 45510. |
| H2 | 2. | 30 | 02 | | | .78 | | H20 | | 6 | . 0 | H: | 202 | 6.6 |
| END | | | | | | | | | | • | •• | | | |
| H2 | + | OH | | = | H20 | | + | H | | 4.1 | 74E+ | 13 | 0. | 6098. |
| н | + | 02 | | = | H02 | | + | M | | 1.4 | 46 E+ | 15 | Ο. | -1000. |
| THIRDE | ODY | | | | | | | | | | | | | |
| 02 | . 1. | .30 | N2 | | | 1.3 | | H20 | | 2 | 1.3 | H | 2 | 3.0 |
| END | - | | | | •• | | | | | | | | - | |
| M | + | H20 | | - | н | | + | OH | | 1 | 50E+ | -15 | υ. | 105140. |
| INTERNE | זעטי | ** | | | | ч с | | 420 | | | ~ ~ | M | • | 1 6 |
| 72 FND | 4. | | 02 | | | 1.3 | | n20 | | ~ | 0.0 | R. | 2 | 1.5 |
| - CR <i>U</i> | + | n | | = | 0H | | + | м | | 7 | 15+ | 18 | -1 | n |
| M | ÷ | H2 | | . = | Ř. | | ÷ | H | | 2 | .2F+ | 14 | â. | 96000. |
| THIRDE | ODY | | | | | | | | | _ | | • | ••• | |
| H2 | 4. | 10 | 02 | | | 2.0 | | H20 | | 1 | 5.0 | N | 2 | 2.0 |
| END | | | | | | | | | | | | | | |
| M | + | 02 | | z | 0 | | + | 0 | | 1.3 | BOEt | 18 | -1. | 118020. |
| CQ | + | 0 | | 2 | COS | | | - | | 8. | 43E+ | -09 | 001 | 1000. |
| C 11 D | | C02 | | > | Cū | | Ŧ | U | | 9. | 08E4 | .12 | ~1.84 | - 130/54. |
| END | | | | | | _ 1 | | | _ | | | | | |
| TIME | | | | | | - 1 | PLA | NK LINE | - | | | | | |
| 2PPOR L | IFI ST | 2= TRIS | F. | | SEND | | | CJIID | | | | | | |
| AWSPROB | | | , | | | | | | | | | | | |
| DELM | D= 10 | 10., D | OTMA | X= 1 | 160. | MPR | =1, | | | | | | | |
| VOLI | ME= | 500., | | &EN | D | | | | | | | | | |
| &START 1 | = 880 |).,P=5 | .5,M | DOT= | 140 | .0, 4 | era | tio =1.5 | , scc | Ξ. | 3.0, | sc | h = 8.0, | &END |
| END | | | | | | | | | | | | | | |
| FINIS | | | | | | | | | | | | | | |

LENIS SENSITIVITY AND GENERAL KINETICS PROGRAM

NASA LEWIS RESEARCH CENTER

GLOBAL AND MOLECULAR REACTIONS; MOLECULAR REACTIONS ADDED CASE 7

| NUMBER REACTION REACTION REACTION RATE VAR | RIABLES N ACTIVATION |
|--|-------------------------------|
| 1 1×0 + 1×H20 = 2×0H 6.80000F+13 0 | 0 0000 18365 00 |
| 2 1XH + 1XO2 = 1XOH + 1XO 1 89000F+16 2 | 1 1110 16305.00 |
| 3 1×0 + 1×H2 = 1×0H + 1×H 62000F+14 0 | 0 8000 13750 00 |
| 4 1XH + 1XH02 = 1XH2 + 1XD2 7 28000F+13 0 | 0 0000 23730.00 |
| 5 1×0 + 1×H02 = 1×0H + 1×02 5 0000E+13 0 | 0 0000 1000 00 |
| $6 1 \times 102 + 1 \times 101 = 1 \times 120 + 1 \times 12 $ | 0 0000 0 000.00 |
| 7 1×H + 1×H02 = 2×0H 1 36000F+16 0 | 0.0000 0.00 0.0000 1070.00 |
| 8 1¥H2 + 1¥H02 = 1¥H202 + 1¥H 7 01000E413 0 | |
| 9 IX0H + IXH202 = IXH20 + IXH02 (771000-11) | 0 0000 20000.00 |
| | |
| | |
| $12 M + 1 \times 1/2 = 2 \times 1/1 $ 1 66 00 0 5 1 1 0 | |
| 13 1¥H2 + 1¥0H = 1¥H20 + 1¥K 6 76000F413 n | |
| | |
| | |
| | |
| | |
| | |
| | 1.0000 116020.00 |
| 20 1¥CO2 > 1¥CO + 1¥O 9.08000E+18 -1 | 1.8400 130754.00 |
| ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING | |
| M(H2 , 12) = 2,30000 M(02 , 12) = 0,78000 M(H20 , 12) = 6,00000 M(H202 | 12) = 6 60000 |
| M(02, 14) = 1.30000 $M(N2, 14) = 1.30000$ $M(H20, 14) = 21.30000$ $M(H22)$ | 161 = 3.00000 |
| M(H2 , 15) = 4.00000 M(O2 , 15) = 1.50000 M(H20 , 15) = 20.00000 M(H2 | (15) = 150000 |
| M(H2 , 17) = 4,10000 M(O2 , 17) = 2,00000 M(H20 , 17) = 15,00000 M(H2 | (17) = 2.00000 |

| , 12) = 2.30000 M(02 | , 12) = 0.78000 | M(H20 | , 12) = 6.00000 | M(H202 | · 12) = | 6.60000 |
|----------------------|-----------------|-------|-----------------|--------|---------|---------|
| , 14) = 1.30000 M(N2 | , 14) = 1.30000 | M(H20 | (14) = 21.30000 | M(H2 | (14) = | 3.00000 |
| , 15) = 4.00000 M(02 | , 15) = 1.50000 | M(H2D | 15) = 20.00000 | M(N2 | 155 = | 1 50000 |
| , 17) = 4.10000 M(02 | , 17) = 2.00000 | MCH20 | 17) = 15,00000 | MCN2 | . 17) = | 2 00000 |

| XXX GLOBAL R | EACTIONS XXX |
|--------------|--------------|
|--------------|--------------|

| NUMBER | | | | | | | |
|----------------|-----------------------------|-------------|----------------------------|-------------|-----------------------------|--------|----------------------------|
| 21 22 23 | 1.0×H20 1.0×C0 1.0×C0 | + + + | 1.0×0 1.0×H20 1.0×H2 | > > > | 1.0×H2 1.0×C02 1.0×C0 | + + | 1.0×02 1.0×H2 1.0×H2 |
| 24 25 26 | 1.0×N2 1.0×CN | + | 1.0×02 2.0×N0 2.0×0 | > > > | 2.0×N0 1.0×N2 1.0×N0 | + | 1.0×02 1.0×C0 |

| 27 28 29 30 31 32 33 1 34 | . O¥0H | + | 1.0×CN 2.0×CH2 1.0×CH2 1.0×H2 1.0×H2 1.0×C3H8 1.0×H2 1.0×H2 1.0×H2 | + + + + + + + | 1.0×N0 1.0×N2 1.0×02 1.0×C3H8 1.0×02 2.0×0H 1.0×02 1.0×0 1.0×0 | > > > > > > > > > > > > > > > > > > > | 1.0%C0 2.0%CN 1.0%C0 3.0%CH2 2.0%OH 1.0%H20 1.0%H20 1.0%H20 | | + 1.0%N2 + 2.0%H2 + 1.0%H20 + 2.0%OH + 1.0%C0H + 1.0%C0 + 1.0%O2 | * + | 1.0×8 1.0×0H | | |
|--|--------|-----------|--|---------------|--|---|--|----|--|---------------|-----------------|--------|------------|
| PEACTION | | | DEACTANT ET | PONEN | re | | | | RE | ACTION | RATE VAL | TARI F | · s |
| NUMBER | | REXP 1 | REXP | 2 | REXP | 3 | | | A | | N | | ACTIVATION |
| 21 | | 0.000 | 1.00 | 0 | 1.000 | I | | | 4.90000E+10 | | 0.1800 | | -510.00 |
| 22 | | 0.000 | 1.00 | ő | 1.000 | 1 | | | 1.30000E+05 | | 1.3100 | | -7000.00 |
| 23 | | 0.000 | 1.00 | Ő | 1.000 | l I | | | 4.41000E+10 | | 0.1900 | | 3527.00 |
| 24 | | 0.000 | 1.00 | Ŭ. | 1.000 |) | | | 4.00000E+14 | | 0.0300 | | 100000.00 |
| 25 | | 0.000 | 0.00 | 0 | 2.000 | 1 | | | 2.00000E+11 | | 0.0000 | | 38000.00 |
| 26 | | 0.000 | 1.00 | 0 | 1.000 | 1 | | | 8.30000E+11 | | 0.0000 | | 0.00 |
| 27 | | 0.000 | 1.00 | 0 | 1.000 | l i i i i i i i i i i i i i i i i i i i | | | 1.25000E+12 | | 0.0000 | | 0.00 |
| 28 | | 0.000 | 1.00 | 0 | 1.000 | 1 | | | 5.00000E+13 | | 0.0000 | | 54000.00 |
| 29 | | 0.000 | 1.00 | 0 | 0.500 | l i | | | 3.50000E+07 | | 0.0000 | | 5000.00 |
| 30 | | 0.000 | 1.60 | 0 | 0.100 |) | | | 1.10000E+12 | | 0.0000 | | 41000.00 |
| 31 | | 0.000 | 1.00 | 0 | 1.000 | ł | | | 1.00000E+00 | | 0.0000 | | 49080.00 |
| 32 | | 0.000 | 9.15 | 0 | 1.000 | 1 | | | 1.98000E+06 | | 0.0000 | | 4000.00 |
| 33 | | 1.000 | 8.00 | 0 | 1.000 | 1 | | | 9.60000E+11 | | -0.1000 | | 1013.00 |
| 34 | | 0.000 | 1.00 | 0 | 1.000 | 1 | | | 4.9000E+10 | | 0.1800 | ~~~ | ~510.00 |
| | ¥X | NEW INPUT | DATA GIVEN | IN COS | S UNITS | ¥X | | Ж¥ | OUTPUT REQUIRED | IN CGS | 5 UNITS | 天天 | |

TABLE A.8.—Continued.

** ASSIGNED VARIABLE PROFILE **

WELL - STIRRED REACTOR CASE

VOLUME OF REACTOR = 5.00000E+02 CMXX3 Mass flow rate to start iteration = 1.40000E+02 G/S

ASSIGNED MASS FLOW RATE PROBLEM: MASS FLOW RATE INCREMENT = 1.000000E+02 G/S Maximum Mass Flow Rate = 1.16000E+03 G/S

FUEL-AIR REACTION, FUEL-AIR EQUIVALENCE RATIO = 1.5000 DXYGEN FRACTION IN AIR = 0.2095

NUMBER OF REACTING SPECIES: 15 NUMBER OF INERT SPECIES: 1 ** INITIAL CONDITIONS **

| TIME | 0.0000CE+00 | SEC | AREA | 0.00000E+00 | SQ CM | AXIAL POSITION | 0.00000E+00 CM |
|------|-------------------------------|-----|-------------|-------------|-------|------------------------|----------------|
| F | LOW PROPERTIES | | | | | INTEGRATION INDICATORS | |
| | PRESSURE | | 5.50000 | | | STEPS FROM LAST PRINT | 0 |
| | VELOCITY | | 0.00 | | | AVERAGE STEP SIZE | 0.0000E+00 |
| | DENSITY (G/CM##3) | | 2.50173E-03 | | | METHOD ORDER | 0 |
| | TEMPERATURE | | 800.00 | | | | |
| | MASS FLOW RAT | E | 1.40000E+02 | | | TOTAL NUMBER OF STEPS | 0 |
| | ENTROPY | ` | 1.8011 | | | FUNCT EVALUATIONS | 0 |
| | MACH NUMBER | , | 0.0000 | | | JACOBIAN EVALUATIONS | 0 |
| | GAMMA | | 1.2701 | | | | |
| | ENTHALPY | | 9.23468E+01 | | | | |
| | SP. HEAT (CP) (CAL/G/DEG K |) | 3.12948E-01 | | | | |

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 |
| H20 | 0.0000E+00 | 0.00000E+00 | 0.0000E+00 | 1 | 6.5377E+08 | 0.00000E+00 | 0.00000 |
| 0 | 0.00000E+00 | 0.00000E+00 | 3.57038E-26 | 2 | 6.2545E+09 | 0.00000E+00 | 0.00000. |
| H2 | 0.00000E+00 | C.00000E+DC | 0.00002+00 | 3 | 7.3608E+10 | 0.00000E+00 | 0.0000 |
| 02 | 1.65148E-05 | 1.97112E-01 | -4.55842E-08 | 4 | 1.9113E+13 | 0.00000E+00 | 0.00000 |
| C0 | 0.00000E+00 | 0.00000E+D0 | 1.86163E-30 | 5 | 2.6655E+13 | 0.00000E+00 | 0.00000. |
| C02 | 2.36493E-08 | 2.82264E-04 | -1.86163E-30 | 6 | 8.0000E+12 | 0.0000CE+00 | 6.0000 |
| N2 | 6.15566E-05 | 7.34704E-01 | -2.38549E-22 | 7 | 6.8359E+13- | 0.00000E+00 | 0.00000 |
| NO | 0.00000E+00 | C.00000E+00 | 4.77899E-22 | 8 | 1.1708E+07 | 0.00C0CE+00 | 0.00000 |
| CN | 0.00000E+00 | 0.00000E+00 | 0,0000E+09 | 9 | 2.4813E+12 | 0.0000E+00 | 0.00000 |
| CH2 | 0.00000E+00 | 0.00000E+00 | 1.36753E-07 | 10 | 1.8000E+12 | 0.0000E+00 | 8.00000 |
| C3H8 | 4.95445E-D6 | 5.91335E-02 | -4.55842E-08 | 11 | 7.8000E+11 | 0.00000E+00 | 0.0000 |
| OH | 0.00000E+00 | C.00000E+00 | 9.11685E-08 | 12 | 5.3163E+04 | 0.0000CE+00 | 0.0000 |
| н | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 13 | 1.0230E+12 | 0.00000E+00 | 0.00000 |
| H02 | 0.00000E+00 | C.00000E+CC | 0.00000E+00 | 14 | 2.7387E+15 | 0.00000E+00 | 0.00000 |
| H202 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 15 | 2.4606E-14 | 0.00000E+00 | 0.0000 |
| AR | 7.34696E-07 | 8.76890E-03 | 0.00000E+00 | 16 | 8.8750E+15 | 0.00000E+00 | 0.00000 |
| | | | | 17 | 1.3075E-12 | 0.00000E+00 | 0.00000 |
| | | | | 18 | 1.2901E-17 | 2.85221E-21 | 1.00000 |

TABLE A.8.—Continued.

| | 19 | 4.4641E+89 | 0.0000E+00 | 0.00000 |
|-----|------|-------------|-------------------|------------|
| | 20 | 7.8718E-23 | 2.97450E-25 | 1.00000 |
| | 21 | 2.2495F+11 | 0.0000F+08 | 0.0000 |
| | 22 | 6.7500E+10 | 0.00000E+00 | 0.00000 |
| | 23 | 1.7080E+10 | 8.00000E+00 | 0.0000 |
| | 24 | 2.3465E-13 | 3.81152E-17 | 1.00000 |
| | 25 | 8.3160E+00 | 8.0000F+0B | <u> </u> |
| | 26 | 8.3000F+11 | 0.000005+00 | 0.0000 |
| | 27 | 1.2500F+12 | 0 000005+00 | 0.0000 |
| | 28 | 8 8483F-02 | 0 000005+00 | 0.0000 |
| | 29 | 1.5071E+06 | 0.000005+00 | 0.0000 |
| | 36 | 6 9297F+00 | 7 283415-83 | 1 80000 |
| | 31 | 3.9081F-14 | 0.0000F+00 | 0.0000 |
| | 32 | 1.5992F+85 | 0.00000E+00 | 0,0000 |
| | 33 | 2 6015F+11 | 0 000005+00 | 0 0000 |
| | 34 | 2.2495E+11 | 0.00000E+00 | 0.00000 |
| | DATE | 7 107505-14 | MARE EDICTION SUM | 1 00000000 |
| 105 | KA15 | 3,377376-10 | MADD LEADITON DOW | T.00000000 |

TOTAL ENERGY EXCHANGE RATE 3.39759E-16 (CAL-CM**3/G**2/SEC)

MIXTURE MOLECULAR WEIGHT 29.85916

CPU TIME FOR INITIALIZATION OF LSENS = 0.516666 S **Equilibrium conditions **

| TIME | 0.00000E+00 | SEC | AREA | 0.00D00E+00 | SQ CM | AXIAL POSITION | 0.00000E+00 CM |
|------|-------------------------------|--------------|------|-------------|-------|------------------------|----------------|
| F | LOW PROPERTIES | | | | | INTEGRATION INDICATORS | |
| | PRESSURE | 5.500 | 00 | | | STEPS FROM LAST PRINT | 0 |
| | VELOCITY (CM/SEC) | 8.00 | | | | AVERAGE STEP SIZE | 0.00008E+80 |
| | DENSITY (G/CMHH3) | 7.34828E-0 |)4 | | | METHOD ORDER | 0 |
| | TEMPERATURE | 2350.3 | 51 | | | | |
| | MASS FLOW RAT | E 1.40000E+0 | 2 | | | TOTAL NUMBER OF STEPS | 0 |
| | ENTROPY | 2.360 | 14 | | | FUNCT EVALUATIONS | C |
| | MACH NUMBER | , D.000 | 0 | | | JACOBIAN EVALUATIONS | G |
| | GAMMA | 1.264 | 11 | | | | |
| | ENTHALPY | 9.23468E+I | 01 | | | | |
| | SP. HEAT (CP) (CAL/G/DEG K | 3.69088E-1 |)1 | | | | |

CHEMICAL PROPERTIES

| SPECIES | CONCENTRATION (MOLES/CMXX3) | MOLE FRACTION | NET SPECIES PRODUCTION RATE (MOLE/CMXX3/SEC) | REACTION NUMBER | A RATE CONST CGS UNITS | NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC) | NET RATE/POSI- TIVE DIR RATE |
|---------|--------------------------------|---------------|---|--------------------|---------------------------|---|---------------------------------|
| H20 | 4.05534E-06 | 1.42200E-01 | 8.67144E-03 | 1 | 1.3329E+12 | -7.60162E-04 | 0.00000 |
| 0 | 2.17893E-10 | 7.64039E-06 | -2.74022E-04 | 2 | 5.6424E+12 | -2.68460E-05 | 0.00000 |
| H2 | 1.73940E-06 | 6.09920E-02 | -8.55648E-03 | 3 | 2.2114E+13 | -6.59110E-04 | 0.00000 |
| 02 | 2.11927E-10 | 7.43118E-06 | 3.89333E-04 | 4 | 4.6178E+13 | 1.43082E-06 | 0.0000 |
| C0 | 3.10378E-06 | 1.08834E-01 | 8.94626E-03 | 5 | 4.0363E+13 | 7.03729E-09 | 0.00000 |
| CO2 | 1.26895E-06 | 4.44958E-D2 | -8.94626E-03 | 6 | 8.0000E+12 | 1.29043E~07 | 0.0000 |
| N2 | 1.80796E-05 | 6.33959E-01 | -1.08608E-07 | 7 | 1.0656E+14 | - 2.24499E-06 | 0.00000 |
| NO | 2.64686E-09 | 9.28118E-05 | 8.94819E-10 | 8 | 3.7453E+11 | 1.99374E-01 | 0.42297 |
| CN | 7.34828E-14 | 2.57667E-09 | 2.16320E-07 | 9 | 4.4911E+12 | -6.86707E-03 | 0.42297 |
| CH2 | 7.34828E-14 | 2.57667E-09 | -2.04669E-07 | 10 | 1.8000E+12 | 2.15231E-07 | 0.42297 |
| C3H8 | 7.34828E-14 | 2.57667E-09 | -2.73798E-09 | 11 | 7.8000E+11 | -2.90148E-03 | 0.42297 |
| OH | 1.53281E-08 | 5.37479E-04 | -2.76262E-04 | 12 | 8.4429E+12 | -4.30001E+01 | 0.42297 |
| H | 3.72907E-08 | 1.30759E-03 | 2.13187E-07 | 13 | 1.2845E+13 | 1.94110E-01 | 0.00000 |
| H02 | 3.90703E-13 | 1.37000E-08 | -1.11365E-07 | 14 | 1.8086E+15 | 3.66684E-06 | 0.00000 |
| H202 | 7.34828E-14 | 2.57667E-09 | 2.33318E-05 | 15 | 2.1738E+05 | -5.10833E-04 | 0.00000 |
| AR | 2.15801E-07 | 7.56703E-03 | 0.0000E+00 | 16 | 3.0209E+15 | 2.93337E-06 | 0.00000 |
| | | | | 17 | 2.6038E+05 | -2.10296E-04 | 0.00000 |
| | | | | 18 | 8.1234E+03 | -2.35297E-10 | 0.00000 |
| | | | | 19 | 6.7526E+09 | 8.45/30E+00 | 1.00000 |
| | | | | 20 | 3.9510E+00 | 9.28491E+00 | 1.00000 |
| | | | | 21 | 2.2102E+11 | 3.61677E+02 | 1.00000 |
| | | | | 22 | 1.5172E+10 | 3.53653E+05 | 1.00000 |
| | | | | 23 | 9.0570E+10 | 3.70220E+05 | 1.00000 |
| | | | | 24 | 2.5376E+05 | I.80064E-03 | 1.00000 |
| | | | | 25 | 5.8546E+07 | 7.59605E-04 | 1.00090 |
| | | | | 26 | 8.3000E+11 | 2.46114E-05 | 1.00000 |
| | | | | 27 | 1.2500E+12 | 4.50252E-04 | 1.00000 |
| | | | | 28 | 4.7603E+08 | 1.17122E-03 | 1.00000 |
| | | | | 29 | 1.1999E+07 | 2.37704E-05 | 1.00000 |
| | | | | 30 | 1.6939E+08 | 5.07039E-03 | 1.00000 |
| | | | | 31 | 2.7300E-05 | 1.86371E-14 | 1.00000 |
| | | | | 32 | 8.4084E+05 | 2.55717E+02 | 1.00000 |
| | | | | 33 | 3.5560E+11 | 2.13927E+00 | 1.00000 |
| | | | | 34 | 2.2102E+11 | 3.61677E+02 | 1.00000 |
| MIXTUR | E MOLECULAR NEIGH | T 25.76666 | TOTAL ENERGY EXCHANGE (CAL-CM**3/G**2/SI | RATE C) | 1.05177E+05 | MASS FRACTION SUM | 1.0000010 |

COMPUTATIONAL WORK REQUIRED FOR EQUILIBRIUM CALCULATION: NO. OF ITERATIONS = 12 CPU TIME = 3.333282E-02 S

INITIAL ESTIMATES (SIGMAS) AT TEMPERATURE = 2350.31 K:

| H20 | 5.51876F-03 |
|------|--------------|
| 0 | |
| Ų | 2.965235-07 |
| HZ | 2.36709E-03 |
| 02 | 2 226035-07 |
| 02 | 2.0040JL-07 |
| CO | 4.223826-03 |
| C02 | 1.72687E-03 |
| N2 | 2.46038E-02 |
| | 7 (000) 6 07 |
| NU | 2.005016-00 |
| CN | 1.00000E-10 |
| CH2 | 1.00000E~10 |
| CTUR | 1 000005-10 |
| Cono | 1.000002-10 |
| OH | 2.08595E-05 |
| н | 5.07475E-05 |
| H02. | 5 31693F-10 |
| | 2.210/32 10 |
| 1202 | 1.000002-10 |
| AR | 2.93675E-84 |
| **** | |

(WSR) *** FOR CONV. NO. 1, CONVERGED TEMP. (AFTER 17 ITERATIONS) IS GREATER THAN OR EQUAL TO THE PREVIOUS TEMP. *** MASS FLOW RATE = 1.4000DE+02 G/S, TEMPERATURE = 2.44550E+03 K, PREVIOUS TEMPERATURE = 2.35031E+03 K

(WSR) ** RESTART: MASS FLOW RATE = 2.80000E+02 G/S, TEMPERATURE = 2.35031E+03 K **

(WSR) *** FOR CONV. NO. 1, CONVERGED TEMP. (AFTER 21 ITERATIONS) IS GREATER THAN OR EQUAL TO THE PREVIOUS TEMP. *** Mass flom rate = 2.800000=+02 G/S, temperature = 2.41194E+03 K, previous temperature = 2.35031E+03 K

(WSR) ** RESTART: MASS FLON RATE = 5.60000E+02 G/S, TEMPERATURE = 2.35031E+03 K ** Wellstirred reactor calculation....global and molecular reactions; molecular reactions added case 7

| | INITIAL STATE | | FINAL STATE | FINAL/INITIAL RATIO |
|---|---|--|--|---|
| PRESSURE ATM TEMP. DEG K ENTROPY CAL/GM/K DENSITY GM/CM**3 ENTHALPY CAL/GM SP. HEAT (CP) CAL/GM/K MOL. NT. OF MIXT GAMMA | 5.50000 800.000 1.80111 2.50173E-03 92.3468 3.12948E-01 29.8592 1.2701 | | 5.50000 2342.87 2.25627 8.03853E-04 92.3468 3.76201E-01 28.0978 1.2315 | 1.00000 2.92859 1.25271 0.32132 1.00000 1.20212 |
| SPECIES | MOLE FRACT | MASS FRACT | MOLE FRACT | MASS FRACT |
| H20 D H2 D2 C02 N2 N0 CN CN CN CN CN CN CN CN CN CN CN CN CN | 0.00000E+00 0.0000E+00 1.97112E-01 2.82264E-04 7.34704E-01 0.0000E+00 0.0000E+00 0.0000E+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 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 | 0.000000000000000000000000000000000000 | $\begin{array}{c} 1.41886E-01\\ 7.861884E-04\\ 6.16159E-03\\ 1.12541E-02\\ 1.91345E-02\\ 9.07499E-02\\ 6.90019E-01\\ 3.92059E-04\\ 2.29878E-03\\ 6.28177E-03\\ 1.62455E-03\\ 1.62455E-03\\ 3.43037E-06\\ 4.4354E-07\\ 8.25163E-03\\ \end{array}$ | 9.09717E-02 4.47668E-04 1.28166E-02 1.90750E-02 1.42142E-01 6.87946E-01 4.18686E-04 2.12860E-03 3.13594E-03 3.19292E-03 3.19292E-03 4.50232E-05 9.90322E-05 5.37925E-07 1.17317E-02 |
| VOLUME 500.000 CM× | ×3 MASS FLO | 560.000 | GM/ SEC | |
| NDOT/VOLUME = 1.1200 Nellstirred reactor Cal | 0 RESIDENCE TIME = CulationGlobal An | 0.718 ID MOLECULAR RE | MSEC ITERATIONS = Actions; Molecular Re | 17 ACTIONS ADDED CASE |
| | INITIAL STATE | | FINAL STATE | FINAL/INITIAL RATIO |
| PRESSURE ATM TEMP: DEG K ENTROPY CAL/GM/K DENSITY GM/CMXX3 ENTHALPY CAL/GM/K SP. HEAT (CP) CAL/GM/K MDL. WT. OF NIXT GAMMA | 5.50000 800.000 1.80111 2.50173E-03 92.3468 3.12948E-01 29.8592 1.2701 | | 5.50000 2192.26 2.23090 8.61527E-04 92.3468 3.73834E-01 28.1779 1.2325 | 1.00000 2.74032 1.23863 0.34437 1.00000 1.19456 |
| SPECIES | MOLE FRACT | MASS FRACT | MOLE FRACT | MASS FRACT |
| H20 0 H2 02 C0 C02 N2 N0 CN CH2 C3H8 OH H H02 H202 AR | 0.00000E+00 0.00000E+00 1.97112E-01 2.82264E-04 7.34704E-01 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.91353E-02 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 8.76890E-03 | $\begin{array}{c} 0.00000000000000000000000000000000000$ | 1.32976E-01 1.05479E-03 3.60083E-03 2.23110E-02 1.16951E-02 8.83688E-02 6.92506E-01 1.91990E-04 1.46599E-03 1.39672E-02 1.73936E-02 5.24581E-03 9.30158E-04 1.68549E-05 9.35949E-03 | 8.50163E-02 5.98908E-04 2.57598E-04 2.53364E-02 1.16256E-02 1.38019E-01 6.88463E-01 2.04446E-04 1.35360E-03 6.95280E-03 3.16621E-03 3.32733E-05 1.97433E-05 1.12982E-06 1.17317E-02 |

7

TABLE A.8.—Concluded.

| VOLUME | 500.000 | CMXX3 | MASS FLO | 1060.00 | GM/SEC | | | | |
|--|--|--|--|---|---|--|---|---|-------------------|
| MDOT/VOL WELLST | UME = 2. Irred reactor | 12000 RESII Calculation. | ENCE TIME = Global An | D.400 D MOLECULAR RE | 6 MSEC Eactions | ITERATION: ; MOLECULAR | S = 4 REACTIONS | ADDED | CASE 7 |
| | | IN | ITIAL STATE | | FINAL | STATE | FINAL | /INITIAL | RATIO |
| PRESSURI TEMP. ENTROPY DENSITY ENTHALPY SP. HEA MOL. WT GAMMA | E ATM DEG K CAL/G GM/CM Y CAL/G T (CP) CAL/G . OF MIXT | 5 M/K 8 XX3 2 M 9 M/K 3 | .50000 00.000 .80111 .50173E-03 2.3468 .12948E-01 29.8592 1.2701 | | 5.5 212 2.2 8.769 92. 3.731 28. 1. | 0000 4.84 2440 49E-04 3468 52E-01 1927 2329 | | 1.00000 2.69355 1.23502 0.35054 1.00000 1.19238 | |
| SPECIES | | MOLE FR | ACT | MASS FRACT | | MOLE FRACT | I | MASS FRAC | т |
| H20 0 H2 C0 C02 N2 N0 CN CN CH2 C3H8 H4 H02 H202 AR VOLUME MDOT/VOLU | 500.000 UME = 2. | 0.00000 0.00000 0.97112 0.00000 0.282264 7.34704 0.000000 | E+00 E+00 E+00 E-01 E+00 E-04 E+00 E+00 E+00 E+00 E+00 E+00 E+00 E+ | 0.00000E+00 0.00000E+00 2.11236E-01 0.00000E+00 4.16032E-04 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 1.17317E-02 1160.00 0.378 | GM/SEC 3 MSEC | 1.30743E-01 1.07475E-03 3.10814E-03 1.54944E-02 1.37071E-02 6.93073E-01 1.214869E-05 1.23144E-03 1.55465E-02 1.77430E-02 5.07489E-03 4.30841E-05 8.27951E-03 ITERATIONS | 8 6 2 2 1 1 6 2 2 1 7 7 2 3 2 2 1 1 1 5 5 | .35451E=0 .09921E=0 .22234E=0 .89352E=0 .35891E=0 .35891E=0 .35891E=0 .13645E=0 .73488E=0 .73488E=0 .73488E=0 .061749E=0 .234628E=0 .234628E=0 .234628E=0 .23472E=0 .17317E=0 | 24422115332235562 |
| | | NO. OF | MPUTATIONAL I | NORK REQUIRED = 89 CF | FOR PSR PU TIME | CALCULATIO | 1:- +00 S | | |

(LSENS) END OF THIS CASE

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 2.400001 S

(LSENS) READ DATA FOR NEXT CASE

References

- Radhakrishnan, K.: LSENS—A General Chemical Kinetics and Sensitivity Analysis Code for Homogeneous Gas-Phase Reactions, Part I: Theory and Numerical Solution Procedures. NASA RP–1328, 1994.
- Radhakrishnan, K.; and Bittker, D.A.: LSENS—A General Chemical Kinetics and Sensitivity Analysis Code for Homogeneous Gas-Phase Reactions, Part II: Code Description and Usage. NASA RP–1329, 1994.
- Bittker, D.A.; and Radhakrishnan, K.: LSENS—A General Chemical Kinetics and Sensitivity Analysis Code for Homogeneous Gas-Phase Reactions, Part III: Illustrative Test Problems. NASA RP–1330, 1994.
- Bittker, D.A.: Mathematical Description of Complex Chemical Kinetics and Application to CFD Modeling Codes. Computing Sys. Eng., vol. 4, no. 1, 1993, pp. 1–12.
- Bittker, D. A.: Detailed Mechanism of Toluene Oxidation and Comparison With Benzene. NASA TM–100261, 1988.
- Bittker, D.A.: Detailed Mechanism for Oxidation of Benzene. Comb. Sci. Tech., vol. 79, nos. 1–3, 1991, pp. 49–72, and Errata, vol. 86, 1992, p. 337.
- Emdee, J.L.; Brezinsky, K.; and Glassman, I.: A Kinetic Model for the Oxidation of Toluene Near 1200 K. J. Phys. Chem., vol. 96, 1992, pp. 2151–2161.
- Daguet, P., et al.: Kinetic Modeling of Ethylene Oxidation. Comb. Flame, vol. 71, 1988, pp. 295–312.

- Daguet, P., et al.: Kinetic Modeling of Propane Oxidation. Comb. Sci. Tech., vol. 56, 1987, pp. 23–63.
- Westbrook, C.K., et al.: A Kinetic Modeling Study of *n*-Pentane Oxidation in a Well-Stirred Reactor. Comb. Flame, vol. 72, 1988, pp. 45–62.
- Daguet, P.; Boettner, J.C.; and Cathonnet, M.: Ethylene Pyrolysis and Oxidation: A Kinetic Modeling Study. Int. J. Chem. Kinet., vol. 22, no. 6, June 1990, pp. 641–664.
- Glasstone, S.: Textbook of Physical Chemistry. Second ed., D. Van Nostrand, 1946, p. 232.
- Gordon, S.; and McBride, B.J.: Computer Program for Calculation of Complex Chemical Equilibrium Compositions and Applications, Part I—Analysis. NASA RP–1311, 1994.
- McBride, B.J.; and Gordon, S.: Computer Program for Calculating and Fitting Thermodynamic Functions. NASA RP–1271, 1992.
- Kundu, K.P.; and Deur, J.M.: A Simplified Reaction Mechanism for Prediction of NO_x in the Combustion of Hydrocarbons. AIAA Paper 92–3340, July 1992.
- Brabbs, T.A.; and Musiak, J.D.: Ignition Delay Measurements and Proposed Kinetic Model for Hydrogen-Oxygen. NASPCR-1030, 1988.
- Brabbs, T.A., et al.: Hydrogen Oxidation Mechanism With Applications to (1) Chaperon Efficiency of Carbon Dioxide and (2) Vitiated Air Testing. NASA TM-100186, 1987.

| REPORT I | Form Approved OMB No. 0704-0188 | | | | | |
|--|--|--|--|--|--|--|
| Public reporting burden for this collection of ir gathering and maintaining the data needed, a collection of information, including suggestions Davis Highway, Suite 1204, Arlington, VA 22 | nformation is estimated to average 1 hour per nd completing and reviewing the collection of i s for reducing this burden, to Washington Head 202-4302, and to the Office of Management ar | esponse, including the time for rev nformation. Send comments regar lquarters Services, Directorate for id Budget, Paperwork Reduction P | viewing instructions, searching existing data sources, ding this burden estimate or any other aspect of this Information Operations and Reports, 1215 Jefferson roject (0704-0188), Washington, DC 20503. | | | |
| 1. AGENCY USE ONLY (Leave blank) |) 2. REPORT DATE | 3. REPORT TYPE AND | ND DATES COVERED | | | |
| | March 1990 | | | | | |
| GLSENS, A Generalized E Added Sensitivity Analysis | xtension of LSENS Including Gl for the Perfectly Stirred Reactor | obal Reactions and | | | | |
| 6. AUTHOR(S) | WU-505-62-52 | | | | | |
| David A. Bittker | | | | | | |
| 7. PERFORMING ORGANIZATION N | AME(S) AND ADDRESS(ES) | | 8. PERFORMING ORGANIZATION REPORT NUMBER | | | |
| National Aeronautics and S Lewis Research Center Cleveland, Ohio 44135–3 | pace Administration | | E-9496 | | | |
| 9. SPONSORING/MONITORING AGE | ENCY NAME(S) AND ADDRESS(ES) | | 10. SPONSORING/MONITORING AGENCY REPORT NUMBER | | | |
| National Aeronautics and S Washington, D.C. 20546–0 | pace Administration 0001 | | NASA RP-1362 | | | |
| 11. SUPPLEMENTARY NOTES David A. Bittker, Distinguis (216) 433–5850. | shed Research Associate. Respor | sible person, Edward J. | Mularz, organization code 2650, | | | |
| 12a. DISTRIBUTION/AVAILABILITY | STATEMENT | | 12b. DISTRIBUTION CODE | | | |
| Unclassified - Unlimited | | | | | | |
| Subject Categories 25 and 6 | 51 | | | | | |
| This publication is available from ABSTBACT (Maximum 200 word) | m the NASA Center for Aerospace Inf | ormation, (301) 621–0390. | | | | |
| A generalized version of the global reactions as well as a performing sensitivity analy the main kinetics calculation accurate and efficient. Nine ties. This report is to be use | e NASA Lewis general kinetics of molecular processes in a chemica ysis calculations for a perfectly s ons are being done. The GLSENS e example problems are presented and in conjunction with the docum | code, LSENS, is describ al mechanism. The code tirred reactor rapidly and code has been extensive and complete user instr entation for the original | ed. The new code allows the use of also incorporates the capability of d conveniently at the same time that ely tested and has been found to be ructions are given for the new capabili LSENS code. | | | |
| 14. SUBJECT TERMS | | | 15. NUMBER OF PAGES 93 | | | |
| General chemical kinetics c | computations; Global reactions; S | sensitivity analysis | 16. PRICE CODE A05 | | | |
| 17. SECURITY CLASSIFICATION OF REPORT Unclassified | 18. SECURITY CLASSIFICATION OF THIS PAGE Unclassified | 19. SECURITY CLASSIFICA OF ABSTRACT Unclassified | TION 20. LIMITATION OF ABSTRACT | | | |
| NSN 7540-01-280-5500 | | I | Standard Form 298 (Rev. 2-89) | | | |