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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 species-composition 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

Symbols

A_j	preexponential factor in rate coefficient equations (2.6) and (2.7) for reaction j
A_s	preexponential factor for reaction s (eq. (2.43))
a_j	sum of all a_{lj} values over all rate-controlling species for reaction j
a_{ij}	empirically determined power of $\rho\sigma_i$ in global reaction rate equation (2.9) for reaction j
a_{lj}	empirical global rate equation exponent for species l in reaction j (eq. (2.35))
C_{pl}	molar heat capacity of species l
c_j	exponential constant in special rate coefficient equation (2.7) for reaction j
c_p	mass specific heat of reacting mixture
c_s	exponential constant for reaction s (eq. (2.46))
E_j	activation energy in rate coefficient equation for reaction j
E_s	activation energy for reaction s (eq. (2.45))
ΔG_j°	Gibbs function change for reaction j
GLADD	logical variable which, if true, indicates that global reactions are being added when multiple cases are being performed
GLCHNG	logical variable which, if true, indicates that global reaction rates are being changed when multiple cases are being performed
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 in reacting mixture
H_i°	standard molar enthalpy of species i (298.15 K)
ΔH_j°	enthalpy change for reaction j at 298.15 K
H_l	molar enthalpy of species l at reactor temperature T
$H_{l,0}$	molar enthalpy of species l at initial reactor temperature T_0
K_j	equilibrium constant for jth chemical reaction, in concentration units
k_j	reaction rate coefficient for jth molecular chemical reaction (eqs. (2.6) and (2.7))
$k_j(T)$	reaction rate coefficient for jth global chemical reaction (eq. (2.9))
k_s	reaction rate coefficient for sth 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 previous case mechanism contains only molecular reactions when multiple cases are being performed
M_j	collisional efficiency factor for collisionally catalyzed reaction j (eq. (2.8))
M_W	molecular weight of mixture
m_{ij}	relative collisional efficiency of species i in collisionally catalyzed reaction j
$\dot{m}$	mass flow rate through reactor
NR	number of reactions in chemical mechanism
NRS	number of reacting species in reacting mixture
NS	total number of species (including inert ones) in reacting mixture
n_j	temperature exponent in rate coefficient equations (2.6) and (2.7) for reaction j
n_s	temperature exponent in rate coefficient equation for reaction s (eq. (2.44))
p	pressure
$\dot{Q}$	rate of heat transfer from reactor
R	universal gas constant
R_j	forward rate of molecular chemical reaction j per unit volume
R_{-j}	backward rate of molecular chemical reaction j per unit volume
r_j	net molar rate of molecular or global reaction j per unit volume
S_{ij}	unnormalized sensitivity coefficient
$\langle S_{ij} \rangle$	normalized sensitivity coefficient (eq. (2.54))
$\mathcal{S}_i$	symbol for species i as reactant or product in chemical reaction
T	absolute temperature
v	volume of reactor
W_i	net molar formation rate of species i per unit volume
y_i	ith dependent variable (species concentration or temperature) of PSR problem
$\bar{y}_i$	value of ith dependent variable for standard value of changed parameter in brute-force sensitivity coefficient calculation
η_j	rate coefficient parameter of jth chemical reaction
ν'_j	sum of stoichiometric coefficients for reactants in reaction j
ν''_j	sum of stoichiometric coefficients for products in reaction j
ν'_{ij}	stoichiometric coefficient of reactant species i in reaction j
ν''_{ij}	stoichiometric coefficient of product species i in reaction j
ν'_{lj}	stoichiometric coefficient of reactant species l in reaction j
ν''_{lj}	stoichiometric coefficient of product species l in reaction j
$\Delta\nu_j$	change in number of molecules (products minus reactants) for reaction j
ρ	mass density of gas mixture
σ_i	mole number (moles per unit mass of mixture) of species i
σ_l	mole number of species l
φ	equivalence ratio
ω_{ij}	net rate of formation of species i by reaction j per unit volume
ω_{is}	rate of formation of species i by reaction s

Subscript:

0	initial-mixture condition

Superscript:

$\circ$	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 one-dimensional 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 heat-release 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 heat-release 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 one-dimensional 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_{ij} 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

$$M + \sum_{i=1}^{\mathrm{NRS}} \nu'_{ij} \mathcal{S}_i = \sum_{i=1}^{\mathrm{NRS}} \nu''_{ij} \mathcal{S}_i + M \qquad j = 1, 2, \ldots, \mathrm{NR} \quad (2.1)$$

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, $\mathcal{S}_i$ is the name of species i, and ν'_{ij} and ν''_{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

$$W_i = \sum_{j=1}^{\mathrm{NR}} \omega_{ij} = \sum_{j=1}^{\mathrm{NR}} \left(\nu''_{ij} - \nu'_{ij} \right) r_j \qquad (2.2)$$

where

$$r_j = R_j - R_{-j} \qquad (2.3)$$

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

$$R_j = M_j k_j \prod_{i=1}^{\mathrm{NRS}} \left(\rho\sigma_i \right)^{\nu'_i} \qquad (2.4)$$

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

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

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

or, for a few reactions, by the equation

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

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

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

where m_{ij} is the collisional efficiency of species i in the jth 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

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

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

$$r_j = k_j \left\{ [C_2HO]^2 - \frac{[C_2H_2][CO]^2}{K_j} \right\}$$

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

$$\frac{\dot{m}}{v}\left(\sigma_{i,0} - \sigma_i\right) + W_i = 0 \qquad i = 1, 2, \ldots, \mathrm{NRS} \qquad (2.10)$$

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

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

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 $\sigma_1, \sigma_2, ..., \sigma_{NRS}$ 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

$$y_i = \sigma_i \quad i = 1,2,3,...,\text{NRS}$$

and

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

2.2.1 Sensitivity Coefficients With Respect to Rate Parameters

The following unnormalized sensitivity coefficients are defined:

$$S_{ij} = \frac{\partial y_i}{\partial \eta_j} \qquad j = 1,2...,\text{NR}$$

$$i = 1,2,...,\text{NRS}+1 \qquad (2.12)$$

where η_j represents any of the rate coefficient parameters of the jth 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

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

$$i = 1,2,...,\text{NRS} \qquad (2.13)$$

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

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

$$i = 1,2,...,\text{NRS} \qquad (2.14)$$

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

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

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

$$c_p = \sum_{l=1}^{NS} \sigma_l C_{pl} \qquad (2.16)$$

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:

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

*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

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

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

$$\frac{\partial r_s}{\partial \eta_s} = r_s \frac{\partial \ln k_s}{\partial \eta_s} \quad (2.20)$$

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

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

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 $\{\sigma_i\}$ through the ideal-gas law.

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

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:

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

$$\left.\frac{\partial W_i}{\partial T}\right|_{\substack{\text{all}\\ \sigma_i}} = \left.\frac{\partial W_i}{\partial T}\right|_{\substack{\text{all }\sigma_i,\\ \rho}} - \frac{\rho}{T}\left.\frac{\partial W_i}{\partial \rho}\right|_{\substack{\text{all }\sigma_i,\\ T}} \quad (2.24)$$

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

$$\frac{\partial \rho}{\partial \sigma_l} = -\rho M_w \quad (2.25)$$

$$\frac{\partial \rho}{\partial T} = \frac{-\rho}{T} \quad (2.26)$$

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

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

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

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

*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,

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

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:

$$\frac{\partial r_j}{\partial \sigma_l} = \frac{\nu'_{lj} R_j}{\sigma_l} - \frac{\nu''_{lj} R_{-j}}{\sigma_l} \tag{2.31}$$

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

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

where ν'_j is the sum of the reactant stoichiometric coefficients in the jth reaction and ν''_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,

$$\frac{\partial r_j}{\partial \sigma_l} = \frac{\nu'_{lj} R_j}{\sigma_l} - \frac{\nu''_{lj} R_{-j}}{\sigma_l} + \frac{r_j \rho m_{lj}}{M_j} \tag{2.33}$$

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

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

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

$$\frac{\partial r_j}{\partial \rho} = \frac{a_j r_j}{\rho} \tag{2.36}$$

where a_j is the sum of all the a_{lj} 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 calculated. 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

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

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

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

where ΔG_j° is the Gibbs function change for the reaction and $\Delta\nu_j$ 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

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

where ΔH_j° is the heat of reaction given by

$$\Delta H_j^\circ = \sum_{i=1}^{\text{NRS}} \left(\nu''_{ij} - \nu'_{ij}\right) H_i^\circ \tag{2.41}$$

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

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

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:

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

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

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)

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

The second term can be written out as follows:

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

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

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

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

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

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

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

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

$$S_{i,T_0} = \frac{\partial y_i}{\partial T_0} \qquad i = 1,2,\ldots,\text{NRS}+1 \tag{2.52}$$

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

$$\left.\begin{aligned} &\sum_{l=1}^{\text{NRS}} \left\{ \left.\frac{\partial W_i}{\partial \sigma_l}\right|_T - \frac{\dot{m}}{v}\delta_{il} \right\} S_{l,T_0} + \left.\frac{\partial W_i}{\partial T}\right|_{\substack{\text{all}\\ \sigma_i}} S_{\text{NRS}+1,T_0} = 0 \\ &\qquad\qquad\qquad\qquad i = 1,2,\ldots,\text{NRS} \\ &\sum_{l=1}^{\text{NRS}} H_l S_{l,T_0} + \left(c_p + \frac{1}{\dot{m}}\frac{\partial \dot{Q}}{\partial T}\right) S_{\text{NRS}+1,T_0} = c_{p,0} \end{aligned}\right\} \tag{2.53}$$

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

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

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 $\delta y_i/\delta\eta_j$, 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

TABLE 2.1.—NORMALIZATION FACTORS FOR RATE COEFFICIENT PARAMETER SENSITIVITY COEFFICIENTS

[R is the universal gas constant in calories per mole-K and T_0 is the gas mixture's initial temperature.]

Rate coefficient parameter	Sensitivity coefficient normalization factor in eq. (2.54)
A_j [a,b]	$0.01\ A_j$
n_j [a,b]	$0.01/\ln T_0$
E_j [a]	$-0.01\ RT_0$
c_j [b]	$0.01/T_0$

[a]See eq. (2.6).
[b]See eq. (2.7).

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

where

$\bar{y}_i$ — y_i value for standard value of A_j

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

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

and

$$\Delta = 0.01A_j$$

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

$$\left\langle S_{i,T_0} \right\rangle = \frac{T_0}{y_i}\left\{\frac{\partial y_i}{\partial T_0}\right\} \qquad i = 1,2,\ldots,\text{NRS}+1 \tag{2.56}$$

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

$$\left\langle S_{i,T_0} \right\rangle = \frac{T_0\left[y_i\left(T_0 + 2\text{K}\right) - y_i\left(T_0 - 2\text{K}\right)\right]}{4\bar{y}_i} \tag{2.57}$$

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

TABLE 3.1.—DESCRIPTION OF LOGICAL VARIABLES IN NAMELIST RTYPE

Variable name	Value[a]	Explanation
GLOBAL	TRUE	Global reactions are present in current case mechanism.
	FALSE	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.

[a]Default 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 in the first two product fields. The reactant species listed on this line include all whose concentrations 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_{ij} 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_j, n_j, and E_j 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

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

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 coefficients and add molecular reactions.	FALSE[b]	FALSE[b]	TRUE	TRUE
Change molecular rate coefficients and add global reactions.	FALSE[b]	TRUE	TRUE	FALSE[b]
Change molecular rate coefficients 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

[a]The variables GLOBAL, GRONLY, and MRPREV are set according to the makeup of the mechanisms of the previous and current cases; see table 3.1.
[b]Default value.

TABLE 3.3.—FORMATS OF TWO REACTION LINES FOR EACH GLOBAL REACTION

(a) Line 1.

Columns	Variable type	Format	Content and explanation
1–4	Real	F4.2	Stoichiometric coefficient of left reactant (default value = 1)
5–12	Character	A8	Name of left reactant (third one)
14–17	Real	F4.2	Stoichiometric coefficient of center reactant (default value = 1)
18–25	Character	A8	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 precision	F10.4	Concentration exponent of left (third) reactant
11–20		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_j in eq. (2.6)
41–50		F10.4	Temperature exponent n_j in eq. (2.6)
51–60		F10.4	Activation energy E_j in eq. (2.6)

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 cm^3. 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 H_2 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 (φ = 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 H_2 and O_2.

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 (φ = 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_j factor for the most controlling reaction, which is (global) reaction 14, the reaction of C_3H_8 with O_2. 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 brute-force 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 brute-force 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 CH_4 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 ($OH + C_2H_6$ and $CH_3 + CH_2$) significantly controlled the concentrations of CH_4, CH_3, and C_2H_6. 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, WSRHT0, and WSRHT1 in namelist WSPROB. Sensitivity coefficients for 10 species concentration variables and temperature are requested with respect to all reaction A_j factors and initial temperature.

Sensitivity coefficients calculated by GLSENS and the brute-force 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:

$$C_6H_6 + O_2 = C_6H_5O + OH$$

$$C_5H_6 + O_2 = C_5H_5O + OH$$

$$C_6H_5O = C_5H_5 + CO$$

$$C_6H_5OH = C_6H_5O + H$$

$$C_6H_6 + OH = C_6H_5 + H_2O$$

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 C_4H_2 and C_5H_5 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.

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

```
TAPE
GLOBAL CODE-EXAMPLE PROB 1; ALL GLOBAL REACTIONS; PSR PROBLEM
 &rtype  global=.true.,gronly=.true., &end
                 H2O      +    O         >     H2       +    O2
            1.          1.       4.90E+10   .18       -510.
                 CO       +    H2O       >     CO2      +    H2
             1.          1.       1.30E+05   1.31      -7000.
                 CO2      +    H2        >     CO       +    H2O
             1.          1.       4.41E+10   .19        3527.
                 N2       +    O2        >2.0  NO
             1.          1.       4.00E+14   .03      100000.
                             2.0 NO      >     N2       +    O2
                         2.       2.00E+11   0.       38000.
                 CN       +2.0 O         >     NO       +    CO
             1.          1.       8.30E+11   0.          0.
                 CN       +    NO        >     CO       +    N2
             1.          1.       1.25E+12   0.          0.
             2.0 CH2      +    N2        >2.0  CN       +2.0 H2
             1.      1.           5.00E+13   0.       54000.
                 CH2      +    O2        >     CO       +    H2O
             1.        .5         3.50E+07   0.        5000.
                 O2       +    C3H8      >3.0  CH2      +2.0 OH
             1.6       .1         1.10E+12   0.       41000.
                 H2       +    O2        >2.0  OH
             1.      1.           1.00E+00   0.       49080.
                 C3H8     +2.0 OH        >     H2O      +    C3H8     +    O
              .15    1.           1.98E+06   0.        4000.
      OH        +    H2       +    O2        >     H2O      +    O        +    OH
  1.            0.   1.           0.96E+12   -.1       1013.

AR
DISTANCE  AREA                             C3H8
 &prob  welstr=.true.,
  conc=.true.,   &end
 &wsprob
     delmd=200., dotmax=1600.,mpr=2,
     volume=2500.,        &end
 &start t= 800.,p=5.5,mdot= 100.,eratio=2.0,
 scc=3,sch=8,   &end
END
FINIS
```

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 φ = 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 mole fractions				
C_3H_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_2O	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}
O	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
              H2O      +    O         >     H2      +    O2
          1.        1.       4.90E+10   .18      -510.
              CO       +    H2O       >     CO2     +    H2
          1.        1.       1.30E+05   1.31     -7000.
              CO2      +    H2        >     CO      +    H2O
          1.        1.       4.41E+10   .19      3527.
  H2      +   N2       +    O2       >2.0 NO      +    H2
 -.05     1.        1.       4.00E+14   .03     100000.
          2.0 NO       +    H2        >     N2      +    O2      +    H2
          2.        0.       2.00E+11   0.       38000.
  H2      +   CN      +2.0 O         >     NO      +    CO      +    H2
 -.05     1.        1.       8.30E+11   0.          0.
              CN       +    NO        >     CO      +    N2
          1.        1.       1.25E+12   0.          0.
  O2     +2.0 CH2      +    N2       >2.0 CN     +2.0 H2      +    O2
 -.05     1.      1.         5.00E+13   0.       54000.
              CH2      +    O2        >     CO      +    H2O
          1.      .5         3.50E+07   0.       5000.
  H2          O2       +    C3H8     >3.0 CH2    +2.0 OH      +    H2
 0.5      1.6     .1         1.10E+12   0.       41000.
  C3H8    +   H2       +    O2       >2.0 OH      +    C3H8
 0.5      1.      1.         1.00E+00   0.       49080.
              C3H8    +2.0 OH        >     H2O     +    C3H8    +    O
         .15      1.         1.98E+06   0.       4000.
  OH      +   H2       +    O2        >     H2O     +    O       +    OH
 1.       0.      1.         0.96E+12   -.1      1013.

AR
DISTANCE  AREA                         C3H8
 &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 φ = 1.5; equilibrium temperature, 2357.42 K.]

Variable	Convergence number			
	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_3H_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_2O	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}
O	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 MOLECULAR REACTIONS; EXAMPLE PROBLEM 3
 &rtype  global=.true.,gronly=.false., &end
   O        +   H2O      =   OH      +   OH            6.8E+13    0.        18365.
   H        +   O2       =   OH      +   O            1.89E+14   0.        16400.
   O        +   H2       =   OH      +   H            4.20E+14   0.        13750.
   H        +   HO2      =   H2      +   O2           7.28E+13   0.        2126.
   O        +   HO2      =   OH      +   O2            5.0E+13   0.        1000.
   HO2      +   OH       =   H2O     +   O2            8.0E+12   0.        0.
   H        +   HO2      =2.0OH                       1.34E+14   0.        1070.
   H2       +   HO2      =   H2O2    +   H            7.91E+13   0.        25000.
   OH       +   H2O2     =   H2O     +   HO2           6.1E+12   0.        1430.
   HO2      +   HO2      =   H2O2    +   O2            1.8E+12   0.         0.
   H        +   H2O2     =   OH      +   H2O           7.8E+11   0.         0.
   M        +   H2O2     =2.0OH                       1.44E+17   0.        45510.
   THIRDBODY
H2          2.30    O2          .78     H2O          6.0    H2O2          6.6
END
   H2       +   OH       =   H2O     +   H            4.74E+13   0.        6098.
   H        +   O2       =   HO2     +   M            1.46E+15   0.        -1000.
   THIRDBODY
O2          1.30    N2          1.3     H2O          21.3   H2            3.0
END
   M        +   H2O      =   H       +   OH           1.30E+15   0.        105140.
   THIRDBODY
H2          4.00    O2          1.5     H2O          20.0   N2            1.5
END
   H        +   O        =   OH      +   M            7.1E+18   -1.        0.
   M        +   H2       =   H       +   H            2.2E+14    0.        96000.
   THIRDBODY
H2          4.10    O2          2.0     H2O          15.0   N2            2.0
END
   M        +   O2       =   O       +   O            1.80E+18    -1.       118020.
   END
                N2      +    O2       >2.0 NO
            1.          1.       4.00E+14   .03    100000.
                     2.0 NO       >     N2      +   O2
                        2.       2.00E+11    0.     38000.
                CN      +2.0 O        >     NO      +   CO
            1.          1.       8.30E+11   0.        0.
                CN      +    NO       >     CO      +   N2
            1.          1.       1.25E+12    0.        0.
            2.0 CH2     +    N2       >2.0 CN      +2.0 H2
            1.      1.           5.00E+13    0.     54000.
                CH2     +    O2       >     CO      +   H2O
            1.       .5          3.50E+07    0.     5000.
                O2      +    C3H8     >3.0 CH2     +2.0 OH
            1.6      .1          1.10E+12    0.     41000.
                H2      +    O2       >2.0 OH
            1.      1.           1.00E+00    0.     49080.
                C3H8    +2.0 OH       >     H2O     +   C3H8    +    O
            .15     1.           1.98E+06    0.     4000.
    OH       +  H2      +    O2       >     H2O     +   O       +    OH
  1.0       0.      1.           0.96E+12   -.1     1013.

AR
DISTANCE  AREA                          C3H8
 &prob  welstr=.true.,       conc=.true.,  &end
 &wsprob      delmd= 50., dotmax=2500.,mpr=1,  volume= 500.,      &end
 &start t= 800.,p=5.5,mdot= 200.,eratio=1.5,
    scc=3,sch=8,  &end
END
FINIS
```

TABLE 4.6.—COMPUTED RESULTS FOR EXAMPLE PROBLEM 3 (PROPANE-AIR COMBUSTION IN PERFECTLY STIRRED REACTOR)

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

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	3	3	3
Species mole fractions				
C_3H_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}
O_2	1.0693×10^{-2}	1.3130×10^{-2}	1.8679×10^{-2}	2.1946×10^{-2}
H_2O	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}
O	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}

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

```
TAPE
  GLOBAL LSENS CODE-EXAMPLE PROBLEM 4; INTEGRATION CASE BOTH TYPES OF REACTION
 &rtype  global=.true.,gronly=.false., &end
  H2O     +   O         >   H2     +   O2              4.90E+10    .18      -510.
           2.00         >   O2                         4.56E+11    .027     -1849.
              O2        >2.00                          2.78E+16    -.92     118954.
  CO      +   O         >   CO2                        8.43E+09    -.001    1000.
              CO2       >   CO     +   O               9.08E+18    -1.84    130754.
  CH2     +   O         >   CO     +   H2              0.69E+11    1.       0.
  CO      +   H2        >   CH2    +   O               5.38E+10    1.44     177439.

                N2       +     O2       >2.0 NO
            1.        1.        4.00E+14   .03     100000.
                          2.0 NO        >    N2      +    O2
                      2.        2.00E+11    0.      38000.
                CN       +2.0 O         >    NO      +    CO
            1.       1.         8.30E+11    0.        0.
                CN       +     NO       >    CO      +    N2
            1.       1.         1.25E+12    0.        0.
            2.0 CH2      +     N2       >2.0 CN      +2.0 H2
            1.      1.          5.00E+13    0.      54000.
                CH2      +     O2       >    CO      +    H2O
            1.        .5        3.50E+07    0.      5000.
                O2       +     C3H8     >3.0 CH2     +2.0 OH
            1.6       .1        1.10E+12    0.      41000.
   C3H8     +   H2       +     O2       >2.0 OH      +    C3H8
   0.0      1.      1.          1.00E+00    0.      49080.
                C3H8     +2.0 OH        >    H2O     +    C3H8    +    O
            .15     1.          1.98E+06    0.      4000.

AR
TIME                                         C3H8
 &prob rhocon = .true., print = 1.e-6, 1.e-4, 0.2, .3, .5, .575, .580,
   .585, .590, .592, .5923, .5925, .5927, .593,
     sencal = .true., tiny =1.e-3, &end
 &start t=  850., p=5.5,     eratio=2.0,
        scc=3,sch=8,   &end
END
 &solver   emax = 1.e-7,  atolsp = 1.e-16,      &end
SENSVAR
H2O      C3H8      OH        NO        CO        CO2       CH2       TEMP
END
REAC
 &senrxn allrxn = .true.,  output = .false., order = .true.,
           sensaj = .true.,     &end
FINIS
```

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

[Initial temperature T_0 = 850 K; initial pressure p_0 = 5.5 atm; equivalence ratio φ = 2.0; reaction time t = 592.5 ms.]

Variable	EMAX value (ATOLSP = 10^{-9}EMAX)					
	10^{-4}		10^{-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_3H_8	3.8686×10^{-2}	−1250	5.1507×10^{-2}	−215	5.1539×10^{-2}	−214
H_2O	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

TABLE 4.9.—DATA FILE FOR EXAMPLE PROBLEM 5 (HYDROGEN-OXYGEN PSR SENSITIVITY)

```
TAPE
  LSENS    HYDROGEN - OXYGEN  PSR WITH SENSITIVITY ANALYSIS
 &rtype       &end
   O       +   H2O       =   OH      +   OH            6.8E+13    0.        18365.
   H       +   O2        =   OH      +   O            1.89E+14    0.        16400.
   O       +   H2        =   OH      +   H            4.20E+14    0.        13750.
   H       +   HO2       =   H2      +   O2           7.28E+13    0.        2126.
   O       +   HO2       =   OH      +   O2            5.0E+13    0.        1000.
   HO2     +   OH        =   H2O     +   O2            8.0E+12    0.        0.
   H       +   HO2       =2.0OH                       1.34E+14    0.        1070.
   H2      +   HO2       =   H2O2    +   H            7.91E+13    0.        25000.
   OH      +   H2O2      =   H2O     +   HO2           6.1E+12    0.        1430.
   HO2     +   HO2       =   H2O2    +   O2            1.8E+12    0.         0.
   H       +   H2O2      =   OH      +   H2O           7.8E+11    0.         0.
   M       +   H2O2      =2.0OH                       1.44E+17    0.        45510.
   THIRDBODY
H2          2.30     O2          .78     H2O           6.0     H2O2         6.6
END
   H2      +   OH        =   H2O     +   H            4.74E+13    0.        6098.
   H       +   O2        =   HO2     +   M            1.46E+15    0.        -1000.
   THIRDBODY
O2          1.30                         H2O          21.3     H2           3.0
END
   M       +   H2O       =   H       +   OH           1.30E+15    0.        105140.
   THIRDBODY
H2          4.00     O2          1.5     H2O          20.0     END
   H       +   O         =   OH      +   M            7.1E+18   -1.          0.
   M       +   H2        =   H       +   H            2.2E+14    0.          96000.
   THIRDBODY
H2          4.10     O2          2.0     H2O          15.0     END
   M       +   O2        =   O       +   O            1.80E+18   -1.        118020.


TIME
 &prob  welstr = .true.,  sencal = .true., tiny = 1.e-3, &end
 &wsprob  dotmax=10200., delmd=2000., mpr = 1, volume= 2000.,   &end
 &start    t = 298.,  p = 2.0,   mdot = 200.,       &end
H2          0.6667
O2          0.3333
END
SENSVAR
O        H2O        OH        H        O2        H2        HO2        H2O2
TEMP     END
INIT
TEMP     END
REAC
 &senrxn   sensaj = .true., allrxn = .true., order = .true.,
      output = .false.,    &end
FINIS
```

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.]

Reaction number	Reaction	H_2		O		H_2O		OH		HO_2		Temperature	
		GLSENS	Brute force	GLSENS	Brute force	GLSENS	Brute force	GLSENS	Brute force	GLSENS	Brute force	GLSENS	Brute force
	(a) Sensitivity coefficient $\langle S_{ij} \rangle$ with respect to A_j, n_j, or E_j												
15	$H_2O + M = H + OH + M$	-1.77×10^{-2}	-1.77×10^{-2}	-6.79×10^{-2}	-6.80×10^{-2}	1.04×10^{-2}	1.04×10^{-2}	6.54×10^{-3}	6.36×10^{-3}	2.11×10^{-2}	2.11×10^{-2}	2.69×10^{-2}	2.69×10^{-2}
14	$H + O_2 + M = HO_2 + M$	-1.22×10^{-2}	-1.23×10^{-2}	-4.42×10^{-2}	-4.42×10^{-2}	6.88×10^{-3}	6.86×10^{-3}	5.48×10^{-3}	5.58×10^{-3}	0.312	0.312	1.78×10^{-2}	1.77×10^{-2}
17	$H_2 + M = H + H + M$	-2.79×10^{-3}	-2.73×10^{-3}	-1.11×10^{-2}	-1.11×10^{-2}	1.66×10^{-3}	1.69×10^{-3}	1.11×10^{-3}	1.03×10^{-3}	3.53×10^{-3}	3.47×10^{-3}	4.35×10^{-3}	4.35×10^{-3}
2	$H + O_2 = OH + O$	-4.85×10^{-3}	-4.88×10^{-3}	1.09×10^{-2}	1.09×10^{-2}	------	------	5.66×10^{-3}	5.69×10^{-3}	-7.31×10^{-3}	-7.30×10^{-3}	------	------
4	$H + HO_2 = H_2 + O_2$	------	------	-3.80×10^{-3}	-3.82×10^{-3}	------	------	------	------	-7.85×10^{-2}	-7.87×10^{-2}	1.38×10^{-3}	1.42×10^{-3}
16	$H + O + M = OH + M$	-1.34×10^{-3}	-1.31×10^{-3}	-5.24×10^{-3}	-5.21×10^{-3}	------	------	------	------	1.65×10^{-3}	1.74×10^{-3}	2.04×10^{-3}	2.09×10^{-3}
13	$H_2 + OH = H_2O + H$	-2.40×10^{-3}	-2.38×10^{-3}	1.78×10^{-3}	1.78×10^{-3}	------	------	-1.33×10^{-3}	-1.23×10^{-3}	-2.85×10^{-3}	-2.89×10^{-3}	------	------
	(b) Sensitivity coefficient $\langle S_{i,T_0} \rangle$ with respect to initial temperature												
--	-------------	5.18×10^{-2}	5.17×10^{-2}	0.126	0.126	-2.91×10^{-2}	-2.92×10^{-2}	7.70×10^{-2}	7.71×10^{-2}	5.85×10^{-2}	5.86×10^{-2}	2.11×10^{-2}	2.12×10^{-2}

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

```
TAPE
  GLOBAL AND MOLECULAR REACTIONS;  EXAMPLE PROB. 6 FOR PSR
 &rtype  global=.true.,gronly=.false., &end
   O      +   H2O      =   OH      +   OH          6.8E+13    0.         18365.
   H      +   O2       =   OH      +   O           1.89E+14   0.         16400.
   O      +   H2       =   OH      +   H           4.20E+14   0.         13750.
   H      +   HO2      =   H2      +   O2          7.28E+13   0.         2126.
   O      +   HO2      =   OH      +   O2          5.0E+13    0.         1000.
   HO2    +   OH       =   H2O     +   O2          8.0E+12    0.         0.
   H      +   HO2      =2.0OH                      1.34E+14   0.         1070.
   H2     +   HO2      =   H2O2    +   H           7.91E+13   0.         25000.
   OH     +   H2O2     =   H2O     +   HO2         6.1E+12    0.         1430.
   HO2    +   HO2      =   H2O2    +   O2          1.8E+12    0.          0.
   H      +   H2O2     =   OH      +   H2O         7.8E+11    0.          0.
   M      +   H2O2     =2.0OH                      1.44E+17   0.         45510.
   THIRDBODY
H2         2.30     O2          .78     H2O         6.0    H2O2          6.6
END
   H2     +   OH       =   H2O     +   H           4.74E+13   0.         6098.
   H      +   O2       =   HO2     +   M           1.46E+15   0.         -1000.
   THIRDBODY
O2         1.30     N2          1.3     H2O         21.3   H2            3.0
END
   M      +   H2O      =   H       +   OH          1.30E+15   0.         105140.
   THIRDBODY
H2         4.00     O2          1.5     H2O         20.0   N2            1.5
END
   H      +   O        =   OH      +   M           7.1E+18   -1.          0.
   M      +   H2       =   H       +   H           2.2E+14    0.          96000.
   THIRDBODY
H2         4.10     O2          2.0     H2O         15.0   N2            2.0
END
   M      +   O2       =   O       +   O           1.80E+18   -1.        118020.
   END
              N2      +     O2      >2.0 NO
         1.        1.       4.00E+14    .03     100000.
                    2.0 NO      >     N2      +   O2
                  2.        2.00E+11    0.      38000.
              CN    +2.0 O      >     NO      +   CO
         1.        1.       8.30E+11   0.        0.
              CN      +     NO      >     CO      +   N2
         1.        1.       1.25E+12    0.       0.
         2.0 CH2      +     N2      >2.0 CN     +2.0 H2
         1.      1.         5.00E+13   0.       54000.
              CH2     +     O2      >     CO      +   H2O
         1.      .5         3.50E+07   0.       5000.
              O2      +     C3H8    >3.0 CH2    +2.0 OH
         1.6     .1         1.10E+12   0.       41000.
              H2      +     O2      >2.0 OH
         1.      1.         1.00E+00   0.       49080.
              C3H8    +2.0 OH      >     H2O    +   C3H8    +   O
        .15      1.         1.98E+06   0.       4000.
    OH      +    H2     +   O2      >     H2O    +   O       +   OH
  1.0       0.      1.         0.96E+12   -.1      1013.

AR
DISTANCE  AREA                       C3H8
 &prob  welstr=.true., sencal = .true., tiny = 1.0e-3,
  conc=.true.,   &end
 &wsprob
     delmd= 50., dotmax= 800.,mpr=1,
     volume=500.,       &end
 &start t= 800.,p=5.5,mdot=  200.,eratio=1.5,
 scc=3,sch=8,   &end
END
SENSVAR
C3H8      H2        O2        OH        H2O       NO        TEMP      END
INIT
TEMP      END
REAC
 &senrxn  sensaj = .true.,  order = .true., allrxn = .true.,
     output = .false.,      &end
FINIS
```

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.]

(a) Sensitivity coefficient $\langle S_{ij} \rangle$ with respect to A_j, n_j, or E_j

Reaction number	Reaction	C_3H_8		O_2		OH		H_2O		NO		Temperature	
		GLSENS	Brute force	GLSENS	Brute force	GLSENS	Brute force	GLSENS	Brute force	GLSENS	Brute force	GLSENS	Brute force
28	$OH + H_2 + O_2 \rightarrow H_2O + O + OH$	7.60×10^{-2}	7.68×10^{-2}	4.08×10^{-3}	3.30×10^{-3}	0.302	0.302	-8.58×10^{-3}	-8.33×10^{-3}	0.643	0.643	-3.01×10^{-3}	-2.90×10^{-3}
25	$O_2 + C_3H_8 \rightarrow 3CH_2 + 2OH$	−0.863	−0.865	−0.731	−0.730	-6.54×10^{-2}	-6.56×10^{-2}	9.45×10^{-2}	9.42×10^{-2}	−0.449	−0.449	4.61×10^{-2}	4.58×10^{-2}
24	$CH_2 + O_2 \rightarrow CO + H_2O$	5.30×10^{-2}	5.25×10^{-2}	−0.262	−0.261	6.76×10^{-2}	6.93×10^{-2}	2.48×10^{-2}	2.46×10^{-2}	−0.112	−0.114	4.92×10^{-2}	4.92×10^{-2}
23	$2CH_2 + N_2 \rightarrow 2CN + 2H_2$	3.37×10^{-2}	3.35×10^{-2}	-9.86×10^{-2}	-9.85×10^{-2}	1.48×10^{-2}	1.47×10^{-2}	1.20×10^{-2}	1.21×10^{-2}	-4.88×10^{-2}	-4.86×10^{-2}	1.81×10^{-2}	1.81×10^{-2}
22	$CN + NO \rightarrow CO + N_2$	-1.68×10^{-2}	-1.68×10^{-2}	-6.63×10^{-3}	-6.61×10^{-3}	5.00×10^{-3}	5.01×10^{-3}	2.04×10^{-3}	2.08×10^{-3}	−0.981	−0.982	1.78×10^{-3}	1.93×10^{-3}
21	$CN + 2O \rightarrow NO + CO$	7.95×10^{-3}	7.91×10^{-3}	-3.11×10^{-2}	-3.11×10^{-2}	2.23×10^{-3}	2.31×10^{-3}	------	------	0.963	0.963	5.80×10^{-3}	5.79×10^{-3}
2	$H + O_2 \rightleftharpoons OH + O$	-7.07×10^{-2}	-7.09×10^{-2}	-1.13×10^{-2}	-1.10×10^{-2}	−0.316	−0.316	1.07×10^{-2}	1.04×10^{-2}	−0.625	−0.625	4.21×10^{-3}	4.10×10^{-3}

(b) Sensitivity coefficient $\langle S_{i,T_0} \rangle$ with respect to initial temperature

		−2.12	−2.13	−2.23	−2.23	0.819	0.817	0.265	0.263	−0.798	−0.796	0.496	0.495

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

```
TAPE
 LSENS    PROPANE - AIR WELL-STIRRED REACTOR  WITH SENSITIVITY
&rtype      &end
              C3H8     =    C2H5     +    CH3          5.0E+15   0.          83500.
  CH3    +    C3H8     =    CH4      +    C3H7         3.55E+12  0.          10300.
              C3H7     =    C2H4     +    CH3          3.0E+14   0.          33200.
  M      +    CH4      =    CH3      +    H            2.0E+17   0.          88000.
  H      +    CH4      =    CH3      +    H2           1.26E+14  0.          11900.
  CH4    +    O2       =    CH3      +    HO2          7.94E+13  0.          56000.
  O      +    CH4      =    CH3      +    OH           1.9E+14   0.          11720.
  OH     +    CH4      =    CH3      +    H2O          2.5E+13   0.          5010.
  CH3    +    O2       =    CH3O     +    O            2.4E+13    0.         28680.
  CH3    +    OH       =    CH3O     +    H            6.3E+12   0.           0.
  M      +    CH3O     =    CH2O     +    H            5.0E+13   0.          21000.
  CH3    +    CH3      =    C2H6                      2.4E+14   -.4         0.
  H      +    C2H6     =    C2H5     +    H2           1.32E+14  0.          9700.
  O      +    C2H6     =    C2H5     +    OH           1.13E+14  0.          7850.
  OH     +    C2H6     =    C2H5     +    H2O          8.7E+13   0.          3520.
  M      +    C2H5     =    C2H4     +    H            1.0E+17   0.          31000.
  C2H5   +    O2       =    C2H4     +    HO2          2.0E+12   0.          5000.
  H      +    C2H5     =    C2H4     +    H2           4.8E+13   0.           0.
  CH3    +    CH2      =    C2H4     +    H            2.0E+13   0.           0.
  H      +    C2H4     =    H2       +    C2H3         1.5E+14   0.          10200.
  M      +    C2H4     =    C2H2     +    H2           2.6E+17    0.         79300.
  C2H4   +    OH       =    C2H3     +    H2O          4.8E+12   0.           1230.
  C2H4   +    OH       =    CH3      +    CH2O         2.0E+12   0.           960.
  C2H4   +    O        =    CH3      +    HCO          3.3E+12   0.           1130.
  C2H4   +    O        =    CH2O     +    CH2          2.5E+13   0.          5000.
  M      +    C2H3     =    C2H2     +    H            3.0E+15   0.          32000.
  C2H3   +    O2       =    CH2O     +    HCO          3.98E+12  0.           -250.
  C2H3   +    H        =    C2H2     +    H2           6.0E+12  0.              0.
  C2H3   +    O        =    C2H2O    +    H            3.3E+13  0.              0.
  C2H3   +    OH       =    C2H2     +    H2O          5.0E+12   0.          0.
  C2H3   +    CH2      =    C2H2     +    CH3          3.0E+13    0.         0.
  C2H3   +    C2H      =2.0C2H2                       3.0E+13   0.          0.
  M      +    C2H2     =    C2H      +    H            4.2E+16   0.          107000.
  C2H2   +    O        =    CH2      +    CO           1.6E+14    .0          9890.
  C2H2   +    O        =    C2HO     +    H            4.0E+14   0.0         10660.
  C2H2   +    OH       =    C2H      +    H2O          6.3E+12   0.0          7000.
  C2H2   +    OH       =    C2H2O    +    H            3.2E+11   0.0          200.
  C2H    +    O2       =    C2HO     +    O            5.00E+13  0.          1500.
  C2H    +    OH       =    C2HO     +    H            2.0E+13    0.         0.
  C2HO   +    O2       =2.0CO        +    OH           1.46E+12  0.          2500.
  C2HO   +    O        =2.0CO        +    H            1.202E+12  0.         0.
  C2HO   +    OH       =2.0HCO                        1.0E+13   0.          0.
  C2HO   +    H        =    CH2      +    CO           5.0E+13    0.         0.
  C2HO   +    CH2      =    C2H3     +    CO           3.0E+13    0.         0.
  C2HO   +    CH2      =    CH2O     +    C2H          1.0E+13   0.          2000.
           2.0C2HO     =    C2H2     +2.0CO            1.0E+13    0.         0.
  C2H2O  +    OH       =    CH2O     +    HCO          2.8E+13    0.         0.
  C2H2O  +    OH       =    C2HO     +    H2O          7.5E+12    0.         3000.
  C2H2O  +    H        =    CH3      +    CO           1.13E+13  0.          3428.
  C2H2O  +    H        =    C2HO     +    H2           7.5E+13   0.          8000.
  C2H2O  +    O        =    C2HO     +    OH           5.0E+13    0.         8000.
  C2H2O  +    O        =    CH2O     +    CO           2.0E+13   0.          0.
  M      +    C2H2O    =    CH2      +    CO           2.0E+16   0.          60000.
  C2H    +    O        =    CO       +    CH           5.0E+13   0.           0.
  CH3O   +    O2       =    CH2O     +    HO2          1.0E+13   0.           7170.
  CH3O   +    H        =    CH2O     +    H2           2.0E+13    0.          0.
  M      +    CH2O     =    HCO      +    H            5.0E+16   0.          81000.
  CH2O   +    OH       =    HCO      +    H2O          3.0E+13    0.          1200.
  CH2O   +    H        =    HCO      +    H2           2.5E+13   0.          3990.
  CH2O   +    O        =    HCO      +    OH           3.5E+13   0.          3510.
  CH3    +    CH2O     =    CH4      +    HCO          1.0E+10   0.5          6000.
  CH3    +    HCO      =    CH4      +    CO           3.0E+11   .5           0.
  CH3    +    HO2      =    CH3O     +    OH           2.0E+13   0.           0.
  M      +    CH3      =    CH2      +    H            1.95E+16   0.         91600.
  H      +    CH3      =    H2       +    CH2          2.7E+11   .67         25700.
  O      +    CH3      =    OH       +    CH2          1.9E+11    .68        25700.
```

TABLE 4.13.—Continued.

OH	+	CH3	=	H2O	+	CH2	2.7E+11	.67	25700.
CH	+	CO2	=	HCO	+	CO	3.7E+12	0.	0.
CH	+	O2	=	HCO	+	O	1.0E+13	0.	0.
CH2	+	O2	=	CH2O	+	O	5.0E+11	0.5	6960.
CH2	+	O	=	CH	+	OH	2.0E+11	.7	25800.
CH2	+	OH	=	CH	+	H2O	5.0E+11	.5	5900.
CH2	+	H	=	CH	+	H2	3.2E+11	0.7	4970.
CH2	+	CH2	=	C2H3	+	H	5.0E+12	0.	0.
CH2	+	CH2	=	C2H2	+	H2	4.0E+13	0.	0.
HCO	+	O2	=	CO	+	HO2	3.0E+13	0.	0.
HCO	+	O	=	CO	+	OH	3.0E+13	0.	0.
HCO	+	OH	=	CO	+	H2O	3.0E+13	0.	0.
HCO	+	H	=	CO	+	H2	2.0E+13	0.	0.
M	+	HCO	=	H	+	CO	2.9E+14	0.	15570.
CO	+	O	=	CO2	+	M	2.4E+15	0.	4100.
CO	+	O2	=	CO2	+	O	2.5E+12	0.	47690.
CO	+	OH	=	CO2	+	H	4.17E+11	0.	1000.
CO	+	HO2	=	CO2	+	OH	5.75E+13	0.	22930.
O	+	H2O	=	OH	+	OH	6.8E+13	0.	18365.
H	+	O2	=	OH	+	O	1.89E+14	0.	16400.
O	+	H2	=	OH	+	H	4.20E+14	0.	13750.
H	+	HO2	=	H2	+	O2	7.28E+13	0.	2126.
O	+	HO2	=	OH	+	O2	5.0E+13	0.	1000.
HO2	+	OH	=	H2O	+	O2	8.0E+12		0.
H	+	HO2	=2.0OH				1.34E+14	0.	1070.
H2	+	HO2	=	H2O2	+	H	7.91E+13	0.	25000.
OH	+	H2O2	=	H2O	+	HO2	6.1E+12	0.	1430.
HO2	+	HO2	=	H2O2	+	O2	1.8E+12	0.	0.
H	+	H2O2	=	OH	+	H2O	7.8E+11	0.	0.
M	+	H2O2	=2.0OH				1.44E+17	0.	45510.
THIRDBODY									
H2		2.30	O2	.78		H2O	6.0	H2O2	6.6
END									
H2	+	OH	=	H2O	+	H	4.74E+13	0.	6098.
H	+	O2	=	HO2	+	M	1.46E+15	0.	-1000.
THIRDBODY									
O2		1.30	N2	1.3		H2O	21.3	CO2	7.0
END									
M	+	H2O	=	H	+	OH	1.30E+15	0.	105140.
THIRDBODY									
H2		4.00	O2	1.5		H2O	20.0	N2	1.5
CO2		4.0	END						
H	+	O	=	OH	+	M	7.1E+18	-1.	0.
M	+	H2	=	H	+	H	2.2E+14	0.	96000.
THIRDBODY									
H2		4.10	O2	2.0		H2O	15.0	N2	2.0
END									
M	+	O2	=	O	+	O	1.80E+18	-1.	118020.
CH	+	N2	=	HCN	+	N	1.0E+11	0.	19000.
CN	+	H2	=	HCN	+	H	6.0E+13	0.	5300.
O	+	HCN	=	OH	+	CN	1.4E+11	.68	16900.
OH	+	HCN	=	HNCO	+	H	4.0E+11	0.	2800.
CN	+	O	=	CO	+	N	1.2E+13	0.	0.
CN	+	OH	=	NCO	+	H	2.5E+14	0.	6000.
H2	+	NCO	=	HNCO	+	H	1.0E+14	0.	9000.
HNCO	+	H	=	NH2	+	CO	1.0E+14	0.	8500.
CN	+	O2	=	NCO	+	O	3.2E+13	0.	1000.
CN	+	CO2	=	NCO	+	CO	3.7E+12	0.	0.
O	+	NCO	=	NO	+	CO	2.0E+13	0.	0.
N	+	NCO	=	N2	+	CO	1.0E+13	0.	0.
H	+	NCO	=	NH	+	CO	2.0E+13	0.	0.
CH	+	NO	=	N	+	HCO	1.6E+13	0.	9940.
CH	+	NO	=	O	+	HCN	2.0E+12	0.	0.
NH	+	OH	=	N	+	H2O	5.0E+11	0.5	2000.
HO2	+	NO	=	NO2	+	OH	2.09E+12	0.	-477.
O	+	NO2	=	NO	+	O2	1.0E+13	0.	596.
NO	+	O	=	NO2	+	M	5.62E+15	0.	-1160.
NO2	+	H	=	NO	+	OH	3.47E+14	0.	1470.

TABLE 4.13.—Concluded.

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

AR
TIME
 &prob  welstr=.true.,  conc=.false., sencal = .true.,
     tiny = 1.e-3,             &end
 &wsprob  dotmax=1600.0, delmd=800.0,   volume=300.0,
   wsrhtr=.true., wsrht1=0.05, wsrht0=-42.88,  &end
 &start  t=614.0, p=5.0, mdot=10.0, molef=.false.,    &end
C3H8       0.0873262
N2         0.6892887
O2         0.211232
AR         0.011737
CO2        0.0004162
END
INIT
TEMP       END
SENSVAR
C3H8       CH4        CH3        H2         OH         H2O        C2H2       C2H6
CO         TEMP       END
REAC
 &senrxn  sensaj = .true., order = .true., rxnum =1.,4.,5.,11, 13.,15.,19.,
     35., 37., 49.,  64., 83., 86.,       &end
FINIS
```

TABLE 4.14.—COMPARISON OF GLSENS AND BRUTE-FORCE SENSITIVITY COEFFICIENTS FOR EXAMPLE PROBLEM 7 (PROPANE-AIR PSR)

[Equivalence ratio $\varphi = 1.5$; temperature $T = 2148.7$ K.]

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

Reaction number	Reaction	C_3H_8 concentration		CH_4 concentration		CH_3 concentration		H_2 concentration	
		GLSENS	Brute force	GLSENS	Brute force	GLSENS	Brute force	GLSENS	Brute force
1	$C_3H_8 \rightleftharpoons C_2H_5 + CH_3$	–0.996	–0.996	1.56×10^{-3}	1.60×10^{-3}	----	----	1.63×10^{-3}	1.63×10^{-3}
4	$CH_4 + M \rightleftharpoons CH_3 + H + M$	–0.208	–0.208	0.859	0.859	0.217	0.217	–0.162	–0.162
15	$OH + C_2H_6 \rightleftharpoons C_2H_5 + H_2O$	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	$CH_3 + CH_2 \rightleftharpoons C_2H_4 + H$	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 temperature

--	---------------	-3.96	-3.96	3.83×10^{-2}	3.81×10^{-2}	0.979	0.979	8.67×10^{-2}	8.69×10^{-2}

TABLE 4.14.—Concluded.

(a) Concluded.

Reaction number	Reaction	OH concentration		H_2O concentration		CO concentration		C_2H_6 concentration		Temperature	
		GLSENS	Brute force	GLSENS	Brute force	GLSENS	Brute force	GLSENS	Brute force	GLSENS	Brute force
1	$C_3H_8 = C_2H_5 + CH_3$	-2.21×10^{-3}	-2.37×10^{-3}	------	------	------	------	2.38×10^{-3}	2.45×10^{-3}	------	------
4	$CH_4 + M = CH_3 + H + M$	−0.458	−0.458	3.14×10^{-2}	3.12×10^{-2}	-6.25×10^{-2}	-6.25×10^{-2}	0.322	0.322	1.07×10^{-2}	1.07×10^{-2}
15	$OH + C_2H_6 = C_2H_5 + H_2O$	5.51×10^{-2}	5.52×10^{-2}	-4.01×10^{-3}	-3.95×10^{-3}	1.58×10^{-2}	1.59×10^{-2}	−0.428	−0.428	-1.91×10^{-3}	-2.09×10^{-3}
19	$CH_3 + CH_2 = C_2H_4 + H$	9.71×10^{-2}	9.70×10^{-2}	-7.94×10^{-3}	-7.89×10^{-3}	1.42×10^{-2}	1.45×10^{-2}	−0.472	−0.472	-2.48×10^{-3}	-2.56×10^{-3}

(b) Concluded.

--	---------------	1.27	1.27	-3.12×10^{-2}	-3.18×10^{-2}	9.16×10^{-2}	9.16×10^{-2}	−2.08	−2.08	0.214	0.214

TABLE 4.15.—DATA FILE FOR EXAMPLE PROBLEM 8 (BENZENE-OXYGEN PSR)

```
TAPE
C6H6 OXYGEN     NO ARGON   PSR SENSITIVITY TEST CASE; MECHANISM K-72
 &rtype          &end
   C6H6     +   O2       =   C6H5O    +   OH          4.0E+13  0.          34000.
   C6H6     +   C6H5     =   C12H10   +   H           4.0E+11  0.          4000.
                C6H6     =   C6H5     +   H           5.0E+15  0.          108000.
   C6H6     +   H        =   C6H5     +   H2          2.5E+14  0.          16000.
   C6H6     +   O        =   C6H5O    +   H         2.783E+13   0.         4910.
   C6H6     +   OH       =   C6H5     +   H2O       2.132E+13   0.         4580.
   M        +   C4H3     =   C4H2     +   H           1.0E+16   0.0        60000.
                C6H5O    =   C5H5     +   CO         2.51E+11  0.          43900.
   C6H5     +   O2       =   C6H5O    +   O           2.1E+12  0.           7470.
   C6H5     +   HO2      =   C6H5O    +   OH          2.0E+13  0.          1000.
                C6H5     =   C4H3     +   C2H2       4.50E+13  0.          72530.
                C6H5OH   =   C6H5O    +   H          2.00E+16  0.          88000.
   C6H5OH   +   H        =   C6H6     +   OH         2.20E+13  0.           7910.
   C6H5OH   +   H        =   C6H5O    +   H2         1.15E+14  0.          12400.
   C5H5     +   C6H5OH   =   C6H5O    +   C5H6       2.67E+14  0.          25227.
                C5H6     =   C5H5     +   H          8.13E+24  -2.981      78682.
   C5H6     +   O2       =   C5H5O    +   OH          1.0E+13   0.         20716.
   C6H5OH   +   OH       =   C6H5O    +   H2O         3.0E+13   0.         0.
   C6H5OH   +   HO2      =   C6H5O    +   H2O2        3.0E+13   0.         1500.
                C5H5O    =   C4H5     +   CO          3.0E+16   0.         15000.
   C5H5     +   O        =   C5H5O                    1.0E+13   0.          0.
   C5H5     +   OH       =   C5H4OH   +   H           1.0E+13   0.          0.
                C5H4OH   =   C4H4     +   HCO         1.0E+15   0.         22000.
   C5H5     +   HO2      =   C5H5O    +   OH          2.0E+13   0.           0.
   C5H6     +   HO2      =   C5H5O    +   H2O         5.0E+13   0.          0.
              2.0C6H5    =   C12H10                   3.1E+12   0.         0.
                C4H5     =   C2H3     +   C2H2        1.4E+13   0.         32900.
   C4H2     +   O        =   C2HO     +   C2H         1.0E+13   0.          0.
   C4H2     +   OH       =   HCO      +   C3H2        3.0E+13    0.        0.
   C4H2     +   O        =   CO       +   C3H2        1.2E+12    0.        0.
   M        +   C2H4     =   C2H2     +   H2         9.33E+16    0.        77200.
   C2H4     +   OH       =   C2H3     +   H2O       4.786E+12  0.           1230.
   C2H4     +   O        =   CH3      +   HCO       3.311E+12  0.           1130.
   C2H4     +   O        =   CH2O     +   CH2       2.512E+13  0.           5000.
   C2H4     +   OH       =   CH3      +   CH2O      1.995E+12  0.           960.
   M        +   C2H3     =   C2H2     +   H           3.0E+15  0.          32000.
   C2H3     +   O2       =   CH2O     +   HCO        3.98E+12  0.          -250.
   C2H3     +   H        =   C2H2     +   H2          6.0E+12 0.             0.
   C2H3     +   OH       =   C2H2     +   H2O       5.012E+12  0.          0.
   C2H3     +   CH2      =   C2H2     +   CH3       3.020E+13   0.          0.
   C2H3     +   C2H      =2.0C2H2                   3.020E+13  0.           0.
   C2H3     +   O        =   C2H2O    +   H           3.3E+13  0.          0.
   CH2      +   CH2      =   C2H2     +   H2          4.0E+13  0.           0.
   CH2      +   CH2      =   C2H3     +   H         5.012E+12  0.          0.
   CH2      +   OH       =   CH       +   H2O        2.51E+11  .67         25700.
   CH2      +   O        =   CH       +   OH          2.0E+11  .68         25000.
   CH2      +   O2       =   CO2      +2.0H          1.59E+12  0.          1000.
   M        +   C2H2     =   C2H      +   H         4.169E+16  0.          107000.
   C2H2     +   C2H2     =   C4H3     +   H           2.0E+12  0.          45900.
   C2H2     +   O        =   CH2      +   CO          1.6E+14  0.0          9890.
   C2H2     +   O        =   C2HO     +   H           4.0E+14  0.0         10660.
   C2H2     +   OH       =   C2H      +   H2O       6.310E+12   0.          7000.
   C2H2     +   OH       =   C2H2O    +   H           3.2E+11  0.           200.
   C2H2     +   C2H      =   C4H2     +   H           3.0E+13  0.          0.
   C2H2O    +   OH       =   CH2O     +   HCO         2.8E+13   0.          0.
   C2H2O    +   OH       =   C2HO     +   H2O         7.5E+12   0.         3000.
   C2H2O    +   H        =   CH3      +   CO         1.13E+13  0.          3428.
   C2H2O    +   H        =   C2HO     +   H2          7.5E+13  0.          8000.
   C2H2O    +   O        =   C2HO     +   OH          5.0E+13   0.         8000.
   C2H2O    +   O        =   CH2O     +   CO          2.0E+13  0.           0.
   M        +   C2H2O    =   CH2      +   CO          2.0E+16  0.          60000.
```

C2HO	+	O2	=	2.0CO	+	OH	1.46E+12	0.	2500.
C2HO	+	O	=	2.0CO	+	H	1.202E+12	0.	0.
C2HO	+	OH	=	2.0HCO			1.0E+13	0.	0.
C2HO	+	H	=	CH2	+	CO	5.0E+13	0.	0.
C2HO	+	CH2	=	C2H3	+	CO	3.0E+13	0.	0.
C2HO	+	CH2	=	CH2O	+	C2H	1.0E+13	0.	2000.
2.0C2HO			=	C2H2	+	2.0CO	1.0E+13	0.	0.
C2H	+	OH	=	C2HO	+	H	2.0E+13	0.	0.
C2H	+	O2	=	C2HO	+	O	5.00E+13	0.	1500.
C2H	+	O	=	CO	+	CH	5.012E+13	0.	0.
M	+	CH4	=	CH3	+	H	2.0E+17	0.	88000.
CH4	+	O2	=	CH3	+	HO2	7.943E+13	0.	56000.
CH4	+	H	=	CH3	+	H2	1.26E+14	0.	11900.
OH	+	CH4	=	CH3	+	H2O	2.5E+13	0.	5010.
O	+	CH4	=	CH3	+	OH	1.9E+14	0.	11720.
CH3	+	O2	=	CH3O	+	O	4.786E+13	0.	29000.
CH3	+	OH	=	CH3O	+	H	6.3E+12	0.	0.
M	+	CH3O	=	CH2O	+	H	5.0E+13	0.	21000.
CH3O	+	O2	=	CH2O	+	HO2	1.0E+12	0.	6000.
CH3O	+	H	=	CH2O	+	H2	2.0E+13	0.	0.
CH3	+	CH3	=	C2H4	+	H2	1.0E+16	0.	32000.
CH3	+	O	=	CH2O	+	H	1.288E+14	0.	2000.
CH3	+	CH2O	=	CH4	+	HCO	1.0E+10	0.5	6000.
CH3	+	HCO	=	CH4	+	CO	3.020E+11	.5	0.
CH3	+	HO2	=	CH3O	+	OH	2.00E+13	0.	0.
M	+	CH2O	=	HCO	+	H	5.0E+16	0.	81000.
CH2O	+	OH	=	HCO	+	H2O	3.0E+13	0.	1200.
CH2O	+	H	=	HCO	+	H2	2.5E+13	0.	3990.
CH2O	+	O	=	HCO	+	OH	3.5E+13	0.	3510.
HCO	+	HO2	=	CH2O	+	O2	1.0E+14	0.	3000.
M	+	HCO	=	H	+	CO	2.94E+14	0.	15569.
HCO	+	O2	=	CO	+	HO2	3.311E+12	0.	7000.
HCO	+	OH	=	CO	+	H2O	1.0E+14	0.	0.
HCO	+	H	=	CO	+	H2	1.995E+14	0.	0.
HCO	+	O	=	CO	+	OH	1.0E+14	0.	0.
CH	+	O2	=	HCO	+	O	1.0E+13	0.	0.
CO	+	O	=	CO2	+	M	5.9E+15	0.	4100.
CO	+	O2	=	CO2	+	O	2.5E+12	0.	47690.
CO	+	OH	=	CO2	+	H	4.17E+11	0.	1000.
CO	+	HO2	=	CO2	+	OH	5.75E+13	0.	22930.
O	+	H2O	=	OH	+	OH	6.8E+13	0.	18365.
H	+	O2	=	OH	+	O	1.89E+14	0.	16400.
O	+	H2	=	OH	+	H	4.20E+14	0.	13750.
H	+	HO2	=	H2	+	O2	7.28E+13	0.	2126.
O	+	HO2	=	OH	+	O2	5.0E+13	0.	1000.
HO2	+	OH	=	H2O	+	O2	8.0E+12		0.
H	+	HO2	=	2.0OH			1.34E+14	0.	1070.
H2	+	HO2	=	H2O2	+	H	7.91E+13	0.	25000.
OH	+	H2O2	=	H2O	+	HO2	6.1E+12	0.	1430.
HO2	+	HO2	=	H2O2	+	O2	1.8E+12	0.	0.
H	+	H2O2	=	OH	+	H2O	7.8E+11	0.	0.
M	+	H2O2	=	OH	+	OH	1.44E+17	0.	45510.
THIRDBODY									
H2	2.30	O2		.78		H2O	6.0	H2O2	6.6
END									
H2	+	OH	=	H2O	+	H	4.74E+13	0.	6098.
H	+	O2	=	HO2	+	M	1.46E+15	0.	-1000.
THIRDBODY									
O2	1.30	CO2		7.0		H2O	21.3	H2	3.0
C6H6	20.0	CH4		5.0		END			
M	+	H2O	=	H	+	OH	1.30E+15	0.	105140.
THIRDBODY									
H2	4.00	O2		1.5		H2O	20.0	C6H6	20.0
CO2	4.00	END							
H	+	O	=	OH	+	M	7.1E+18	-1.	0.
M	+	H2	=	H	+	H	2.2E+14	0.	96000.
THIRDBODY									
H2	4.10	O2		2.0		H2O	15.0	END	
M	+	O2	=	O	+	O	1.80E+18	-1.	118020.

TABLE 4.15.—Concluded.

```
DISTANCE  AREA
 &prob welstr=.true.,  sencal = .true., tiny = 1.e-3,  &end
 &wsprob dotmax= 6000., delmd= 1000., mpr= 1,  volume = 1000.,
        wsrhtr =.true., wsrhtl= .05, wsrht0 = -42.88,   &end
 &start t= 614., p = 5.0,   mdot= 1000.,         &end
C6H6       .11765
O2         .88235
END
INIT
TEMP       END
SENSVAR
C6H6       C6H5O     OH        C6H5      H2O       CO        C6H5OH    C2H2
C5H5       CH2O      TEMP      END
REAC
 &senrxn  sensaj=.true., order =.true., output =.false., allrxn=.true., &end
FINIS
```

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

[Equivalence ratio $\varphi = 1.0$; mass flow rate $\dot{m} = 6000$ g/s; temperature $T = 3168.7$ K.]

Reaction number	Reaction	C_6H_6		C_6H_5O		C_6H_5		C_6H_5OH		CO		Temperature	
		GLSENS	Brute force	GLSENS	Brute force	GLSENS	Brute force	GLSENS	Brute force	GLSENS	Brute force	GLSENS	Brute force
		Sensitivity coefficient (S_{ij}) with respect to A_j, n_j, or E_j											
29	$C_4H_2 + OH = HCO + C_3H_2$	0.876	0.876	1.00	1.00	0.563	0.563	1.12	1.12	−0.707	−0.707	-6.64×10^{-2}	-6.64×10^{-2}
3	$C_6H_6 = C_6H_5 + H$	−0.843	−0.843	−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}
8	$C_6H_5O = C_5H_5 + CO$	------	------	−0.996	−0.996	------	------	−0.923	−0.924	------	------	------	------
54	$C_2H_2 + C_2H = C_4H_2 + H$	−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}
28	$C_4H_2 + O = C_2HO + C_2H$	−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}
49	$C_2H_2 + C_2H_2 = C_4H_3 + H$	−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}
22	$C_5H_5 + OH = C_5H_4OH + H$	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}
11	$C_6H_5 = C_4H_3 + C_2H_2$	-3.39×10^{-2}	-3.38×10^{-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}

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

```
TAPE
C6H6-O2-N2 PLUS ARGON PSR CASE WITH SENSITIVITY - MECHANISM K-72
 &rtype        &end
   C6H6     +  O2      =  C6H5O   +  OH          4.0E+13  0.          34000.
   C6H6     +  C6H5    =  C12H10  +  H           4.0E+11  0.          4000.
               C6H6    =  C6H5    +  H           5.0E+15  0.          108000.
   C6H6     +  H       =  C6H5    +  H2          2.5E+14  0.          16000.
   C6H6     +  O       =  C6H5O   +  H         2.783E+13   0.         4910.
   C6H6     +  OH      =  C6H5    +  H2O       2.132E+13   0.         4580.
   M        +  C4H3    =  C4H2    +  H           1.0E+16   0.0        60000.
               C6H5O   =  C5H5    +  CO         2.51E+11   0.         43900.
   C6H5     +  O2      =  C6H5O   +  O           2.1E+12   0.          7470.
   C6H5     +  HO2     =  C6H5O   +  OH          2.0E+13   0.         1000.
               C6H5    =  C4H3    +  C2H2       4.50E+13   0.         72530.
               C6H5OH  =  C6H5O   +  H          2.00E+16   0.         88000.
   C6H5OH   +  H       =  C6H6    +  OH         2.20E+13   0.          7910.
   C6H5OH   +  H       =  C6H5O   +  H2         1.15E+14   0.         12400.
   C5H5     +  C6H5OH  =  C6H5O   +  C5H6       2.67E+14   0.         25227.
               C5H6    =  C5H5    +  H          8.13E+24  -2.981      78682.
   C5H6     +  O2      =  C5H5O   +  OH          1.0E+13   0.         20716.
   C6H5OH   +  OH      =  C6H5O   +  H2O         3.0E+13   0.         0.
   C6H5OH   +  HO2     =  C6H5O   +  H2O2        3.0E+13   0.         1500.
               C5H5O   =  C4H5    +  CO          3.0E+16   0.         15000.
   C5H5     +  O       =  C5H5O                  1.0E+13   0.          0.
   C5H5     +  OH      =  C5H4OH  +  H           1.0E+13   0.          0.
               C5H4OH  =  C4H4    +  HCO         1.0E+15   0.         22000.
   C5H5     +  HO2     =  C5H5O   +  OH          2.0E+13   0.           0.
   C5H6     +  HO2     =  C5H5O   +  H2O         5.0E+13   0.           0.
            2.0C6H5    =  C12H10                 3.1E+12   0.         0.
               C4H5    =  C2H3    +  C2H2        1.4E+13   0.         32900.
   C4H2     +  O       =  C2HO    +  C2H         1.0E+13   0.          0.
   C4H2     +  OH      =  HCO     +  C3H2        3.0E+13    0.        0.
   C4H2     +  O       =  CO      +  C3H2        1.2E+12    0.        0.
   M        +  C2H4    =  C2H2    +  H2         9.33E+16    0.        77200.
   C2H4     +  OH      =  C2H3    +  H2O       4.786E+12  0.           1230.
   C2H4     +  O       =  CH3     +  HCO       3.311E+12  0.           1130.
   C2H4     +  O       =  CH2O    +  CH2       2.512E+13  0.           5000.
   C2H4     +  OH      =  CH3     +  CH2O      1.995E+12  0.           960.
   M        +  C2H3    =  C2H2    +  H           3.0E+15  0.          32000.
   C2H3     +  O2      =  CH2O    +  HCO        3.98E+12  0.          -250.
   C2H3     +  H       =  C2H2    +  H2          6.0E+12 0.              0.
   C2H3     +  OH      =  C2H2    +  H2O       5.012E+12  0.          0.
   C2H3     +  CH2     =  C2H2    +  CH3       3.020E+13   0.          0.
   C2H3     +  C2H     =2.0C2H2                3.020E+13  0.           0.
   C2H3     +  O       =  C2H2O   +  H           3.3E+13  0.          0.
   CH2      +  CH2     =  C2H2    +  H2          4.0E+13  0.           0.
   CH2      +  CH2     =  C2H3    +  H         5.012E+12  0.          0.
   CH2      +  OH      =  CH      +  H2O        2.51E+11  .67         25700.
   CH2      +  O       =  CH      +  OH          2.0E+11  .68         25000.
   CH2      +  O2      =  CO2     +2.0H         1.59E+12  0.          1000.
   M        +  C2H2    =  C2H     +  H         4.169E+16  0.          107000.
   C2H2     +  C2H2    =  C4H3    +  H           2.0E+12  0.          45900.
   C2H2     +  O       =  CH2     +  CO          1.6E+14  0.0          9890.
   C2H2     +  O       =  C2HO    +  H           4.0E+14  0.0         10660.
   C2H2     +  OH      =  C2H     +  H2O       6.310E+12   0.          7000.
   C2H2     +  OH      =  C2H2O   +  H           3.2E+11  0.           200.
   C2H2     +  C2H     =  C4H2    +  H           3.0E+13  0.          0.
   C2H2O    +  OH      =  CH2O    +  HCO         2.8E+13   0.          0.
   C2H2O    +  OH      =  C2HO    +  H2O         7.5E+12   0.         3000.
   C2H2O    +  H       =  CH3     +  CO         1.13E+13  0.          3428.
   C2H2O    +  H       =  C2HO    +  H2          7.5E+13  0.          8000.
   C2H2O    +  O       =  C2HO    +  OH          5.0E+13   0.         8000.
   C2H2O    +  O       =  CH2O    +  CO          2.0E+13  0.           0.
   M        +  C2H2O   =  CH2     +  CO          2.0E+16  0.          60000.
```

TABLE 4.17.—Continued.

```
    C2HO     +    O2        =2.0CO       +   OH          1.46E+12    0.          2500.
    C2HO     +    O         =2.0CO       +   H           1.202E+12   0.          0.
    C2HO     +    OH        =2.0HCO                      1.0E+13     0.          0.
    C2HO     +    H         =   CH2      +   CO          5.0E+13     0.          0.
    C2HO     +    CH2       =   C2H3     +   CO          3.0E+13     0.          0.
    C2HO     +    CH2       =   CH2O     +   C2H         1.0E+13     0.          2000.
             2.0C2HO        =   C2H2     +2.0CO          1.0E+13     0.          0.
    C2H      +    OH        =   C2HO     +   H           2.0E+13     0.          0.
    C2H      +    O2        =   C2HO     +   O           5.00E+13    0.          1500.
    C2H      +    O         =   CO       +   CH          5.012E+13   0.          0.
    M        +    CH4       =   CH3      +   H           2.0E+17     0.          88000.
    CH4      +    O2        =   CH3      +   HO2         7.943E+13   0.          56000.
    CH4      +    H         =   CH3      +   H2          1.26E+14    0.          11900.
    OH       +    CH4       =   CH3      +   H2O         2.5E+13     0.          5010.
    O        +    CH4       =   CH3      +   OH          1.9E+14     0.          11720.
    CH3      +    O2        =   CH3O     +   O           4.786E+13   0.          29000.
    CH3      +    OH        =   CH3O     +   H           6.3E+12     0.          0.
    M        +    CH3O      =   CH2O     +   H           5.0E+13     0.          21000.
    CH3O     +    O2        =   CH2O     +   HO2         1.0E+12     0.          6000.
    CH3O     +    H         =   CH2O     +   H2          2.0E+13     0.          0.
    CH3      +    CH3       =   C2H4     +   H2          1.0E+16     0.          32000.
    CH3      +    O         =   CH2O     +   H           1.288E+14   0.          2000.
    CH3      +    CH2O      =   CH4      +   HCO         1.0E+10     0.5         6000.
    CH3      +    HCO       =   CH4      +   CO          3.020E+11   .5          0.
    CH3      +    HO2       =   CH3O     +   OH          2.00E+13    0.          0.
    M        +    CH2O      =   HCO      +   H           5.0E+16     0.          81000.
    CH2O     +    OH        =   HCO      +   H2O         3.0E+13     0.          1200.
    CH2O     +    H         =   HCO      +   H2          2.5E+13     0.          3990.
    CH2O     +    O         =   HCO      +   OH          3.5E+13     0.          3510.
    HCO      +    HO2       =   CH2O     +   O2          1.0E+14     0.          3000.
    M        +    HCO       =   H        +   CO          2.94E+14    0.          15569.
    HCO      +    O2        =   CO       +   HO2         3.311E+12   0.          7000.
    HCO      +    OH        =   CO       +   H2O         1.0E+14     0.          0.
    HCO      +    H         =   CO       +   H2          1.995E+14   0.          0.
    HCO      +    O         =   CO       +   OH          1.0E+14     0.          0.
    CH       +    O2        =   HCO      +   O           1.0E+13     0.          0.
    CO       +    O         =   CO2      +   M           5.9E+15     0.          4100.
    CO       +    O2        =   CO2      +   O           2.5E+12     0.          47690.
    CO       +    OH        =   CO2      +   H           4.17E+11    0.          1000.
    CO       +    HO2       =   CO2      +   OH          5.75E+13    0.          22930.
    O        +    H2O       =   OH       +   OH          6.8E+13     0.          18365.
    H        +    O2        =   OH       +   O           1.89E+14    0.          16400.
    O        +    H2        =   OH       +   H           4.20E+14    0.          13750.
    H        +    HO2       =   H2       +   O2          7.28E+13    0.          2126.
    O        +    HO2       =   OH       +   O2          5.0E+13     0.          1000.
    HO2      +    OH        =   H2O      +   O2          8.0E+12     0.          0.
    H        +    HO2       =2.0OH                       1.34E+14    0.          1070.
    H2       +    HO2       =   H2O2     +   H           7.91E+13    0.          25000.
    OH       +    H2O2      =   H2O      +   HO2         6.1E+12     0.          1430.
    HO2      +    HO2       =   H2O2     +   O2          1.8E+12     0.          0.
    H        +    H2O2      =   OH       +   H2O         7.8E+11     0.          0.
    M        +    H2O2      =   OH       +   OH          1.44E+17    0.          45510.
     THIRDBODY
H2          2.30     O2          .78     H2O         6.0     H2O2        6.6
END
    H2       +    OH        =   H2O      +   H           4.74E+13    0.          6098.
    H        +    O2        =   HO2      +   M           1.46E+15    0.          -1000.
     THIRDBODY
O2          1.30     N2          1.3     H2O         21.3    CO2         7.0
C6H6        20.0     CH4         5.0     H2          3.0     END
    M        +    H2O       =   H        +   OH          1.30E+15    0.          105140.
     THIRDBODY
H2          4.00     O2          1.5     H2O         20.0    N2          1.5
CO2         4.00     C6H6        20.0    END
    H        +    O         =   OH       +   M           7.1E+18     -1.         0.
    M        +    H2        =   H        +   H           2.2E+14     0.          96000.

     THIRDBODY
H2          4.10     O2          2.0     H2O         15.0    N2          2.0
END
```

TABLE 4.17.—Concluded.

```
   M      +   O2      =   O       +   O        1.80E+18   -1.       118020.
   HO2    +   NO      =   NO2     +   OH       2.09E+12    0.       -477.
   O      +   NO2     =   NO      +   O2        1.0E+13     0.      596.
   NO     +   O       =   NO2     +   M        5.62E+15   0.        -1160.
   NO2    +   H       =   NO      +   OH       3.47E+14   0.         1470.
   NO     +   O       =   N       +   O2         3.8E+9   1.        41370.
   O      +   N2      =   NO      +   N         1.8E+14   0.        76250.
   NO     +   H       =   N       +   OH       2.63E+14   0.        50410.
   M      +   N2O     =   N2      +   O        6.92E+23   -2.5      65000.
   O      +   N2O     =   N2      +   O2        1.0E+14   0.        28020.
   O      +   N2O     =2.0NO                   6.92E+13   0.        26630.
   N      +   NO2     =2.0NO                    4.0E+12   0.        0.
   N2O    +   H       =   N2      +   OH       7.59E+13   0.        15100.
   NO2    +   H2      =   HNO2    +   H         2.4E+13  0.         29000.
   OH     +   NO2     =   HNO3    +   M         3.0E+15  0.         -3800.
   THIRDBODY
O2         0.70    H2          1.4    END
   OH     +   NO      =   HNO2    +   M         5.6E+15  0.         -1700.
   HNO    +   H       =   H2      +   NO        5.0E+12   0.        0.
   H      +   NO      =   HNO     +   M         5.4E+15   0.        -600.
   HNO    +   OH      =   H2O     +   NO        3.6E+13   0.        0.

AR
DISTANCE  AREA
 &prob welstr=.true.,  sencal = .true., tiny = 1.e-3,  &end
 &wsprob dotmax= 6000., delmd= 1000., mpr= 1,  volume = 200.,
        wsrhtr =.true., wsrht1= .05, wsrht0 = -42.88,   &end
 &start t= 614., p = 5.0,   mdot= 1500.,        &end
C6H6       .058825
O2         .441175
N2         .2500
AR         .2500
END
SENSVAR
C6H6       C6H5O     C6H5      H2O       C6H5OH    C2H2      C5H6      CH2O
OH         CO        NO        TEMP      END
INIT
TEMP       END
REAC
 &senrxn   sensaj=.true., order =.true., output =.false., allrxn =.true.,&end
FINIS
```

TABLE 4.18.—COMPARISON OF GLSENS AND BRUTE-FORCE SENSITIVITY COEFFICIENTS FOR PSR EXAMPLE PROBLEM 9 (REACTION OF BENZENE, O_2, N_2, AND Ar)

[Equivalence ratio $\varphi = 1.0$; mass flow rate $\dot{m} = 6000$ g/s; temperature $T = 2586.1$ K.]

Reaction number	Reaction	C_6H_6		C_6H_5O		C_6H_5		C_6H_5OH		CO		Temperature	
		GLSENS	Brute force	GLSENS	Brute force	GLSENS	Brute force	GLSENS	Brute force	GLSENS	Brute force	GLSENS	Brute force
		Sensitivity coefficient (S_{ij}) with respect to A_j, n_j, or E_j											
22	$C_5H_5 + OH = C_5H_4OH + H$	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}
6	$C_6H_6 + OH = C_6H_5 + H_2O$	−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}
8	$C_6H_5O = C_5H_5 + CO$	-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}	------	------
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}
5	$C_6H_6 + O = C_6H_5O + H$	−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	$C_4H_2 + O = C_2HO + C_2H$	−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}
11	$C_6H_5 = C_4H_3 + C_2H_2$	−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}

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

Variable	Example problem 8[a]		Example problem 9[b]	
	GLSENS	Brute force	GLSENS	Brute force
	Sensitivity coefficients (S_{i,T_0}) with respect to initial temperature			
C_6H_6	−0.775	−0.776	−0.876	−0.876
C_6H_5O	−0.812	−0.812	−1.42	−1.42
C_6H_5	−0.503	−0.503	−1.08	−1.08
C_6H_5OH	−1.00	−1.00	−2.84	−2.84
CO	0.438	0.438	0.297	0.297
Temperature	5.79×10^{-2}	5.81×10^{-2}	0.118	0.118

[a] C_6H_6–O_2; initial temperature $T_0 = 614$ K; mass flow rate $\dot{m} = 6000$ g/s; temperature $T = 3168.7$ K.

[b] C_6H_6–O_2–N_2–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 least-squares 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 three-volume 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-flow-rate 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 μs. 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 all-global 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.

TABLE A.1.—DATA FILE FOR MULTIPLE CASES WITH GLOBAL CODE

```
TAPE
 GLOBAL CODE TEST CASE: MOLECULAR REACTIONS ONLY AND NO INERTS     CASE 1
 &rtype            &end
   O       +   H2O       =   OH       +   OH            6.8E+13    0.         18365.
   H       +   O2        =   OH       +   O            1.89E+14   0.         16400.
   O       +   H2        =   OH       +   H            4.20E+14   0.         13750.
   H       +   HO2       =   H2       +   O2           7.28E+13   0.         2126.
   O       +   HO2       =   OH       +   O2            5.0E+13   0.         1000.
   HO2     +   OH        =   H2O      +   O2            8.0E+12   0.         0.
   H       +   HO2       =2.0OH                        1.34E+14   0.         1070.
   H2      +   HO2       =   H2O2     +   H            7.91E+13   0.         25000.
   OH      +   H2O2      =   H2O      +   HO2           6.1E+12   0.         1430.
   HO2     +   HO2       =   H2O2     +   O2            1.8E+12   0.           0.
   H       +   H2O2      =   OH       +   H2O           5.0E+11   0.           0.


TIME
 &prob  welstr=.true.,              &end
 &wsprob       delmd=  100., dotmax= 1000.,   mpr=2, volume= 2000., &end
 &start t= 800.,p=5.5,mdot=  0.1, &end
O2          .193301
H2          .806699
END
FINIS
 GLOBAL TEST CASE: CHANGE AND ADD GLOBAL AND MOLECULAR REACTIONS  CASE 2
CHANGE
 &rtype global=.true.,gronly=.false.,
    mrchng=.true.,  mradd = .true., gladd = .true., &end
   H       +   H2O2      =   OH       +   H2O           7.8E+11   0.           0.

ADD
   M       +   H2O2      =2.0OH                        1.44E+17   0.         45510.
   THIRDBODY
H2          2.30     O2            .78      H2O         6.0    H2O2          6.6
END
   H2      +   OH        =   H2O      +   H            4.74E+13   0.         6098.
   H       +   O2        =   HO2      +   M            1.46E+15   0.         -1000.
   THIRDBODY
O2          1.30     N2            1.3      H2O         21.3   H2            3.0
END
   M       +   H2O       =   H        +   OH           1.30E+15   0.         105140.
   THIRDBODY
H2          4.00     O2            1.5      H2O         20.0   N2            1.5
END
   H       +   O         =   OH       +   M             7.1E+18  -1.           0.
   M       +   H2        =   H        +   H             2.2E+14   0.          96000.
   THIRDBODY
H2          4.10     O2            2.0      H2O         15.0   N2            2.0
END
   M       +   O2        =   O        +   O            1.80E+18   -1.        118020.
   CO      +   O         >   CO2                       8.43E+09   -.001      1000.
               CO2       >   CO       +   O            9.08E+18   -1.84      130754.
   END
                 H2O     +     O        >     H2      +   O2
             1.        1.       4.90E+10   .18      -510.
                 CO      +    H2O       >    CO2      +   H2
             1.        1.       1.30E+05   1.31     -7000.
                 CO2     +    H2        >    CO       +   H2O
             1.        1.       4.41E+10   .19      3527.
                 N2      +    O2        >2.0 NO
             1.        1.       4.00E+14   .03     100000.
                    2.0 NO              >    N2       +   O2
                       2.       2.00E+11   0.       38000.
                 CN      +2.0 O         >    NO       +   CO
             1.       1.        8.30E+11   0.          0.
                 CN      +    NO        >    CO       +   N2
             1.       1.        1.25E+12   0.          0.
             2.0 CH2     +    N2        >2.0 CN       +2.0 H2
             1.    1.           5.00E+13   0.       54000.
                 CH2     +    O2        >    CO       +   H2O
             1.       .5        3.50E+07   0.       5000.
                 O2      +    C3H8      >3.0 CH2      +2.0 OH
             1.6      .1        1.10E+12   0.       41000.
                 H2      +    O2        >2.0 OH
             1.    1.           1.00E+00   0.       49080.
                 C3H8    +2.0 OH        >    H2O      +   C3H8      +     O
             .15   1.           1.98E+06   0.       4000.
    OH      +    H2      +    O2        >    H2O      +   O         +     OH
  1.        0.    1.            0.96E+12   -.1      1013.
                 H2O     +    O         >    H2       +   O2
             1.        1.       4.90E+10   .18      -510.
    END
```

TABLE A.1.—Continued.

```
 AR
 TIME                                   C3H8
  &prob                 &end
  &wsprob
      delmd= 50., dotmax= 4000.,mpr=2,
      volume= 500.,      &end
  &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
  &rtype global=.true.,gronly=.false., gladd = .false., glchng = .false.,
      mrprev = .false., mrchng = .false., mradd=.true.,  &end
    H2      +   O2      =   OH      +   OH          1.7E+13   0.       47780.
    O       +   H2O2    =   OH      +   HO2         8.0E+13   0.       1000.
    END

 TIME                                   C3H8
  &PROB  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.,                    &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,      welstr = .false.,  &end
  &start t= 1600., p=5.5,    &end
 H2          .0573205
 N2          .720502
 CO2         .0002768
 O2          .193301
 C3H8        .02
 AR          .0085997
 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
                  H2O     +    O         >    H2      +    O2
            1.        1.       4.90E+10   .18      -510.
                  CO      +    H2O       >    CO2     +    H2
            1.        1.       1.30E+05   1.31     -7000.
                  CO2     +    H2        >    CO      +    H2O
            1.        1.       4.41E+10   .19      3527.
                  N2      +    O2       >2.0  NO
            1.        1.       3.00E+14   .03     100000.
                         2.0 NO          >    N2      +    O2
                          2.       2.00E+11   0.      38000.
                  CN     +2.0 O          >    NO      +    CO
            1.       1.        8.30E+11   0.         0.
                  CN      +    NO        >    CO      +    N2
            1.       1.        1.25E+12   0.         0.
            2.0 CH2       +    N2       >2.0  CN     +2.0  H2
            1.    1.           5.00E+13   0.      54000.
                  CH2     +    O2        >    CO      +    H2O
            1.      .5         3.50E+07   0.      5000.
                  O2      +    C3H8     >3.0  CH2    +2.0  OH
            1.6     .1         1.10E+12   0.      41000.
                  H2      +    O2       >2.0  OH
            1.    1.           1.00E+00   0.      49080.
                  C3H8   +2.0  OH        >    H2O     +    C3H8    +    O
            .15   1.           1.98E+06   0.      4000.
    OH      +     H2      +    O2        >    H2O     +    O       +    OH
  1.        0.    1.           0.96E+12   -.1     1013.

 AR
 TIME                                   C3H8
  &prob  welstr=.true.,             &end
  &wsprob       delmd= 10., dotmax= 1600.,   mpr=1, volume= 200., &end
  &start t= 800.,p=5.5,mdot=  100.,  &end
 O2          .193301
 N2          .720502
 C3H8        .0773205
 AR          .0088765
 END
 FINIS
```

TABLE A.1.—Concluded.

```
 ALL GLOBAL REACTIONS - CHANGE AND ADD ONE GLOBAL REACTION      CASE 6
CHANGE
 &rtype  global=.true.,gronly=.true., glchng=.true.,
         gladd = .true., mrprev = .false., &end
                 N2       +     O2        >2.0 NO
            1.         1.        4.00E+14    .03     100000.

ADD
                 H2O      +     O         >     H2      +    O2
            1.         1.        4.90E+10    .18      -510.
    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
O2          .193301
N2          .720502
C3H8        .0773205
AR          .0088765
END
FINIS
GLOBAL AND MOLECULAR REACTIONS; MOLECULAR REACTIONS ADDED      CASE 7
ADD
 &rtype global=.true.,gronly=.false.,  mrprev = .false.,
      mradd=.true., &end
   O        +   H2O      =   OH       +   OH             6.8E+13    0.          18365.
   H        +   O2       =   OH       +   O             1.89E+14   0.          16400.
   O        +   H2       =   OH       +   H             4.20E+14   0.          13750.
   H        +   HO2      =   H2       +   O2            7.28E+13   0.          2126.
   O        +   HO2      =   OH       +   O2             5.0E+13   0.          1000.
   HO2      +   OH       =   H2O      +   O2             8.0E+12   0.          0.
   H        +   HO2      =2.0OH                         1.34E+14   0.          1070.
   H2       +   HO2      =   H2O2     +   H             7.91E+13   0.          25000.
   OH       +   H2O2     =   H2O      +   HO2            6.1E+12   0.          1430.
   HO2      +   HO2      =   H2O2     +   O2             1.8E+12   0.           0.
   H        +   H2O2     =   OH       +   H2O            7.8E+11   0.           0.
   M        +   H2O2     =2.0OH                         1.44E+17   0.          45510.
   THIRDBODY
H2          2.30     O2          .78      H2O           6.0     H2O2         6.6
END
   H2       +   OH       =   H2O      +   H             4.74E+13   0.          6098.
   H        +   O2       =   HO2      +   M             1.46E+15   0.          -1000.
   THIRDBODY
O2          1.30     N2          1.3      H2O           21.3    H2           3.0
END
   M        +   H2O      =   H        +   OH            1.30E+15   0.          105140.
   THIRDBODY
H2          4.00     O2          1.5      H2O           20.0    N2           1.5
END
   H        +   O        =   OH       +   M              7.1E+18   -1.          0.
   M        +   H2       =   H        +   H              2.2E+14   0.           96000.
   THIRDBODY
H2          4.10     O2          2.0      H2O           15.0    N2           2.0
END
   M        +   O2       =   O        +   O             1.80E+18   -1.         118020.
   CO       +   O        >   CO2                        8.43E+09   -.001       1000.
                CO2      >   CO       +   O             9.08E+18   -1.84       130754.
   END

TIME                                   C3H8
 &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)

```
                              ** DATA LINES **

             1         2         3         4         5         6         7         8
CC  12345678901234567890123456789012345678901234567890123456789012345678901234567890

  GLOBAL CODE TEST CASE: MOLECULAR REACTIONS ONLY AND NO INERTS    CASE 1
  &rtype           &end
    O      +   H2O     =   OH     +   OH          6.8E+13   0.       18365.
    H      +   O2      =   OH     +   O          1.89E+14   0.       16400.
    O      +   H2      =   OH     +   H          4.20E+14   0.       13750.
    H      +   HO2     =   H2     +   O2         7.28E+13   0.       2126.
    O      +   HO2     =   OH     +   O2          5.0E+13   0.       1000.
    HO2    +   OH      =   H2O    +   O2          8.0E+12   0.       0.
    H      +   HO2     =2.0OH                    1.34E+14   0.       1070.
    H2     +   HO2     =   H2O2   +   H          7.91E+13   0.       25000.
    OH     +   H2O2    =   H2O    +   HO2         6.1E+12   0.       1430.
    HO2    +   HO2     =   H2O2   +   O2          1.8E+12   0.         0.
    H      +   H2O2    =   OH     +   H2O         5.0E+11   0.         0.
                                 -  BLANK LINE  -
                                 -  BLANK LINE  -
 TIME
  &prob  welstr=.true.,                &end
  &wsprob        delmd=  100., dotmax= 1000.,   mpr=2, volume= 2000., &end
  &start t= 800.,p=5.5,mdot=  0.1, &end
 O2          .193301
 H2          .806699
 END
 FINIS
```

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM   NASA LEWIS RESEARCH CENTER

GLOBAL CODE TEST CASE: MOLECULAR REACTIONS ONLY AND NO INERTS   CASE 1

REACTION NUMBER	REACTION							REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1*O	+	1*H2O	=	2*OH			6.80000E+13	0.0000	18365.00
2	1*H	+	1*O2	=	1*OH	+	1*O	1.89000E+14	0.0000	16400.00
3	1*O	+	1*H2	=	1*OH	+	1*H	4.20000E+14	0.0000	13750.00
4	1*H	+	1*HO2	=	1*H2	+	1*O2	7.28000E+13	0.0000	2126.00
5	1*O	+	1*HO2	=	1*OH	+	1*O2	5.00000E+13	0.0000	1000.00
6	1*HO2	+	1*OH	=	1*H2O	+	1*O2	8.00000E+12	0.0000	0.00
7	1*H	+	1*HO2	=	2*OH			1.34000E+14	0.0000	1070.00
8	1*H2	+	1*HO2	=	1*H2O2	+	1*H	7.91000E+13	0.0000	25000.00
9	1*OH	+	1*H2O2	=	1*H2O	+	1*HO2	6.10000E+12	0.0000	1430.00
10			2*HO2	=	1*H2O2	+	1*O2	1.80000E+12	0.0000	0.00
11	1*H	+	1*H2O2	=	1*OH	+	1*H2O	5.00000E+11	0.0000	0.00

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

** ASSIGNED VARIABLE PROFILE **

WELL - STIRRED REACTOR CASE

VOLUME OF REACTOR = 2.00000E+03 CM**3
MASS FLOW RATE TO START ITERATION = 1.00000E-01 G/S

ASSIGNED MASS FLOW RATE PROBLEM: MASS FLOW RATE INCREMENT = 1.00000E+02 G/S
MAXIMUM MASS FLOW RATE = 1.00000E+03 G/S

NUMBER OF REACTING SPECIES: 8

NUMBER OF INERT SPECIES: 0

** INITIAL CONDITIONS **

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

FLOW PROPERTIES		INTEGRATION INDICATORS	
PRESSURE (ATM)	5.50000	STEPS FROM LAST PRINT	0
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE	0.00000E+00
DENSITY (G/CM**3)	6.54484E-04	METHOD ORDER	0
TEMPERATURE (DEG K)	800.00		
MASS FLOW RATE (G/SEC)	1.00000E-01	TOTAL NUMBER OF STEPS	0
ENTROPY (CAL/G/DEG K)	5.0211	FUNCT EVALUATIONS	0
MACH NUMBER	0.0000	JACOBIAN EVALUATIONS	0
GAMMA	1.3762		
ENTHALPY (CAL/G)	4.56525E+02		
SP. HEAT (CP) (CAL/G/DEG K)	9.30602E-01		

TABLE A.2.—Continued.

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
O	0.00000E+00	0.00000E+00	0.00000E+00	1	6.5377E+08	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	0.00000E+00	2	6.2545E+09	0.00000E+00	0.00000
OH	0.00000E+00	0.00000E+00	0.00000E+00	3	7.3608E+10	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	2.25347E-10	4	1.9113E+13	-5.26082E-04	1.00000
O2	1.61956E-05	1.93301E-01	-2.25347E-10	5	2.6655E+13	0.00000E+00	0.00000
H2	6.75887E-05	8.06699E-01	-2.25347E-10	6	8.0000E+12	0.00000E+00	0.00000
HO2	0.00000E+00	0.00000E+00	2.25347E-10	7	6.8359E+13	0.00000E+00	0.00000
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	8	1.1708E+07	0.00000E+00	0.00000
				9	2.4813E+12	0.00000E+00	0.00000
				10	1.8000E+12	0.00000E+00	0.00000
				11	5.0000E+11	0.00000E+00	0.00000

MIXTURE MOLECULAR WEIGHT 7.81154 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 2.76731E+01 MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 0.433333 S

**EQUILIBRIUM CONDITIONS **

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

FLOW PROPERTIES		INTEGRATION INDICATORS	
PRESSURE (ATM)	5.50000	STEPS FROM LAST PRINT	0
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE	0.00000E+00
DENSITY (G/CM**3)	1.99835E-04	METHOD ORDER	0
TEMPERATURE (DEG K)	3103.95		
MASS FLOW RATE (G/SEC)	1.00000E-01	TOTAL NUMBER OF STEPS	0
ENTROPY (CAL/G/DEG K)	6.0245	FUNCT EVALUATIONS	0
MACH NUMBER	0.0000	JACOBIAN EVALUATIONS	0
GAMMA	1.2304		
ENTHALPY (CAL/G)	4.56525E+02		
SP. HEAT (CP) (CAL/G/DEG K)	1.14667E+00		

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
O	3.57432E-08	1.65522E-03	1.07622E-06	1	3.4628E+12	-1.03879E+01	0.00000
H2O	9.37412E-06	4.34104E-01	4.15227E-07	2	1.3235E+13	-1.93939E+00	0.00000
OH	4.54298E-07	2.10379E-02	-1.62916E-06	3	4.5197E+13	-1.85043E+01	0.00000
H	1.36271E-06	6.31051E-02	-6.76196E-07	4	5.1575E+13	1.41732E-01	0.00000
O2	1.28850E-08	5.96686E-04	8.35931E-08	5	4.2517E+13	2.95487E-03	0.00000
H2	1.03544E-05	4.79498E-01	7.45053E-07	6	8.0000E+12	9.19158E-03	0.00000
HO2	6.53034E-11	3.02412E-06	-1.42663E-08	7	1.1266E+14	2.14840E-01	0.00000
H2O2	1.02949E-11	4.76743E-07	-4.69738E-10	8	1.3738E+12	-1.10281E-02	0.00000
				9	4.8377E+12	4.46155E-04	0.00000
				10	1.8000E+12	1.45917E-07	0.00000
				11	5.0000E+11	2.88632E-04	0.00000

MIXTURE MOLECULAR WEIGHT 9.25413 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) -2.58138E+05 MASS FRACTION SUM 1.00000071

COMPUTATIONAL WORK REQUIRED FOR EQUILIBRIUM CALCULATION:
NO. OF ITERATIONS = 8 CPU TIME = 1.666665E-02 S

INITIAL ESTIMATES (SIGMAS) AT TEMPERATURE = 3103.95 K:

O	1.78863E-04
H2O	4.69092E-02
OH	2.27336E-03
H	6.81913E-03
O2	6.44778E-05
H2	5.18145E-02
HO2	3.26786E-07
H2O2	5.15168E-08

WELLSTIRRED REACTOR CALCULATION.... GLOBAL CODE TEST CASE: MOLECULAR REACTIONS ONLY AND NO INERTS CASE 1

		INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE	ATM	5.50000	5.50000	1.00000
TEMP.	DEG K	800.000	1102.07	1.37758
ENTROPY	CAL/GM/K	5.02109	5.50757	1.09689
DENSITY	GM/CM**3	6.54484E-04	4.75096E-04	0.72591
ENTHALPY	CAL/GM	456.525	456.525	1.00000
SP. HEAT (CP)	CAL/GM/K	9.30602E-01	9.62486E-01	1.03426
MOL. WT. OF MIXT		7.8115	7.8115	
GAMMA		1.3762	1.3593	

TABLE A.2.—Concluded.

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
O	0.00000E+00	0.00000E+00	4.12446E-03	8.44761E-03
H2O	0.00000E+00	0.00000E+00	3.73312E-01	8.60942E-01
OH	0.00000E+00	0.00000E+00	2.61348E-03	5.69007E-03
H	0.00000E+00	0.00000E+00	3.69187E-01	4.76385E-02
O2	1.93301E-01	7.91828E-01	3.27611E-03	1.34201E-02
H2	8.06699E-01	2.08172E-01	2.47487E-01	6.38649E-02
HO2	0.00000E+00	0.00000E+00	7.81154E-10	3.30067E-09
H2O2	0.00000E+00	0.00000E+00	7.81154E-10	3.40146E-09

VOLUME 2000.00 CM**3 MASS FLO 0.100000 GM/SEC

MDOT/VOLUME = 0.00005 RESIDENCE TIME = 9501.925 MSEC ITERATIONS = 10

WELLSTIRRED REACTOR CALCULATION.... GLOBAL CODE TEST CASE: MOLECULAR REACTIONS ONLY AND NO INERTS CASE 1

		INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE	ATM	5.50000	5.50000	1.00000
TEMP.	DEG K	800.000	1098.26	1.37282
ENTROPY	CAL/GM/K	5.02109	5.50748	1.09687
DENSITY	GM/CM**3	6.54484E-04	4.76743E-04	0.72843
ENTHALPY	CAL/GM	456.525	456.525	1.00000
SP. HEAT (CP)	CAL/GM/K	9.30602E-01	9.61760E-01	1.03348
MOL. WT. OF MIXT		7.8115	7.8115	
GAMMA		1.3762	1.3596	

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
O	0.00000E+00	0.00000E+00	4.66892E-03	9.56277E-03
H2O	0.00000E+00	0.00000E+00	3.69883E-01	8.53035E-01
OH	0.00000E+00	0.00000E+00	3.01596E-03	6.56636E-03
H	0.00000E+00	0.00000E+00	3.65214E-01	4.71258E-02
O2	1.93301E-01	7.91828E-01	4.51704E-03	1.85034E-02
H2	8.06699E-01	2.08172E-01	2.52701E-01	6.52105E-02
HO2	0.00000E+00	0.00000E+00	7.81154E-10	3.30067E-09
H2O2	0.00000E+00	0.00000E+00	7.81154E-10	3.40146E-09

VOLUME 2000.00 CM**3 MASS FLO 900.100 GM/SEC

MDOT/VOLUME = 0.45005 RESIDENCE TIME = 1.059 MSEC ITERATIONS = 2

WELLSTIRRED REACTOR CALCULATION.... GLOBAL CODE TEST CASE: MOLECULAR REACTIONS ONLY AND NO INERTS CASE 1

		INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE	ATM	5.50000	5.50000	1.00000
TEMP.	DEG K	800.000	1097.88	1.37235
ENTROPY	CAL/GM/K	5.02109	5.50746	1.09687
DENSITY	GM/CM**3	6.54484E-04	4.76907E-04	0.72868
ENTHALPY	CAL/GM	456.525	456.525	1.00000
SP. HEAT (CP)	CAL/GM/K	9.30602E-01	9.61689E-01	1.03341
MOL. WT. OF MIXT		7.8115	7.8115	
GAMMA		1.3762	1.3597	

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
O	0.00000E+00	0.00000E+00	4.71882E-03	9.66496E-03
H2O	0.00000E+00	0.00000E+00	3.69536E-01	8.52233E-01
OH	0.00000E+00	0.00000E+00	3.05414E-03	6.64948E-03
H	0.00000E+00	0.00000E+00	3.64817E-01	4.70745E-02
O2	1.93301E-01	7.91828E-01	4.64676E-03	1.90347E-02
H2	8.06699E-01	2.08172E-01	2.53228E-01	6.53465E-02
HO2	0.00000E+00	0.00000E+00	7.81154E-10	3.30067E-09
H2O2	0.00000E+00	0.00000E+00	7.81154E-10	3.40146E-09

VOLUME 2000.00 CM**3 MASS FLO 1000.00 GM/SEC

MDOT/VOLUME = 0.50000 RESIDENCE TIME = 0.954 MSEC ITERATIONS = 2

COMPUTATIONAL WORK REQUIRED FOR PSR CALCULATION:
NO. OF ITERATIONS = 30 CPU TIME = 3.666667E-01 S

(LSENS) END OF THIS CASE

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 0.833333 S

(LSENS) READ DATA FOR NEXT CASE

TABLE A.3.—COMPUTED RESULTS FOR TEST CASE 2 (PROPANE-AIR PSR PROBLEM USING GLOBAL AND MOLECULAR REACTIONS)

```
                                    **  DATA LINES  **

              1         2         3         4         5         6         7         8
CC  1234567890123456789012345678901234567890123456789012345678901234567890123456789 0

  GLOBAL TEST CASE: CHANGE AND ADD GLOBAL AND MOLECULAR REACTIONS  CASE 2
 CHANGE
  &rtype global=.true.,gronly=.false.,
     mrchng=.true.,  mradd = .true., gladd = .true., &end
    H       +   H2O2      =    OH       +   H2O         7.8E+11   0.          0.
                                     -  BLANK LINE  -
 ADD
    M       +   H2O2      =2.0OH                        1.44E+17   0.          45510.
    THIRDBODY
 H2         2.30     O2          .78      H2O            6.0    H2O2           6.6
 END
    H2      +   OH        =    H2O      +   H           4.74E+13   0.          6098.
    H       +   O2        =    HO2      +   M           1.46E+15   0.          -1000.
    THIRDBODY
 O2         1.30     N2          1.3      H2O            21.3   H2             3.0
 END
    M       +   H2O       =    H        +   OH          1.30E+15   0.          105140.
    THIRDBODY
 H2         4.00     O2          1.5      H2O            20.0   N2             1.5
 END
    H       +   O         =    OH       +   M            7.1E+18  -1.           0.
    M       +   H2        =    H        +   H            2.2E+14   0.           96000.
    THIRDBODY
 H2         4.10     O2          2.0      H2O            15.0   N2             2.0
 END
    M       +   O2        =    O        +   O           1.80E+18   -1.         118020.
    CO      +   O         >    CO2                      8.43E+09   -.001       1000.
                CO2       >    CO       +   O           9.08E+18   -1.84       130754.
    END
                   H2O     +     O          >     H2      +   O2
              1.          1.       4.90E+10    .18      -510.
                   CO      +     H2O        >     CO2     +   H2
              1.          1.       1.30E+05    1.31     -7000.
                   CO2     +     H2         >     CO      +   H2O
              1.          1.       4.41E+10    .19      3527.
                   N2      +     O2         >2.0 NO
              1.          1.       4.00E+14    .03     100000.
                             2.0 NO         >     N2      +   O2
                          2.       2.00E+11    0.       38000.
                   CN      +2.0 O           >     NO      +   CO
              1.         1.        8.30E+11    0.          0.
                   CN      +     NO         >     CO      +   N2
              1.         1.        1.25E+12    0.          0.
              2.0 CH2      +     N2         >2.0 CN      +2.0 H2
              1.      1.           5.00E+13    0.       54000.
                   CH2     +     O2         >     CO      +   H2O
              1.         .5        3.50E+07    0.       5000.
                   O2      +     C3H8       >3.0 CH2     +2.0 OH
              1.6        .1        1.10E+12    0.       41000.
                   H2      +     O2         >2.0 OH
              1.      1.           1.00E+00    0.       49080.
                   C3H8    +2.0 OH          >     H2O     +   C3H8     +   O
              .15     1.           1.98E+06    0.       4000.
    OH       +     H2      +     O2         >     H2O     +   O        +   OH

  1.          0.      1.           0.96E+12    -.1      1013.
                   H2O     +     O          >     H2      +   O2
              1.          1.       4.90E+10    .18      -510.
     END
 AR
 TIME                                          C3H8
  &prob                   &end
  &wsprob
      delmd= 50., dotmax= 4080.,mpr=2,
      volume= 500.,       &end
  &START T= 800.,P=5.5,MDOT= 140.0, eratio =1.5, scc = 3.0, sch = 8.0,  &END
 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 NUMBER	REACTION							REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1*O	+	1*H2O	=	2*OH			6.80000E+13	0.0000	18365.00
2	1*H	+	1*O2	=	1*OH	+	1*O	1.89000E+14	0.0000	16400.00
3	1*O	+	1*H2	=	1*OH	+	1*H	4.20000E+14	0.0000	13750.00
4	1*H	+	1*HO2	=	1*H2	+	1*O2	7.28000E+13	0.0000	2126.00
5	1*O	+	1*HO2	=	1*OH	+	1*O2	5.00000E+13	0.0000	1000.00
6	1*HO2	+	1*OH	=	1*H2O	+	1*O2	8.00000E+12	0.0000	0.00
7	1*H	+	1*HO2	=	2*OH			1.34000E+14	0.0000	1070.00
8	1*H2	+	1*HO2	=	1*H2O2	+	1*H	7.91000E+13	0.0000	25000.00
9	1*OH	+	1*H2O2	=	1*H2O	+	1*HO2	6.10000E+12	0.0000	1430.00
10			2*HO2	=	1*H2O2	+	1*O2	1.80000E+12	0.0000	0.00
11	1*H	+	1*H2O2	=	1*OH	+	1*H2O	7.80000E+11	0.0000	0.00
12	M	+	1*H2O2	=	2*OH			1.44000E+17	0.0000	45510.00
13	1*H2	+	1*OH	=	1*H2O	+	1*H	4.74000E+13	0.0000	6098.00
14	1*H	+	1*O2	=	1*HO2	+	M	1.46000E+15	0.0000	-1000.00
15	M	+	1*H2O	=	1*H	+	1*OH	1.30000E+15	0.0000	105140.00
16	1*H	+	1*O	=	1*OH	+	M	7.10000E+18	-1.0000	0.00
17	M	+	1*H2	=	2*H			2.20000E+14	0.0000	96000.00
18	M	+	1*O2	=	2*O			1.80000E+18	-1.0000	118020.00
19	1*CO	+	1*O	>	1*CO2			8.43000E+09	-0.0010	1000.00
20			1*CO2	>	1*CO	+	1*O	9.08000E+18	-1.8400	130754.00

TABLE A.3.—Continued.

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

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

*** GLOBAL REACTIONS ***

NUMBER	REACTION											
21			1.0*H2O	+	1.0*O	>	1.0*H2	+	1.0*O2		
22			1.0*CO	+	1.0*H2O	>	1.0*CO2	+	1.0*H2		
23			1.0*CO2	+	1.0*H2	>	1.0*CO	+	1.0*H2O		
24			1.0*N2	+	1.0*O2	>	2.0*NO				
25					2.0*NO	>	1.0*N2	+	1.0*O2		
26			1.0*CN	+	2.0*O	>	1.0*NO	+	1.0*CO		
27			1.0*CN	+	1.0*NO	>	1.0*CO	+	1.0*N2		
28			2.0*CH2	+	1.0*N2	>	2.0*CN	+	2.0*H2		
29			1.0*CH2	+	1.0*O2	>	1.0*CO	+	1.0*H2O		
30			1.0*O2	+	1.0*C3H8	>	3.0*CH2	+	2.0*OH		
31			1.0*H2	+	1.0*O2	>	2.0*OH				
32			1.0*C3H8	+	2.0*OH	>	1.0*H2O	+	1.0*C3H8	+	1.0*O
33	1.0*OH	+	1.0*H2	+	1.0*O2	>	1.0*H2O	+	1.0*O	+	1.0*OH
34			1.0*H2O	+	1.0*O	>	1.0*H2	+	1.0*O2		

REACTION NUMBER	REACTANT EXPONENTS REXP 1	REXP 2	REXP 3	REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
21	0.000	1.000	1.000	4.90000E+10	0.1800	-510.00
22	0.000	1.000	1.000	1.30000E+05	1.3100	-7000.00
23	0.000	1.000	1.000	4.41000E+10	0.1900	3527.00
24	0.000	1.000	1.000	4.00000E+14	0.0300	100000.00
25	0.000	0.000	2.000	2.00000E+11	0.0000	38000.00
26	0.000	1.000	1.000	8.30000E+11	0.0000	0.00
27	0.000	1.000	1.000	1.25000E+12	0.0000	0.00
28	0.000	1.000	1.000	5.00000E+13	0.0000	54000.00
29	0.000	1.000	0.500	3.50000E+07	0.0000	5000.00
30	0.000	1.600	0.100	1.10000E+12	0.0000	41000.00
31	0.000	1.000	1.000	1.00000E+00	0.0000	49080.00
32	0.000	0.150	1.000	1.98000E+06	0.0000	4000.00
33	1.000	0.000	1.000	9.60000E+11	-0.1000	1013.00
34	0.000	1.000	1.000	4.90000E+10	0.1800	-510.00

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

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

FLOW PROPERTIES		INTEGRATION INDICATORS	
PRESSURE (ATM)	5.50000	STEPS FROM LAST PRINT	0
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE	0.00000E+00
DENSITY (G/CM**3)	2.50173E-03	METHOD ORDER	0
TEMPERATURE (DEG K)	800.00		
MASS FLOW RATE (G/SEC)	1.40000E+02	TOTAL NUMBER OF STEPS	0
ENTROPY (CAL/G/DEG K)	1.8011	FUNCT EVALUATIONS	0
MACH NUMBER	0.0000	JACOBIAN EVALUATIONS	0
GAMMA	1.2701		
ENTHALPY (CAL/G)	9.23468E+01		
SP. HEAT (CP) (CAL/G/DEG K)	3.12948E-01		

TABLE A.3.—Continued.

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSI-TIVE DIR RATE
O	0.00000E+00	0.00000E+00	3.57038E-26	1	6.5377E+08	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	0.00000E+00	2	6.2545E+09	0.00000E+00	0.00000
OH	0.00000E+00	0.00000E+00	9.11685E-08	3	7.3608E+10	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	0.00000E+00	4	1.9113E+13	0.00000E+00	0.00000
O2	1.65148E-05	1.97112E-01	-4.55842E-08	5	2.6655E+13	0.00000E+00	0.00000
H2	0.00000E+00	0.00000E+00	0.00000E+00	6	8.0000E+12	0.00000E+00	0.00000
HO2	0.00000E+00	0.00000E+00	0.00000E+00	7	6.8359E+13	0.00000E+00	0.00000
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	8	1.1708E+07	0.00000E+00	0.00000
CO	0.00000E+00	0.00000E+00	1.86163E-30	9	2.4813E+12	0.00000E+00	0.00000
CO2	2.36493E-08	2.82264E-04	-1.86163E-30	10	1.8000E+12	0.00000E+00	0.00000
N2	6.15566E-05	7.34704E-01	-2.38549E-22	11	7.8000E+11	0.00000E+00	0.00000
NO	0.00000E+00	0.00000E+00	4.77099E-22	12	5.3163E+04	0.00000E+00	0.00000
CN	0.00000E+00	0.00000E+00	0.00000E+00	13	1.0230E+12	0.00000E+00	0.00000
CH2	0.00000E+00	0.00000E+00	1.36753E-07	14	2.7387E+15	0.00000E+00	0.00000
C3H8	4.95445E-06	5.91335E-02	-4.55842E-08	15	2.4606E-14	0.00000E+00	0.00000
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
				19	4.4641E+09	0.00000E+00	0.00000
				20	7.8718E-23	2.97450E-25	1.00000
				21	2.2495E+11	0.00000E+00	0.00000
				22	6.7500E+10	0.00000E+00	0.00000
				23	1.7080E+10	0.00000E+00	0.00000
				24	2.3465E-13	3.81152E-17	1.00000
				25	8.3160E+00	0.00000E+00	0.00000
				26	8.3000E+11	0.00000E+00	0.00000
				27	1.2500E+12	0.00000E+00	0.00000
				28	8.8483E-02	0.00000E+00	0.00000
				29	1.5071E+06	0.00000E+00	0.00000
				30	6.9297E+00	7.28341E-03	1.00000
				31	3.9081E-14	0.00000E+00	0.00000
				32	1.5992E+05	0.00000E+00	0.00000
				33	2.6015E+11	0.00000E+00	0.00000
				34	2.2495E+11	0.00000E+00	0.00000

MIXTURE MOLECULAR WEIGHT 29.85916 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 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 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES		INTEGRATION INDICATORS	
PRESSURE (ATM)	5.50000	STEPS FROM LAST PRINT	0
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE	0.00000E+00
DENSITY (G/CM**3)	7.34828E-04	METHOD ORDER	0
TEMPERATURE (DEG K)	2350.31		
MASS FLOW RATE (G/SEC)	1.40000E+02	TOTAL NUMBER OF STEPS	0
ENTROPY (CAL/G/DEG K)	2.3604	FUNCT EVALUATIONS	0
MACH NUMBER	0.0000	JACOBIAN EVALUATIONS	0
GAMMA	1.2641		
ENTHALPY (CAL/G)	9.23468E+01		
SP. HEAT (CP) (CAL/G/DEG K)	3.69088E-01		

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSI-TIVE DIR RATE
O	2.17893E-10	7.64039E-06	-2.50908E-04	1	1.3329E+12	-7.60162E-04	0.00000
H2O	4.05534E-06	1.42200E-01	8.69456E-03	2	5.6424E+12	-2.68460E-05	0.00000
OH	1.53281E-08	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
O2	2.11927E-10	7.43118E-06	3.89433E-04	5	4.0363E+13	7.03729E-09	0.00000
H2	1.73940E-06	6.09920E-02	-8.55659E-03	6	8.0000E+12	1.29043E-07	0.00000
HO2	3.90703E-13	1.37000E-08	-1.11365E-07	7	1.0656E+14	2.24499E-06	0.00000
H2O2	7.34828E-14	2.57667E-09	2.33318E-05	8	3.7453E+11	1.99374E-01	0.42297
CO	3.10378E-06	1.08834E-01	8.94626E-03	9	4.4911E+12	-6.86707E-03	0.42297
CO2	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	2.1738E+05	-5.10833E-04	0.00000
AR	2.15801E-07	7.56703E-03	0.00000E+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	8.45730E+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	1.80064E-03	1.00000
				25	5.8546E+07	7.59605E-04	1.00000
				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

TABLE A.3.—Continued.

31	2.7300E-05	1.86571E-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

MIXTURE MOLECULAR WEIGHT 25.76666 TOTAL ENERGY EXCHANGE RATE -2.09583E+06 MASS FRACTION SUM 1.00000010
(CAL-CM**3/GM**2/SEC)

COMPUTATIONAL WORK REQUIRED FOR EQUILIBRIUM CALCULATION:
NO. OF ITERATIONS = 12 CPU TIME = 4.999995E-02 S

INITIAL ESTIMATES (SIGMAS) AT TEMPERATURE = 2350.31 K:

O	2.96523E-07
H2O	5.51876E-03
OH	2.08595E-05
H	5.07475E-05
O2	2.88403E-07
H2	2.36709E-03
HO2	5.31693E-10
H2O2	1.00000E-10
CO	4.22382E-03
CO2	1.72687E-03
N2	2.46038E-02
NO	3.60201E-06
CN	1.00000E-10
CH2	1.00000E-10
C3H8	1.00000E-10
AR	2.93675E-04

(WSR) *** FOR CONV. NO. 1, CONVERGED TEMP. (AFTER 13 ITERATIONS) IS GREATER THAN OR EQUAL TO THE PREVIOUS TEMP. ***
MASS FLOW RATE = 1.40000E+02 G/S, TEMPERATURE = 2.43751E+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 13 ITERATIONS) IS GREATER THAN OR EQUAL TO THE PREVIOUS TEMP. ***
MASS FLOW RATE = 2.80000E+02 G/S, TEMPERATURE = 2.39895E+03 K, PREVIOUS TEMPERATURE = 2.35031E+03 K

(WSR) ** RESTART: MASS FLOW RATE = 5.60000E+02 G/S, TEMPERATURE = 2.35031E+03 K **

WELLSTIRRED REACTOR CALCULATION.... GLOBAL TEST CASE: CHANGE AND ADD GLOBAL AND MOLECULAR REACTIONS CASE 2

		INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE	ATM	5.50000	5.50000	1.00000
TEMP.	DEG K	800.000	2322.08	2.90260
ENTROPY	CAL/GM/K	1.80111	2.25758	1.25344
DENSITY	GM/CM**3	2.50173E-03	8.08713E-04	0.32326
ENTHALPY	CAL/GM	92.3468	92.3468	1.00000
SP. HEAT (CP)	CAL/GM/K	3.12948E-01	3.75502E-01	1.19989
MOL. WT. OF MIXT		29.8592	28.0169	
GAMMA		1.2701	1.2329	

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
O	0.00000E+00	0.00000E+00	6.87192E-04	3.92430E-04
H2O	0.00000E+00	0.00000E+00	1.43809E-01	9.24711E-02
OH	0.00000E+00	0.00000E+00	4.89021E-03	2.96854E-03
H	0.00000E+00	0.00000E+00	1.11930E-03	4.02695E-05
O2	1.97112E-01	2.11236E-01	1.18479E-02	1.35318E-02
H2	0.00000E+00	0.00000E+00	5.94161E-03	4.27496E-04
HO2	0.00000E+00	0.00000E+00	8.82955E-06	1.04021E-05
H2O2	0.00000E+00	0.00000E+00	4.21885E-07	5.12200E-07
CO	0.00000E+00	0.00000E+00	2.30038E-02	2.29985E-02
CO2	2.82264E-04	4.16032E-04	8.69366E-02	1.36563E-01
N2	7.34704E-01	6.89288E-01	6.87537E-01	6.87452E-01
NO	0.00000E+00	0.00000E+00	4.51698E-04	4.83769E-04
CN	0.00000E+00	0.00000E+00	3.22026E-03	2.99047E-03
CH2	0.00000E+00	0.00000E+00	6.69793E-03	3.35335E-03
C3H8	5.91335E-02	8.73286E-02	1.56204E-02	2.45852E-02
AR	8.76890E-03	1.17317E-02	8.22787E-03	1.17317E-02

VOLUME 500.000 CM**3 MASS FLO 560.000 GM/SEC

MDOT/VOLUME = 1.12000 RESIDENCE TIME = 0.722 MSEC ITERATIONS = 14

WELLSTIRRED REACTOR CALCULATION.... GLOBAL TEST CASE: CHANGE AND ADD GLOBAL AND MOLECULAR REACTIONS CASE 2

		INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE	ATM	5.50000	5.50000	1.00000
TEMP.	DEG K	800.000	1955.97	2.44496
ENTROPY	CAL/GM/K	1.80111	2.18426	1.21273
DENSITY	GM/CM**3	2.50173E-03	9.72001E-04	0.38853
ENTHALPY	CAL/GM	92.3468	92.3468	1.00000
SP. HEAT (CP)	CAL/GM/K	3.12948E-01	3.69334E-01	1.18018
MOL. WT. OF MIXT		29.8592	28.3646	
GAMMA		1.2701	1.2341	

TABLE A.3.—Concluded.

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
O	0.00000E+00	0.00000E+00	1.13807E-03	6.41940E-04
H2O	0.00000E+00	0.00000E+00	1.15773E-01	7.35311E-02
OH	0.00000E+00	0.00000E+00	3.95050E-03	2.36870E-03
H	0.00000E+00	0.00000E+00	4.24100E-04	1.50709E-05
O2	1.97112E-01	2.11236E-01	4.59855E-02	5.18773E-02
H2	0.00000E+00	0.00000E+00	1.20109E-03	8.53581E-05
HO2	0.00000E+00	0.00000E+00	3.05287E-05	3.55250E-05
H2O2	0.00000E+00	0.00000E+00	2.20101E-06	2.63944E-06
CO	0.00000E+00	0.00000E+00	7.41554E-03	7.32294E-03
CO2	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-02	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 CM**3 MASS FLO 1510.00 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

WELLSTIRRED REACTOR CALCULATION.... GLOBAL TEST CASE: CHANGE AND ADD GLOBAL AND MOLECULAR REACTIONS CASE 2

		INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE	ATM	5.50000	5.50000	1.00000
TEMP.	DEG K	800.000	1878.52	2.34815
ENTROPY	CAL/GM/K	1.80111	2.16364	1.20128
DENSITY	GM/CM**3	2.50173E-03	1.01711E-03	0.40656
ENTHALPY	CAL/GM	92.3468	92.3468	1.00000
SP. HEAT (CP)	CAL/GM/K	3.12948E-01	3.67837E-01	1.17539
MOL. WT. OF MIXT		29.8592	28.5056	
GAMMA		1.2701	1.2338	

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
O	0.00000E+00	0.00000E+00	1.18240E-03	6.63646E-04
H2O	0.00000E+00	0.00000E+00	1.07409E-01	6.78813E-02
OH	0.00000E+00	0.00000E+00	3.47916E-03	2.07577E-03
H	0.00000E+00	0.00000E+00	3.12397E-04	1.10465E-05
O2	1.97112E-01	2.11236E-01	5.66938E-02	6.36412E-02
H2	0.00000E+00	0.00000E+00	6.34489E-04	4.48684E-05
HO2	0.00000E+00	0.00000E+00	3.34605E-05	3.87439E-05
H2O2	0.00000E+00	0.00000E+00	2.93797E-06	3.50576E-06
CO	0.00000E+00	0.00000E+00	5.47125E-03	5.37620E-03
CO2	2.82264E-04	4.16032E-04	7.26205E-02	1.12119E-01
N2	7.34704E-01	6.89288E-01	7.00907E-01	6.88804E-01
NO	0.00000E+00	0.00000E+00	6.48177E-04	6.82296E-04
CN	0.00000E+00	0.00000E+00	3.35483E-04	3.06203E-04
CH2	0.00000E+00	0.00000E+00	1.72462E-02	8.48636E-03
C3H8	5.91335E-02	8.73286E-02	2.46516E-02	3.81342E-02
AR	8.76890E-03	1.17317E-02	8.37140E-03	1.17317E-02

VOLUME 500.000 CM**3 MASS FLO 1610.00 GM/SEC

MDOT/VOLUME = 3.22000 RESIDENCE TIME = 0.316 MSEC ITERATIONS = 4

(WSR) *** 75 ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREMENTS ***
MDOT = 1.66000E+03 G/S TEMPERATURE = 1.85438E+03 K
PSR SOLUTION ABANDONED

ITERATION NUMBER: 75 CURRENT TEMPERATURE = 1854.38 K CURRENT MDOT = 1.66000E+03 G/S

I	W(I)	TZ(I)
1	-0.16762E-02	-0.18179E-02
2	0.18781E-01	0.75625E-02
3	-0.25667E-02	-0.29014E-02
4	0.81832E-02	0.81588E-02
5	-0.14576E-01	-0.88945E-03
6	-0.10196E-01	-0.10227E-01
7	-0.25369E-04	-0.29400E-04

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

** DATA LINES **

```
             1         2         3         4         5         6         7         8
CC  12345678901234567890123456789012345678901234567890123456789012345678901234567890

    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      +   O2       =   OH      +   OH              1.7E+13   0.        47780.
       O       +   H2O2     =   OH      +   HO2             8.0E+13   0.        1000.
       END
                                 - BLANK LINE -
    TIME                                C3H8
     &PROB  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
```

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM   NASA LEWIS RESEARCH CENTER

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

REACTION NUMBER	REACTION	REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1*O + 1*H2O = 2*OH	6.80000E+13	0.0000	18365.00
2	1*H + 1*O2 = 1*OH + 1*O	1.89000E+14	0.0000	16400.00
3	1*O + 1*H2 = 1*OH + 1*H	4.20000E+14	0.0000	13750.00
4	1*H + 1*HO2 = 1*H2 + 1*O2	7.28000E+13	0.0000	2126.00
5	1*O + 1*HO2 = 1*OH + 1*O2	5.00000E+13	0.0000	1000.00
6	1*HO2 + 1*OH = 1*H2O + 1*O2	8.00000E+12	0.0000	0.00
7	1*H + 1*HO2 = 2*OH	1.34000E+14	0.0000	1070.00
8	1*H2 + 1*HO2 = 1*H2O2 + 1*H	7.91000E+13	0.0000	25000.00
9	1*OH + 1*H2O2 = 1*H2O + 1*HO2	6.10000E+12	0.0000	1430.00
10	2*HO2 = 1*H2O2 + 1*O2	1.80000E+12	0.0000	0.00
11	1*H + 1*H2O2 = 1*OH + 1*H2O	7.80000E+11	0.0000	0.00
12	M + 1*H2O2 = 2*OH	1.44000E+17	0.0000	45510.00
13	1*H2 + 1*OH = 1*H2O + 1*H	4.74000E+13	0.0000	6098.00
14	1*H + 1*O2 = 1*HO2 + M	1.46000E+15	0.0000	-1000.00
15	M + 1*H2O = 1*H + 1*OH	1.30000E+15	0.0000	105140.00
16	1*H + 1*O = 1*OH + M	7.10000E+18	-1.0000	0.00
17	M + 1*H2 = 2*H	2.20000E+14	0.0000	96000.00
18	M + 1*O2 = 2*O	1.80000E+18	-1.0000	118020.00
19	1*CO + 1*O > 1*CO2	8.43000E+09	-0.0010	1000.00
20	1*CO2 > 1*CO + 1*O	9.08000E+18	-1.8400	130754.00
21	1*H2 + 1*O2 = 2*OH	1.70000E+13	0.0000	47780.00
22	1*O + 1*H2O2 = 1*OH + 1*HO2	8.00000E+13	0.0000	1000.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2 , 12) = 2.50000	M(O2 , 12) = 0.78000	M(H2O , 12) = 6.00000	M(H2O2 , 12) = 6.60000
M(O2 , 14) = 1.30000	M(N2 , 14) = 1.30000	M(H2O , 14) = 21.30000	M(H2 , 14) = 3.00000
M(H2 , 15) = 4.00000	M(O2 , 15) = 1.50000	M(H2O , 15) = 20.00000	M(N2 , 15) = 1.50000
M(H2 ,.17) = 4.10000	M(O2 , 17) = 2.00000	M(H2O , 17) = 15.00000	M(N2 , 17) = 2.00000

*** GLOBAL REACTIONS ***

NUMBER	REACTION
23	1.0*H2O + 1.0*O > 1.0*H2 + 1.0*O2
24	1.0*CO + 1.0*H2O > 1.0*CO2 + 1.0*H2
25	1.0*CO2 + 1.0*H2 > 1.0*CO + 1.0*H2O
26	1.0*N2 + 1.0*O2 > 2.0*NO
27	2.0*NO > 1.0*N2 + 1.0*O2
28	1.0*CN + 2.0*O > 1.0*NO + 1.0*CO
29	1.0*CN + 1.0*NO > 1.0*CO + 1.0*N2
30	2.0*CH2 + 1.0*N2 > 2.0*CN + 2.0*H2
31	1.0*CH2 + 1.0*O2 > 1.0*CO + 1.0*H2O
32	1.0*O2 + 1.0*C3H8 > 3.0*CH2 + 2.0*OH
33	1.0*H2 + 1.0*O2 > 2.0*OH
34	1.0*C3H8 + 2.0*OH > 1.0*H2O + 1.0*C3H8 + 1.0*O
35	1.0*OH + 1.0*H2 + 1.0*O2 > 1.0*H2O + 1.0*O + 1.0*OH
36	1.0*H2O + 1.0*O > 1.0*H2 + 1.0*O2

REACTION NUMBER	REACTANT EXPONENTS REXP 1	REXP 2	REXP 3	REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
23	0.000	1.000	1.000	4.90000E+10	0.1800	-510.00
24	0.000	1.000	1.000	1.30000E+05	1.3100	-7000.00
25	0.000	1.000	1.000	4.41000E+10	0.1900	3527.00
26	0.000	1.000	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	5.00000E+13	0.0000	54000.00
31	0.000	1.000	0.500	3.50000E+07	0.0000	5000.00
32	0.000	1.600	0.100	1.10000E+12	0.0000	41000.00
33	0.000	1.000	1.000	1.00000E+00	0.0000	49080.00
34	0.000	0.150	1.000	1.98000E+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	4.90000E+10	0.1800	-510.00

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

TABLE A.4.—Continued.

** ASSIGNED VARIABLE PROFILE **

WELL - STIRRED REACTOR CASE

VOLUME OF REACTOR = 5.00000E+02 CM**3
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 0.00000E+00 CM

FLOW PROPERTIES		INTEGRATION INDICATORS	
PRESSURE (ATM)	5.50000	STEPS FROM LAST PRINT	0
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE	0.00000E+00
DENSITY (G/CM**3)	2.50173E-03	METHOD ORDER	0
TEMPERATURE (DEG K)	800.00		
MASS FLOW RATE (G/SEC)	4.50000E+02	TOTAL NUMBER OF STEPS	0
ENTROPY (CAL/G/DEG K)	1.8011	FUNCT EVALUATIONS	0
MACH NUMBER	0.0000	JACOBIAN EVALUATIONS	0
GAMMA	1.2701		
ENTHALPY (CAL/G)	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/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
O	0.00000E+00	0.00000E+00	3.57038E-26	1	6.5377E+08	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	0.00000E+00	2	6.2545E+09	0.00000E+00	0.00000
OH	0.00000E+00	0.00000E+00	9.11685E-08	3	7.3608E+10	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	0.00000E+00	4	1.9113E+13	0.00000E+00	0.00000
O2	1.65148E-05	1.97112E-01	-4.55842E-08	5	2.6655E+13	0.00000E+00	0.00000
H2	0.00000E+00	0.00000E+00	0.00000E+00	6	8.0000E+12	0.00000E+00	0.00000
HO2	0.00000E+00	0.00000E+00	0.00000E+00	7	6.8359E+13	0.00000E+00	0.00000
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	8	1.1708E+07	0.00000E+00	0.00000
CO	0.00000E+00	0.00000E+00	1.86163E-30	9	2.4813E+12	0.00000E+00	0.00000
CO2	2.36493E-08	2.82264E-04	-1.86163E-30	10	1.8000E+12	0.00000E+00	0.00000
N2	6.15566E-05	7.34704E-01	-2.38549E-22	11	7.8000E+11	0.00000E+00	0.00000
NO	0.00000E+00	0.00000E+00	4.77099E-22	12	5.3163E+04	0.00000E+00	0.00000
CN	0.00000E+00	0.00000E+00	0.00000E+00	13	1.0230E+12	0.00000E+00	0.00000
CH2	0.00000E+00	0.00000E+00	1.36753E-07	14	2.7387E+15	0.00000E+00	0.00000
C3H8	4.95445E-06	5.91335E-02	-4.55842E-08	15	2.4606E-14	0.00000E+00	0.00000
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
				19	4.4641E+09	0.00000E+00	0.00000
				20	7.8718E-23	2.97450E-25	1.00000
				21	1.5051E+00	0.00000E+00	0.00000
				22	4.2648E+13	0.00000E+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	0.00000E+00	0.00000
				29	1.2500E+12	0.00000E+00	0.00000
				30	8.8483E-02	0.00000E+00	0.00000
				31	1.5071E+06	0.00000E+00	0.00000
				32	6.9297E+00	7.28341E-03	1.00000
				33	3.9081E-14	0.00000E+00	0.00000
				34	1.5992E+05	0.00000E+00	0.00000
				35	2.6015E+11	0.00000E+00	0.00000
				36	2.2495E+11	0.00000E+00	0.00000

MIXTURE MOLECULAR WEIGHT 29.85916 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 3.39759E-16 MASS FRACTION SUM 1.00000000

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 0.00000E+00 CM

FLOW PROPERTIES	
PRESSURE (ATM)	5.50000
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	7.34828E-04
TEMPERATURE (DEG K)	2350.31
MASS FLOW RATE (G/SEC)	4.50000E+02
ENTROPY (CAL/G/DEG K)	2.3604
MACH NUMBER	0.0000
GAMMA	1.2641
ENTHALPY (CAL/G)	9.23468E+01
SP. HEAT (CP) (CAL/G/DEG K)	3.69088E-01

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

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
O	2.17893E-10	7.64039E-06	-2.50907E-04
H2O	4.05534E-06	1.42200E-01	8.69456E-03
OH	1.53281E-08	5.37479E-04	-3.22698E-04
H	3.72907E-08	1.30759E-03	2.13187E-07
O2	2.11927E-10	7.43118E-06	3.89433E-04
H2	1.73940E-06	6.09920E-02	-8.55659E-03
HO2	3.90703E-13	1.37000E-08	-1.12123E-07
H2O2	7.34828E-14	2.57667E-09	2.33325E-05
CO	3.10378E-06	1.08834E-01	8.94626E-03
CO2	1.26895E-06	4.44958E-02	-8.94626E-03
N2	1.80796E-05	6.33959E-01	-9.51429E-10
NO	2.64686E-09	9.28118E-05	8.94424E-10
CN	7.34828E-14	2.57667E-09	1.00844E-09
CH2	7.34828E-14	2.57667E-09	6.93592E-09
C3H8	7.34828E-14	2.57667E-09	-2.73787E-09
AR	2.15801E-07	7.56703E-03	0.00000E+00

REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
1	1.3329E+12	-7.60162E-04	0.00000
2	5.6424E+12	-2.68460E-05	0.00000
3	2.2114E+13	-6.59110E-04	0.00000
4	4.6178E+13	1.43082E-06	0.00000
5	4.0363E+13	7.03729E-09	0.00000
6	8.0000E+12	1.29043E-07	0.00000
7	1.0656E+14	2.24499E-06	0.00000
8	3.7453E+11	1.99374E-01	0.42297
9	4.4911E+12	-6.86707E-03	0.42297
10	1.8000E+12	2.15231E-07	0.42297
11	7.8000E+11	-2.90148E-03	0.42297
12	8.4429E+12	-4.30001E+01	0.42297
13	1.2845E+13	1.94110E-01	0.00000
14	1.8086E+15	3.66684E-06	0.00000
15	2.1738E+05	-5.10833E-04	0.00000
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	8.45730E+00	1.00000
20	3.9510E+00	9.28491E+00	1.00000
21	6.1305E+08	-1.53826E-07	0.00000
22	6.4581E+13	-1.40369E-03	0.42297
23	2.2102E+11	3.61677E+02	1.00000
24	1.5172E+10	3.53653E+05	1.00000
25	9.0570E+10	3.70220E+05	1.00000
26	2.5376E+05	1.80064E-03	1.00000
27	5.8546E+07	7.59605E-04	1.00000
28	8.3000E+11	2.46114E-05	1.00000
29	1.2500E+12	4.50252E-04	1.00000
30	4.7603E+08	1.17122E-03	1.00000
31	1.1999E+07	2.37704E-05	1.00000
32	1.6939E+08	5.07039E-03	1.00000
33	2.7300E-05	1.86371E-14	1.00000
34	8.4084E+05	2.55717E+02	1.00000
35	3.5560E+11	2.13927E+00	1.00000
36	2.2102E+11	3.61677E+02	1.00000

MIXTURE MOLECULAR WEIGHT 25.76666　　TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) -2.09583E+06　　MASS FRACTION SUM 1.00000010

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

INITIAL ESTIMATES (SIGMAS) AT TEMPERATURE = 2350.31 K:

O	2.96523E-07
H2O	5.51876E-03
OH	2.08595E-05
H	5.07475E-05
O2	2.88403E-07
H2	2.36709E-03
HO2	5.31693E-10
H2O2	1.00000E-10
CO	4.22382E-03
CO2	1.72687E-03
N2	2.46038E-02
NO	3.60201E-06
CN	1.00000E-10
CH2	1.00000E-10
C3H8	1.00000E-10
AR	2.93675E-04

TABLE A.4.—Continued.

(WSR) *** FOR CONV. NO. 1, CONVERGED TEMP. (AFTER 14 ITERATIONS) IS GREATER THAN OR EQUAL TO THE PREVIOUS TEMP. ***
MASS FLOW RATE = 4.50000E+02 G/S, TEMPERATURE = 2.35274E+03 K, PREVIOUS TEMPERATURE = 2.35031E+03 K

(WSR) ** RESTART: MASS FLOW RATE = 9.00000E+02 G/S, TEMPERATURE = 2.35031E+03 K **

WELLSTIRRED REACTOR CALCULATION....GLOBAL TEST CASE; ADD MOLECULAR REACTIONS TO PREV. CASE CASE 3

		INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE	ATM	5.50000	5.50000	1.00000
TEMP.	DEG K	800.000	2217.39	2.77173
ENTROPY	CAL/GM/K	1.80111	2.23959	1.24345
DENSITY	GM/CM**3	2.50173E-03	8.49004E-04	0.33937
ENTHALPY	CAL/GM	92.3468	92.3468	1.00000
SP. HEAT (CP)	CAL/GM/K	3.12948E-01	3.73920E-01	1.19483
MOL. WT. OF MIXT		29.8592	28.0866	
GAMMA		1.2701	1.2334	

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
O	0.00000E+00	0.00000E+00	8.92493E-04	5.08405E-04
H2O	0.00000E+00	0.00000E+00	1.37250E-01	8.80343E-02
OH	0.00000E+00	0.00000E+00	5.01543E-03	3.03700E-03
H	0.00000E+00	0.00000E+00	9.33721E-04	3.35094E-05
O2	1.97112E-01	2.11236E-01	1.93856E-02	2.20858E-02
H2	0.00000E+00	0.00000E+00	4.09560E-03	2.93945E-04
HO2	0.00000E+00	0.00000E+00	1.48347E-05	1.74334E-05
H2O2	0.00000E+00	0.00000E+00	7.46335E-07	9.03859E-07
CO	0.00000E+00	0.00000E+00	1.70515E-02	1.70052E-02
CO2	2.82264E-04	4.16032E-04	8.58796E-02	1.34568E-01
N2	7.34704E-01	6.89288E-01	6.89512E-01	6.87716E-01
NO	0.00000E+00	0.00000E+00	5.80529E-04	6.20204E-04
CN	0.00000E+00	0.00000E+00	2.57135E-03	2.38194E-03
CH2	0.00000E+00	0.00000E+00	1.20367E-02	6.01129E-03
C3H8	5.91335E-02	8.73286E-02	1.65318E-02	2.59551E-02
AR	8.76890E-03	1.17317E-02	8.24834E-03	1.17317E-02

VOLUME 500.000 CM**3 MASS FLO 900.000 GM/SEC

MDOT/VOLUME = 1.80000 RESIDENCE TIME = 0.472 MSEC ITERATIONS = 13

WELLSTIRRED REACTOR CALCULATION....GLOBAL TEST CASE; ADD MOLECULAR REACTIONS TO PREV. CASE CASE 3

		INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE	ATM	5.50000	5.50000	1.00000
TEMP.	DEG K	800.000	1991.29	2.48912
ENTROPY	CAL/GM/K	1.80111	2.19287	1.21751
DENSITY	GM/CM**3	2.50173E-03	9.52978E-04	0.38093
ENTHALPY	CAL/GM	92.3468	92.3468	1.00000
SP. HEAT (CP)	CAL/GM/K	3.12948E-01	3.69995E-01	1.18229
MOL. WT. OF MIXT		29.8592	28.3117	
GAMMA		1.2701	1.2341	

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
O	0.00000E+00	0.00000E+00	1.10597E-03	6.25001E-04
H2O	0.00000E+00	0.00000E+00	1.19266E-01	7.58908E-02
OH	0.00000E+00	0.00000E+00	4.13083E-03	2.48146E-03
H	0.00000E+00	0.00000E+00	4.74856E-04	1.69061E-05
O2	1.97112E-01	2.11236E-01	4.15614E-02	4.69740E-02
H2	0.00000E+00	0.00000E+00	1.47633E-03	1.05115E-04
HO2	0.00000E+00	0.00000E+00	2.92002E-05	3.40426E-05
H2O2	0.00000E+00	0.00000E+00	1.85824E-06	2.23256E-06
CO	0.00000E+00	0.00000E+00	8.30454E-03	8.21617E-03
CO2	2.82264E-04	4.16032E-04	7.88301E-02	1.22539E-01
N2	7.34704E-01	6.89288E-01	6.95879E-01	6.88548E-01
NO	0.00000E+00	0.00000E+00	6.75110E-04	7.15515E-04
CN	0.00000E+00	0.00000E+00	8.20074E-04	7.53627E-04
CH2	0.00000E+00	0.00000E+00	1.84359E-02	9.13391E-03
C3H8	5.91335E-02	8.73286E-02	2.06945E-02	3.22322E-02
AR	8.76890E-03	1.17317E-02	8.31444E-03	1.17317E-02

VOLUME 500.000 CM**3 MASS FLO 1450.00 GM/SEC

MDOT/VOLUME = 2.90000 RESIDENCE TIME = 0.329 MSEC ITERATIONS = 3

(WSR) CONV..NO. = 13 NO. ITERATIONS = 3
MASS FLOW RATE = 1.50000E+03 G/S TEMPERATURE = 1.96365E+03 K RESIDENCE TIME = 3.22616E-04 S

WELLSTIRRED REACTOR CALCULATION....GLOBAL TEST CASE; ADD MOLECULAR REACTIONS TO PREV. CASE CASE 3

		INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE	ATM	5.50000	5.50000	1.00000
TEMP.	DEG K	800.000	1932.21	2.41526
ENTROPY	CAL/GM/K	1.80111	2.17798	1.20924
DENSITY	GM/CM**3	2.50173E-03	9.85460E-04	0.39391
ENTHALPY	CAL/GM	92.3468	92.3468	1.00000
SP. HEAT (CP)	CAL/GM/K	3.12948E-01	3.68893E-01	1.17877
MOL. WT. OF MIXT		29.8592	28.4080	
GAMMA		1.2701	1.2340	

TABLE A.4.—Concluded.

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
O	0.00000E+00	0.00000E+00	1.14023E-03	6.42178E-04
H2O	0.00000E+00	0.00000E+00	1.13272E-01	7.18329E-02
OH	0.00000E+00	0.00000E+00	3.78670E-03	2.26702E-03
H	0.00000E+00	0.00000E+00	3.78780E-04	1.34370E-05
O2	1.97112E-01	2.11236E-01	4.91890E-02	5.54067E-02
H2	0.00000E+00	0.00000E+00	9.93964E-04	7.05307E-05
HO2	0.00000E+00	0.00000E+00	3.23518E-05	3.75890E-05
H2O2	0.00000E+00	0.00000E+00	2.28914E-06	2.74093E-06
CO	0.00000E+00	0.00000E+00	6.65623E-03	6.56308E-03
CO2	2.82264E-04	4.16032E-04	7.58156E-02	1.17454E-01
N2	7.34704E-01	6.89288E-01	6.98398E-01	6.88698E-01
NO	0.00000E+00	0.00000E+00	6.66088E-04	7.03560E-04
CN	0.00000E+00	0.00000E+00	5.29466E-04	4.84917E-04
CH2	0.00000E+00	0.00000E+00	1.81714E-02	8.97238E-03
C3H8	5.91335E-02	8.73286E-02	2.26247E-02	3.51192E-02
AR	8.76890E-03	1.17317E-02	8.34272E-03	1.17317E-02

```
VOLUME      500.000        CM**3         MASS FLO    1550.00       GM/SEC
  MDOT/VOLUME =      3.10000    RESIDENCE TIME =          0.318  MSEC    ITERATIONS =   3


(WSR)     CONV.. NO. =  15      NO. ITERATIONS =   4
          MASS FLOW RATE =  1.60000E+03 G/S      TEMPERATURE =  1.89288E+03 K      RESIDENCE TIME =  3.15163E-04 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           W(I)          TZ(I)

                                1        -0.36271E-02    -0.37634E-02
```

TABLE A.5.—COMPUTED RESULTS FOR TEST CASE 4 (PROPANE-HYDROGEN-AIR, CONSTANT-VOLUME COMBUSTION WITH MECHANISM OF CASE 3)

** DATA LINES **

```
                1         2         3         4         5         6         7         8
CC  12345678901234567890123456789012345678901234567890123456789012345678901234567890

    GLOBAL TEST CASE; INTEGRATION CASE WITH PREVIOUS MECHANISM;     CASE 4
    REPEAT
     &rtype 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,      welstr = .false.,  &end
     &start t= 1600., p=5.5,    &end
    H2          .0573205
    N2          .720502
    CO2         .0002768
    O2          .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 NUMBER	REACTION								REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1*O	+	1*H2O	=	2*OH				6.80000E+13	0.0000	18365.00
2	1*H	+	1*O2	=	1*OH	+	1*O		1.89000E+14	0.0000	16400.00
3	1*O	+	1*H2	=	1*OH	+	1*H		4.20000E+14	0.0000	13750.00
4	1*H	+	1*HO2	=	1*H2	+	1*O2		7.28000E+13	0.0000	2126.00
5	1*O	+	1*HO2	=	1*OH	+	1*O2		5.00000E+13	0.0000	1000.00
6	1*HO2	+	1*OH	=	1*H2O	+	1*O2		8.00000E+12	0.0000	0.00
7	1*H	+	1*HO2	=	2*OH				1.34000E+14	0.0000	1070.00
8	1*H2	+	1*HO2	=	1*H2O2	+	1*H		7.91000E+13	0.0000	25000.00
9	1*OH	+	1*H2O2	=	1*H2O	+	1*HO2		6.10000E+12	0.0000	1430.00
10			2*HO2	=	1*H2O2	+	1*O2		1.80000E+12	0.0000	0.00
11	1*H	+	1*H2O2	=	1*OH	+	1*H2O		7.80000E+11	0.0000	0.00
12	M	+	1*H2O2	=	2*OH				1.44000E+17	0.0000	45510.00
13	1*H2	+	1*OH	=	1*H2O	+	1*H		4.74000E+13	0.0000	6098.00
14	1*H	+	1*O2	=	1*HO2	+	M		1.46000E+15	0.0000	-1000.00
15	M	+	1*H2O	=	1*H	+	1*OH		1.30000E+15	0.0000	105140.00
16	1*H	+	1*O	=	1*OH	+	M		7.10000E+18	-1.0000	0.00
17	M	+	1*H2	=	2*H				2.20000E+14	0.0000	96000.00
18	M	+	1*O2	=	2*O				1.80000E+18	-1.0000	118020.00
19	1*CO	+	1*O	>	1*CO2				8.43000E+09	-0.0010	1000.00
20			1*CO2	>	1*CO	+	1*O		9.08000E+18	-1.8400	130754.00
21	1*H2	+	1*O2	=	2*OH				1.70000E+13	0.0000	47780.00
22	1*O	+	1*H2O2	=	1*OH	+	1*HO2		8.00000E+13	0.0000	1000.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

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

*** GLOBAL REACTIONS ***

NUMBER	REACTION										
23			1.0*H2O	+	1.0*O	>	1.0*H2	+	1.0*O2		
24			1.0*CO	+	1.0*H2O	>	1.0*CO2	+	1.0*H2		
25			1.0*CO2	+	1.0*H2	>	1.0*CO	+	1.0*H2O		
26			1.0*N2	+	1.0*O2	>	2.0*NO				
27					2.0*NO	>	1.0*N2	+	1.0*O2		
28			1.0*CN	+	2.0*O	>	1.0*NO	+	1.0*CO		
29			1.0*CN	+	1.0*NO	>	1.0*CO	+	1.0*N2		
30			2.0*CH2	+	1.0*N2	>	2.0*CN	+	2.0*H2		
31			1.0*CH2	+	1.0*O2	>	1.0*CO	+	1.0*H2O		
32			1.0*O2	+	1.0*C3H8	>	3.0*CH2	+	2.0*OH		
33			1.0*H2	+	1.0*O2	>	2.0*OH				
34			1.0*C3H8	+	2.0*OH	>	1.0*H2O	+	1.0*C3H8	+	1.0*O
35	1.0*OH	+	1.0*H2	+	1.0*O2	>	1.0*H2O	+	1.0*O	+	1.0*OH
36			1.0*H2O	+	1.0*O	>	1.0*H2	+	1.0*O2		

REACTION NUMBER	REACTANT EXPONENTS REXP 1	REXP 2	REXP 3	REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
23	0.000	1.000	1.000	4.90000E+10	0.1800	-510.00
24	0.000	1.000	1.000	1.30000E+05	1.3100	-7000.00
25	0.000	1.000	1.000	4.41000E+10	0.1900	3527.00
26	0.000	1.000	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	5.00000E+13	0.0000	54000.00
31	0.000	1.000	0.500	3.50000E+07	0.0000	5000.00
32	0.000	1.600	0.100	1.10000E+12	0.0000	41000.00
33	0.000	1.000	1.000	1.00000E+00	0.0000	49080.00
34	0.000	0.150	1.000	1.98000E+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	4.90000E+10	0.1800	-510.00

TABLE A.5.—Continued.

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

** ASSIGNED VARIABLE PROFILE **

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

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 **

STATION	TIME (SEC)
1	1.00000E-06
2	2.00000E-06
3	3.00000E-06
4	3.50000E-06
5	4.00000E-06
6	5.00000E-06

** INITIAL CONDITIONS **

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

FLOW PROPERTIES		INTEGRATION INDICATORS	
PRESSURE (ATM)	5.50000	STEPS FROM LAST PRINT	0
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE	0.00000E+00
DENSITY (G/CM**3)	1.16135E-03	METHOD ORDER	0
TEMPERATURE (DEG K)	1600.00		
MASS FLOW RATE (G/SEC)	0.00000E+00	TOTAL NUMBER OF STEPS	0
ENTROPY (CAL/G/DEG K)	2.0791	FUNCT EVALUATIONS	0
MACH NUMBER	0.0000	JACOBIAN EVALUATIONS	0
GAMMA	1.2740		
ENTHALPY (CAL/G)	3.72713E+02		
SP. HEAT (CP) (CAL/G/DEG K)	3.33274E-01		

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
O	0.00000E+00	0.00000E+00	-9.83591E-05	1	2.1085E+11	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	1.54676E-03	2	1.0872E+12	0.00000E+00	0.00000
OH	0.00000E+00	0.00000E+00	9.91942E-03	3	5.5602E+12	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	1.31087E-04	4	3.7302E+13	-9.71879E+01	1.00000
O2	8.09779E-06	1.93301E-01	-4.99243E-03	5	3.6507E+13	0.00000E+00	0.00000
H2	2.40128E-06	5.73205E-02	-1.77620E-03	6	8.0000E+12	0.00000E+00	0.00000
HO2	0.00000E+00	0.00000E+00	1.31080E-04	7	9.5708E+13	0.00000E+00	0.00000
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	8	3.0432E+10	0.00000E+00	0.00000
CO	0.00000E+00	0.00000E+00	1.64512E-03	9	3.8905E+12	0.00000E+00	0.00000
CO2	1.15957E-08	2.76800E-04	-1.64512E-03	10	1.8000E+12	0.00000E+00	0.00000
N2	3.01834E-05	7.20502E-01	-2.67274E-09	11	7.8000E+11	0.00000E+00	0.00000
NO	0.00000E+00	0.00000E+00	5.34547E-09	12	8.7496E+10	0.00000E+00	0.00000
CN	0.00000E+00	0.00000E+00	0.00000E+00	13	6.9635E+12	0.00000E+00	0.00000
CH2	0.00000E+00	0.00000E+00	1.45841E-02	14	1.9996E+15	0.00000E+00	0.00000
C3H8	8.37842E-07	2.00000E-02	-4.86135E-03	15	5.6558E+00	0.00000E+00	0.00000
AR	3.60260E-07	8.59970E-03	0.00000E+00	16	4.4375E+15	0.00000E+00	0.00000
				17	1.6960E+01	2.64572E-03	1.00000
				18	8.5187E-02	2.14264E-05	1.00000
				19	6.1098E+09	0.00000E+00	0.00000
				20	1.5935E-05	1.36999E-07	1.00000
				21	5.0583E+06	7.29275E+01	1.00000
				22	5.8411E+13	0.00000E+00	0.00000
				23	2.1707E+11	0.00000E+00	0.00000
				24	1.8514E+10	0.00000E+00	0.00000
				25	5.9082E+10	1.21976E+03	1.00000

TABLE A.5.—Continued.

26	1.0935E+01	1.98168E-03	1.00000
27	1.2897E+06	0.00000E+00	0.00000
28	8.3000E+11	0.00000E+00	0.00000
29	1.2500E+12	0.00000E+00	0.00000
30	2.1034E+06	0.00000E+00	0.00000
31	7.2627E+06	0.00000E+00	0.00000
32	2.7609E+06	3.60441E+03	1.00000
33	1.9769E-07	2.85017E-12	1.00000
34	5.6272E+05	0.00000E+00	0.00000
35	3.3380E+11	0.00000E+00	0.00000
36	2.1707E+11	0.00000E+00	0.00000

DERIVATIVES (CGS UNITS): T -5.04396E+06 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 27.72230 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 5.11257E+06 MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 0.833333 S

TIME 1.00000E-06 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES		INTEGRATION INDICATORS	
PRESSURE (ATM)	5.58525	STEPS FROM LAST PRINT	107
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE	0.94404E-08
DENSITY (G/CM**3)	1.16135E-03	METHOD ORDER	5
TEMPERATURE (DEG K)	1627.92		
MASS FLOW RATE (G/SEC)	0.00000E+00	TOTAL NUMBER OF STEPS	107
ENTROPY (CAL/G/DEG K)	2.0928	FUNCT EVALUATIONS	128
MACH NUMBER	0.0000	JACOBIAN EVALUATIONS	13
GAMMA	1.2726		
ENTHALPY (CAL/G)	3.74490E+02		
SP. HEAT (CP) (CAL/G/DEG K)	3.33980E-01		

CHEMICAL PROPERTIES

PECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
O	3.19217E-07	7.63461E-03	1.53419E+00	1	2.3280E+11	-2.67982E+05	0.84410
H2O	8.98284E-07	2.14840E-02	3.60541E+00	2	1.1878E+12	1.63230E+06	0.63751
OH	3.16661E-07	7.57348E-03	1.02544E+00	3	5.9882E+12	1.17971E+06	0.72556
H	3.96981E-07	9.49446E-03	1.00269E+00	4	3.7732E+13	7.31763E+04	0.99923
O2	7.32362E-06	1.75156E-01	-3.09190E+00	5	3.6704E+13	5.72712E+04	0.99979
H2	1.14721E-06	2.74374E-02	-4.61715E+00	6	8.0000E+12	1.23849E+04	0.99997
HO2	6.59396E-09	1.57705E-04	1.37949E-03	7	9.6262E+13	1.86817E+05	0.99992
H2O2	6.23618E-10	1.49149E-05	2.43739E-03	8	3.4826E+10	-6.22012E+03	0.96955
CO	5.46803E-10	1.30777E-05	-1.05386E-02	9	3.9206E+12	5.73291E+02	0.99870
CO2	1.11953E-08	2.67755E-04	1.08272E-02	10	1.8000E+12	5.65545E+01	0.97460
N2	3.01834E-05	7.21885E-01	-1.21742E-06	11	7.8000E+11	1.43173E+02	1.00000
NO	3.49233E-14	8.35247E-10	2.54611E-07	12	1.1184E+11	-1.72828E+04	0.87858
CN	9.29669E-13	2.22346E-08	2.18022E-06	13	7.1964E+12	1.85540E+06	0.95721
CH2	1.42817E-08	3.41571E-04	1.51918E-02	14	1.9889E+15	3.15396E+05	0.99963
C3H8	8.33033E-07	1.99234E-02	-5.16088E-03	15	9.9719E+00	-4.42463E+04	1.00000
AR	3.60260E-07	8.61621E-03	0.00000E+00	16	4.3614E+15	1.71340E+04	1.00000
				17	2.8465E+01	-8.12522E+03	1.00000
				18	1.5824E-01	-1.66840E+02	1.00000
				19	6.1428E+09	7.94984E-01	1.00000
				20	3.1247E-05	2.59373E-07	1.00000
				21	6.5453E+06	3.67170E+01	0.90052
				22	5.8727E+13	8.59561E+03	0.99164
				23	2.1715E+11	4.61673E+04	1.00000
				24	1.8236E+10	6.64142E+00	1.00000
				25	6.0415E+10	5.75309E+02	1.00000
				26	1.8763E+01	3.07515E-03	1.00000
				27	1.5830E+06	1.43151E-15	1.00000
				28	8.3000E+11	1.82629E-01	1.00000
				29	1.2500E+12	3.00905E-08	1.00000
				30	2.8146E+06	8.99568E-01	1.00000
				31	7.4613E+06	2.13812E+02	1.00000
				32	3.4443E+06	3.82649E+03	1.00000
				33	2.5761E-07	1.60472E-12	1.00000
				34	5.7499E+05	1.65361E+04	1.00000
				35	3.3505E+11	5.76115E+05	1.00000
				36	2.1715E+11	4.61673E+04	1.00000

DERIVATIVES (CGS UNITS): T 1.87387E+08 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 27.77552 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) -4.19411E+10 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

TABLE A.5.—Continued.

TIME 3.50000E-06 SEC   AREA 0.00000E+00 SQ CM   AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES		INTEGRATION INDICATORS	
PRESSURE (ATM)	6.37810	STEPS FROM LAST PRINT	5
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE	0.10023E-06
DENSITY (G/CM**3)	1.16135E-03	METHOD ORDER	5
TEMPERATURE (DEG K)	1889.71		
MASS FLOW RATE (G/SEC)	0.00000E+00	TOTAL NUMBER OF STEPS	206
ENTROPY (CAL/G/DEG K)	2.1179	FUNCT EVALUATIONS	248
MACH NUMBER	0.0000	JACOBIAN EVALUATIONS	25
GAMMA	1.2609		
ENTHALPY (CAL/G)	3.91023E+02		
SP. HEAT (CP) (CAL/G/DEG K)	3.40096E-01		

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
O	4.16265E-07	1.01201E-02	-1.01451E-01	1	5.1115E+11	7.40454E+04	0.20840
H2O	2.25224E-06	5.47555E-02	8.82441E-02	2	2.3975E+12	-2.30157E+05	0.20324
OH	2.88228E-07	7.00729E-03	-3.38176E-02	3	1.0790E+13	-8.06954E+04	0.61815
H	7.69813E-08	1.87154E-03	-3.78435E-02	4	4.1329E+13	8.36789E+03	0.99914
O2	6.59377E-06	1.60305E-01	1.86437E-02	5	3.8310E+13	4.18851E+04	0.99775
H2	1.49682E-08	3.63900E-04	-2.34895E-02	6	8.0000E+12	6.05258E+03	0.99716
HO2	3.55038E-09	8.63153E-05	-5.47249E-04	7	1.0078E+14	2.03640E+04	0.99717
H2O2	3.08885E-10	7.50948E-06	-6.48815E-05	8	1.0159E+11	-7.48349E+02	0.99468
CO	-3.59652E-08	-8.74372E-04	-4.33519E-03	9	4.1682E+12	2.70299E+02	0.98240
CO2	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
NO	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	1.36053E-07	3.30766E-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	0.99997
AR	3.60260E-07	8.75849E-03	0.00000E+00	16	3.7572E+15	3.67174E+03	0.99998
				17	1.7368E+03	-2.43455E+02	0.99999
				18	2.1357E+01	-2.37434E+02	0.99998
				19	6.4106E+09	-7.11586E+01	1.00000
				20	6.4189E-03	2.44378E-04	1.00000
				21	5.0648E+07	-8.47581E+00	0.69576
				22	6.1297E+13	5.76218E+03	0.98607
				23	2.1824E+11	1.51702E+05	1.00000
				24	1.6428E+10	0.00000E+00	0.00000
				25	7.2285E+10	4.11927E+01	1.00000
				26	1.3648E+03	2.01396E-01	1.00000
				27	8.0580E+06	1.19576E-08	1.00000
				28	8.3000E+11	4.13550E+01	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+04	1.00000
				35	3.4473E+11	4.85761E+05	1.00000
				36	2.1824E+11	1.51702E+05	1.00000

DERIVATIVES (CGS UNITS): T 2.23588E+07 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 28.23417   TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) -1.04075E+10   MASS FRACTION SUM 1.00000002

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 (ATM)	6.42873	STEPS FROM LAST PRINT	32
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE	0.30449E-07
DENSITY (G/CM**3)	1.16135E-03	METHOD ORDER	4
TEMPERATURE (DEG K)	1905.03		
MASS FLOW RATE (G/SEC)	0.00000E+00	TOTAL NUMBER OF STEPS	243
ENTROPY (CAL/G/DEG K)	2.1205	FUNCT EVALUATIONS	305
MACH NUMBER	0.0000	JACOBIAN EVALUATIONS	37
GAMMA	1.2608		
ENTHALPY (CAL/G)	3.92079E+02		
SP. HEAT (CP) (CAL/G/DEG K)	3.40164E-01		

TABLE A.5.—Concluded.

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
O	3.08932E-07	7.51191E-03	-4.98532E-02	1	5.3165E+11	8.05900E+04	0.28005
H2O	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	4	4.1518E+13	3.76540E+03	0.99856
O2	6.60548E-06	1.60617E-01	-8.75174E-04	5	3.8393E+13	2.54683E+04	0.99645
H2	-9.99808E-09	-2.43110E-04	-1.17148E-02	6	8.0000E+12	4.23605E+03	0.99506
HO2	2.90641E-09	7.06716E-05	-3.34401E-04	7	1.0101E+14	9.10169E+03	0.99499
H2O2	2.39983E-10	5.83537E-06	-3.12076E-05	8	1.0718E+11	-3.24528E+02	0.99283
CO	-3.75646E-08	-9.13411E-04	1.70741E-03	9	4.1810E+12	1.79205E+02	0.97551
CO2	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	9.4667E+12	-7.65536E+04	0.70740
CH2	2.48428E-07	6.04071E-03	7.56509E-02	14	1.9014E+15	3.85206E+04	0.98317
C3H8	7.51243E-07	1.82670E-02	-2.73648E-02	15	1.1272E+03	-2.48217E+03	0.99992
AR	3.60260E-07	8.75997E-03	0.00000E+00	16	3.7270E+15	1.47538E+03	0.99994
				17	2.1333E+03	-7.22141E+01	0.99998
				18	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	2.1832E+11	1.18169E+05	1.00000
				24	1.6356E+10	0.00000E+00	0.00000
				25	7.2945E+10	0.00000E+00	0.00000
				26	1.6912E+03	2.50003E-01	1.00000
				27	8.7412E+06	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
				33	2.3411E-06	0.00000E+00	0.00000
				34	6.8830E+05	1.51986E+04	1.00000
				35	3.4520E+11	4.17478E+05	1.00000
				36	2.1832E+11	1.18169E+05	1.00000

DERIVATIVES (CGS UNITS): T 2.08524E+06 RHO 0.00000E+00

MIXTURE MOLECULAR WEIGHT 28.23896 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) -5.92238E+09 MASS FRACTION SUM 1.00000001

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 - 2.133333 S

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

(LSENS) READ DATA FOR NEXT CASE

TABLE A.6.—COMPUTED RESULTS FOR TEST CASE 5 (PROPANE-AIR PSR PROBLEM USING ALL-GLOBAL REACTIONS)

```
                                   **  DATA LINES  **

              1         2         3         4         5         6         7         8
 CC  12345678901234567890123456789012345678901234567890123456789012345678901234567890

      GLOBAL CODE TEST CASE: ALL GLOBAL REACTIONS; NEW CASE      CASE 5
     NEW
      &rtype  global=.true.,gronly=.true., &end
                    H2O      +    O         >      H2        +    O2
                 1.         1.       4.90E+10   .18       -510.
                    CO       +    H2O       >      CO2       +    H2
                  1.         1.       1.30E+05   1.31      -7000.
                    CO2      +    H2        >      CO        +    H2O
                  1.         1.       4.41E+10   .19       3527.
                    N2       +    O2        >2.0 NO
                  1.         1.       3.00E+14   .03     100000.
                          2.0 NO        >      N2        +    O2
                           2.         2.00E+11   0.       38000.
                    CN       +2.0 O         >      NO        +    CO
                  1.        1.        8.30E+11   0.           0.
                    CN       +    NO        >      CO        +    N2
                  1.        1.        1.25E+12   0.           0.
                  2.0 CH2    +    N2        >2.0 CN       +2.0 H2
                  1.     1.         5.00E+13   0.       54000.
                    CH2      +    O2        >      CO        +    H2O
                  1.      .5         3.50E+07   0.       5000.
                    O2       +    C3H8      >3.0 CH2      +2.0 OH
                  1.6     .1         1.10E+12   0.       41000.
                    H2       +    O2        >2.0 OH
                  1.     1.         1.00E+00   0.       49080.
                    C3H8     +2.0 OH        >      H2O       +    C3H8     +    O
                   .15   1.         1.98E+06   0.       4000.
        OH        +    H2       +    O2        >      H2O       +    O        +    OH
       1.         0.     1.         0.96E+12   -.1      1013.
                                       -  BLANK LINE  -
     AR
     TIME                                          C3H8
      &prob  welstr=.true.,               &end
      &wsprob       delmd=  10., dotmax= 1600.,    mpr=1, volume= 200., &end
      &start t= 800.,p=5.5,mdot=  100.,  &end
     O2           .193301
     N2           .720502
     C3H8         .0773205
     AR           .0088765
     END
     FINIS
```

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM   NASA LEWIS RESEARCH CENTER

GLOBAL CODE TEST CASE: ALL GLOBAL REACTIONS; NEW CASE   CASE 5

*** GLOBAL REACTIONS ***

NUMBER	REACTION										
1			1.0*H2O	+	1.0*O	>	1.0*H2	+	1.0*O2		
2			1.0*CO	+	1.0*H2O	>	1.0*CO2	+	1.0*H2		
3			1.0*CO2	+	1.0*H2	>	1.0*CO	+	1.0*H2O		
4			1.0*N2	+	1.0*O2	>	2.0*NO				
5					2.0*NO	>	1.0*N2	+	1.0*O2		
6			1.0*CN	+	2.0*O	>	1.0*NO	+	1.0*CO		
7			1.0*CN	+	1.0*NO	>	1.0*CO	+	1.0*N2		
8			2.0*CH2	+	1.0*N2	>	2.0*CN	+	2.0*H2		
9			1.0*CH2	+	1.0*O2	>	1.0*CO	+	1.0*H2O		
10			1.0*O2	+	1.0*C3H8	>	3.0*CH2	+	2.0*OH		
11			1.0*H2	+	1.0*O2	>	2.0*OH				
12			1.0*C3H8	+	2.0*OH	>	1.0*H2O	+	1.0*C3H8	+	1.0*O
13	1.0*OH	+	1.0*H2	+	1.0*O2	>	1.0*H2O	+	1.0*O	+	1.0*OH

REACTION NUMBER	REACTANT EXPONENTS REXP 1	REXP 2	REXP 3	REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	0.000	1.000	1.000	4.90000E+10	0.1800	-510.00
2	0.000	1.000	1.000	1.30000E+05	1.3100	-7000.00
3	0.000	1.000	1.000	4.41000E+10	0.1900	3527.00
4	0.000	1.000	1.000	3.00000E+14	0.0300	100000.00
5	0.000	0.000	2.000	2.00000E+11	0.0000	38000.00
6	0.000	1.000	1.000	8.30000E+11	0.0000	0.00
7	0.000	1.000	1.000	1.25000E+12	0.0000	0.00
8	0.000	1.000	1.000	5.00000E+13	0.0000	54000.00
9	0.000	1.000	0.500	3.50000E+07	0.0000	5000.00
10	0.000	1.600	0.100	1.10000E+12	0.0000	41000.00
11	0.000	1.000	1.000	1.00000E+00	0.0000	49080.00
12	0.000	0.150	1.000	1.98000E+06	0.0000	4000.00
13	1.000	0.000	1.000	9.60000E+11	-0.1000	1013.00

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

** ASSIGNED VARIABLE PROFILE **

WELL - STIRRED REACTOR CASE

VOLUME OF REACTOR = 2.00000E+02 CM**3
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 0.00000E+00 SEC   AREA 0.00000E+00 SQ CM   AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES		INTEGRATION INDICATORS	
PRESSURE (ATM)	5.50000	STEPS FROM LAST PRINT	0
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE	0.00000E+00
DENSITY (G/CM**3)	2.52469E-03	METHOD ORDER	0
TEMPERATURE (DEG K)	800.00		
MASS FLOW RATE (G/SEC)	1.00000E+02	TOTAL NUMBER OF STEPS	0
ENTROPY (CAL/G/DEG K)	1.8096	FUNCT EVALUATIONS	0
MACH NUMBER	0.0000	JACOBIAN EVALUATIONS	0
GAMMA	1.2519		
ENTHALPY (CAL/G)	8.37665E+01		
SP. HEAT (CP) (CAL/G/DEG K)	3.27783E-01		

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
H2O	0.00000E+00	0.00000E+00	0.00000E+00	1	2.2495E+11	0.00000E+00	0.00000
O	0.00000E+00	0.00000E+00	0.00000E+00	2	6.7500E+10	0.00000E+00	0.00000
H2	0.00000E+00	0.00000E+00	0.00000E+00	3	1.7080E+10	0.00000E+00	0.00000
O2	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	0.00000E+00	5	8.3160E+00	0.00000E+00	0.00000
CO2	0.00000E+00	0.00000E+00	0.00000E+00	6	8.3000E+11	0.00000E+00	0.00000
N2	6.03667E-05	7.20502E-01	-1.72062E-22	7	1.2500E+12	0.00000E+00	0.00000
NO	0.00000E+00	0.00000E+00	3.44124E-22	8	8.8483E-02	0.00000E+00	0.00000
CN	0.00000E+00	0.00000E+00	0.00000E+00	9	1.5071E+06	0.00000E+00	0.00000
CH2	0.00000E+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
OH	0.00000E+00	0.00000E+00	9.07666E-08	12	1.5992E+05	0.00000E+00	0.00000
AR	7.43711E-07	8.87650E-03	0.00000E+00	13	2.6015E+11	0.00000E+00	0.00000

MIXTURE MOLECULAR WEIGHT 30.13325   TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 0.00000E+00   MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 0.500000 S

**EQUILIBRIUM CONDITIONS **

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

FLOW PROPERTIES		INTEGRATION INDICATORS	
PRESSURE (ATM)	5.50000	STEPS FROM LAST PRINT	0
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE	0.00000E+00
DENSITY (G/CM**3)	7.86509E-04	METHOD ORDER	0
TEMPERATURE (DEG K)	2021.03		
MASS FLOW RATE (G/SEC)	1.00000E+02	TOTAL NUMBER OF STEPS	0
ENTROPY (CAL/G/DEG K)	2.4443	FUNCT EVALUATIONS	0
MACH NUMBER	0.0000	JACOBIAN EVALUATIONS	0
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/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
H2O	3.26171E-06	9.83480E-02	1.59430E-02	1	2.1895E+11	1.23633E+00	1.00000
O	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
O2	7.86509E-14	2.37151E-09	7.64769E-07	4	5.7878E+03	1.38388E-08	1.00000
CO	5.28064E-06	1.59223E-01	1.59381E-02	5	1.5552E+07	5.88118E-08	1.00000
CO2	7.73802E-07	2.33319E-02	-1.59381E-02	6	8.3000E+11	1.13011E-07	1.00000
N2	1.88058E-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	7.86509E-14	2.37151E-09	-2.14286E-10	10	4.0527E+07	3.45965E-09	1.00000
C3H8	7.86509E-14	2.37151E-09	-2.14013E-15	11	4.9272E-06	3.01360E-18	1.00000
OH	7.22352E-10	2.17806E-05	-1.14353E-05	12	7.3133E+05	9.24295E+00	1.00000
AR	2.31686E-07	6.98587E-03	0.00000E+00	13	3.4847E+11	3.20048E-05	1.00000

MIXTURE MOLECULAR WEIGHT 23.71507 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC) 0.00000E+00 MASS FRACTION SUM 1.00000009

COMPUTATIONAL WORK REQUIRED FOR EQUILIBRIUM CALCULATION:
NO. OF ITERATIONS = 12 CPU TIME = 1.666737E-02 S
INITIAL ESTIMATES (SIGMAS) AT TEMPERATURE = 2021.03 K:

H2O	4.14707E-03
O	1.36158E-09
H2	6.11629E-03
O2	1.00000E-10
CO	6.71402E-03
CO2	9.83843E-04
N2	2.39105E-02
NO	6.14944E-08
CN	1.00000E-10
CH2	1.00000E-10
C3H8	1.00000E-10
OH	9.18427E-07
AR	2.94575E-04

WELLSTIRRED REACTOR CALCULATION.... GLOBAL CODE TEST CASE: ALL GLOBAL REACTIONS; NEW CASE CASE 5

		INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE	ATM	5.50000	5.50000	1.00000
TEMP.	DEG K	800.000	1866.72	2.33340
ENTROPY	CAL/GM/K	1.80955	2.32614	1.28548
DENSITY	GM/CM**3	2.52469E-03	9.22862E-04	0.36553
ENTHALPY	CAL/GM	83.7665	83.7665	1.00000
SP. HEAT (CP)	CAL/GM/K	3.27783E-01	3.82394E-01	1.16661
MOL. WT. OF MIXT		30.1332	25.7019	
GAMMA		1.2519	1.2534	

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
H2O	0.00000E+00	0.00000E+00	1.06379E-01	7.45646E-02
O	0.00000E+00	0.00000E+00	1.52775E-04	9.51022E-05
H2	0.00000E+00	0.00000E+00	8.14109E-02	6.38507E-03
O2	1.93301E-01	2.05268E-01	2.62297E-02	3.26560E-02
CO	0.00000E+00	0.00000E+00	1.06128E-01	1.15661E-01
CO2	0.00000E+00	0.00000E+00	3.20966E-02	5.49597E-02
N2	7.20502E-01	6.69815E-01	6.14077E-01	6.69305E-01
NO	0.00000E+00	0.00000E+00	1.00021E-04	1.16771E-04
CN	0.00000E+00	0.00000E+00	8.36062E-04	8.46336E-04
CH2	0.00000E+00	0.00000E+00	7.63022E-03	4.16420E-03
C3H8	7.73205E-02	1.13149E-01	1.70527E-02	2.92570E-02
OH	0.00000E+00	0.00000E+00	3.35137E-04	2.21765E-04
AR	8.87650E-03	1.17677E-02	7.57112E-03	1.17677E-02

VOLUME 200.000 CM**3 MASS FLO 100.000 GM/SEC

MDOT/VOLUME = 0.50000 RESIDENCE TIME = 1.846 MSEC ITERATIONS = 16
WELLSTIRRED REACTOR CALCULATION.... GLOBAL CODE TEST CASE: ALL GLOBAL REACTIONS; NEW CASE CASE 5

		INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE	ATM	5.50000	5.50000	1.00000
TEMP.	DEG K	800.000	1840.61	2.30077
ENTROPY	CAL/GM/K	1.80955	2.31665	1.28023
DENSITY	GM/CM**3	2.52469E-03	9.39340E-04	0.37206
ENTHALPY	CAL/GM	83.7665	83.7665	1.00000
SP. HEAT (CP)	CAL/GM/K	3.27783E-01	3.81967E-01	1.16530
MOL. WT. OF MIXT		30.1332	25.7948	
GAMMA		1.2519	1.2526	

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
H2O	0.00000E+00	0.00000E+00	1.03756E-01	7.24638E-02
O	0.00000E+00	0.00000E+00	1.86020E-04	1.15380E-04
H2	0.00000E+00	0.00000E+00	7.98767E-02	6.24216E-03
O2	1.93301E-01	2.05268E-01	2.96722E-02	3.68087E-02
CO	0.00000E+00	0.00000E+00	1.03451E-01	1.12336E-01
CO2	0.00000E+00	0.00000E+00	3.18636E-02	5.43640E-02
N2	7.20502E-01	6.69815E-01	6.16417E-01	6.69433E-01
NO	0.00000E+00	0.00000E+00	1.20874E-04	1.40607E-04
CN	0.00000E+00	0.00000E+00	5.82636E-04	5.87670E-04
CH2	0.00000E+00	0.00000E+00	7.84543E-03	4.26621E-03
C3H8	7.73205E-02	1.13149E-01	1.82743E-02	3.12398E-02
OH	0.00000E+00	0.00000E+00	3.55798E-04	2.34588E-04
AR	8.87650E-03	1.17677E-02	7.59852E-03	1.17677E-02

VOLUME 200.000 CM**3 MASS FLO 110.000 GM/SEC

MDOT/VOLUME = 0.55000 RESIDENCE TIME = 1.708 MSEC ITERATIONS = 3
WELLSTIRRED REACTOR CALCULATION.... GLOBAL CODE TEST CASE: ALL GLOBAL REACTIONS; NEW CASE CASE 5

		INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE	ATM	5.50000	5.50000	1.00000
TEMP.	DEG K	800.000	1810.12	2.26265
ENTROPY	CAL/GM/K	1.80955	2.30522	1.27392
DENSITY	GM/CM**3	2.52469E-03	9.59338E-04	0.37998
ENTHALPY	CAL/GM	83.7665	83.7665	1.00000
SP. HEAT (CP)	CAL/GM/K	3.27783E-01	3.81447E-01	1.16372
MOL. WT. OF MIXT		30.1332	25.9076	
GAMMA		1.2519	1.2517	

TABLE A.6.—Continued.

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
H2O	0.00000E+00	0.00000E+00	1.00629E-01	6.99736E-02
O	0.00000E+00	0.00000E+00	2.25408E-04	1.39202E-04
H2	0.00000E+00	0.00000E+00	7.80868E-02	6.07572E-03
O2	1.93301E-01	2.05268E-01	3.38253E-02	4.17780E-02
CO	0.00000E+00	0.00000E+00	1.00260E-01	1.08397E-01
CO2	0.00000E+00	0.00000E+00	3.15536E-02	5.36008E-02
N2	7.20502E-01	6.69815E-01	6.19200E-01	6.69529E-01
NO	0.00000E+00	0.00000E+00	1.46619E-04	1.67497E-04
CN	0.00000E+00	0.00000E+00	3.84734E-04	3.86369E-04
CH2	0.00000E+00	0.00000E+00	7.91299E-03	4.28422E-03
C3H8	7.73205E-02	1.13149E-01	1.97741E-02	3.36566E-02
OH	0.00000E+00	0.00000E+00	3.71866E-04	2.44115E-04
AR	8.87650E-03	1.17677E-02	7.63173E-03	1.17677E-02

VOLUME 200.000 CM**3 MASS FLO 120.000 GM/SEC

MDOT/VOLUME = 0.60000 RESIDENCE TIME = 1.599 MSEC ITERATIONS = 3

WELLSTIRRED REACTOR CALCULATION.... GLOBAL CODE TEST CASE: ALL GLOBAL REACTIONS; NEW CASE CASE 5

		INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE	ATM	5.50000	5.50000	1.00000
TEMP.	DEG K	800.000	1771.71	2.21464
ENTROPY	CAL/GM/K	1.80955	2.29023	1.26564
DENSITY	GM/CM**3	2.52469E-03	9.85816E-04	0.39047
ENTHALPY	CAL/GM	83.7665	83.7665	1.00000
SP. HEAT (CP)	CAL/GM/K	3.27783E-01	3.80763E-01	1.16163
MOL. WT. OF MIXT		30.1332	26.0577	
GAMMA		1.2519	1.2504	

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
H2O	0.00000E+00	0.00000E+00	9.65660E-02	6.67616E-02
O	0.00000E+00	0.00000E+00	2.74493E-04	1.68538E-04
H2	0.00000E+00	0.00000E+00	7.57757E-02	5.86193E-03
O2	1.93301E-01	2.05268E-01	3.92916E-02	4.82499E-02
CO	0.00000E+00	0.00000E+00	9.61201E-02	1.03323E-01
CO2	0.00000E+00	0.00000E+00	3.11090E-02	5.25411E-02
N2	7.20502E-01	6.69815E-01	6.22854E-01	6.69600E-01
NO	0.00000E+00	0.00000E+00	1.71843E-04	1.97881E-04
CN	0.00000E+00	0.00000E+00	2.29289E-04	2.28936E-04
CH2	0.00000E+00	0.00000E+00	7.76221E-03	4.17838E-03
C3H8	7.73205E-02	1.13149E-01	2.17894E-02	3.68731E-02
OH	0.00000E+00	0.00000E+00	3.80663E-04	2.48450E-04
AR	8.87650E-03	1.17677E-02	7.67596E-03	1.17677E-02

VOLUME 200.000 CM**3 MASS FLO 130.000 GM/SEC

MDOT/VOLUME = 0.65000 RESIDENCE TIME = 1.517 MSEC ITERATIONS = 4

WELLSTIRRED REACTOR CALCULATION.... GLOBAL CODE TEST CASE: ALL GLOBAL REACTIONS; NEW CASE CASE 5

		INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE	ATM	5.50000	5.50000	1.00000
TEMP.	DEG K	800.000	1705.10	2.13138
ENTROPY	CAL/GM/K	1.80955	2.26265	1.25039
DENSITY	GM/CM**3	2.52469E-03	1.03540E-03	0.41011
ENTHALPY	CAL/GM	83.7665	83.7665	1.00000
SP. HEAT (CP)	CAL/GM/K	3.27783E-01	3.79479E-01	1.15771
MOL. WT. OF MIXT		30.1332	26.3395	
GAMMA		1.2519	1.2481	

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
H2O	0.00000E+00	0.00000E+00	8.91865E-02	6.10001E-02
O	0.00000E+00	0.00000E+00	3.51692E-04	2.13628E-04
H2	0.00000E+00	0.00000E+00	7.15417E-02	5.47518E-03
O2	1.93301E-01	2.05268E-01	4.93907E-02	6.00026E-02
CO	0.00000E+00	0.00000E+00	8.86313E-02	9.42537E-02
CO2	0.00000E+00	0.00000E+00	3.02031E-02	5.04653E-02
N2	7.20502E-01	6.69815E-01	6.29643E-01	6.69657E-01
NO	0.00000E+00	0.00000E+00	2.03736E-04	2.32097E-04
CN	0.00000E+00	0.00000E+00	9.40160E-05	9.28673E-05
CH2	0.00000E+00	0.00000E+00	7.02425E-03	3.74068E-03
C3H8	7.73205E-02	1.13149E-01	2.56018E-02	4.28611E-02
OH	0.00000E+00	0.00000E+00	3.68789E-04	2.38125E-04
AR	8.87650E-03	1.17677E-02	7.75897E-03	1.17677E-02

VOLUME 200.000 CM**3 MASS FLO 140.000 GM/SEC

MDOT/VOLUME = 0.70000 RESIDENCE TIME = 1.479 MSEC ITERATIONS = 5

(WSR) *** IN COMPUTING CONV. NO. 6, MASS FRACTION SUM = 1.38003E+00 ON ITERATION NO. 17 ***
TEMPERATURE = 1.12164E+03 K, MASS FLOW RATE = 1.50000E+02 G/S

(WSR) ** RESTART: MASS FLOW RATE = 2.80000E+02 G/S, TEMPERATURE = 1.70510E+03 K **

(WSR) *** IN COMPUTING CONV. NO. 6, MASS FRACTION SUM = 1.23801E+00 ON ITERATION NO. 1 ***
TEMPERATURE = 1.24041E+03 K, MASS FLOW RATE = 2.80000E+02 G/S

TABLE A.6.—Concluded.

```
(WSR)    ** RESTART: MASS FLOW RATE =  5.60000E+02 G/S,      TEMPERATURE =  1.70510E+03 K **


(WSR)    *** IN COMPUTING CONV. NO.   6, MASS FRACTION SUM =  1.40184E+00 ON ITERATION NO.   1 ***
                             TEMPERATURE =  1.15180E+03 K,      MASS FLOW RATE =  5.60000E+02 G/S
 WSR)    ** RESTART: MASS FLOW RATE =  1.12000E+03 G/S,      TEMPERATURE =  1.70510E+03 K **


:WSR)    *** IN COMPUTING CONV. NO.   6, MASS FRACTION SUM =  1.40026E+00 ON ITERATION NO.   1 ***
                             TEMPERATURE =  1.14817E+03 K,      MASS FLOW RATE =  1.12000E+03 G/S

:WSR)    *** ABOVE PROBLEM ENCOUNTERED   4 TIMES ***
             PSR SOLUTION ABANDONED

:LSENS)    A FATAL ERROR HAS OCCURRED  -  CASE TERMINATED
```

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

```
                                 ** DATA LINES **

             1         2         3         4         5         6         7         8
CC  12345678901234567890123456789012345678901234567890123456789012345678901234567890

  ALL GLOBAL REACTIONS - CHANGE AND ADD ONE GLOBAL REACTION      CASE 6
 CHANGE
  &rtype  global=.true.,gronly=.true., glchng=.true.,
          gladd = .true., mrprev = .false., &end
                  N2      +    O2       >2.0 NO
              1.         1.       4.00E+14   .03    100000.
                                  -  BLANK LINE  -
 ADD
                  H2O     +    O          >    H2      +    O2
              1.         1.       4.90E+10   .18      -510.
     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
 O2           .193301
 N2           .720502
 C3H8         .0773205
 AR           .0088765
 END
 FINIS
```

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM   NASA LEWIS RESEARCH CENTER

ALL GLOBAL REACTIONS - CHANGE AND ADD ONE GLOBAL REACTION   CASE 6

*** GLOBAL REACTIONS ***

NUMBER	REACTION												
1			1.0*H2O	+	1.0*O	>	1.0*H2	+	1.0*O2		
2			1.0*CO	+	1.0*H2O	>	1.0*CO2	+	1.0*H2		
3			1.0*CO2	+	1.0*H2	>	1.0*CO	+	1.0*H2O		
4			1.0*N2	+	1.0*O2	>	2.0*NO				
5					2.0*NO	>	1.0*N2	+	1.0*O2		
6			1.0*CN	+	2.0*O	>	1.0*NO	+	1.0*CO		
7			1.0*CN	+	1.0*NO	>	1.0*CO	+	1.0*N2		
8			2.0*CH2	+	1.0*N2	>	2.0*CN	+	2.0*H2		
9			1.0*CH2	+	1.0*O2	>	1.0*CO	+	1.0*H2O		
10			1.0*O2	+	1.0*C3H8	>	3.0*CH2	+	2.0*OH		
11			1.0*H2	+	1.0*O2	>	2.0*OH				
12			1.0*C3H8	+	2.0*OH	>	1.0*H2O	+	1.0*C3H8	+	1.0*O
13	1.0*OH	+	1.0*H2	+	1.0*O2	>	1.0*H2O	+	1.0*O	+	1.0*OH
14			1.0*H2O	+	1.0*O	>	1.0*H2	+	1.0*O2		

REACTION NUMBER	REACTANT EXPONENTS REXP 1	REXP 2	REXP 3	REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	0.000	1.000	1.000	4.90000E+10	0.1800	-510.00
2	0.000	1.000	1.000	1.30000E+05	1.3100	-7000.00
3	0.000	1.000	1.000	4.41000E+10	0.1900	3527.00
4	0.000	1.000	1.000	4.00000E+14	0.0300	100000.00
5	0.000	0.000	2.000	2.00000E+11	0.0000	38000.00
6	0.000	1.000	1.000	8.30000E+11	0.0000	0.00
7.	0.000	1.000	1.000	1.25000E+12	0.0000	0.00
8	0.000	1.000	1.000	5.00000E+13	0.0000	54000.00
9	0.000	1.000	0.500	3.50000E+07	0.0000	5000.00
10	0.000	1.600	0.100	1.10000E+12	0.0000	41000.00
11	0.000	1.000	1.000	1.00000E+00	0.0000	49080.00
12	0.000	0.150	1.000	1.98000E+06	0.0000	4000.00
13	1.000	0.000	1.000	9.60000E+11	-0.1000	1013.00
14	0.000	1.000	1.000	4.90000E+10	0.1800	-510.00

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

** 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 **

TABLE A.7.—Continued.

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

FLOW PROPERTIES		INTEGRATION INDICATORS	
PRESSURE (ATM)	5.50000	STEPS FROM LAST PRINT	0
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE	0.00000E+00
DENSITY (G/CM**3)	2.52469E-03	METHOD ORDER	0
TEMPERATURE (DEG K)	800.00		
MASS FLOW RATE (G/SEC)	1.00000E+02	TOTAL NUMBER OF STEPS	0
ENTROPY (CAL/G/DEG K)	1.8096	FUNCT EVALUATIONS	0
MACH NUMBER	0.0000	JACOBIAN EVALUATIONS	0
GAMMA	1.2519		
ENTHALPY (CAL/G)	8.37665E+01		
SP. HEAT (CP) (CAL/G/DEG K)	3.27783E-01		

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
H2O	0.00000E+00	0.00000E+00	0.00000E+00	1	2.2495E+11	0.00000E+00	0.00000
O	0.00000E+00	0.00000E+00	0.00000E+00	2	6.7500E+10	0.00000E+00	0.00000
H2	0.00000E+00	0.00000E+00	0.00000E+00	3	1.7080E+10	0.00000E+00	0.00000
O2	1.61956E-05	1.93301E-01	-4.53833E-08	4	2.3465E-13	3.59921E-17	1.00000
CO	0.00000E+00	0.00000E+00	0.00000E+00	5	8.3160E+00	0.00000E+00	0.00000
CO2	0.00000E+00	0.00000E+00	0.00000E+00	6	8.3000E+11	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	0.00000E+00	4.58832E-22	8	8.8483E-02	0.00000E+00	0.00000
CN	0.00000E+00	0.00000E+00	0.00000E+00	9	1.5071E+06	0.00000E+00	0.00000
CH2	0.00000E+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
OH	0.00000E+00	0.00000E+00	9.07666E-08	12	1.5992E+05	0.00000E+00	0.00000
AR	7.43711E-07	8.87650E-03	0.00000E+00	13	2.6015E+11	0.00000E+00	0.00000
				14	2.2495E+11	0.00000E+00	0.00000

MIXTURE MOLECULAR WEIGHT 30.13325 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 0.00000E+00 MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 0.150000 S

**EQUILIBRIUM CONDITIONS **

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

FLOW PROPERTIES		INTEGRATION INDICATORS	
PRESSURE (ATM)	5.50000	STEPS FROM LAST PRINT	0
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE	0.00000E+00
DENSITY (G/CM**3)	7.86509E-04	METHOD ORDER	0
TEMPERATURE (DEG K)	2021.03		
MASS FLOW RATE (G/SEC)	1.00000E+02	TOTAL NUMBER OF STEPS	0
ENTROPY (CAL/G/DEG K)	2.4443	FUNCT EVALUATIONS	0
MACH NUMBER	0.0000	JACOBIAN EVALUATIONS	0
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/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
H2O	3.26171E-06	9.83480E-02	1.59423E-02	1	2.1895E+11	1.23633E+00	1.00000
O	1.07090E-12	3.22900E-08	4.18810E-06	2	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
O2	7.86509E-14	2.37151E-09	1.52956E-06	4	7.7170E+03	1.84517E-08	1.00000
CO	5.28064E-06	1.59223E-01	1.59381E-02	5	1.5552E+07	5.88118E-08	1.00000
CO2	7.73802E-07	2.33319E-02	-1.59381E-02	6	8.3000E+11	1.13011E-07	1.00000
N2	1.88058E-05	5.67039E-01	-1.02255E-10	7	1.2500E+12	7.68680E-06	1.00000
NO	4.83659E-11	1.45834E-06	-4.73505E-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
CH2	7.86509E-14	2.37151E-09	-2.14286E-10	10	4.0527E+07	3.45965E-09	1.00000
C3H8	7.86509E-14	2.37151E-09	-2.14013E-15	11	4.9272E-06	3.01360E-18	1.00000
OH	7.22352E-10	2.17806E-05	-1.14353E-05	12	7.3133E+05	9.24295E+00	1.00000
AR	2.31686E-07	6.98587E-03	0.00000E+00	13	3.4847E+11	3.20048E-05	1.00000
				14	2.1895E+11	1.23633E+00	1.00000

MIXTURE MOLECULAR WEIGHT 23.71507 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 0.00000E+00 MASS FRACTION SUM 1.00000009

TABLE A.7.—Continued.

COMPUTATIONAL WORK REQUIRED FOR EQUILIBRIUM CALCULATION:
NO. OF ITERATIONS = 12 CPU TIME = 1.666641E-02 S

INITIAL ESTIMATES (SIGMAS) AT TEMPERATURE = 2021.03 K:

H2O	4.14707E-03
O	1.36158E-09
H2	6.11629E-03
O2	1.00000E-10
CO	6.71402E-03
CO2	9.83843E-04
N2	2.39105E-02
NO	6.14944E-08
CN	1.00000E-10
CH2	1.00000E-10
C3H8	1.00000E-10
OH	9.18427E-07
AR	2.94575E-04

WELLSTIRRED REACTOR CALCULATION.... ALL GLOBAL REACTIONS - CHANGE AND ADD ONE GLOBAL REACTION CASE 6

		INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE	ATM	5.50000	5.50000	1.00000
TEMP.	DEG K	800.000	1934.60	2.41824
ENTROPY	CAL/GM/K	1.80955	2.38309	1.31695
DENSITY	GM/CM**3	2.52469E-03	8.59087E-04	0.34027
ENTHALPY	CAL/GM	83.7665	83.7665	1.00000
SP. HEAT (CP)	CAL/GM/K	3.27783E-01	3.81218E-01	1.16302
MOL. WT. OF MIXT		30.1332	24.7956	
GAMMA		1.2519	1.2662	

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
H2O	0.00000E+00	0.00000E+00	1.22126E-01	8.87304E-02
O	0.00000E+00	0.00000E+00	1.84123E-06	1.18805E-06
H2	0.00000E+00	0.00000E+00	1.02900E-01	8.36539E-03
O2	1.93301E-01	2.05268E-01	5.22441E-03	6.74211E-03
CO	0.00000E+00	0.00000E+00	1.22134E-01	1.37969E-01
CO2	0.00000E+00	0.00000E+00	3.16861E-02	5.62397E-02
N2	7.20502E-01	6.69815E-01	5.85567E-01	6.61558E-01
NO	0.00000E+00	0.00000E+00	1.22333E-06	1.48040E-06
CN	0.00000E+00	0.00000E+00	1.46165E-02	1.53369E-02
CH2	0.00000E+00	0.00000E+00	1.38415E-03	7.83007E-04
C3H8	7.73205E-02	1.13149E-01	7.01732E-03	1.24795E-02
OH	0.00000E+00	0.00000E+00	3.69903E-05	2.53717E-05
AR	8.87650E-03	1.17677E-02	7.50416E-03	1.17677E-02

VOLUME 2500.00 CM**3 MASS FLO 100.000 GM/SEC

MDOT/VOLUME = 0.04000 RESIDENCE TIME = 21.477 MSEC ITERATIONS = 14

(WSR) *** FOR CONV. NO. 2, CONVERGED TEMP. (AFTER 5 ITERATIONS) IS GREATER THAN OR EQUAL TO THE PREVIOUS TEMP. ***
MASS FLOW RATE = 3.00000E+02 G/S, TEMPERATURE = 1.94931E+03 K, PREVIOUS TEMPERATURE = 1.93460E+03 K

(WSR) ** RESTART: MASS FLOW RATE = 2.00000E+02 G/S, TEMPERATURE = 2.02103E+03 K **

(WSR) *** FOR CONV. NO. 1, CONVERGED TEMP. (AFTER 13 ITERATIONS) IS GREATER THAN OR EQUAL TO THE PREVIOUS TEMP. ***
MASS FLOW RATE = 2.00000E+02 G/S, TEMPERATURE = 1.94694E+03 K, PREVIOUS TEMPERATURE = 1.93460E+03 K

(WSR) ** RESTART: MASS FLOW RATE = 4.00000E+02 G/S, TEMPERATURE = 2.02103E+03 K **

(WSR) *** FOR CONV. NO. 1, CONVERGED TEMP. (AFTER 13 ITERATIONS) IS GREATER THAN OR EQUAL TO THE PREVIOUS TEMP. ***
MASS FLOW RATE = 4.00000E+02 G/S, TEMPERATURE = 1.94721E+03 K, PREVIOUS TEMPERATURE = 1.93460E+03 K

(WSR) ** RESTART: MASS FLOW RATE = 8.00000E+02 G/S, TEMPERATURE = 2.02103E+03 K **

WELLSTIRRED REACTOR CALCULATION.... ALL GLOBAL REACTIONS - CHANGE AND ADD ONE GLOBAL REACTION CASE 6

		INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE	ATM	5.50000	5.50000	1.00000
TEMP.	DEG K	800.000	1916.92	2.39616
ENTROPY	CAL/GM/K	1.80955	2.34918	1.29821
DENSITY	GM/CM**3	2.52469E-03	8.88948E-04	0.35210
ENTHALPY	CAL/GM	83.7665	83.7665	1.00000
SP. HEAT (CP)	CAL/GM/K	3.27783E-01	3.82830E-01	1.16794
MOL. WT. OF MIXT		30.1332	25.4231	
GAMMA		1.2519	1.2566	

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
H2O	0.00000E+00	0.00000E+00	1.12731E-01	7.98830E-02
O	0.00000E+00	0.00000E+00	3.61974E-05	2.27799E-05
H2	0.00000E+00	0.00000E+00	8.72016E-02	6.91422E-03
O2	1.93301E-01	2.05268E-01	1.79598E-02	2.26050E-02
CO	0.00000E+00	0.00000E+00	1.12675E-01	1.24142E-01
CO2	0.00000E+00	0.00000E+00	3.22747E-02	5.58705E-02
N2	7.20502E-01	6.69815E-01	6.06071E-01	6.67822E-01
NO	0.00000E+00	0.00000E+00	2.39898E-05	2.83144E-05
CN	0.00000E+00	0.00000E+00	3.59355E-03	3.67759E-03
CH2	0.00000E+00	0.00000E+00	5.97986E-03	3.29930E-03
C3H8	7.73205E-02	1.13149E-01	1.37268E-02	2.38090E-02
OH	0.00000E+00	0.00000E+00	2.36778E-04	1.58398E-04
AR	8.87650E-03	1.17677E-02	7.48901E-03	1.17677E-02

TABLE A.7.—Concluded.

```
VOLUME     2500.00      CM**3          MASS FLO   800.000      GM/SEC

 MDOT/VOLUME =      0.32000   RESIDENCE TIME =          2.778  MSEC   ITERATIONS =  15
   WELLSTIRRED REACTOR CALCULATION.... ALL GLOBAL REACTIONS - CHANGE AND ADD ONE GLOBAL REACTION     CASE 6

                                 INITIAL STATE                   FINAL STATE          FINAL/INITIAL RATIO

   PRESSURE       ATM            5.50000                          5.50000                1.00000
   TEMP.          DEG K          800.000                          1825.55                2.28194
   ENTROPY        CAL/GM/K       1.80955                          2.31250                1.27794
   DENSITY        GM/CM**3       2.52469E-03                   9.48045E-04               0.37551
   ENTHALPY       CAL/GM         83.7665                          83.7665                1.00000
   SP. HEAT (CP)  CAL/GM/K       3.27783E-01                   3.81622E-01               1.16425
   MOL. WT. OF MIXT                30.1332                        25.8208
   GAMMA                            1.2519                         1.2526


  SPECIES                    MOLE FRACT         MASS FRACT          MOLE FRACT         MASS FRACT

   H2O                       0.00000E+00        0.00000E+00         1.02509E-01        7.15205E-02
   O                         0.00000E+00        0.00000E+00         9.95728E-05        6.16984E-05
   H2                        0.00000E+00        0.00000E+00         7.97738E-02        6.22784E-03
   O2                        1.93301E-01        2.05268E-01         3.13087E-02        3.87997E-02
   CO                        0.00000E+00        0.00000E+00         1.02345E-01        1.11024E-01
   CO2                       0.00000E+00        0.00000E+00         3.16403E-02        5.39286E-02
   N2                        7.20502E-01        6.69815E-01         6.16901E-01        6.69284E-01
   NO                        0.00000E+00        0.00000E+00         6.52160E-05        7.57868E-05
   CN                        0.00000E+00        0.00000E+00         9.13986E-04        9.20954E-04
   CH2                       0.00000E+00        0.00000E+00         7.78644E-03        4.22987E-03
   C3H8                      7.73205E-02        1.13149E-01         1.86930E-02        3.19235E-02
   OH                        0.00000E+00        0.00000E+00         3.57854E-04        2.35706E-04
   AR                        8.87650E-03        1.17677E-02         7.60617E-03        1.17677E-02
VOLUME     2500.00      CM**3          MASS FLO   1400.00      GM/SEC

 MDOT/VOLUME =      0.56000   RESIDENCE TIME =          1.693  MSEC   ITERATIONS =   3
   WELLSTIRRED REACTOR CALCULATION.... ALL GLOBAL REACTIONS - CHANGE AND ADD ONE GLOBAL REACTION     CASE 6

                                 INITIAL STATE                   FINAL STATE          FINAL/INITIAL RATIO

   PRESSURE       ATM            5.50000                          5.50000                1.00000
   TEMP.          DEG K          800.000                          1802.65                2.25332
   ENTROPY        CAL/GM/K       1.80955                          2.30347                1.27295
   DENSITY        GM/CM**3       2.52469E-03                   9.63525E-04               0.38164
   ENTHALPY       CAL/GM         83.7665                          83.7665                1.00000
   SP. HEAT (CP)  CAL/GM/K       3.27783E-01                   3.81246E-01               1.16310
   MOL. WT. OF MIXT                30.1332                        25.9133
   GAMMA                            1.2519                         1.2518


  SPECIES                    MOLE FRACT         MASS FRACT          MOLE FRACT         MASS FRACT

   H2O                       0.00000E+00        0.00000E+00         1.00036E-01        6.95461E-02
   O                         0.00000E+00        0.00000E+00         1.15417E-04        7.12606E-05
   H2                        0.00000E+00        0.00000E+00         7.82734E-02        6.08890E-03
   O2                        1.93301E-01        2.05268E-01         3.46098E-02        4.27376E-02
   CO                        0.00000E+00        0.00000E+00         9.98464E-02        1.07927E-01
   CO2                       0.00000E+00        0.00000E+00         3.13991E-02        5.33265E-02
   N2                        7.20502E-01        6.69815E-01         6.19230E-01        6.69414E-01
   NO                        0.00000E+00        0.00000E+00         7.51465E-05        8.70153E-05
   CN                        0.00000E+00        0.00000E+00         6.66980E-04        6.69667E-04
   CH2                       0.00000E+00        0.00000E+00         7.83380E-03        4.24041E-03
   C3H8                      7.73205E-02        1.13149E-01         1.99102E-02        3.38809E-02
   OH                        0.00000E+00        0.00000E+00         3.70383E-04        2.43088E-04
   AR                        8.87650E-03        1.17677E-02         7.63341E-03        1.17677E-02
VOLUME     2500.00      CM**3          MASS FLO   1500.00      GM/SEC

 MDOT/VOLUME =      0.60000   RESIDENCE TIME =          1.606  MSEC   ITERATIONS =   3


                        COMPUTATIONAL WORK REQUIRED FOR PSR CALCULATION:
                     NO. OF ITERATIONS =    72       CPU TIME =  8.666668E-01 S


(LSENS)     END OF THIS CASE


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


(LSENS)     READ DATA FOR NEXT CASE
```

TABLE A.8.—COMPUTED RESULTS FOR TEST CASE 7 (PROPANE-AIR PSR PROBLEM WITH MOLECULAR REACTIONS ADDED TO GLOBAL MECHANISM OF CASE 6)

```
                                    ** DATA LINES **

             1         2         3         4         5         6         7         8
CC  12345678901234567890123456789012345678901234567890123456789012345678901234567890

    GLOBAL AND MOLECULAR REACTIONS; MOLECULAR REACTIONS ADDED      CASE 7
    ADD
     &rtype global=.true.,gronly=.false.,  mrprev = .false.,
          mradd=.true., &end
       O       +   H2O      =   OH      +   OH            6.8E+13    0.        18365.
       H       +   O2       =   OH      +   O            1.89E+14   0.        16400.
       O       +   H2       =   OH      +   H            4.20E+14   0.        13750.
       H       +   HO2      =   H2      +   O2           7.28E+13   0.        2126.
       O       +   HO2      =   OH      +   O2            5.0E+13   0.        1000.
       HO2     +   OH       =   H2O     +   O2            8.0E+12   0.        0.
       H       +   HO2      =2.0OH                       1.34E+14   0.        1070.
       H2      +   HO2      =   H2O2    +   H            7.91E+13   0.        25000.
       OH      +   H2O2     =   H2O     +   HO2           6.1E+12   0.        1430.
       HO2     +   HO2      =   H2O2    +   O2            1.8E+12   0.         0.
       H       +   H2O2     =   OH      +   H2O           7.8E+11   0.         0.
       M       +   H2O2     =2.0OH                       1.44E+17   0.        45510.
       THIRDBODY
    H2          2.30    O2         .78      H2O           6.0   H2O2          6.6
    END
       H2      +   OH       =   H2O     +   H            4.74E+13   0.        6098.
       H       +   O2       =   HO2     +   M            1.46E+15   0.        -1000.
       THIRDBODY
    O2          1.30    N2         1.3      H2O           21.3  H2            3.0
    END
       M       +   H2O      =   H       +   OH           1.30E+15   0.        105140.
       THIRDBODY
    H2          4.00    O2         1.5      H2O           20.0  N2            1.5
    END
       H       +   O        =   OH      +   M            7.1E+18  -1.          0.
       M       +   H2       =   H       +   H            2.2E+14   0.         96000.
       THIRDBODY
    H2          4.10    O2         2.0      H2O           15.0  N2            2.0
    END
       M       +   O2       =   O       +   O            1.80E+18   -1.       118020.
       CO      +   O        >   CO2                      8.43E+09   -.001     1000.
                   CO2      >   CO      +   O            9.08E+18   -1.84-    130754.
       END
                                    - BLANK LINE -
    TIME                                 C3H8
     &PROB  HELSTR=.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
```

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM   NASA LEWIS RESEARCH CENTER

GLOBAL AND MOLECULAR REACTIONS; MOLECULAR REACTIONS ADDED   CASE 7

REACTION NUMBER			REACTION					REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	1*O	+	1*H2O	=	2*OH			6.80000E+13	0.0000	18365.00
2	1*H	+	1*O2	=	1*OH	+	1*O	1.89000E+14	0.0000	16400.00
3	1*O	+	1*H2	=	1*OH	+	1*H	4.20000E+14	0.0000	13750.00
4	1*H	+	1*HO2	=	1*H2	+	1*O2	7.28000E+13	0.0000	2126.00
5	1*O	+	1*HO2	=	1*OH	+	1*O2	5.00000E+13	0.0000	1000.00
6	1*HO2	+	1*OH	=	1*H2O	+	1*O2	8.00000E+12	0.0000	0.00
7	1*H	+	1*HO2	=	2*OH			1.34000E+14	0.0000	1070.00
8	1*H2	+	1*HO2	=	1*H2O2	+	1*H	7.91000E+13	0.0000	25000.00
9	1*OH	+	1*H2O2	=	1*H2O	+	1*HO2	6.10000E+12	0.0000	1430.00
10			2*HO2	=	1*H2O2	+	1*O2	1.80000E+12	0.0000	0.00
11	1*H	+	1*H2O2	=	1*OH	+	1*H2O	7.80000E+11	0.0000	0.00
12	M	+	1*H2O2	=	2*OH			1.44000E+17	0.0000	45510.00
13	1*H2	+	1*OH	=	1*H2O	+	1*H	4.74000E+13	0.0000	6098.00
14	1*H	+	1*O2	=	1*HO2	+	M	1.46000E+15	0.0000	-1000.00
15	M	+	1*H2O	=	1*H	+	1*OH	1.30000E+15	0.0000	105140.00
16	1*H	+	1*O	=	1*OH	+	M	7.10000E+18	-1.0000	0.00
17	M	+	1*H2	=	2*H			2.20000E+14	0.0000	96000.00
18	M	+	1*O2	=	2*O			1.80000E+18	-1.0000	118020.00
19	1*CO	+	1*O	>	1*CO2			8.43000E+09	-0.0010	1000.00
20			1*CO2	>	1*CO	+	1*O	9.08000E+18	-1.8400	130754.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

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

*** GLOBAL REACTIONS ***

NUMBER			REACTION				
21	1.0*H2O	+	1.0*O	>	1.0*H2	+	1.0*O2
22	1.0*CO	+	1.0*H2O	>	1.0*CO2	+	1.0*H2
23	1.0*CO2	+	1.0*H2	>	1.0*CO	+	1.0*H2O
24	1.0*N2	+	1.0*O2	>	2.0*NO		
25			2.0*NO	>	1.0*N2	+	1.0*O2
26	1.0*CN	+	2.0*O	>	1.0*NO	+	1.0*CO

TABLE A.8.—Continued.

27			1.0*CN	+	1.0*NO	>	1.0*CO	+	1.0*N2		
28			2.0*CH2	+	1.0*N2	>	2.0*CN	+	2.0*H2		
29			1.0*CH2	+	1.0*O2	>	1.0*CO	+	1.0*H2O		
30			1.0*O2	+	1.0*C3H8	>	3.0*CH2	+	2.0*OH		
31			1.0*H2	+	1.0*O2	>	2.0*OH				
32			1.0*C3H8	+	2.0*OH	>	1.0*H2O	+	1.0*C3H8	+	1.0*O
33	1.0*OH	+	1.0*H2	+	1.0*O2	>	1.0*H2O	+	1.0*O	+	1.0*OH
34			1.0*H2O	+	1.0*O	>	1.0*H2	+	1.0*O2		

REACTION NUMBER	REACTANT EXPONENTS REXP 1	REXP 2	REXP 3	REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
21	0.000	1.000	1.000	4.90000E+10	0.1800	-510.00
22	0.000	1.000	1.000	1.30000E+05	1.3100	-7000.00
23	0.000	1.000	1.000	4.41000E+10	0.1900	3527.00
24	0.000	1.000	1.000	6.00000E+14	0.0300	100000.00
25	0.000	0.000	2.000	2.00000E+11	0.0000	38000.00
26	0.000	1.000	1.000	8.30000E+11	0.0000	0.00
27	0.000	1.000	1.000	1.25000E+12	0.0000	0.00
28	0.000	1.000	1.000	5.00000E+13	0.0000	54000.00
29	0.000	1.000	0.500	3.50000E+07	0.0000	5000.00
30	0.000	1.600	0.100	1.10000E+12	0.0000	41000.00
31	0.000	1.000	1.000	1.00000E+00	0.0000	49080.00
32	0.000	0.150	1.000	1.98000E+06	0.0000	4000.00
33	1.000	0.000	1.000	9.60000E+11	-0.1000	1013.00
34	0.000	1.000	1.000	4.90000E+10	0.1800	-510.00

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

** 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 = 1.00000E+02 G/S
MAXIMUM MASS FLOW RATE = 1.16000E+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 0.00000E+00 CM

FLOW PROPERTIES		INTEGRATION INDICATORS	
PRESSURE (ATM)	5.50000	STEPS FROM LAST PRINT	0
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE	0.00000E+00
DENSITY (G/CM**3)	2.50173E-03	METHOD ORDER	0
TEMPERATURE (DEG K)	800.00		
MASS FLOW RATE (G/SEC)	1.40000E+02	TOTAL NUMBER OF STEPS	0
ENTROPY (CAL/G/DEG K)	1.8011	FUNCT EVALUATIONS	0
MACH NUMBER	0.0000	JACOBIAN EVALUATIONS	0
GAMMA	1.2701		
ENTHALPY (CAL/G)	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/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
H2O	0.00000E+00	0.00000E+00	0.00000E+00	1	6.5377E+08	0.00000E+00	0.00000
O	0.00000E+00	0.00000E+00	3.57038E-26	2	6.2545E+09	0.00000E+00	0.00000
H2	0.00000E+00	0.00000E+00	0.00000E+00	3	7.3608E+10	0.00000E+00	0.00000
O2	1.65148E-05	1.97112E-01	-4.55842E-08	4	1.9113E+13	0.00000E+00	0.00000
CO	0.00000E+00	0.00000E+00	1.86163E-30	5	2.6655E+13	0.00000E+00	0.00000
CO2	2.36493E-08	2.82264E-04	-1.86163E-30	6	8.0000E+12	0.00000E+00	0.00000
N2	6.15566E-05	7.34704E-01	-2.38549E-22	7	6.8359E+13	0.00000E+00	0.00000
NO	0.00000E+00	0.00000E+00	4.77099E-22	8	1.1708E+07	0.00000E+00	0.00000
CN	0.00000E+00	0.00000E+00	0.00000E+00	9	2.4813E+12	0.00000E+00	0.00000
CH2	0.00000E+00	0.00000E+00	1.36753E-07	10	1.8000E+12	0.00000E+00	0.00000
C3H8	4.95445E-06	5.91335E-02	-4.55842E-08	11	7.8000E+11	0.00000E+00	0.00000
OH	0.00000E+00	0.00000E+00	9.11685E-08	12	5.3163E+04	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	0.00000E+00	13	1.0230E+12	0.00000E+00	0.00000
HO2	0.00000E+00	0.00000E+00	0.00000E+00	14	2.7387E+15	0.00000E+00	0.00000
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	15	2.4606E-14	0.00000E+00	0.00000
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+09	0.00000E+00	0.00000
20	7.8718E-23	2.97450E-25	1.00000
21	2.2495E+11	0.00000E+00	0.00000
22	6.7500E+10	0.00000E+00	0.00000
23	1.7080E+10	0.00000E+00	0.00000
24	2.3465E-13	3.81152E-17	1.00000
25	8.3160E+00	0.00000E+00	0.00000
26	8.3000E+11	0.00000E+00	0.00000
27	1.2500E+12	0.00000E+00	0.00000
28	8.8483E-02	0.00000E+00	0.00000
29	1.5071E+06	0.00000E+00	0.00000
30	6.9297E+00	7.28341E-03	1.00000
31	3.9081E-14	0.00000E+00	0.00000
32	1.5992E+05	0.00000E+00	0.00000
33	2.6015E+11	0.00000E+00	0.00000
34	2.2495E+11	0.00000E+00	0.00000

MIXTURE MOLECULAR WEIGHT 29.85916 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 3.39759E-16 MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSENS = 0.516666 S

**EQUILIBRIUM CONDITIONS **

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

FLOW PROPERTIES		INTEGRATION INDICATORS	
PRESSURE (ATM)	5.50000	STEPS FROM LAST PRINT	0
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE	0.00000E+00
DENSITY (G/CM**3)	7.34828E-04	METHOD ORDER	0
TEMPERATURE (DEG K)	2350.31		
MASS FLOW RATE (G/SEC)	1.40000E+02	TOTAL NUMBER OF STEPS	0
ENTROPY (CAL/G/DEG K)	2.3604	FUNCT EVALUATIONS	0
MACH NUMBER	0.0000	JACOBIAN EVALUATIONS	0
GAMMA	1.2641		
ENTHALPY (CAL/G)	9.23468E+01		
SP. HEAT (CP) (CAL/G/DEG K)	3.69088E-01		

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
H2O	4.05534E-06	1.42200E-01	8.67144E-03	1	1.3329E+12	-7.60162E-04	0.00000
O	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
O2	2.11927E-10	7.43118E-06	3.89333E-04	4	4.6178E+13	1.43082E-06	0.00000
CO	3.10378E-06	1.08834E-01	8.94626E-03	5	4.0363E+13	7.03729E-09	0.00000
CO2	1.26895E-06	4.44958E-02	-8.94626E-03	6	8.0000E+12	1.29043E-07	0.00000
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
HO2	3.90703E-13	1.37000E-08	-1.11365E-07	14	1.8086E+15	3.66684E-06	0.00000
H2O2	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	0.00000E+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	8.45730E+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	1.80064E-03	1.00000
				25	5.8546E+07	7.59605E-04	1.00000
				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

MIXTURE MOLECULAR WEIGHT 25.76666 TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 1.05177E+05 MASS FRACTION SUM 1.00000010

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

TABLE A.8.—Continued.

INITIAL ESTIMATES (SIGMAS) AT TEMPERATURE = 2350.31 K:

H2O	5.51876E-03
O	2.96523E-07
H2	2.36709E-03
O2	2.88403E-07
CO	4.22382E-03
CO2	1.72687E-03
N2	2.46038E-02
NO	3.60201E-06
CN	1.00000E-10
CH2	1.00000E-10
C3H8	1.00000E-10
OH	2.08595E-05
H	5.07475E-05
HO2	5.31693E-10
H2O2	1.00000E-10
AR	2.93675E-04

(HSR) *** FOR CONV. NO. 1, CONVERGED TEMP. (AFTER 17 ITERATIONS) IS GREATER THAN OR EQUAL TO THE PREVIOUS TEMP. ***
MASS FLOW RATE = 1.40000E+02 G/S, TEMPERATURE = 2.44550E+03 K, PREVIOUS TEMPERATURE = 2.35031E+03 K

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

(HSR) *** FOR CONV. NO. 1, CONVERGED TEMP. (AFTER 21 ITERATIONS) IS GREATER THAN OR EQUAL TO THE PREVIOUS TEMP. ***
MASS FLOW RATE = 2.80000E+02 G/S, TEMPERATURE = 2.41194E+03 K, PREVIOUS TEMPERATURE = 2.35031E+03 K

(HSR) ** RESTART: MASS FLOW 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	5.50000	5.50000	1.00000
TEMP.	DEG K	800.000	2342.87	2.92859
ENTROPY	CAL/GM/K	1.80111	2.25627	1.25271
DENSITY	GM/CM**3	2.50173E-03	8.03853E-04	0.32132
ENTHALPY	CAL/GM	92.3468	92.3468	1.00000
SP. HEAT (CP)	CAL/GM/K	3.12948E-01	3.76201E-01	1.20212
MOL. WT. OF MIXT		29.8592	28.0978	
GAMMA		1.2701	1.2315	

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
H2O	0.00000E+00	0.00000E+00	1.41886E-01	9.09717E-02
O	0.00000E+00	0.00000E+00	7.86184E-04	4.47668E-04
H2	0.00000E+00	0.00000E+00	6.16159E-03	4.42046E-04
O2	1.97112E-01	2.11236E-01	1.12541E-02	1.28166E-02
CO	0.00000E+00	0.00000E+00	1.91345E-02	1.90750E-02
CO2	2.82264E-04	4.16032E-04	9.07499E-02	1.42142E-01
N2	7.34704E-01	6.89288E-01	6.90019E-01	6.87946E-01
NO	0.00000E+00	0.00000E+00	3.92059E-04	4.18686E-04
CN	0.00000E+00	0.00000E+00	2.29878E-03	2.12860E-03
CH2	0.00000E+00	0.00000E+00	6.28177E-03	3.13594E-03
C3H8	5.91335E-02	8.73286E-02	1.62455E-02	2.54954E-02
OH	0.00000E+00	0.00000E+00	5.27503E-03	3.19292E-03
H	0.00000E+00	0.00000E+00	1.25505E-03	4.50232E-05
HO2	0.00000E+00	0.00000E+00	8.43037E-06	9.90322E-06
H2O2	0.00000E+00	0.00000E+00	4.44354E-07	5.37925E-07
AR	8.76890E-03	1.17317E-02	8.25163E-03	1.17317E-02

VOLUME 500.000 CM**3 MASS FLO 560.000 GM/SEC

MDOT/VOLUME = 1.12000 RESIDENCE TIME = 0.718 MSEC ITERATIONS = 17

WELLSTIRRED REACTOR CALCULATION....GLOBAL AND MOLECULAR REACTIONS; MOLECULAR REACTIONS ADDED CASE 7

		INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE	ATM	5.50000	5.50000	1.00000
TEMP.	DEG K	800.000	2192.26	2.74032
ENTROPY	CAL/GM/K	1.80111	2.23090	1.23863
DENSITY	GM/CM**3	2.50173E-03	8.61527E-04	0.34437
ENTHALPY	CAL/GM	92.3468	92.3468	1.00000
SP. HEAT (CP)	CAL/GM/K	3.12948E-01	3.73834E-01	1.19456
MOL. WT. OF MIXT		29.8592	28.1779	
GAMMA		1.2701	1.2325	

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
H2O	0.00000E+00	0.00000E+00	1.32976E-01	8.50163E-02
O	0.00000E+00	0.00000E+00	1.05479E-03	5.98908E-04
H2	0.00000E+00	0.00000E+00	3.60083E-03	2.57598E-04
O2	1.97112E-01	2.11236E-01	2.23110E-02	2.53364E-02
CO	0.00000E+00	0.00000E+00	1.16951E-02	1.16256E-02
CO2	2.82264E-04	4.16032E-04	8.83688E-02	1.38019E-01
N2	7.34704E-01	6.89288E-01	6.92506E-01	6.88463E-01
NO	0.00000E+00	0.00000E+00	1.91990E-04	2.04446E-04
CN	0.00000E+00	0.00000E+00	1.46599E-03	1.35360E-03
CH2	0.00000E+00	0.00000E+00	1.39672E-02	6.95280E-03
C3H8	5.91335E-02	8.73286E-02	1.73936E-02	2.72196E-02
OH	0.00000E+00	0.00000E+00	5.24581E-03	3.16621E-03
H	0.00000E+00	0.00000E+00	9.30158E-04	3.32733E-05
HO2	0.00000E+00	0.00000E+00	1.68549E-05	1.97433E-05
H2O2	0.00000E+00	0.00000E+00	9.35949E-07	1.12982E-06
AR	8.76890E-03	1.17317E-02	8.27515E-03	1.17317E-02

TABLE A.8.—Concluded.

```
VOLUME     500.000      CM**3          MASS FLO    1060.00       GM/SEC
 MDOT/VOLUME =      2.12000   RESIDENCE TIME =           0.406  MSEC   ITERATIONS =    4
 WELLSTIRRED REACTOR CALCULATION....GLOBAL AND MOLECULAR REACTIONS; MOLECULAR REACTIONS ADDED     CASE 7
                                    INITIAL STATE                    FINAL STATE         FINAL/INITIAL RATIO

  PRESSURE        ATM               5.50000                          5.50000                 1.00000
  TEMP.           DEG K             800.000                          2154.84                 2.69355
  ENTROPY         CAL/GM/K          1.80111                          2.22440                 1.23502
  DENSITY         GM/CM**3          2.50173E-03                     8.76949E-04              0.35054
  ENTHALPY        CAL/GM            92.3468                          92.3468                 1.00000
  SP. HEAT (CP)   CAL/GM/K          3.12948E-01                     3.73152E-01              1.19238
  MOL. WT. OF MIXT                     29.8592                          28.1927
  GAMMA                                1.2701                           1.2329
```

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
H2O	0.00000E+00	0.00000E+00	1.30743E-01	8.35451E-02
O	0.00000E+00	0.00000E+00	1.07475E-03	6.09921E-04
H2	0.00000E+00	0.00000E+00	3.10814E-03	2.22234E-04
O2	1.97112E-01	2.11236E-01	2.54944E-02	2.89362E-02
CO	0.00000E+00	0.00000E+00	1.07071E-02	1.06379E-02
CO2	2.82264E-04	4.16032E-04	8.70521E-02	1.35891E-01
N2	7.34704E-01	6.89288E-01	6.93073E-01	6.88665E-01
NO	0.00000E+00	0.00000E+00	2.14869E-05	2.28689E-05
CH	0.00000E+00	0.00000E+00	1.23144E-03	1.13644E-03
CH2	0.00000E+00	0.00000E+00	1.55465E-02	7.73488E-03
C3H8	5.91335E-02	8.73286E-02	1.77430E-02	2.77518E-02
OH	0.00000E+00	0.00000E+00	5.07489E-03	3.06144E-03
H	0.00000E+00	0.00000E+00	8.30086E-04	2.96779E-05
HO2	0.00000E+00	0.00000E+00	1.90841E-05	2.23428E-05
H2O2	0.00000E+00	0.00000E+00	1.07477E-06	1.29672E-06
AR	8.76890E-03	1.17317E-02	8.27951E-03	1.17317E-02

```
VOLUME     500.000      CM**3          MASS FLO    1160.00       GM/SEC
 MDOT/VOLUME =      2.32000   RESIDENCE TIME =           0.378  MSEC   ITERATIONS =    5

                          COMPUTATIONAL WORK REQUIRED FOR PSR CALCULATION:-
                       NO. OF ITERATIONS =     89      CPU TIME =  1.833334E+00 S

(LSENS)     END OF THIS CASE

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

(LSENS)     READ DATA FOR NEXT CASE
```

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13. ABSTRACT ***(Maximum 200 words)***
A generalized version of the NASA Lewis general kinetics code, LSENS, is described. The new code allows the use of global reactions as well as molecular processes in a chemical mechanism. The code also incorporates the capability of performing sensitivity analysis calculations for a perfectly stirred reactor rapidly and conveniently at the same time that the main kinetics calculations are being done. The GLSENS code has been extensively tested and has been found to be accurate and efficient. Nine example problems are presented and complete user instructions are given for the new capabilities. This report is to be used in conjunction with the documentation for the original LSENS code.

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