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# PREMIX

A PROGRAM FOR MODELING STEADY, LAMINAR,  
ONE-DIMENSIONAL PREMIXED FLAMES

Reaction Design

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## PREMIX: A PROGRAM FOR MODELING STEADY, LAMINAR, ONE-DIMENSIONAL PREMIXED FLAMES

### ABSTRACT

PREMIX computes species and temperature profiles in steady-state burner-stabilized and freely propagating premixed laminar flames. The program accounts for finite-rate chemical kinetics and multicomponent molecular transport. This manual provides details on the governing equations and boundary conditions, the finite-difference discretization and the Newton method employed in solving the boundary-value problem. Steady-state convergence of the premixed-flame solution is aided by invoking time integration procedures when the Newton method has convergence difficulties. The PREMIX program runs in conjunction with the Gas-phase CHEMKIN and TRANSPORT software packages for processing the chemical reaction mechanism and for calculating the transport properties. Transport property formulations include the option of using multicomponent or mixture-averaged formulas for molecular diffusion. Discussion of two example problems illustrates many of the program's capabilities.



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## NOMENCLATURE

		<u>CGS Units</u>
$A$	Cross-sectional area of the stream tube encompassing the flame	$\text{cm}^2$
$A$	Pre-exponential factor in an Arrhenius rate expression	---
$c_p$	Specific heat at constant pressure of gas mixture	$\text{ergs}/(\text{g K})$
$c_{pk}$	Specific heat at constant pressure of the $k$ th species	$\text{ergs}/(\text{g K})$
$D_{kj}$	Binary diffusion coefficient of species $k$ in species $j$	$\text{cm}^2/\text{sec}$
$D_{km}$	Mixture-averaged diffusion coefficient of the $k$ th species	$\text{cm}^2/\text{sec}$
$D_{kj}$	Multicomponent diffusion coefficient of the species $k$ in species $j$	$\text{cm}^2/\text{sec}$
$D_k^T$	Thermal diffusion coefficient of the $k$ th species	$\text{cm}^2/\text{sec}$
$E_A$	Activation energy in an Arrhenius rate expression	$\text{ergs}/\text{mole}$
$h_k$	Specific enthalpy of the $k$ th species	$\text{ergs}/\text{g}$
$j$	Grid-point index	---
$J$	Jacobian matrix	---
$k$	Species index	---
$k_f$	Forward rate constant	---
$K$	Total number of species	---
$\dot{M}$	Mass flow rate	$\text{g}/\text{sec}$
$p$	Pressure	$\text{dynes}/\text{cm}^2$
$R$	Universal gas constant	$\text{ergs}/(\text{mole K})$
$t$	Time	$\text{sec}$
$T$	Temperature	$\text{K}$
$u$	Velocity of the fluid mixture	$\text{cm}/\text{sec}$
$V_c$	Correction velocity	$\text{cm}/\text{sec}$
$V_k$	Diffusion velocity of the $k$ th species	$\text{cm}/\text{sec}$
$v_k$	Ordinary diffusion velocity of the $k$ th species	$\text{cm}/\text{sec}$
$W_k$	Molecular weight of $k$ th species	$\text{g}/\text{mole}$
$W_k$	Thermal diffusion velocity of $k$ th species	$\text{cm}/\text{sec}$
$\bar{W}$	Mean molecular weight of a mixture	$\text{g}/\text{mole}$
$x$	Spatial coordinate	$\text{cm}$
$X_k$	Mole fraction of the $k$ th species	---
$Y_k$	Mass fraction of the $k$ th species	---

**GREEK**

		<b><u>CGS Units</u></b>
$\beta$	Temperature exponent in the rate constant	---
$\gamma$	User-specified parameter for solution curvature resolution	---
$\delta$	User-specified parameter for solution gradient resolution	---
$\varepsilon_k$	Inlet mass fraction of the $k$ th species	---
$\lambda$	Thermal conductivity of the gas mixture	ergs/(cm K sec)
$\lambda^{(n)}$	Damping parameter for the $n$ th iterate in the solution algorithm	---
$\rho$	Mass density	g/cm <sup>3</sup>
$\phi$	Solution vector	---
$\dot{\omega}_k$	Production rate of the $k$ th species from gas-phase reactions	mole/(cm <sup>2</sup> sec)
$\Theta_k$	Thermal diffusion ratio for mixture-averaged formula	---



# 1. INTRODUCTION

Many practical combustors, such as internal combustion engines, rely on premixed flame propagation. Moreover, burner-stabilized laminar premixed flames are very often used to study chemical kinetics in a combustion environment. Such flames are effectively one-dimensional and can be made very steady, thus facilitating detailed experimental measurements of temperature and species profiles. Also, laminar flame speed is often used to characterize the combustion of various fuel-oxidizer combinations. Therefore, the ability to model chemical kinetics and transport processes in these flames is critical to interpreting flame experiments and to understanding the combustion process itself. Examples of the use of flame modeling to interpret experimental observations and to understand combustion chemistry and pollution formation can be found in Miller, et al.<sup>2-4</sup>

The earliest efforts at solving premixed flame problems with realistic chemical kinetics made use of shooting techniques (e.g. Hirschfelder, et al.<sup>5</sup>). However, as the kinetics becomes more complex the shooting methods are not useable. Spalding<sup>6</sup> introduced the use of implicit finite difference methods, obtaining the solution of the steady-state problem as the asymptotic limit of a transient problem. Using implicit methods relieved the stiffness and instability problems that caused the shooting methods to fail. Most subsequent treatments of the problem have utilized some variation of Spalding's approach. Much of the early work in premixed flame modeling is summarized in the proceedings of a GAMM-workshop, edited by Peters and Warnatz.<sup>7</sup> Wilde<sup>8</sup> and Kendall and Kelly<sup>9</sup> introduced the idea of solving the steady-state problem directly by finite-difference boundary-value-problem techniques. PREMIX draws on both of these ideas, using a combination of time-dependent and steady-state methods. Furthermore, we have introduced the idea of coarse-to-fine grid refinement as a means to enhance the convergence properties of the steady-state approach and as a means to provide optimal mesh placement.

This model is capable of predicting temperature and species profiles in two laminar premixed flame configurations. The first, and the one most often used for analyzing species profiles in flame experiments, is the burner-stabilized flame with a known mass flow rate. We consider two cases of the burner-stabilized flame -- one where the temperature profile is known and one in which the temperature profile is determined by the energy conservation equation. We have most often used the program when the temperatures were obtained from experiment. In this case, only the species transport equations are solved. In many flames there can be significant heat losses to the external environment, which are of unknown or questionable origin and thus are troublesome to model. However, since the chemistry depends strongly on temperature, it is essential to know the temperatures accurately in order to draw conclusions about the chemical kinetics behavior. We have discovered that if a temperature profile can be measured accurately, then it is often better to use this measurement than the temperature profile obtained by solving an energy conservation equation. For cases where the heat losses are known to be negligible, the program can solve a burner-stabilized flame problem in which the temperatures are determined from

the energy conservation equation. Comparing the two types of burner-stabilized models may provide some indication of the heat losses.

The second flame configuration that we consider is the freely propagating adiabatic flame. In this case there are no heat losses (by definition) and thus the temperatures should be computed from the energy equation. Flame speed depends, in part, on the transport of heat, and predicting the temperature distribution is an integral part of the flame speed calculation.

Chapter 2 presents the conservation equations and associated boundary conditions that are solved in each of the flame configurations we consider. Chapter 3 describes the numerical method used to solve these boundary value problems; it is a combination of a Newton's method and time integration. Chapter 4 then explains how to use the program itself, which is designed to be run in conjunction with two CHEMKIN preprocessors, the CHEMKIN Gas-phase Interpreter, which processes the chemical reaction mechanism, and the TRANSPORT Property preprocessor, which calculates polynomial fits for transport property calculations. After describing how these packages work together, Chapter 5 describes the Keyword input needed to define and solve a particular flame problem, while Chapter 6 discusses post-processing options. Finally, Chapter 7 presents two sample problems.

## 2. PREMIXED FLAME EQUATIONS

The equations governing steady, isobaric, quasi-one-dimensional flame propagation may be written as follows:

$$\text{Continuity:} \quad \dot{M} = \rho u A \quad (1)$$

$$\text{Energy:} \quad \dot{M} \frac{dT}{dx} - \frac{1}{c_p} \frac{d}{dx} \left( \lambda A \frac{dT}{dx} \right) + \frac{A}{c_p} \sum_{k=1}^K \rho Y_k V_k c_{pk} \frac{dT}{dx} + \frac{A}{c_p} \sum_{k=1}^K \dot{\omega}_k h_k W_k = 0, \quad (2)$$

$$\text{Species:} \quad \dot{M} \frac{dY_k}{dx} + \frac{d}{dx} (\rho A Y_k V_k) - A \dot{\omega}_k W_k = 0 \quad (k = 1, \dots, K), \quad (3)$$

$$\text{Equation of State:} \quad \rho = \frac{p \bar{W}}{RT}. \quad (4)$$

In these equations  $x$  denotes the spatial coordinate;  $\dot{M}$  the mass flow rate (which is independent of  $x$ );  $T$  the temperature;  $Y_k$  the mass fraction of the  $k$ th species (there are  $K$  species);  $p$  the pressure;  $u$  the velocity of the fluid mixture;  $\rho$  the mass density;  $W_k$  the molecular weight of the  $k$ th species;  $\bar{W}$  the mean molecular weight of the mixture;  $R$  the universal gas constant;  $\lambda$  the thermal conductivity of the mixture;  $c_p$  the constant-pressure heat capacity of the mixture;  $c_{pk}$  the constant pressure heat capacity of the  $k$ th species;  $\dot{\omega}_k$  the molar rate of production by chemical reaction of the  $k$ th species per unit volume;  $h_k$  the specific enthalpy of the  $k$ th species;  $V_k$  the diffusion velocity of the  $k$ th species; and  $A$  the cross-sectional area of the stream tube encompassing the flame (normally increasing due to thermal expansion). The user may provide a subroutine to specify the area as a function of the spatial coordinate. By default, the stream tube area is taken to be constant and equal to unity.

The net chemical production rate  $\dot{\omega}_k$  of each species results from a competition between all the chemical reactions involving that species. We presume that each reaction proceeds according to the law of mass action and the forward rate coefficients are in the modified Arrhenius form,

$$k_f = AT^\beta \exp\left(\frac{-E_A}{RT}\right). \quad (5)$$

The details of the chemical reaction equations and the thermochemical properties are found in the user's manuals for Gas-phase CHEMKIN, which evaluates these expressions.

In addition to chemical reaction rates, we must also be concerned with the transport properties of the species, i.e., thermal conductivities and diffusion coefficients. Stockmayer potentials are used throughout in evaluating transport properties, as described in the TRANSPORT User's Manual. The user has the option of evaluating transport properties using mixture-averaged formulas or a multicomponent diffusion model (see descriptions of the user Keywords MIX and MULT). Although details of the calculation of transport properties are available in the TRANSPORT manual, a brief description is provided here.

## 2.1 Mixture-Averaged Transport Properties

For the mixture-averaged formula, we assume the diffusion velocity  $V_k$  to be composed of three parts:

$$V_k = V_k^o + W_k + V_c. \quad (6)$$

$V_k^o$  is the ordinary diffusion velocity and is given in the Curtiss-Hirschfelder<sup>10</sup> approximation by

$$V_k^o = -D_{km} \frac{1}{X_k} \frac{dX_k}{dx}, \quad (7)$$

where  $X_k$  is the mole fraction, and where the mixture-averaged diffusion coefficient  $D_{km}$  is given explicitly in terms of the binary diffusion coefficients  $D_{kj}$

$$D_{km} = \frac{1 - Y_k}{\sum_{j \neq k}^K X_j / D_{kj}}. \quad (8)$$

A non-zero thermal diffusion velocity  $W_k$  is included only for the low molecular weight species H, H<sub>2</sub>, and He. The trace, light-component limit is employed in determining  $W_k$ , i.e.,

$$W_k = -\frac{D_{km} \Theta_k}{X_k} \frac{1}{T} \frac{dT}{dx}, \quad (9)$$

where  $\Theta_k$  is the thermal diffusion ratio.<sup>11</sup> The sign of  $\Theta_k$  makes the lower molecular weight species diffuse from low to high temperature regions.

The correction velocity  $V_c$  (independent of species but a function of the distance  $x$ ) is included to insure that the mass fractions sum to unity (or equivalently  $\sum_{k=1}^K Y_k V_k = 0$ ). This formulation of the correction velocity is the one recommended by Coffee and Heimerl<sup>12, 13</sup> in their extensive investigation of approximate transport models in hydrogen and methane flames.

## 2.2 Multicomponent Transport Properties

For the multicomponent option, the transport property evaluation follows the method described by Dixon-Lewis.<sup>14</sup> Multicomponent diffusion coefficients, thermal conductivities and thermal diffusion coefficients are computed through the solution of a system of equations involving the binary diffusion coefficients, the species mole fractions, and the thermodynamic and molecular properties of the species. Details of the matrix of equations, the solution algorithms, and the subsequent determination of multicomponent transport properties are provided by Kee, et al.<sup>15</sup> These equations result in the determination of ordinary multicomponent diffusion coefficients,  $D_{k,j}$ , for species  $k$  diffusing in species  $j$ , as well as species thermal diffusion coefficients and thermal conductivities.

For the multicomponent formulation, the correction velocity,  $V_c$ , is not required and the diffusion velocity is defined as

$$V_k = V_c + W_k. \quad (10)$$

Now, the ordinary diffusion velocity term becomes:

$$W_k = \frac{1}{X_k \bar{M}} \sum_{j \neq k}^K W_j D_{k,j} \mathbf{d}_j, \quad (11)$$

where  $\bar{M}$  is the mean molar mass,  $W_j$  is the molar mass of species  $j$ , and  $\mathbf{d}_j$  is defined as:

$$\mathbf{d}_j = \nabla X_k + (X_k - Y_k) \frac{1}{p} \nabla p.$$

The thermal diffusion velocity is given as:

$$W_k = -\frac{D_k^T}{\rho Y_k} \frac{1}{T} \nabla T, \quad (12)$$

where  $D_k^T$  is the thermal diffusion coefficient for species  $k$ .

## 2.3 Boundary Conditions

We consider two different types of flames: burner-stabilized flames and adiabatic, freely propagating flames. The conservation equations governing the two are the same, but the boundary conditions differ. In both cases the appropriate boundary conditions may be deduced from the early work of Curtiss and Hirschfelder.<sup>10</sup> For burner-stabilized flames  $\dot{M}$  is a known constant, the temperature and mass flux fractions ( $\varepsilon_k = Y_k + \rho Y_k V_k A / \dot{M}$ ) are specified at the cold boundary, and vanishing gradients are imposed at the hot boundary.

For freely propagating flames  $\dot{M}$  is an eigenvalue and must be determined as part of the solution.<sup>16</sup> Therefore, an additional boundary condition is required, or alternatively one degree of freedom must be removed from the problem. We choose to fix the location of the flame by specifying the temperature at one point. This is sufficient to allow for the solution of the flame speed eigenvalue  $\dot{M}$ . The user must select this point in such a way as to insure that the temperature and species gradients “nearly” vanish at the cold boundary. If this condition is not met then the resultant  $\dot{M}$  will be too low because some heat will be lost through the cold boundary. The details of the fixed temperature condition are explained more fully in Chapter 3.

### 3. NUMERICAL SOLUTION METHOD

The numerical solution procedure begins by making finite difference approximations to reduce the boundary value problem to a system of algebraic equations. The initial approximations are usually on a very coarse mesh that may have as few as five or six points. After obtaining a solution on the coarse mesh, new mesh points are added in regions where the solution or its gradients change rapidly. We obtain an initial guess for the solution on the finer mesh by interpolating the coarse mesh solution. This procedure continues until no new mesh points are needed to resolve the solution to the degree specified by the user. This continuation from coarse to fine meshes has several important benefits that are explained later in this chapter. We attempt to solve the system of algebraic equations by the damped modified Newton algorithm. However, if the Newton algorithm fails to converge, the solution estimate is conditioned by integration in time. This provides a new starting point for the Newton algorithm that is closer to the solution, and thus more likely to be in the domain of convergence for Newton's method. As the mesh becomes finer we normally find that the estimate interpolated from the previous mesh is within the domain of convergence of Newton's method. This point is key to the solution strategy.

#### 3.1 Finite Difference Approximations

The first task in solving the flame problem is to discretize the governing conservation equations. We use finite difference approximations on a nonuniform grid with points numbered from 1 at the cold boundary to  $J$  at the hot boundary. On the convective terms the user has the choice of using either first order windward differences or central differences. Both cases are illustrated using the convective term in the energy equation. The windward difference is given as

$$\left( \dot{M} \frac{dT}{dx} \right)_j \approx \dot{M}_j \left( \frac{T_j - T_{j-1}}{x_j - x_{j-1}} \right), \quad (13)$$

where the index  $j$  refers to the mesh point. The central difference formula is

$$\left( \dot{M} \frac{dT}{dx} \right)_j \approx \dot{M}_j \left( \frac{h_{j-1}}{h_j(h_j + h_{j-1})} T_{j+1} + \frac{h_j - h_{j-1}}{h_j h_{j-1}} T_j - \frac{h_j}{h_{j-1}(h_j + h_{j-1})} T_{j-1} \right), \quad (11)$$

where  $h_j = x_{j+1} - x_j$ . The windward difference formulas introduce artificial diffusion on a coarse mesh; this has the effect of spreading out the solution and making the convergence of Newton's method less sensitive to the starting estimate. However, because the mesh is refined in regions of high gradient, the artificial diffusion becomes relatively unimportant after the solution has progressed to the fine meshes.

Nevertheless, for a given mesh, the windward difference approximation is less accurate than the central difference formula. Therefore, the user may want to select the central difference formula on finer meshes or in cases where the solution is converging without difficulty.

The first derivative in the summation term in the energy equation (2) is always approximated by a central difference formula,

$$\left(\frac{dT}{dx}\right)_j \approx \left(\frac{h_{j-1}}{h_j(h_j + h_{j-1})}T_{j+1} + \frac{h_j - h_{j-1}}{h_j h_{j-1}}T_j - \frac{h_j}{h_{j-1}(h_j + h_{j-1})}T_{j-1}\right), \quad (15)$$

and the coefficients in the summation are evaluated at  $j$ .

The second derivative term in the energy equation is approximated by the following second order central difference.

$$\frac{d}{dx}\left(\lambda A \frac{dT}{dx}\right)_j \approx \left(\frac{2}{x_{j+1} - x_{j-1}}\right) \left[ \lambda A_{j+1/2} \left(\frac{T_{j+1} - T_j}{x_{j+1} - x_j}\right) - \lambda A_{j-1/2} \left(\frac{T_j - T_{j-1}}{x_j - x_{j-1}}\right) \right] \quad (16)$$

The coefficients in this formula (at  $j \pm 1/2$ ) are evaluated using the averages of the dependent variables between mesh points.

The diffusive term in the species conservation equation is approximated in a similar way, but it appears to be different because we have written it using diffusion velocities. The ordinary (Eq. (7)) and thermal (Eq. (9)) diffusion velocities are approximated at the  $j \pm 1/2$  positions as illustrated by the following mixture-averaged evaluation:

$$(Y_k V_k)_{j+1/2} \approx -\left(\frac{W_k D_{km}}{\bar{W}}\right)_{j+1/2} \left(\frac{X_{k,j+1} - X_{k,j}}{x_{j+1} - x_j}\right), \quad (17)$$

and

$$(Y_k W_k)_{j+1/2} \approx \left(\frac{W_k D_{km} \Theta_k}{WT}\right)_{j+1/2} \left(\frac{T_{j+1} - T_j}{x_{j+1} - x_j}\right). \quad (18)$$



Since the mole fraction of a species can be zero, we avoid difficulties by forming  $Y_k V_k$ , which is the expression needed in Eq. (3), rather than  $V_k$  itself ( $Y_k = X_k W_k / \bar{W}$ ). After the diffusion velocities are computed at all the mesh midpoints, the correction velocity  $V_c$  is computed at the midpoints from

$$V_c = -\sum_{k=1}^K Y_k (V_k + W_k). \quad (19)$$

Upon forming the full diffusion velocities  $V_k = V_k + W_k + V_c$  the diffusion term is evaluated with the following difference approximation.

$$\frac{d}{dx} (\rho A Y_k V_k)_j \approx \frac{(\rho A Y_k V_k)_{j+1/2} - (\rho A Y_k V_k)_{j-1/2}}{x_{j+1/2} - x_{j-1/2}} \quad (20)$$

All the non-differentiated terms, such as the chemical production rate terms, are evaluated at the mesh points  $j$ . Coefficients not appearing within derivatives are also evaluated at the mesh points.

### 3.2 Boundary Conditions

The boundary conditions are relatively easily implemented. At the cold boundary we specify the mass flux fractions and the temperature, i.e. we solve

$$\varepsilon_{k,l} - Y_{k,l} - \left( \frac{\rho A Y_k V_k}{\dot{M}} \right)_{j=1/2} = 0, \quad (21)$$

and

$$T_1 - T_b = 0, \quad (22)$$

where  $\varepsilon_{k,l}$  is the inlet reactant fraction of the  $l$ th species (see Keyword REAC) and  $T_b$  is the specified burner temperature. At the hot boundary we specify that all gradients vanish, i.e.,

$$\frac{Y_{k,J} - Y_{k,J-1}}{x_J - x_{J-1}} = 0, \quad (23)$$

and

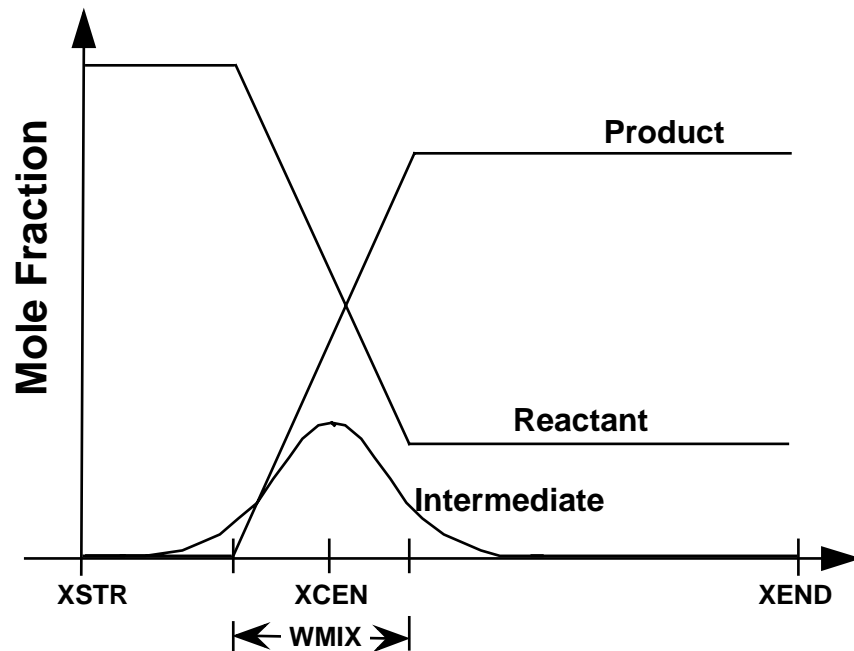
$$\frac{T_J - T_{J-1}}{x_J - x_{J-1}} = 0, \quad (24)$$

The boundary conditions for  $\dot{M}$  depend on whether the given problem is a burner-stabilized or a freely propagating flame. The boundary conditions for each case are discussed in Section 2.3.

### 3.3 Starting Estimates

The program needs a starting estimate of the solution from which to begin its iteration. The general form of this estimate is shown in Figure 1. For this estimate we presume that there is a reaction zone in which the reactants change from their unreacted values (the unburned composition) to the products. The user is asked to provide estimates for the location and thickness of this reaction zone. He also needs to estimate the product species (the fully burned composition). If no product species estimates are given, the program will generate an equilibrium composition for a product estimate; the user can provide a minimum value to be applied to the resulting products.

Within the reaction zone the program uses straight lines between the initial and final values for both the reactants and products. On the cold side of the reaction zone the reactant species profiles are flat at the unburned values. On the hot side, the product species are flat at the estimated product values. Note that any given species can be both a reactant and a product species. For example, the nitrogen in a hydrocarbon-air flame will be both a reactant and a product. The excess fuel in a rich flame will also be both a reactant and a product. Species can also be identified as “intermediates.” Intermediates, such as short-lived radical species, are assumed to have a Gaussian profile that peaks in the center of the reaction zone. The peak height is specified in the input to the program, and the Gaussian’s width is such that the profile is at 1/10 of its peak value at the edges of the reaction zone.



**Figure 1. The general form of the starting estimate.**

We find that the shape of the assumed species profiles is not too important. Smoother functions, such as cubic polynomials and hyperbolic tangents for the reactant and product species, have no apparent effect on the convergence properties of the method. Since the starting profiles are typically evaluated on a very coarse mesh, it makes little difference whether the underlying function is smooth or not. Therefore, in the program we simply use linear starting profiles.

### 3.4 User-Specified Temperature Profile

It is often our preference from a physical point of view to model burner-stabilized flames using a known temperature profile. Doing so eliminates the need to model heat losses in the energy equation, but it does require that the program's user be able to provide a temperature profile. There are also computational advantages to using a known temperature profile. The most severe nonlinearities in chemical kinetics come from the exponential dependence of the reaction rates on temperature. Thus, eliminating the temperature from the iteration makes the flame problem considerably easier to solve.

We find that even if the energy equation is to be solved for the temperature distribution, the iteration converges more reliably if the species profiles are first computed using a fixed temperature profile. Recall that the program begins iterating from a user-specified "guess" at the solution. So, the strategy is to iterate for the species distributions using the "guessed" temperatures. This serves to generate better guesses for the species profiles than the user is typically able to provide. Species profiles computed in this way have some degree of self-consistency. Only after a converged solution is obtained with the

temperatures held fixed is the energy equation included in the iteration. Thus, even in cases where the program attempts to solve the energy equation, we require the program's user to input an estimate of the temperature profile.

The user input for the temperature profiles is in the form of position-temperature pairs. In general, the mesh used by the flame program will not be the same as the one on which the given temperature estimate is defined. The program uses a linear interpolation of the given temperatures onto the current mesh. Thus, especially in the case of a burner-stabilized flame where the energy equation is not included, it is important for the user to provide enough temperature points that the profile is well resolved and relatively smooth.

### 3.5 Modified Damped Newton's Method

The PREMIX uses the modular solver routine TWOPNT to solve the boundary value problem. The method by which TWOPNT arrives at a solution to the governing equations is described here in detail. After discretization on a given mesh, we have a system of nonlinear algebraic equations that TWOPNT attempts to solve by a damped Newton's method. Newton's method determines a sequence of iterations or approximate solutions that approach the true solution. For the sake of notational ease we call these approximate solution vectors  $\phi$ . When any arbitrary  $\phi$  is substituted into the finite difference analog of Eqs. (2) and (3) they do not equal zero as they would if the true solution were substituted; in general they equal a residual vector that we will call  $F$ . Thus our purpose is to find a vector  $\phi$  that satisfies

$$F(\phi) = 0. \quad (25)$$

In our case the vector  $\phi$  is composed as follows:

$$\phi = (T_1, Y_{1,1}, \dots, Y_{K,1}, \dot{M}_1, \dots, T_j, \dots, Y_{k,j}, \dots, \dot{M}_j, \dots, T_J, Y_{1,J}, \dots, Y_{K,J}, \dot{M}_J)^T \quad (26)$$

The corresponding  $F$  vector is composed of the residuals of the energy equation, the species equation, and an equation specifying that  $d\dot{M}/dx = 0$ . The final equation is included for purposes of maintaining a banded Jacobian structure; this is discussed in more detail in Section 3.6. The ordering of the  $F$  vector corresponds to the order of the  $\phi$  vector; it begins with the residuals of the left boundary condition  $j = 1$ , followed by the residuals at the interior mesh points, and finally the residuals at the right boundary,  $j = J$ .

Provided the initial estimate  $\phi^{(0)}$  of the solution is sufficiently good, Newton's method produces a sequence  $\{\phi^{(n)}\}$  that converges to the solution of the nonlinear equations  $F(\phi)$ . The purest form of the algorithm

$$\phi^{(n+1)} = \phi^{(n)} - \left( \frac{\partial F}{\partial \phi} \right)_{\phi^{(n)}}^{-1} F(\phi^{(n)}) \quad (27)$$

is too expensive and delicate to be used in practice. On the one hand, evaluation of the Jacobian matrices  $\partial F / \partial \phi$  by numerical or other means is time consuming, and on the other hand, convergence usually requires a very good initial estimate  $\phi^{(0)}$ . The program employs the usual remedies. First, the Jacobian matrix is replaced by one,  $J^{(n)}$ , inherited from a previous step of the algorithm. Second, the full step from  $\phi^{(n)}$  to  $\phi^{(n+1)}$  may be cut short by a damping parameter  $\lambda^{(n)}$ . In this way the iteration becomes

$$\phi^{(n+1)} = \phi^{(n)} - \lambda^{(n)} (J^{(n)})^{-1} F(\phi^{(n)}) \quad (28)$$

where,  $0 < \lambda^{(n)} \leq 1$ , and

$$J^{(n)} = J^{(n-1)} \text{ or } J^{(n)} = \left( \frac{\partial F}{\partial \phi} \right)_{\phi^{(n)}} \quad (29)$$

Of course, the inverse Jacobian matrix in Eq. (28) is not computed; instead a system of linear equations  $J^{(n)} \Delta \phi^{(n)} = F(\phi^{(n)})$  is solved for the undamped correction vector  $\Delta \phi^{(n)}$ .

Our selection of the matrix  $J^{(n)}$  and of the parameter  $\lambda^{(n)}$  is governed by a look-ahead procedure that forces certain behavior upon the algorithm. Thus, having tentatively chosen  $\phi^{(n+1)}$  the program looks ahead to the calculation of  $\phi^{(n+2)}$ . The criterion<sup>17</sup> for accepting  $\phi^{(n+1)}$  is that the undamped steps decrease in magnitude,

$$\left| (J^{(n)})^{-1} F(\phi^{(n+1)}) \right| < \left| (J^{(n)})^{-1} F(\phi^{(n)}) \right| \quad (30)$$

This prevents the iteration from stepping away from the region where there is good reason to believe a solution lies. Should  $\phi^{(n+1)}$  fail this criterion, the program rejects it and retries the step with a halved

damping parameter or a new Jacobian matrix. The damping parameter  $\lambda^{(n)}$  is initially chosen to be as large as possible so that  $\phi^{(n+1)}$  does not violate various bounds that are set on the solution variables. We know, for example, that the temperature and mass flow rate must be positive, and that the species' mass fractions must be between zero and one. The concentrations of many species, such as fuels downwind of the flame, are close to zero and frequently threaten to place the solution out of bounds.

The Newton iteration continues until the maximum norm of the undamped correction vector  $\Delta\phi$  is reduced to within a user-specified tolerance. Specifically, the criteria for Newton iteration convergence is when the solution correction vector  $\Delta\phi$  satisfies

$$|\Delta\phi| \leq \max(A, R \times |\phi|), \quad (31)$$

The relative  $R$  and absolute  $A$  tolerances are parameters that govern the convergence criteria for the Newton iteration. Roughly speaking the relative tolerance indicates how many significant digits the converged solution should contain, and the absolute tolerance serves to exclude solution components smaller than  $A$  from the relative convergence criteria. Typically, the absolute tolerance  $A$  should be smaller than the maximum mass fraction of any species of interest. The relative tolerance should be in the range of  $10^{-3}$  to  $10^{-4}$ , which will serve to provide 3 to 4 digits of accuracy.

If damping cannot produce a suitable correction, then a new Jacobian is computed. If, after computing a new Jacobian, a damped Newton step still cannot produce a suitable correction, then the program begins to take time steps. This strategy is described further in Section 3.8.

### 3.6 Jacobian Matrix

The Jacobian is a large, banded (actually block tridiagonal) matrix. In principle, we could derive and evaluate analytic expressions for the Jacobian elements. However, because this is a difficult and error-prone task, and because the modified Newton method works well with old (and hence inaccurate) Jacobians, the effort to develop analytic Jacobian expressions is not warranted. Instead, we form the elements of the Jacobian by finite difference perturbations in the manner suggested by Curtis, et al.<sup>18</sup> Specifically, we evaluate a one-sided finite difference formula,

$$J_{i,j} \approx \frac{F_i(\phi_j + \delta) - F_i(\phi_j)}{\delta}, \quad (32)$$

where

$$\delta = r \times \phi_j + a. \quad (33)$$

We choose the relative and absolute perturbations,  $r$  and  $a$ , to be the square root of the computer's unit roundoff.

It can be seen from Eq. (32) that with a single perturbation of  $\phi_j$ , an entire column  $i$  of  $J$  can be computed. Moreover, because the Jacobian is banded, several of its columns can be evaluated at once. When two or more columns share no non-zero rows, then they can be evaluated numerically by a single perturbation of the  $\phi$  vector. Since evaluating the Jacobian and computing its LU decomposition are by far the most expensive parts of the flame computation, taking advantage of the Jacobian's structure is essential to producing an efficient program.

A special treatment of the variable  $\dot{M}$  is important in maintaining the Jacobian's banded structure. For the adiabatic flame problem the mass flow rate  $\dot{M}$  is a dependent variable that must be computed as part of the solution. By looking at Eqs. (2) and (3), one can easily see that the equations at each mesh point depend on  $\dot{M}$ . Moreover,  $\dot{M}$  has no spatial dependence; it is a single number for any given flame. Recall that the Jacobian provides information on how a perturbation of any variable affects the residual of any equation. It is evident that a perturbation of  $\dot{M}$  affects the residuals at each mesh point. Thus, if  $\dot{M}$  were stored as a single variable in the dependent variable vector  $\phi$ , rather than as indicated in Eq. (26), then the Jacobian would not have a banded structure. There would be one full column corresponding to the dependence of each residual equation on  $\dot{M}$ .

We resolve this dilemma by defining a variable  $\dot{M}_j$  at each mesh point, and then solving an additional equation stating that they are all equal, i.e.,

$$\frac{d\dot{M}}{dx} = 0. \quad (34)$$

Equation (34) represents the introduction of a new first-order differential equation to the system and thus requires the introduction of an additional boundary condition. In the case of the burner-stabilized flame, the needed boundary condition is that the incoming flow rate is specified on the left boundary. In this case the finite difference analog of Eq. (34) is simply

$$\frac{\dot{M}_j - \dot{M}_{j-1}}{x_j - x_{j-1}} = 0. \quad (35)$$

For the burner-stabilized problem this whole procedure is trivial because  $\dot{M}$  is not really a variable; it is a parameter that is user-specified and it does not change in the course of the solution. We treat the problem in this way so that the data storage structure in the program is the same for both burner-stabilized and freely propagating flames. Having the same data structure is important in restarting one flame from another and in post-processing the results.

In the case of the freely propagating flame the introduction of Eq. (34) is essential to an efficient solution procedure. Recall that for the freely propagating flame configuration we added an interior boundary condition that anchored the temperature at one mesh point and thus defined a flame-fixed coordinate system. This is the additional boundary condition that is needed to compute the flame speed  $\dot{M}$ , which is now a dependent variable. For the sake of notation, let us say that we fix a temperature  $T_f$  at mesh point  $j_f$ . Then for  $j < j_f$ , the forward-differenced finite difference equation to be solved is

$$\frac{\dot{M}_j - \dot{M}_{j-1}}{x_j - x_{j-1}} = 0, \quad (36)$$

which is the same as Eq. (35). At  $j = j_f$  we solve

$$T_{j_f} - T_f = 0. \quad (37)$$

And, for  $j > j_f$  we use a backward difference formula,

$$\frac{\dot{M}_{j+1} - \dot{M}_j}{x_{j+1} - x_j} = 0. \quad (38)$$

### 3.7 Adaptation

We have found that starting the iteration on a coarse mesh has several important advantages. One is that the Newton iteration is more likely to converge on a coarse mesh than on a fine mesh. Moreover, the number of variables is small on a coarse mesh and thus the cost per iteration is relatively small. Since the iteration begins from a user-specified “guess” at the solution, it is likely that many iterations will be required. Ultimately, of course, to be accurate, the solution must be obtained on a fine mesh. However, as the solution is computed on each successively finer mesh, the starting estimates are better, since they come from the converged solution on the previous coarse mesh. In general, the solution on one mesh lies



within the domain of convergence of Newton's method on the next finer mesh.<sup>19</sup> Thus, even though the cost per iteration is increasing, the number of required iterations is decreasing.

The adaptive placement of the mesh points to form the finer meshes is done in such a way that the total number of mesh points needed to represent the solution accurately is minimized. Specifically, we place the mesh points in the following way. To resolve the gradients we bound the variation in the solution components between mesh points as

$$\left| \phi_{n,j} - \phi_{n,j-1} \right| \leq \delta (\max \phi_n - \min \phi_n), \quad (39)$$

and to resolve the curvature in the solution we bound the variation in the solution's derivatives between mesh points by

$$\left| \left( \frac{d\phi_n}{dx} \right)_j - \left( \frac{d\phi_n}{dx} \right)_{j-1} \right| \leq \gamma \left( \max \frac{d\phi_n}{dx} - \min \frac{d\phi_n}{dx} \right). \quad (40)$$

In the program, we evaluate the above expressions between each of the mesh points. In each of the subintervals where the inequality is not satisfied, a new mesh point is placed at the midpoint of the subinterval. The parameters  $\delta$  and  $\gamma$  are user-specified input parameters. We exclude variables that are below a certain floor value from consideration in the adaptation. This avoids adapting on variables that are essentially zero, but due to rounding errors may show locally high derivatives. The starting estimate for the dependent variable vector  $\phi$  is determined by a linear interpolation of the coarse mesh solution onto the new finer mesh. After determining a converged solution on this new fine mesh, the adaptation procedure is performed once again. A sequence of solutions on successively finer meshes is computed until the inequalities in Eqs. (39) and (40) are satisfied between all mesh points.

### 3.8 Time Stepping

The steady-state flame solution that we seek is the result of some physical transient process. Determining the steady solution by solving the transient equations is a very reliable, but often slow, process. Therefore, we attempt to use a Newton method that converges very rapidly, when it converges. In our earliest programs we only used Newton iteration. When the iteration did not converge, the user had to make a new starting estimate for the initial iterate and try again. This was a time consuming and often frustrating process.

Others who have modeled premixed flames often used a transient computation (see, for example, the proceedings of the GAMM-workshop on Numerical Methods in Laminar Flame<sup>7</sup>). Those who used transient methods reported fewer convergence difficulties, but their computation was less efficient than the Newton method, when the Newton method is convergent. Therefore, we began to use a combination of the two methods. We always try to take a Newton step, but if it is having convergence difficulties, we take some time steps. The time stepping is just a way to go from one trial solution that is not within the domain of Newton convergence to one that is. The user specifies the size of the time step and number of time steps to be taken.

The transient equations are obtained by adding the time derivatives to Eqs. (2) and (3), obtaining,

$$\rho A \frac{\partial T}{\partial t} + \dot{M} \frac{\partial T}{\partial x} - \frac{1}{c_p} \frac{\partial}{\partial x} \left( \lambda A \frac{\partial T}{\partial x} \right) + \frac{A}{c_p} \sum_{k=1}^K \rho Y_k V_k c_{pk} \frac{\partial T}{\partial x} + \frac{A}{c_p} \sum_{k=1}^K \dot{\omega}_k h_k W_k = 0, \quad (41)$$

and

$$\rho A \frac{\partial Y_k}{\partial t} + \dot{M} \frac{\partial Y_k}{\partial x} + \frac{\partial}{\partial x} (\rho A Y_k V_k) - A \dot{\omega}_k W_k = 0 \quad (k = 1, \dots, K). \quad (42)$$

The full system now becomes a system of parabolic partial differential equations, rather than an ordinary differential equation boundary value system. Solution is obtained via the backward Euler method. In this method, the time derivatives are approximated by finite differences as illustrated by

$$\rho A \frac{\partial T}{\partial t} \approx \rho_j^{n+1} A_j \frac{T_j^{n+1} - T_j^n}{h} \quad (43)$$

where the superscript  $n$  indicates the time level and  $h$  represents the size of the time step. All other terms are approximated with finite differences as before, but at time level  $n+1$ . Since all variables are known at time level  $n$ , the discretized problem is just a system of nonlinear algebraic equations for the dependent variable vector  $\phi$  at time level  $n+1$ .

To solve the system for each time step we use the same Newton method as we attempted to use to solve the steady-state boundary value problem in the first place. However, the transient problem is much more likely to converge. It should always converge for a sufficiently small time step. From a physical point of view, as the time step approaches zero, the solution for  $t^{n+1}$  should approach the initial condition or the

solution at  $t^n$ ; thus convergence should be rapid and reliable. From a mathematical point of view, the Jacobian of the transient system has a factor  $1/h$  on the diagonal. Therefore, the condition number of the Jacobian will be reduced as the time step is reduced. The objective is to choose a time step that is large enough to make progress toward the steady solution, but not so large that the transient method also has convergence difficulties. We typically use time steps of around one to ten microseconds, although there are often cases where much smaller time steps are needed.

After taking the specified number of time steps, the program again attempts to solve the steady problem by Newton's method. If it fails again it once again reverts to time stepping. Naturally, the better the user is at making initial guesses at the solution, the less the program will have to time step. If the program fails to converge on a time step, the user has two choices: one is to choose smaller time steps, the other is to try a new starting estimate.

### 3.9 Sensitivity Analysis

Sensitivity analysis is a way to understand quantitatively how the solution to a model depends on parameters in the model. Once the Jacobian has been computed for the purposes of solving the boundary value problem, the sensitivity coefficients can be computed easily. These techniques have been developed and used in the chemical engineering literature for some time (see Stewart and Sørensen,<sup>20</sup> Brown, et al.,<sup>21</sup> and Saito and Scriven<sup>22</sup>). We find that sensitivity analysis is often an invaluable tool in helping to interpret the results of a flame model (see, for example, Miller, et al.<sup>4</sup>). Coffee and Heimerl<sup>13</sup> have also discussed the use of sensitivity analysis in flame modeling, although their computational method is quite different from the one used here. Also, Reuven, et al.,<sup>23</sup> using model problems, have explored various ways that sensitivity analysis can be applied to flames.

Here we consider the first-order sensitivity coefficients of the solution profiles with respect to the reaction rate coefficients. To specify the sensitivity coefficients, let us begin with the boundary-value problem stated in the abstract notation that we introduced in Eq. (25),

$$F(\phi; \alpha) = 0. \quad (44)$$

Note, however, that now we have introduced the idea that the equation may be parameterized by some parameters  $\alpha$ . In our case, these  $\alpha$ 's will be the "A-factors" of the reaction rate coefficients. By differentiating Eq. (44) with respect to  $\alpha$  we obtain a matrix equation for the sensitivity coefficients.

$$\frac{\partial F}{\partial \phi} \frac{\partial \phi}{\partial \alpha} + \frac{\partial F}{\partial \alpha} = 0. \quad (45)$$

The matrix  $\partial F/\partial\phi$  is the Jacobian of the original system and  $\partial F/\partial\alpha$  is the matrix of partial derivatives of  $F$  with respect to the parameters. We will think of the  $\partial F/\partial\alpha$  matrix column by column, with each column indicating the dependence of the residual vector  $F$  on the parameters. There are as many columns as there are parameters, i.e. reactions. The sensitivity coefficients are defined by  $\partial\phi/\partial\alpha$ . This matrix contains quantitative information on how each reaction rate coefficient affects the temperature and species profiles (and the flame speed) at each point in the flame. The sensitivity matrix has a structure similar to that of the  $\partial F/\partial\alpha$  matrix. That is, each column shows the dependence of the solution vector on a particular reaction.

The Jacobian and its LU factorization are already available from the solution of the original system by Newton's method, and the parameter derivatives are computed by finite differences in a manner similar to computation of the Jacobian. Therefore, the linear system of equations (45) is readily solved for each column of the sensitivity matrix, corresponding to the sensitivities of the solution vector to each of the  $I$  reaction rates. The LINPACK software is used to perform these computations. It is set up so that the Jacobian is factored only once, and each column of the sensitivity matrix is computed by back substitution, a relatively inexpensive operation.

We find that some manipulation of the raw sensitivity coefficients makes them more useful. First, we compute normalized sensitivity coefficients in the form of logarithmic derivatives, i.e.

$$\frac{\alpha_i}{Y_k} \frac{\partial Y_k}{\partial \alpha_i} \quad (46)$$

or

$$\frac{\alpha_i}{T} \frac{\partial T}{\partial \alpha_i} \quad (47)$$

In the case that the user specifies that he wants to work in molar quantities, rather than mass quantities, we compute the sensitivity coefficients in terms of mole fractions, i.e.,

$$\frac{\alpha_i}{X_k} \frac{\partial X_k}{\partial \alpha_i} = \frac{\alpha_i}{Y_k} \frac{\partial Y_k}{\partial \alpha_i} - \alpha_i \bar{W} \sum_{j=1}^K \frac{1}{W_j} \frac{\partial Y_j}{\partial \alpha_i} \quad (48)$$

where  $X_k$  are the mole fractions and  $\bar{W}$  is the mean molecular weight. Finally, we find that sensitivity coefficients are more useful when they are normalized by the maximum value of each dependent variable. For example, we might compute

$$\frac{\alpha_i}{Y_k^{\max}} \frac{\partial Y_k}{\partial \alpha_i}, \quad (49)$$

where  $Y_k^{\max}$  is the maximum mass fraction of the  $k$ th species in the flame. This normalization avoids artificially high sensitivity coefficients in regions where the mass fractions are approaching zero, and thus subject to numerical errors. However, the “maximum” normalization is not done in PREMIX and is left as a suggestion to the user in designing a postprocessor for his or her own purposes.

## 4. PROGRAM STRUCTURE

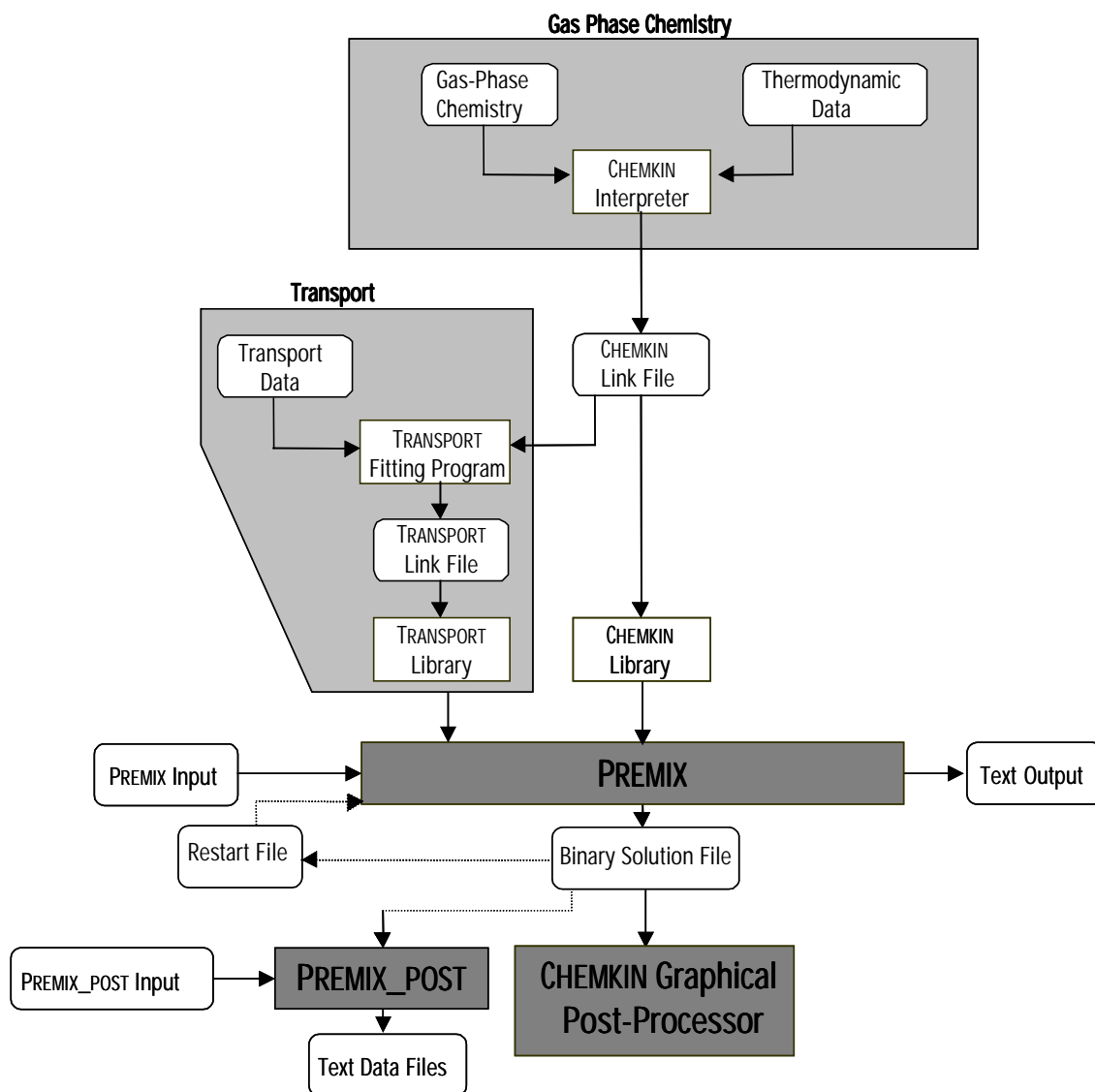
The CHEMKIN Application User Interface runs the PREMIX program automatically through a mouse-driven interface and then allows the user to directly launch visualization of solution results using the CHEMKIN Graphical Post-processor. The PREMIX program has a modular structure with interfaces to the CHEMKIN Utility package for obtaining kinetic, thermodynamic, and transport parameters. In addition to input directly from the user, PREMIX depends on data obtained from the CHEMKIN Gas-phase and TRANSPORT packages. Therefore, to solve a flame problem the user must first execute the two preprocessor programs, “chem” and “tran”, which have access to thermodynamic and transport-property databases. PREMIX then reads input from the user (described in Chapter 5), defines the governing equations, makes calls to the boundary value solver (TWOPT), and prints solutions for the flame problem. The CHEMKIN Graphical Post-processor can then be launched from the Application User Interface to plot solution data. Figure 2 shows the relationships between these components. For more information about the CHEMKIN Application User Interface or Graphical Post-processor, please see the CHEMKIN Getting Started manual.

The first step is to execute the CHEMKIN Interpreter, “chem”. The CHEMKIN Interpreter first reads user-supplied information about the species and chemical reactions for a particular reaction mechanism. It then extracts further information about the species’ thermodynamic properties from a database, “therm.dat”. The user may also optionally input thermodynamic property data directly in the input file to the CHEMKIN Interpreter to override or supplement the database information. The information from the user input and the thermodynamic properties is stored in the CHEMKIN Linking File, “chem.asc”; a file that is needed by the TRANSPORT property fitting program, “tran”, and later by the CHEMKIN subroutine library, which will be accessed by the PREMIX program.

The next program to be executed is the TRANSPORT property-fitting program, “tran”. It needs input from a transport property database, “tran.dat” and from the CHEMKIN subroutine library. The user may also optionally input transport property data directly in a separate input file (e.g. “tran.inp”) to override or supplement the database information. The purpose of the TRANSPORT fitting program is to compute polynomial representations of the temperature-dependent parts of the individual species viscosities, thermal conductivities, and the binary diffusion coefficients. Like the CHEMKIN Interpreter, the TRANSPORT property-fitting program produces a Linking File, “tran.asc” that is later needed in the transport property library routines, which will evaluate mixture properties during the course of the flame computation.

PREMIX makes appropriate calls to the CHEMKIN and the TRANSPORT libraries to initialize the species- and reaction-specific information. The purpose of the initialization is to read the Linking Files and set up the internal working and storage space required by all subroutines in the libraries.

PREMIX reads the input that defines a particular flame and any other needed parameters in a Keyword format from the input file (e.g. "premix.inp"). In addition, there is a provision for the flame program to begin its iteration from a previously computed flame solution. In this case the old solution is read from a binary Restart File, called "rest.bin". The flame program produces printed output (e.g. "premix.out") and it saves the solution in a binary Save File, "save.bin". The Save File can be used to restart PREMIX to provide, for example, a starting estimate for a different flame that may have different unburned species compositions or flow rates. The Restart File is the same format as the Save File; a Restart File can therefore be created simply by copying a Save File, e.g. "save.bin" to the Restart File name, e.g. "rest.bin".



**Figure 2. Relationship of the PREMIX Program to the CHEMKIN and TRANSPORT Preprocessors, and to the Associated Input and Output files.**

## 4.1 Optional User Programming

In addition to using PREMIX through the CHEMKIN Application User Interface, users have the flexibility to write their own interface to the flame model. To facilitate this, the PREMIX program itself is written as a Fortran subroutine that may be called from a user-supplied driver routine. We provide examples of such driver routines as part of the PREMIX software distribution, written in both C++ and Fortran. The driver routine performs the function of allocating total memory usage through definition of array sizes, as well as opening input and output files. PREMIX checks internally to make sure that the allocated work arrays are sufficiently large to address the problem described by the input files. Programs can be linked to the PREMIX subroutine by following the examples in the makefiles provided in the sample driver subdirectories (“drivers\_f77” or “drivers\_cpp”) of the standard distribution. Users taking advantage of this flexibility should be experienced with compiling and linking program files on their operating system and must have either a C++ or Fortran compiler installed.

In addition to the driver routine, the user can provide a function that specifies the stream tube area, relative to the burner area, for a burner-stabilized flame, when this information is available. An example of such an AREA function such as is shown in Figure 3. If the user has no information about the streamtube area, then the area can simply be set to the burner area everywhere. In this case the AREA function returns the area divided by the burner area equal to 1.0, as is shown in Figure 3. However, if the area can be estimated or measured as a function of distance from the burner, then FUNCTION AREA(X) can be used to communicate that information to the flame program. The source-code for the default AREA function that is called by PREMIX is included in the CHEMKIN Collection distribution, with the PREMIX driver programs. As an alternative to writing and compiling a user FUNCTION AREA, the flame-tube area can be specified through the input keyword APRO, as described in Section 5.4. This latter option does not require any compiling or linking of source code.

```
DOUBLE PRECISION FUNCTION AREA(X)
  IMPLICIT DOUBLE PRECISION (A-H, O-Z), INTEGER (I-N)
C
C X is the distance from the burner face in centimeters
C A is the area of the flame streamtube divided by the burner area.
C   In this example, A is constant.
C
  AREA = 1.0
C
  RETURN
END
```

**Figure 3. Example of a user function to pass the local flame streamtube area divided by the burner area to the PREMIX program.**

## 4.2 Save, Restart, and Recover Files

In addition to printed output the program produces a binary Save File (“save.bin”) that contains the solution and the first order sensitivity coefficients, if they were requested. This file has several uses. The



solution in the file can be an initial estimate for a different calculation, through the restart option. It often saves computer time to begin a computation for a given set of conditions by starting with the solution of another set of conditions that are in some way related. In the case of a restart, the PREMIX reads the input keywords to specify some of the parameters, but the initial solution estimate will be read from the Restart file.

The binary solution Save File is written after the solution to a problem is complete. However, another file, the Recover File, is rewound and written after every successful return from a Newton iteration or a sequence of time steps. In the event that the program fails to complete a problem for some reason it may be possible to restart it from the Recover File. Starting from Recover File, but with different keyword inputs (for example a different time step) may be more efficient than restarting the problem from the beginning.

The binary solution file is also used to post-process the solution. Further information on this subject can be found in Chapter 6 of this document.

## 5. PROGRAM INPUT

### 5.1 Keyword Syntax and Rules

The PREMIX program's input is in a Keyword format. On each input line, an identifying Keyword must appear first. For some Keywords only the Keyword itself is required, while for others, additional information is required. Some Keywords have default values associated with them and in such cases the Keyword card need not be included. In the case of restarts or continuation problems, some of the Keywords can be changed. If not changed, they retain their former values. In each Keyword description, we note whether or not it can be changed upon a restart or continuation. The order of the Keyword inputs is generally unimportant, except in the case of some grouped lists that must be ordered. The rules governing the syntax of the Keyword images are listed below:

1. The first four characters of the line are reserved for the Keyword, and it must begin at the first column.
2. Any further input associated with the Keyword can appear anywhere in columns 5 through 80. The specific starting column is not important.
3. When more than one piece of information is required, the order in which the information appears is important.
4. When numbers are required as input, they may be stated in either integer, floating point, or "E" format. The program converts the numbers to the proper type. The double precision specification is not recognized; however, conversion to double precision is done internally as necessary.
5. When species names are required as input, they must appear exactly as they were specified in the CHEMKIN input. This input is case sensitive.
6. When more than one piece of information is required, the pieces are delimited by one or more blank spaces.
7. If more information is input than required, then the inputs that are read last are used. For example, if the same Keyword is encountered twice, the second one read is taken.
8. A "comment" line can be inserted by placing either a period (.) or a slash (/) in the first column. Such a line is ignored by the program, but it is echoed back in the printed output. In addition, on any Keyword line, any input that follows the required input and is enclosed in parentheses is taken as a comment.
9. The Keyword END must be the last input card.

## 5.2 Problem Type Keywords

- BURN**— Inclusion of this Keyword means that the problem is to solve a burner-stabilized flame.  
Default—none, either BURN or FREE is required.  
Restart—can be changed.
- FREE**— Inclusion of this Keyword means that the problem is to solve an adiabatic, freely propagating flame.  
Default—none, either BURN or FREE is required.  
Restart—can be changed.
- MOLE**— Inclusion of this Keyword means that all input (and output) data will be in terms of mole fractions.  
Default—none, either MOLE or MASS is required.
- MASS**— Inclusion of this Keyword means that all input (and output) data will be in terms of mass fractions.  
Default—none, either MOLE or MASS is required.
- TGIV**— Inclusion of this Keyword means that a solution will be obtained for the species equations with a user-supplied temperature profile. This input only has meaning for burner-stabilized flames.  
Default—none, either TGIV or ENRG must be specified.  
Restart—can be changed.
- ENRG**— Inclusion of this Keyword means that a solution will be obtained for the coupled energy-species equations. However, the user must still specify a temperature profile. This profile is used for solving the temperature-fixed problem, whose solution serves as the first iterate for the solution of the full problem including the energy equation.  
Default—none, either TGIV or ENRG must be specified.  
Restart—can be changed.

## 5.3 Solution Method Option Keywords

- ATOL**— Absolute tolerance for the termination of the Newton iteration. The Newton iteration is considered to be converged when the maximum norm of the solution correction vector  $\Delta\phi$  is reduced to below the following criteria:  $|\Delta\phi| \leq \max(\text{ATOL}, \text{RTOL} \times |\phi|)$ . Typically ATOL should be smaller than the maximum mass fraction of any species of interest.  
Default—1.E-9  
Example: ATOL 1.E-8  
Restart—can be changed.
- RTOL**— Relative tolerance for the termination of the Newton iteration. The Newton iteration is considered to be converged when the maximum norm of the solution correction vector  $\Delta\phi$  is reduced to below the following criteria:  $|\Delta\phi| \leq \max(\text{ATOL}, \text{RTOL} \times |\phi|)$ . Typically RTOL should be in the range of  $10^{-3}$ , which would provide roughly three significant digits to  $10^{-6}$ , which would provide roughly six digits.

Default—1.E-4  
Example: RTOL 1.E-3  
Restart—can be changed.

**ATIM**— Absolute tolerance for the termination of the Newton iteration as it is used in the time stepping procedure. For a precise definition see the above description of ATOL. Since we are not seeking accuracy in a transient solution, this convergence criterion typically does not need to be as stringent as for the Newton iteration on the boundary value problem itself.

Default—1.E-9  
Example: ATIM 1.E-8  
Restart—can be changed.

**RTIM**— Relative tolerance for the termination of the Newton iteration as it is used in the time stepping procedure. For a precise definition see the above description of RTOL. Since we are not seeking accuracy in a transient solution, this convergence criterion typically does not need to be as stringent as for the Newton iteration on the boundary value problem itself.

Default—1.E-4  
Example: RTIM 1.E-3  
Restart—can be changed.

**TIME**— If the Newton method fails to converge, then the program takes some time steps, which hopefully will bring the current iterate within the domain of convergence of Newton's method. This input specifies the size of the time step and how many time steps are to be taken. For example, TIME 100 1.E-6, specifies that any time Newton's method fails 100 time steps of 1 microsecond will be taken.

Units—none, seconds  
Default—100, 1.E-6  
Example: TIME 100 3.E-7  
Restart—can be changed.

**TIM2**— This Keyword is the same as TIME except that TIME applies to the fixed-temperature problem and TIM2 is used after the energy equation is included. This input only has meaning in problems that solve for a temperature profile.

Units—none, seconds  
Default—100, 1.E-6  
Example: TIM2 100 3.E-7  
Restart—can be changed.

**ISTP**— Directs TWOPNT to take this number of initial time steps before attempting the Newton search for the steady-state solution.

Default - 0  
Example: ISTP 100

- NJAC**— Number of iterations allowed in TWOPNT's steady-state Newton method before a new Jacobian is calculated (refer to SSAGE in the TWOPNT manual).  
Default—20  
Example: NJAC 10  
Restart—can be changed.
- IRET**— Number of time steps to be taken in TWOPNT's time stepping algorithm before increasing the time step size (refer to STEPS2 in the TWOPNT manual).  
Default—50  
Example: IRET 20  
Restart—can be changed.
- DFAC**— Factor by which to decrease the time step in TWOPNT's time stepping procedure when necessary, i.e., when the current time step does not converge (refer to TDEC in the TWOPNT manual).  
Default—2.2  
Example: DFAC 2.0  
Restart—can be changed.
- DTMN**— Minimum time step tolerated in TWOPNT's time stepping algorithm before flagging an error condition (refer to TMIN in the TWOPNT manual).  
Units—seconds  
Default—1.E-10  
Example: DTMN 1.E-9  
Restart—can be changed.
- DTMX**— Maximum time step allowed in TWOPNT's time stepping algorithm (refer to TMAX in the TWOPNT manual).  
Units—seconds  
Default—1.E-4  
Example: DTMX 1.E-3  
Restart—can be changed.
- TJAC**— Number of iterations allowed in TWOPNT's time-stepping procedure before a new Jacobian is calculated (refer to TDAGE in the TWOPNT manual).  
Default—20  
Example: TJAC 10  
Restart—can be changed.

## 5.4 Grid Parameter Keywords

**NPTS**— The number of initial mesh points. The inclusion of NPTS will generate an equally spaced mesh of NPTS points between 0 and XEND. The user can also specify an initial nonuniform mesh using the Keyword GRID, in which case the NPTS input is not needed.

Default—6

Example: NPTS 10

**GRID**— The use of this Keyword allows the user to input an initial grid. Up to NMAX of these GRID inputs can be included. Each GRID line contains the coordinate of a mesh point. The GRID Keywords are a grouped list and the grid coordinates must appear in ascending order. The use of this Keyword is optional. If no GRID Keywords are included, the grid will have equally spaced grid points based on NPTS.

Units—cm

Default—equally spaced grid based on NPTS.

Example: GRID 0.0

**GRAD**— Adaptive mesh parameter, which controls the number of grid, points inserted in regions of high gradient. Smaller values of GRAD cause more grid points to be used.

Default—0.1

Example: GRAD 0.2

Restart—can be changed.

**CURV**— Adaptive mesh parameter, which controls the number of grid, points inserted in regions of high curvature. Smaller values of CURV cause more grid points to be used.

Default—0.5

Example: CURV 0.7

Restart—can be changed.

**XSTR**— The beginning of the computational interval.

Units—cm

Default—0.0

Example: XSTR -0.2

Restart—can be changed to a smaller value.

**XCEN**— An estimated value for the center of the flame.

Units—cm

Default— $XCEN = 0.35*(XEND-XSTR)$

Example: XCEN 3.0

**XEND**— The end of the computational interval.

Units—cm

Default—XEND is a required input.

Example: XEND 10.0

Restart—can be changed to a larger value.

**WMIX**— An estimated width of the flame zone.

Units—cm

Default— $WMIX = 0.5*(XEND-XSTR)$

Example: WMIX 2.0

**APRO** — Use of the APRO Keyword(s) allow the user to specify a profile as a function of distance for the stream tube area. The stream-tube area is given relative to the burner area and is therefore dimensionless. Each input provides a  $(x, A)$  pair and the  $x$  coordinates must be in ascending order. Example: “APRO 0.1 1.2” assigns a relative area of 1.2 at a position 0.1 cm from the burner surface.

Units— cm, dimensionless

Default—1.0

Example: APRO 1.0 1.0

Restart - can be changed.

**WDIF**— Including this Keyword means that windward differencing is to be used on the convective terms.

Default—WDIF

Restart—can be changed.

**CDIF**— Including this Keyword means that central differencing is to be used on the convective terms.

Default—WDIF

Restart—can be changed.

**SFLR**— This Keyword is used to override the default value for the minimum bounds on the solution variables corresponding to gas-phase mass fractions. TWOPNT will not let the solution variables fall below their minimum bounds during iteration (refer to BELOW in the TWOPNT manual).

Default— - 1.0E-3

Example: SFLR -1.0E-4

Restart—can be changed.

## 5.5 Flame Definition Keywords

**PRES**— The pressure of the flame.

Units—atmospheres

Default—none

Example: PRES 0.5

Restart—can be changed.

- FLRT**— The mass flow rate through the burner (divided by the burner area). For adiabatic flame problems this is the initial estimate of the mass flow rate.  
Units—g/cm<sup>2</sup>-sec  
Default—FLRT is a required input.  
Example: FLRT 10.  
Restart—can be changed.
- REAC**— Mass or mole fraction values of the unburned reactants. One of these REAC inputs must appear for each reactant species. For example, “REAC C2H2 0.5” assigns a mole or mass fraction of 0.5 to C<sub>2</sub>H<sub>2</sub> in the inlet flow. The sum of all the reactant fractions should equal one. However, if they do not, a cautionary message will be printed and the fractions will be normalized so the sum does equal one. Any given species can participate simultaneously as a reactant, intermediate, or product.  
Units—either mass or mole fractions, depending in MASS or MOLE.  
Default—required input.  
Example: REAC C2H2 0.5  
Restart—can be changed.
- INTM**— The estimated peak mass or mole fractions values for “intermediate” species. One of these INTM inputs must appear for each intermediate species. It is usually better to estimate values somewhat higher than those that are actually present in the flame. Example: “INTM HO2 0.001” gives an estimate fraction of 0.001 for the intermediate HO<sub>2</sub>. Any given species can participate simultaneously as a reactant, intermediate, or product.  
Units—either mass or mole fractions, depending in MASS or MOLE.  
Default—0.0  
Example: INTM HO2 0.001
- PROD**— Mass or mole fraction values of the estimated final values of the flame products. For example, “PROD H2O 0.5” estimates the fraction of H<sub>2</sub>O in the post-flame region as 0.5. The sum of the product fractions should equal one. However, if they do not, a cautionary message will be printed and the fractions will be normalized so the sum does equal one. Any given species can participate simultaneously as a reactant, intermediate, or product. If no PROD is given, PROD for each species will be its fraction of the mixture’s equilibrium composition.  
Units—either mass or mole fractions, depending on MASS or MOLE.  
Default—0.0  
Example: PROD H2O 0.5
- PRMN**— Minimum mass or mole fraction value to be applied to the equilibrium-estimated final values of the flame products.  
Units – either mass or mole fractions, depending on MASS or MOLE.  
Default – 0.0  
Example: PRMN 1.0E-10



**XIMN**— Minimum mass or mole fraction value to be applied to intermediate species in the event products are equilibrium-estimated. In that case, a non-initialized intermediate species fraction is initialized to be the average of its PROD and REAC values, or XIMN if smaller.

Units – either mass or mole fractions, depending on MASS or MOLE.

Default – 0.0

Example: XIMN 1.0E-10

**TEMP**— This input allows specification of the initial or given temperature profile. Each input provides an  $(x, T)$  pair and the  $x$  coordinates must be in ascending order. Example: “TEMP 0.1 1000” assigns a temperature of 1000K at a position 0.1 cm from the burner surface.

Units—cm, K

Default—required input, except on a restart.

Example: TEMP 0.0 300.

Restart—can be changed, provided USTG is included.

**USTG**— Including this Keyword on a restart means that the user-specified temperature profile, as given on the TEMP Keywords, is to be used instead of the temperature profile that is on the restart file.

Default—Use the temperature profile on the restart file.

Restart—can be changed.

**TFIX**— When solving a freely propagating adiabatic flame, the problem is posed in a flame-fixed coordinate system. In this case the flame speed becomes an eigenvalue. Therefore, an additional boundary condition is required. We choose to supply this additional condition by fixing the temperature at one point in the flame, and this input allows the specification of that fixed temperature. Given the fixed temperature, the program determines its position from the initial temperature profile as specified by the TEMP inputs. If the fixed temperature is not one of the temperatures specified on a TEMP input, then PREMIX uses a linear interpolation of the TEMP profile to determine the position of TFIX and adds a new mesh point at that point. We find that relatively low temperatures near the unburned side of the flame work best, e.g. 400K.

Units—K

Default—required input for freely propagating flames (see Keyword FREE).

Example: TFIX 500.

## 5.6 Transport Option Keywords

**TDIF**— Inclusion of this Keyword causes the calculation to be run with thermal diffusion (Soret effect).

Default—no thermal diffusion

Restart—can be changed.

**MULT**— Inclusion of this Keyword causes the transport properties to be calculated using the multicomponent formulations.

Default—MIX

Restart—can be changed.

- MIX**— Inclusion of this Keyword causes the transport properties to be calculated using the mixture-averaged formulas.  
Default—MIX  
Restart—can be changed.
- VCOR**— Inclusion of this Keyword causes the use of the correction velocity formalism to ensure mass conservation for gas mixtures.  
Default—VCOR  
Restart—can be changed.
- TRCE**— Inclusion of this Keyword causes the “trace-species” approximation to be used when enforcing mass conservation. In this case all of the transport errors are lumped into the last species in the CHEMKIN list.  
Default—VCOR  
Restart—can be changed.

## 5.7 Sensitivity Option Keywords

- ASEN**— Inclusion of this Keyword causes all the first-order sensitivity coefficients with respect to the rate constants to be determined.  
Default—no sensitivities computed  
Restart—can be changed.
- HSEN**— Inclusion of this Keyword causes all the first order sensitivity coefficients with respect to the species’ heats of formation to be determined.  
Default—no sensitivities computed  
Restart—can be changed.

## 5.8 Miscellaneous Keywords

- PRNT**— Printing control. “PRNT 1” provides less printed output of intermediate solutions than does “PRNT 2.” More printing is often helpful when there are convergence difficulties.  
Default—1  
Restart—can be changed.
- RSTR**— Inclusion of this Keyword causes the program to begin from a previously computed solution as the starting estimate. This previously computed solution will be read from “rest.bin”.  
Default—solution started from input, not a restart file
- SKIP**— This Keyword is used to indicate which solution is used from the Restart file, by telling PREMIX how many solution sets to skip when reading the Restart file.  
Default—no solutions are skipped and the first solution found is taken for the restart.  
Example: SKIP 2

- CNTN**— Inclusion of this Keyword causes the program to expect Keywords for another problem following the END Keyword. The following problem will use the solution of the previous problem as its initial guess. This capability is very similar to that provided by RSTR. However, in the case of CNTN, several related problems can be solved by one job submission without having to manipulate the restart files. Any Keyword that can be changed for a RSTR problem can be changed on continuation.  
Default—no continuation is expected
- JRG**— When restarting or continuing from a previous solution, the user may opt to regrid the solution for the initial guess. This Keyword indicates the number of grid points desired; PREMIX will map the previous solution onto a grid this size.  
Default—no regridding is performed  
Example: JRG 50
- PCAD**— When regridding is requested on a restart or continuation from a previous solution, this Keyword controls the percentage of regrid points dedicated to adaptation.  
Default—0.75 of the grids will be dedicated to adaptation of the solution  
Example: PCAD 0.5
- RGTC**— When regridding is requested on a restart or continuation from a previous solution, this Keyword controls the ratio of gradient regrid points to curvature grid points.  
Default—1.0; equal numbers of grids are dedicated to adapting gradients and curvature.  
Example: RGTC 2.0
- NTOT**— Maximum number of grid points allowed for this job.  
Default—NTOT=maximum grid dimension set by PREMIX driver program  
Example: NTOT 200  
Restart—cannot be changed on restart.
- NADP**— Maximum number of grid points that can be added at a time during grid adaptation.  
Default—no limit is set  
Example: NADP 2  
Restart—can be changed on restart.
- NOFT**— Inclusion of this Keyword causes PREMIX to skip the fixed temperature calculation before solving the full problem including the energy equation.  
Default—the fixed temperature calculation is performed.
- SPOS**— A positive value used to convert any species mass fraction that becomes negative during solution iterations. Any mass fraction calculated that is less than this value is set equal to this value.  
Default— -1.0; i.e. SPOS is not set by default.  
Example: SPOS 1.E-12  
Restart—can be changed.

**GFAC**— This Keyword gives a scalar multiplier that is used to modify all gas-phase reaction rate constants.

Default— 1.0

Example: GFAC 1.1

Restart—can be changed.

**END**— This Keyword signifies the end of a given set of input data. It must appear after each set of data when continuation jobs are indicated using the CNTN Keyword.

## 6. POST PROCESSING

### 6.1 CHEMKIN Graphical Post-processor

The CHEMKIN Graphical Post-processor provides a means for quick visualization of results from PREMIX. Launched from the CHEMKIN Application User Interface, the Graphical Post-processor will automatically read in the solution data from the “save.bin” file in the working directory. Alternatively, the post-processor may be launched independently and a solution file may be opened from within the Post-processor. The user may open one or more solution files in the Post-processor and may also import external data for comparisons with the simulation results. In addition, the Graphical Post-processor can be used to export all of the solution data into comma-, tab-, or space-delimited text for further analysis with other software packages. For more information on the Graphical Post-processor, please see the CHEMKIN Getting Started manual.

### 6.2 Configurable Command-line Post-processor

In addition to the CHEMKIN Graphical Post-processor representation of solution data, we provide the user with a FORTRAN post-processor called PREMIX\_POST. This program reads the binary solution file and prints selected data to text files, which can then be imported by many other graphics programs. The full source-code, `premix_post.f`, is provided in the CHEMKIN “post\_processors” subdirectory. Also in this directory is a makefile script for re-building the PREMIX\_POST program, in case the user makes changes to the source code. In this way, the user may easily configure PREMIX\_POST for their own analysis needs.

To run PREMIX\_POST from the command-line, you will need to do the following:

1. Open a MS-DOS Prompt (PC) or shell (UNIX).
2. Change directories to your working directory, where your “save.bin” solution file resides.
3. Run PREMIX\_POST from the command-line, specifying the full path to the CHEMKIN “bin” directory where the “premix\_post” executable resides, unless this is already in your environment “path” variable:

```
premix_post < premix_post.inp > premix_post.out
```

Here, “premix\_post.inp” is an input file that contains keywords described below. The output “premix\_post.out” will contain diagnostics and error messages for the PREMIX\_POST run. PREMIX\_POST will also create text files containing comma-separated values. The names for these files use a suffix (extension) of “.csv”.

PREMIX\_POST uses keyword input. The available keywords are printed as a banner when the program is invoked; they are also described briefly here:

**PREF** Specifies a character string to be used as a prefix for the text file name.  
 Default - "premix"  
 Example: PREF premix

**NSOL** Requests a particular solution be selected from the binary solution file.  
 Default - the final solution in the binary solution file.  
 Example: NSOL 2.

**SPEC** Requests species fractions for a space-delimited list of species, or "ALL".  
 Default - none  
 Example: SPEC H2 O2 OH H2O HO2 H O

**MOLE** Print species as mole fractions.  
 Default - MOLE.

**MASS** Print species as mass fractions.  
 Default - MOLE.

**SMIN** Do not print species whose maximum fraction is less than SMIN.  
 Default - 0.0.

**SENS** Print rate sensitivity coefficients for space-delimited list of species, or "ALL".  
 Default - none  
 Example: SENS OH NO

**HSEN** Print enthalpy-of-formation sensitivity coefficients for space-delimited list of species, or "ALL".  
 Default - none  
 Example: HSEN OH NO

**RATE** Print chemical production rates for a space-delimited list of species, or "ALL".  
 Default - none  
 Example: RATE OH NO

**DROP** Eliminate reactions where relative (percent) sensitivity coefficients or chemical production rates are low.  
 Default - .10.  
 Example: DROP .20

**HELP** Print a brief guide to keyword input.

**END** Begin post-processing.

## 7. SAMPLE PREMIX PROBLEMS

We show two example problems in this chapter. The first is a low-pressure burner-stabilized hydrogen-oxygen-argon flame. It is relatively easy to solve and requires little computer time. The second problem is an atmospheric-pressure freely propagating stoichiometric methane air flame. This flame is considerably harder to solve, and the example shows some of the procedures we use to get solutions to such problems. Both of the examples were run on a SGI R4400 Indigo workstation.

### 7.1 Burner-Stabilized Hydrogen-Oxygen Flame

We have used low-pressure hydrogen flames with various additives to study several aspects of nitric oxide pollutant formation. One such flame is a hydrogen-oxygen-argon flame that is doped with hydrogen cyanide.<sup>4</sup> This flame is an interesting one to study because all the carbon and nitrogen in the system must come from the HCN. In any case, we use a rich hydrogen flame (without additives) as the first example problem. The unburned reactant mole fractions are:  $H_2=0.28$ ;  $O_2=0.09$ ;  $Ar=0.63$ . The pressure is 25 Torr (0.0329 atmospheres) and the mass flow rate through the burner face is measured to be  $4.63 \times 10^{-3}$  gm/cm<sup>2</sup>-sec. Furthermore, in the computation, a measured temperature profile is used rather than computing the temperatures from the energy equation.

The first file is the input file for the CHEMKIN Interpreter, which defines the hydrogen-oxygen reaction mechanism. This is followed by the corresponding output of the CHEMKIN Interpreter. The third file shows the output of the TRANSPORT fitting routine, which uses the transport data found in the TRANSPORT database. The fourth file shown is the output from PREMIX. After giving statistics on the working space requirements, PREMIX echoes back the Keyword inputs. In this example, the Keyword MOLE is used to indicate that all the species input and printed output are in terms of mole fractions. Following the Keywords, the first thing printed is the initial guess of the solution, which is based on the Keyword inputs. (In the case of a restart this initial guess would come from the restart file.)

The next block of output describes the course of the solution procedure. Since the PRNT Keyword was set to 1, only brief statistics for the progress of the iteration are provided. There are three major functions in the TWOPNT solver, and each reports what it has done at each stage of the solution. These functions are SEARCH (which attempts to solve the steady-state boundary-value problem on the given mesh by Newton's method), EVOLVE (which takes time steps if Newton's method fails), and REFINE (which performs the mesh adaptation). The first column reports the logarithm of the maximum residual norm,  $\|F(\phi)\|$  i.e., the norm of the left-hand side of Eqs. (2) and (3). The second column reports the logarithm of the largest Jacobian condition number encountered during the current iteration. These condition numbers are obtained from the LINPACK condition number estimates. The following column reports the number of mesh points, the number of Newton or time steps, and the number of Jacobian evaluations required, as

well as any remarks about the given operation. For example, the two “GOING OUT OF BOUNDS” remarks indicate that the Newton method failed to converge and thus time steps will be attempted next.

The next block of output is the converged solution. The mesh locations “X” are in centimeters, the temperatures are in Kelvin, the velocities are in cm/sec, the densities are in gm/cm<sup>3</sup>, and, in this case, the species are reported in mole fractions.



## 7.1.1 CHEMKIN INPUT FOR THE HYDROGEN-OXYGEN FLAME EXAMPLE

```

ELEMENTS
H O AR
END
SPECIES
H2 O2 H O OH HO2 H2O2 H2O AR
END
REACTIONS
H2+O2=2OH          1.7E13    0.0    47780.
OH+H2=H2O+H       1.17E9     1.3    3626. !D-L$W
H+O2=OH+O         5.13E16    -0.816 16507. !JAM,JCP 1981
O+H2=OH+H         1.8E10     1.0    8826.
H+O2+M=HO2+M      2.1E18     -1.0    0. !SLACK
    H2O/21./ H2/3.3/ O2/0.0/
H+O2+O2=HO2+O2    6.7E19     -1.42  0. !SLACK,JAN
OH+HO2=H2O+O2     5.0E13     0.0    1000.
H+HO2=2OH         2.5E14     0.0    1900.
O+HO2=O2+OH       4.8E13     0.0    1000.
2OH=O+H2O         6.0E+8     1.3    0. !COHEN-WEST.
H2+M=H+H+M        2.23E12    0.5    92600.
    H2O/6/ H/2/ H2/3/
O2+M=O+O+M        1.85E11    0.5    95560.
H+OH+M=H2O+M      7.5E23    -2.6    0.
    H2O/20/
H+HO2=H2+O2       2.5E13     0.0    700.
HO2+HO2=H2O2+O2   2.0E12     0.0    0.
H2O2+M=OH+OH+M    1.3E17     0.0    45500.
H2O2+H=HO2+H2     1.6E12     0.0    3800.
H2O2+OH=H2O+HO2   1.0E13     0.0    1800.
END

```

## 7.1.2 CHEMKIN OUTPUT FOR THE HYDROGEN-OXYGEN FLAME EXAMPLE

CHEMKIN-III GAS-PHASE MECHANISM INTERPRETER:  
 DOUBLE PRECISION Vers. 6.24 2000/06/18  
 Copyright 1995, Sandia Corporation.  
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```

-----
ELEMENTS      ATOMIC
CONSIDERED   WEIGHT
-----
  1. H        1.00797
  2. O        15.9994
  3. AR       39.9480
-----
  
```

```

-----
C
P H
H A
A R
SPECIES      S G MOLECULAR  TEMPERATURE  ELEMENT COUNT
CONSIDERED  E E  WEIGHT      LOW    HIGH    H  O  AR
-----
  1. H2      G 0   2.01594   300   5000   2  0  0
  2. O2      G 0  31.99880   300   5000   0  2  0
  3. H       G 0   1.00797   300   5000   1  0  0
  4. O       G 0  15.99940   300   5000   0  1  0
  5. OH      G 0  17.00737   300   5000   1  1  0
  6. HO2     G 0  33.00677   300   5000   1  2  0
  7. H2O2    G 0  34.01474   300   5000   2  2  0
  8. H2O     G 0  18.01534   300   5000   2  1  0
  9. AR      G 0  39.94800   300   5000   0  0  1
-----
  
```

```

(k = A T**b exp(-E/RT))
REACTIONS CONSIDERED      A      b      E
-----
  1. H2+O2=2OH            1.70E+13  0.0  47780.0
  2. OH+H2=H2O+H         1.17E+09  1.3   3626.0
  3. H+O2=OH+O           5.13E+16 -0.8  16507.0
  4. O+H2=OH+H           1.80E+10  1.0   8826.0
  5. H+O2+M=HO2+M        2.10E+18 -1.0    0.0
     H2O      Enhanced by  2.100E+01
     H2       Enhanced by  3.300E+00
     O2       Enhanced by  0.000E+00
  6. H+O2+O2=HO2+O2      6.70E+19 -1.4    0.0
  7. OH+HO2=H2O+O2      5.00E+13  0.0  1000.0
  8. H+HO2=2OH           2.50E+14  0.0  1900.0
  9. O+HO2=O2+OH        4.80E+13  0.0  1000.0
 10. 2OH=O+H2O          6.00E+08  1.3    0.0
 11. H2+M=H+H+M         2.23E+12  0.5  92600.0
     H2O      Enhanced by  6.000E+00
     H        Enhanced by  2.000E+00
     H2       Enhanced by  3.000E+00
 12. O2+M=O+O+M         1.85E+11  0.5  95560.0
 13. H+OH+M=H2O+M      7.50E+23 -2.6    0.0
     H2O      Enhanced by  2.000E+01
 14. H+HO2=H2+O2        2.50E+13  0.0   700.0
 15. HO2+HO2=H2O2+O2    2.00E+12  0.0    0.0
 16. H2O2+M=OH+OH+M     1.30E+17  0.0  45500.0
-----
  
```

17. H2O2+H=HO2+H2	1.60E+12	0.0	3800.0
18. H2O2+OH=H2O+HO2	1.00E+13	0.0	1800.0

NOTE: A units mole-cm-sec-K, E units cal/mole

NO ERRORS FOUND ON INPUT:

ASCII Vers. 1.1 CHEMKIN linkfile chem.asc written.

WORKING SPACE REQUIREMENTS ARE

INTEGER: 593

REAL: 399

CHARACTER: 12

Total CPUtime (sec): 0.125

### 7.1.3 TRANSPORT OUTPUT FOR THE HYDROGEN-OXYGEN FLAME EXAMPLE

TRANFIT: CHEMKIN-III Transport property fitting code,  
DOUBLE PRECISION Vers. 3.18 00/08/11  
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WORKING SPACE REQUIREMENTS		
	PROVIDED	REQUIRED
INTEGER	620	620
REAL	1886	1886
CHARACTER	21	21

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DATA HAS BEEN FIT OVER THE RANGE: TLOW= 300.00, THIGH= 5000.00

TRANSPORT PARAMETERS FROM DATA BASE:

AR	0	136.500	3.330	0.000	0.000	0.000	
H	0	145.000	2.050	0.000	0.000	0.000	
H2	1	38.000	2.920	0.000	0.790	280.000	
H2O	2	572.400	2.605	1.844	0.000	4.000	
H2O2	2	107.400	3.458	0.000	0.000	3.800	
HO2	2	107.400	3.458	0.000	0.000	1.000	!(* )
O	0	80.000	2.750	0.000	0.000	0.000	
O2	1	107.400	3.458	0.000	1.600	3.800	
OH	1	80.000	2.750	0.000	0.000	0.000	

COEFFICIENTS FOR SPECIES CONDUCTIVITIES  
MAXIMUM FITTING ERROR = 6.362E-03

H2	0.132E+02	-0.225E+01	0.381E+00	-0.157E-01
O2	-0.213E+01	0.299E+01	-0.287E+00	0.124E-01
H	0.604E+00	0.300E+01	-0.303E+00	0.129E-01
O	0.278E+01	0.144E+01	-0.103E+00	0.440E-02
OH	0.165E+02	-0.432E+01	0.696E+00	-0.314E-01
HO2	0.374E+01	0.153E+00	0.163E+00	-0.103E-01
H2O2	0.709E+00	0.140E+01	0.852E-02	-0.406E-02
H2O	0.163E+02	-0.589E+01	0.109E+01	-0.551E-01
AR	-0.178E+01	0.285E+01	-0.284E+00	0.122E-01

COEFFICIENTS FOR SPECIES VISCOSITIES  
 MAXIMUM FITTING ERROR = 3.645E-03

H2	-0.136E+02	0.884E+00	-0.325E-01	0.147E-02
O2	-0.160E+02	0.217E+01	-0.198E+00	0.854E-02
H	-0.189E+02	0.300E+01	-0.303E+00	0.129E-01
O	-0.140E+02	0.144E+01	-0.103E+00	0.440E-02
OH	-0.140E+02	0.144E+01	-0.103E+00	0.440E-02
HO2	-0.160E+02	0.217E+01	-0.198E+00	0.854E-02
H2O2	-0.160E+02	0.217E+01	-0.198E+00	0.854E-02
H2O	-0.149E+02	0.561E+00	0.137E+00	-0.104E-01
AR	-0.177E+02	0.285E+01	-0.284E+00	0.122E-01

COEFFICIENTS FOR SPECIES DIFFUSION COEFFICIENTS  
 MAXIMUM FITTING ERROR = 2.872E-03

H2	H2	-0.961E+01	0.188E+01	-0.293E-01	0.128E-02
O2	H2	-0.121E+02	0.264E+01	-0.131E+00	0.573E-02
O2	O2	-0.151E+02	0.325E+01	-0.205E+00	0.876E-02
H	H2	-0.108E+02	0.250E+01	-0.109E+00	0.462E-02
H	O2	-0.158E+02	0.426E+01	-0.334E+00	0.143E-01
H	H	-0.141E+02	0.389E+01	-0.283E+00	0.120E-01
O	H2	-0.109E+02	0.231E+01	-0.870E-01	0.386E-02
O	O2	-0.140E+02	0.300E+01	-0.174E+00	0.746E-02
O	H	-0.139E+02	0.366E+01	-0.259E+00	0.111E-01
O	O	-0.125E+02	0.258E+01	-0.119E+00	0.505E-02
OH	H2	-0.109E+02	0.231E+01	-0.870E-01	0.386E-02
OH	O2	-0.140E+02	0.299E+01	-0.173E+00	0.740E-02
OH	H	-0.140E+02	0.367E+01	-0.260E+00	0.112E-01
OH	O	-0.125E+02	0.258E+01	-0.119E+00	0.505E-02
OH	OH	-0.125E+02	0.258E+01	-0.119E+00	0.505E-02
HO2	H2	-0.121E+02	0.265E+01	-0.131E+00	0.574E-02
HO2	O2	-0.151E+02	0.325E+01	-0.205E+00	0.876E-02
HO2	H	-0.158E+02	0.426E+01	-0.334E+00	0.143E-01
HO2	O	-0.140E+02	0.301E+01	-0.174E+00	0.748E-02
HO2	OH	-0.140E+02	0.300E+01	-0.173E+00	0.743E-02
HO2	HO2	-0.151E+02	0.325E+01	-0.205E+00	0.876E-02
H2O2	H2	-0.121E+02	0.265E+01	-0.131E+00	0.574E-02
H2O2	O2	-0.151E+02	0.325E+01	-0.205E+00	0.877E-02
H2O2	H	-0.158E+02	0.426E+01	-0.335E+00	0.143E-01
H2O2	O	-0.140E+02	0.301E+01	-0.175E+00	0.751E-02
H2O2	OH	-0.140E+02	0.300E+01	-0.174E+00	0.746E-02
H2O2	HO2	-0.151E+02	0.325E+01	-0.205E+00	0.876E-02
H2O2	H2O2	-0.151E+02	0.325E+01	-0.205E+00	0.876E-02
H2O	H2	-0.170E+02	0.451E+01	-0.360E+00	0.151E-01
H2O	O2	-0.202E+02	0.514E+01	-0.423E+00	0.171E-01
H2O	H	-0.178E+02	0.480E+01	-0.367E+00	0.143E-01
H2O	O	-0.183E+02	0.467E+01	-0.373E+00	0.154E-01
H2O	OH	-0.183E+02	0.467E+01	-0.373E+00	0.154E-01
H2O	HO2	-0.196E+02	0.491E+01	-0.398E+00	0.162E-01
H2O	H2O2	-0.196E+02	0.491E+01	-0.397E+00	0.162E-01
H2O	H2O	-0.153E+02	0.243E+01	0.200E-01	-0.507E-02
AR	H2	-0.120E+02	0.258E+01	-0.119E+00	0.509E-02
AR	O2	-0.158E+02	0.349E+01	-0.235E+00	0.100E-01
AR	H	-0.163E+02	0.444E+01	-0.354E+00	0.150E-01
AR	O	-0.147E+02	0.330E+01	-0.212E+00	0.907E-02
AR	OH	-0.147E+02	0.329E+01	-0.210E+00	0.901E-02
AR	HO2	-0.158E+02	0.349E+01	-0.235E+00	0.999E-02
AR	H2O2	-0.158E+02	0.349E+01	-0.235E+00	0.999E-02
AR	H2O	-0.200E+02	0.503E+01	-0.406E+00	0.163E-01
AR	AR	-0.166E+02	0.381E+01	-0.274E+00	0.116E-01

COEFFICIENTS FOR THERMAL DIFFUSION RATIOS

MAXIMUM FITTING ERROR = 2.204E-02

H2	H2	0.000E+00	0.000E+00	0.000E+00	0.000E+00
H2	O2	-0.465E+00	-0.114E-04	-0.659E-09	0.204E-12
H2	H	0.166E+00	0.186E-04	-0.611E-08	0.726E-12
H2	O	-0.423E+00	0.113E-04	-0.114E-07	0.174E-11
H2	OH	-0.429E+00	0.115E-04	-0.116E-07	0.177E-11
H2	HO2	-0.466E+00	-0.114E-04	-0.661E-09	0.205E-12
H2	H2O2	-0.468E+00	-0.115E-04	-0.663E-09	0.205E-12
H2	H2O	-0.144E+00	-0.348E-03	0.121E-06	-0.129E-10
H2	AR	-0.457E+00	-0.416E-04	0.128E-07	-0.151E-11
H	H2	-0.166E+00	-0.186E-04	0.611E-08	-0.726E-12
H	O2	-0.304E+00	-0.265E-03	0.971E-07	-0.108E-10
H	H	0.000E+00	0.000E+00	0.000E+00	0.000E+00
H	O	-0.338E+00	-0.185E-03	0.689E-07	-0.782E-11
H	OH	-0.341E+00	-0.187E-03	0.694E-07	-0.787E-11
H	HO2	-0.305E+00	-0.266E-03	0.973E-07	-0.108E-10
H	H2O2	-0.305E+00	-0.266E-03	0.975E-07	-0.108E-10
H	H2O	0.563E-01	-0.552E-03	0.173E-06	-0.172E-10
H	AR	-0.257E+00	-0.326E-03	0.117E-06	-0.128E-10

WORKING SPACE REQUIREMENTS ARE

INTEGER: 38  
 REAL: 1854

Total CPUtime (sec): 0.078125

## 7.1.4 PREMIX OUTPUT FOR THE HYDROGEN-OXYGEN FLAME EXAMPLE

PREMIX: CHEMKIN-III One-dimensional steady premixed laminar flame code,  
DOUBLE PRECISION Vers. 3.39 2000/08/09  
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	WORKING SPACE REQUIREMENTS	
	PROVIDED	REQUIRED
LOGICAL	111	111
INTEGER	2543	2543
REAL	108813	108813
CHARACTER	44	44

CKLIB: CHEMKIN-III GAS-PHASE CHEMICAL KINETICS LIBRARY,  
DOUBLE PRECISION Vers. 5.28 2000/08/05  
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TRANLIB: CHEMKIN-III MULTICOMPONENT TRANSPORT LIBRARY,  
DOUBLE PRECISION Vers. 4.6 1999/06/03  
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### KEYWORD INPUT

```
/ flame configuration, burner stabilized with specified temperature
BURN
TGIV
/ in the event of a Newton failure, take 100 timesteps of 1.E-6
TIME 100 1.00E-6
/ begin on a uniform mesh of 6 points
NPTS 6
/ definition of the computational interval
XEND 10.0
XCEN 5.0
WMIX 10.0
/ pressure and inlet mass flow rate
PRES 0.0329 (atmospheres)
FLRT 4.63E-3 (g/cm**2-sec)
/ adaptive mesh criteria
GRAD 0.2
CURV 0.5
/ unreacted mole fractions
MOLE
REAC O2 0.09
REAC AR .63
REAC H2 0.28
/ estimated products
PROD AR 0.68
PROD H2O 0.12
PROD H2 0.15
PROD OH 0.02
PROD O 0.02
PROD H 0.01
/ estimated intermediate mole fractions
```

```

INTM  H2O2  .00001
INTM  HO2   .001
INTM  H2    .01
/  tolerances for the Newton iteration
ATOL  1.E-10
RTOL  1.E-4
/  tolerances for the time step Newton iteration
ATIM  1.E-5
RTIM  1.E-5
/  print control
PRNT  1
/  given temperature profile
TEMP  0.      373.7
TEMP  .1250  484.5
TEMP  .250   583.7
TEMP  .375   672.2
TEMP  .5     753.5
TEMP  .75    901.4
TEMP  1.0    1027.
TEMP  1.25   1120.
TEMP  1.5    1184.
TEMP  2.0    1260.
TEMP  3.0    1348.
TEMP  6.0    1475.
TEMP  10.0   1524.
END

```

TWOPNT: DOUBLE PRECISION (TWO POINT BOUNDARY VALUE PROBLEM) SOLVER,  
VERSION 3.30 OF APRIL 1998 BY DR. JOSEPH F. GRCAR.

TWOPNT: INITIAL GUESS:

	X	T	V	RHO	H2	O2	H
1	0.0000	3.737E+02	1.508E+02	3.070E-05	2.800E-01	8.999E-02	0.000E+00
2	2.0000	1.260E+03	5.026E+02	9.212E-06	2.539E-01	7.196E-02	1.999E-03
3	4.0000	1.390E+03	5.482E+02	8.447E-06	2.278E-01	5.395E-02	3.996E-03
4	6.0000	1.475E+03	5.749E+02	8.053E-06	2.018E-01	3.597E-02	5.994E-03
5	8.0000	1.500E+03	5.779E+02	8.012E-06	1.759E-01	1.799E-02	7.996E-03
6	10.0000	1.524E+03	5.808E+02	7.971E-06	1.500E-01	0.000E+00	9.998E-03

	X	O	OH	HO2	H2O2	H2O	AR
1	0.0000	0.000E+00	0.000E+00	1.502E-04	1.502E-06	0.000E+00	6.299E-01
2	2.0000	3.998E-03	3.998E-03	5.077E-04	5.077E-06	2.399E-02	6.397E-01
3	4.0000	7.992E-03	7.992E-03	9.356E-04	9.356E-06	4.795E-02	6.494E-01
4	6.0000	1.199E-02	1.199E-02	9.356E-04	9.356E-06	7.193E-02	6.594E-01
5	8.0000	1.599E-02	1.599E-02	5.077E-04	5.077E-06	9.595E-02	6.697E-01
6	10.0000	2.000E-02	2.000E-02	1.502E-04	1.502E-06	1.200E-01	6.799E-01

TWOPNT: SOLVE THE PROBLEM.

TASK	LOG10 NORM F	LOG10 COND J	REMARK
START	-1.72		6 GRID POINTS
SEARCH		5.13	GOING OUT OF BOUNDS
EVOLVE	-2.80	0.83	100 TIME STEPS, 1.0E-06 LAST STRIDE
SEARCH		5.42	GOING OUT OF BOUNDS
EVOLVE	-2.84	1.23	100 TIME STEPS, 2.0E-06 LAST STRIDE
SEARCH	-6.62	5.35	14 SEARCH STEPS
REFINE	-3.01		1.00 AND 1.00 RATIOS, 8 GRID POINTS
SEARCH	-7.84	5.24	9 SEARCH STEPS
REFINE	-2.71		1.00 AND 1.00 RATIOS, 11 GRID POINTS



SEARCH	-8.03	5.16	14 SEARCH STEPS
REFINE	-3.11		0.98 AND 1.00 RATIOS, 15 GRID POINTS
SEARCH	-10.03	4.93	22 SEARCH STEPS
REFINE	-3.56		0.75 AND 1.00 RATIOS, 21 GRID POINTS
SEARCH	-10.10	4.86	24 SEARCH STEPS
REFINE	-3.78		0.92 AND 1.00 RATIOS, 27 GRID POINTS
SEARCH	-9.56	4.78	22 SEARCH STEPS
REFINE	-3.83		0.52 AND 1.00 RATIOS, 31 GRID POINTS
SEARCH	-8.77	4.78	15 SEARCH STEPS
REFINE	-4.39		0.29 AND 0.75 RATIOS, 33 GRID POINTS
SEARCH	-8.84	4.74	6 SEARCH STEPS
REFINE			0.17 AND 0.44 RATIOS

TWOPNT: FINAL SOLUTION:

	X	T	V	RHO	H2	O2	H
1	0.0000	3.737E+02	1.487E+02	3.113E-05	2.680E-01	9.110E-02	3.950E-04
2	0.0156	3.875E+02	1.541E+02	3.004E-05	2.672E-01	9.110E-02	4.088E-04
3	0.0313	4.014E+02	1.595E+02	2.903E-05	2.664E-01	9.109E-02	4.856E-04
4	0.0469	4.153E+02	1.649E+02	2.808E-05	2.656E-01	9.107E-02	6.113E-04
5	0.0625	4.291E+02	1.703E+02	2.719E-05	2.647E-01	9.104E-02	7.810E-04
6	0.0938	4.568E+02	1.810E+02	2.558E-05	2.628E-01	9.095E-02	1.246E-03
7	0.1250	4.845E+02	1.917E+02	2.415E-05	2.606E-01	9.081E-02	1.871E-03
8	0.1563	5.093E+02	2.012E+02	2.301E-05	2.583E-01	9.063E-02	2.648E-03
9	0.1875	5.341E+02	2.107E+02	2.197E-05	2.557E-01	9.040E-02	3.578E-03
10	0.2500	5.837E+02	2.297E+02	2.016E-05	2.500E-01	8.975E-02	5.867E-03
11	0.3125	6.280E+02	2.464E+02	1.879E-05	2.435E-01	8.883E-02	8.663E-03
12	0.3750	6.722E+02	2.631E+02	1.760E-05	2.362E-01	8.753E-02	1.193E-02
13	0.4375	7.129E+02	2.783E+02	1.663E-05	2.281E-01	8.577E-02	1.563E-02
14	0.5000	7.535E+02	2.936E+02	1.577E-05	2.192E-01	8.344E-02	1.971E-02
15	0.5625	7.905E+02	3.073E+02	1.506E-05	2.096E-01	8.046E-02	2.412E-02
16	0.6250	8.275E+02	3.212E+02	1.442E-05	1.993E-01	7.677E-02	2.880E-02
17	0.6875	8.644E+02	3.350E+02	1.382E-05	1.885E-01	7.238E-02	3.365E-02
18	0.7500	9.014E+02	3.489E+02	1.327E-05	1.774E-01	6.735E-02	3.859E-02
19	0.8125	9.328E+02	3.608E+02	1.283E-05	1.663E-01	6.184E-02	4.348E-02
20	0.8750	9.642E+02	3.726E+02	1.243E-05	1.553E-01	5.598E-02	4.825E-02
21	1.0000	1.027E+03	3.965E+02	1.168E-05	1.344E-01	4.390E-02	5.706E-02
22	1.1250	1.074E+03	4.141E+02	1.118E-05	1.166E-01	3.296E-02	6.432E-02
23	1.2500	1.120E+03	4.317E+02	1.072E-05	1.024E-01	2.388E-02	6.985E-02
24	1.3750	1.152E+03	4.437E+02	1.044E-05	9.196E-02	1.704E-02	7.371E-02
25	1.5000	1.184E+03	4.556E+02	1.016E-05	8.458E-02	1.213E-02	7.619E-02
26	1.7500	1.222E+03	4.695E+02	9.861E-06	7.695E-02	6.957E-03	7.802E-02
27	2.0000	1.260E+03	4.835E+02	9.576E-06	7.399E-02	4.553E-03	7.782E-02
28	2.5000	1.304E+03	4.994E+02	9.271E-06	7.384E-02	3.243E-03	7.519E-02
29	3.0000	1.348E+03	5.155E+02	8.981E-06	7.521E-02	2.911E-03	7.228E-02
30	4.0000	1.390E+03	5.305E+02	8.728E-06	7.752E-02	2.664E-03	6.773E-02
31	6.0000	1.475E+03	5.611E+02	8.251E-06	8.106E-02	2.471E-03	6.151E-02
32	8.0000	1.500E+03	5.694E+02	8.131E-06	8.274E-02	2.251E-03	5.813E-02
33	10.0000	1.524E+03	5.787E+02	8.000E-06	8.274E-02	2.251E-03	5.813E-02

	X	O	OH	HO2	H2O2	H2O	AR
1	0.0000	3.322E-08	3.692E-05	1.542E-05	5.281E-07	1.187E-03	6.393E-01
2	0.0156	3.749E-08	4.175E-05	1.859E-05	6.374E-07	1.395E-03	6.398E-01
3	0.0313	7.355E-08	4.667E-05	1.971E-05	7.294E-07	1.627E-03	6.403E-01
4	0.0469	1.542E-07	5.157E-05	1.954E-05	8.034E-07	1.883E-03	6.408E-01
5	0.0625	3.174E-07	5.619E-05	1.858E-05	8.605E-07	2.164E-03	6.412E-01
6	0.0938	1.088E-06	6.393E-05	1.556E-05	9.298E-07	2.806E-03	6.422E-01
7	0.1250	3.135E-06	6.907E-05	1.270E-05	9.598E-07	3.552E-03	6.431E-01
8	0.1563	7.518E-06	7.233E-05	1.054E-05	9.635E-07	4.412E-03	6.439E-01
9	0.1875	1.583E-05	7.413E-05	8.884E-06	9.483E-07	5.398E-03	6.448E-01
10	0.2500	4.937E-05	7.538E-05	6.557E-06	8.773E-07	7.776E-03	6.465E-01
11	0.3125	1.140E-04	7.947E-05	5.156E-06	7.812E-07	1.077E-02	6.481E-01
12	0.3750	2.196E-04	8.923E-05	4.166E-06	6.735E-07	1.451E-02	6.495E-01
13	0.4375	3.727E-04	1.094E-04	3.491E-06	5.652E-07	1.915E-02	6.509E-01
14	0.5000	5.787E-04	1.433E-04	2.971E-06	4.649E-07	2.484E-02	6.521E-01
15	0.5625	8.380E-04	1.941E-04	2.593E-06	3.791E-07	3.167E-02	6.531E-01
16	0.6250	1.150E-03	2.648E-04	2.276E-06	3.112E-07	3.969E-02	6.540E-01
17	0.6875	1.507E-03	3.574E-04	2.001E-06	2.623E-07	4.883E-02	6.547E-01
18	0.7500	1.893E-03	4.711E-04	1.755E-06	2.311E-07	5.891E-02	6.553E-01
19	0.8125	2.281E-03	5.959E-04	1.557E-06	2.146E-07	6.969E-02	6.558E-01
20	0.8750	2.655E-03	7.329E-04	1.366E-06	2.090E-07	8.086E-02	6.563E-01
21	1.0000	3.297E-03	1.033E-03	1.008E-06	2.180E-07	1.033E-01	6.570E-01
22	1.1250	3.639E-03	1.282E-03	7.374E-07	2.316E-07	1.234E-01	6.578E-01
23	1.2500	3.716E-03	1.517E-03	5.122E-07	2.424E-07	1.399E-01	6.587E-01
24	1.3750	3.563E-03	1.677E-03	3.573E-07	2.484E-07	1.526E-01	6.595E-01
25	1.5000	3.327E-03	1.834E-03	2.454E-07	2.526E-07	1.617E-01	6.603E-01
26	1.7500	2.869E-03	2.023E-03	1.349E-07	2.584E-07	1.717E-01	6.615E-01
27	2.0000	2.623E-03	2.255E-03	8.322E-08	2.710E-07	1.763E-01	6.625E-01
28	2.5000	2.468E-03	2.537E-03	5.507E-08	2.905E-07	1.790E-01	6.638E-01
29	3.0000	2.481E-03	2.857E-03	4.567E-08	3.087E-07	1.795E-01	6.647E-01
30	4.0000	2.387E-03	3.095E-03	3.893E-08	3.099E-07	1.803E-01	6.663E-01
31	6.0000	2.365E-03	3.682E-03	3.134E-08	2.897E-07	1.806E-01	6.683E-01
32	8.0000	2.196E-03	3.727E-03	2.759E-08	2.637E-07	1.815E-01	6.695E-01
33	10.0000	2.196E-03	3.727E-03	2.759E-08	2.637E-07	1.815E-01	6.695E-01

TWOPNT: SUCCESS. PROBLEM SOLVED.  
Total CPUtime (sec): 0.609375

## 7.2 Freely Propagating Stoichiometric Methane-Air Flame

In this example we seek to determine the flame speed and structure of an adiabatic, atmospheric-pressure, freely propagating, stoichiometric methane-air flame. This problem is considerably more difficult to solve than the previous example. It is generally true that high-pressure freely propagating flames are more difficult to solve than low-pressure, burner-stabilized flames.

The Keywords `FREE` and `ENRG` indicate that the problem is for a freely propagating flame and that the energy equation will be solved. The Keyword `TFIX` is required in this problem to indicate the temperature that will be held fixed to establish a flame-fixed coordinate system. Unlike in the previous example, the Keyword input for `FLRT` and `TEMP` are simply starting estimates; both will ultimately be computed.

To compute an accurate flame speed, it is important to have the boundaries sufficiently far from the flame itself so that there is negligible diffusion of heat and mass through the boundary. However, in this problem, we had trouble getting a converged solution when an equally spaced coarse mesh and a large solution domain were used at first. Therefore, we used the continuation capabilities of `PREMIX` to make convergence easier (the `CNTN` Keyword). The first problem solved is on a domain of 0.3 cm., much smaller than is appropriate for an accurate flame speed prediction. Moreover, the mesh adaptation parameters `GRAD` and `CURV` are large, meaning that relatively little mesh adaptation will be required.

The initial profiles are also very spread out. We have specified that the initial profiles are centered at 0.1 cm. (`XCEN`) and the width of the flame zone is 1.0 cm. (`WMIX`). Note that this mixing width is larger than the entire domain. These parameters have relatively little physical meaning, but we find that more spread-out guesses are often more likely to lead to convergence than narrow ones. Note that for the initial guess the boundary conditions appear not to be satisfied when the profiles are so spread out. For example, for the initial guess the  $\text{CH}_4$  mole fraction at the left boundary is  $5.103\text{E-}02$  whereas the unreacted methane mole fraction is specified by the `REAC` Keyword to be 0.095. However, while this appears inconsistent, it is not a problem as the boundary condition is specified correctly. When the solution is converged on a sufficiently large domain the unreacted mole fractions will be the same as specified on the Keywords.

The `TWOPNT` solver information follows the printing of the Keywords and the initial guess. First, `SEARCH` indicates that the steady-state Newton iteration failed because one of the variables goes out of the solution bounds. Next, `EVOLVE` takes 100 time steps with the last time step size at  $5.0\text{E-}7$  seconds. After taking the time steps, the next report from `SEARCH` indicates that it was successful. So far in this example, the temperature is still fixed at the user-specified estimate. Now that the Newton iteration is complete on the first mesh, `PREMIX` will include the energy equation and the flame-speed eigenvalue computation. However, before continuing, it reports the converged solution for the fixed temperature problem on the initial mesh.

The computation for the freely propagating flame now begins, using the solution from the fixed-temperature problem as the initial guess. Starting from the fixed-temperature solution, SEARCH is able to quickly find a solution on the coarse mesh. Once the solution is computed, mesh refinement begins. REFINE adds three mesh points and then SEARCH is called again to find a solution on the new mesh. In this case SEARCH has difficulties with the new mesh and EVOLVE is called to take some time steps. EVOLVE takes 200 time steps with 2.0E-6 seconds as the size of the last time-step. SEARCH tries again and this time gets a solution. TWOPNT continues to refine the grid in this manner until a final grid is reached meeting the GRAD and CURV requirements. This grid contains 19 grid points. REFINE shows the final GRAD and CURV values before the final solution is printed out. In this case, we have elected to do a “continuation” calculation, as indicated by the CNTN Keyword, so that after the final solution is obtained, PREMIX goes on to read new Keywords from the user input.

In the first continuation we have reduced GRAD and CURV and have increased the computational interval to  $-0.5 \leq x \leq 8.0$ . Moreover, we have indicated that there will be a further continuation. The continuation calculation uses the converged solution from the first problem as its initial guess. (It follows the very same procedure as if it were a new problem but was started from a restart file.) It first solves the fixed-temperature problem, but with the temperature fixed as computed from the first problem rather than as specified from the user input. In this case the problem is solved easily by Newton’s method with no need for time stepping. However, there were no new mesh points added between the last two mesh points at  $x = 0.3$  and  $x = 8.0$ . As a result, the zero gradient at the hot boundary is still effectively applied at  $x = 0.3$ , which is too close to the flame. One measure of this is a comparison of the independently computed adiabatic flame temperature with the predicted hot-boundary temperature. In this case, the adiabatic flame temperature is 2231K and the burned gas temperature in the flame is 2099K. Therefore, it is clear that another mesh point should be placed near the hot boundary so that the boundary condition is imposed farther from the flame. This is done in the following continuation.

The third and final continuation again reduces GRAD and CURV and further expands the computational interval by adding a new mesh point at  $x = 10$ . Now with the boundary condition applied between  $x = 8$  and 10.0, the flame temperature is free to increase. Several mesh refinements are required to obtain the final solution on 56 mesh points. The flame speed can be seen to be 41.01 cm/sec by looking at the head of the “V” column in the solution. Also it is seen that the unburned mole fractions correspond to the user-specified values as given on the REAC Keywords. Moreover, the species and temperature gradients at both boundaries are seen to be sufficiently small so that there is no appreciable loss of mass or energy through the boundaries. The fact that the burned gas temperature of 2234K is within 3K of the adiabatic flame temperature is further indication that the final solution is an accurate one.

## 7.2.1 CHEMKIN INPUT FOR THE METHANE-AIR FLAME EXAMPLE

```

ELEMENTS  H   O   C   N  END
SPECIES   CH4 CH3 CH2 CH CH2O HCO CO2 CO H2 H O2 O OH HO2 H2O2 H2O
          N2
END
REACTIONS
CH3+H+M=CH4+M          8.0E26      -3.      0.
CH4+O2=CH3+HO2         7.9E13          0.      56000.
CH4+H=CH3+H2           2.2E4            3.      8750.
CH4+O=CH3+OH            1.6E6            2.36    7400.
CH4+OH=CH3+H2O          1.6E6            2.1     2460.
CH3+O=CH2O+H            6.8E13           0.       0.
CH3+OH=CH2O+H2          1.0E12           0.       0.
CH3+OH=CH2+H2O          1.5E13           0.      5000.
CH3+H=CH2+H2            9.0E13           0.     15100.
CH2+H=CH+H2             1.4E19           -2.       0.
CH2+OH=CH2O+H           2.5E13           0.       0.
CH2+OH=CH+H2O           4.5E13           0.      3000.
CH+O2=HCO+O             3.3E13           0.       0.
CH+O=CO+H                5.7E13           0.       0.
CH+OH=HCO+H              3.0E13           0.       0.
CH+CO2=HCO+CO           3.4E12           0.      690.
CH2+CO2=CH2O+CO         1.1E11           0.     1000.
CH2+O=CO+H+H            3.0E13           0.       0.
CH2+O=CO+H2             5.0E13           0.       0.
CH2+O2=CO2+H+H          1.6E12           0.     1000.
CH2+O2=CH2O+O           5.0E13           0.     9000.
CH2+O2=CO2+H2           6.9E11           0.      500.
CH2+O2=CO+H2O           1.9E10           0.    -1000.
CH2+O2=CO+OH+H          8.6E10           0.     -500.
CH2+O2=HCO+OH           4.3E10           0.     -500.
CH2O+OH=HCO+H2O         3.43E9           1.18    -447.
CH2O+H=HCO+H2           2.19E8           1.77    3000.
CH2O+M=HCO+H+M          3.31E16           0.     81000.
CH2O+O=HCO+OH           1.81E13           0.     3082.
HCO+OH=CO+H2O           5.0E12           0.       0.
HCO+M=H+CO+M            1.6E14           0.     14700.
HCO+H=CO+H2             4.0E13           0.       0.
HCO+O=CO2+H             1.0E13           0.       0.
HCO+O2=HO2+CO           3.3E13          -0.4      0.
CO+O+M=CO2+M            3.2E13           0.    -4200.
CO+OH=CO2+H             1.51E7           1.3     -758.
CO+O2=CO2+O             1.6E13           0.     41000.
HO2+CO=CO2+OH           5.8E13           0.    22934.
H2+O2=2OH                1.7E13           0.     47780.
OH+H2=H2O+H             1.17E9           1.3     3626.
H+O2=OH+O               5.13E16          -0.816   16507.
O+H2=OH+H               1.8E10           1.0     8826.
H+O2+M=HO2+M            3.61E17          -0.72    0.
  H2O/18.6/ CO2/4.2/ H2/2.86/ CO/2.11/ N2/1.26/
OH+HO2=H2O+O2           7.5E12           0.       0.
H+HO2=2OH                1.4E14           0.     1073.
O+HO2=O2+OH             1.4E13           0.     1073.
2OH=O+H2O               6.0E8            1.3      0.
H+H+M=H2+M              1.0E18           -1.0     0.
H+H+H2=H2+H2            9.2E16           -0.6     0.
H+H+H2O=H2+H2O          6.0E19           -1.25    0.
H+H+CO2=H2+CO2          5.49E20           -2.0     0.
H+OH+M=H2O+M            1.6E22           -2.0     0.
  H2O/5/
H+O+M=OH+M               6.2E16           -0.6     0.
  H2O/5/
H+HO2=H2+O2             1.25E13           0.       0.

```

$\text{HO}_2 + \text{HO}_2 = \text{H}_2\text{O}_2 + \text{O}_2$	2.0E12	0.	0.
$\text{H}_2\text{O}_2 + \text{M} = \text{OH} + \text{OH} + \text{M}$	1.3E17	0.	45500.
$\text{H}_2\text{O}_2 + \text{H} = \text{HO}_2 + \text{H}_2$	1.6E12	0.	3800.
$\text{H}_2\text{O}_2 + \text{OH} = \text{H}_2\text{O} + \text{HO}_2$	1.0E13	0.	1800.
END			

## 7.2.2 PREMIX OUTPUT FOR THE METHANE-AIR FLAME EXAMPLE

PREMIX: CHEMKIN-III One-dimensional steady premixed laminar flame code,  
DOUBLE PRECISION Vers. 3.39 2000/08/09  
Copyright 1995, Sandia Corporation.  
The U.S. Government retains a limited license in this software.

	WORKING SPACE REQUIREMENTS	
	PROVIDED	REQUIRED
LOGICAL	119	119
INTEGER	5422	5422
REAL	304716	304716
CHARACTER	78	78

CKLIB: CHEMKIN-III GAS-PHASE CHEMICAL KINETICS LIBRARY,  
DOUBLE PRECISION Vers. 5.28 2000/08/05  
Copyright 1995, Sandia Corporation.  
The U.S. Government retains a limited license in this software.

TRANLIB: CHEMKIN-III MULTICOMPONENT TRANSPORT LIBRARY,  
DOUBLE PRECISION Vers. 4.6 1999/06/03  
Copyright 1995, Sandia Corporation.  
The U.S. Government retains a limited license in this software.

### KEYWORD INPUT

```
/ freely propagating flame
FREE
ENRG
/ initial flow-rate estimate
FLRT .04 ! gm/cm**2-sec
/ atmospheric pressure
PRES 1.0 ! atmospheres
/ initial grid and profile specification
NPTS 6
XEND 0.3 ! cm
XCEN 0.1 ! cm
WMLX 1.0 ! cm
/ temperature to fixed for the flame speed computation
TFIX 400.
/ mesh adaptation criteria
GRAD 0.9
CURV 0.9
/ unreacted fuel-oxidizer makeup
MOLE
REAC CH4 0.0950
REAC O2 0.19
REAC N2 0.715
/ estimated product mole fractions
PROD H2O 0.190
PROD CO2 0.095
PROD N2 0.715
/ estimated peak intermediate mole fractions
INTM CO 0.08
INTM HCO 0.00001
INTM HO2 0.0001
INTM O 0.0001
INTM H2O2 0.0001
INTM H 0.02
INTM H2 0.01
INTM OH 0.001
INTM CH2 0.0001
INTM CH 0.00001
INTM CH2O 0.001
INTM CH3 0.0005
```

```

/ convergence tolerance for Newton
ATOL 1.E-9
RTOL 1.E-4
/ convergence tolerance for timestepping
ATIM 1.E-5
RTIM 1.E-5
/ maximum printing
PRNT 1
/ time step control
TIME 100 5.0E-7 ! sec
TIM2 200 1.0E-6 ! sec
/ estimated temperature profile
TEMP 0.0 298.
TEMP 0.03 300.
TEMP 0.05 400.
TEMP 0.06 766.
TEMP 0.07 1512.
TEMP 0.08 1892.
TEMP 0.09 2000.
TEMP 0.1 2030.
TEMP 0.2 2111.
TEMP 0.35 2190.
TEMP 10.0 2190.
/ a continuation run will follow
CNTN
END

```

TWOPNT: DOUBLE PRECISION (TWO POINT BOUNDARY VALUE PROBLEM) SOLVER,  
VERSION 3.30 OF APRIL 1998 BY DR. JOSEPH F. GRGAR.

TWOPNT: INITIAL GUESS:

	X	T	V	RHO	CH4	CH3	CH2
1	0.0000	2.980E+02	3.634E+01	1.101E-03	5.103E-02	4.635E-04	9.269E-05
2	0.0500	4.000E+02	4.886E+01	8.187E-04	4.646E-02	4.906E-04	9.812E-05
3	0.0600	7.660E+02	9.358E+01	4.275E-04	4.558E-02	4.940E-04	9.879E-05
4	0.1200	2.046E+03	2.500E+02	1.600E-04	4.047E-02	4.985E-04	9.970E-05
5	0.1800	2.095E+03	2.556E+02	1.565E-04	3.561E-02	4.763E-04	9.526E-05
6	0.2400	2.132E+03	2.595E+02	1.541E-04	3.087E-02	4.309E-04	8.618E-05
7	0.3000	2.164E+03	2.624E+02	1.524E-04	2.612E-02	3.691E-04	7.382E-05

	X	CH	CH2O	HCO	CO2	CO	H2
1	0.0000	9.269E-06	9.269E-04	9.269E-06	3.402E-02	7.415E-02	9.269E-03
2	0.0500	9.812E-06	9.812E-04	9.812E-06	3.801E-02	7.850E-02	9.812E-03
3	0.0600	9.879E-06	9.879E-04	9.879E-06	3.882E-02	7.903E-02	9.879E-03
4	0.1200	9.970E-06	9.970E-04	9.970E-06	4.384E-02	7.976E-02	9.970E-03
5	0.1800	9.526E-06	9.526E-04	9.526E-06	4.917E-02	7.621E-02	9.526E-03
6	0.2400	8.618E-06	8.618E-04	8.618E-06	5.488E-02	6.894E-02	8.618E-03
7	0.3000	7.382E-06	7.382E-04	7.382E-06	6.096E-02	5.906E-02	7.382E-03

	X	H	O2	O	OH	HO2	H2O2
1	0.0000	1.854E-02	1.021E-01	9.269E-05	9.269E-04	9.269E-05	9.269E-05
2	0.0500	1.962E-02	9.292E-02	9.812E-05	9.812E-04	9.812E-05	9.812E-05
3	0.0600	1.976E-02	9.115E-02	9.879E-05	9.879E-04	9.879E-05	9.879E-05
4	0.1200	1.994E-02	8.093E-02	9.970E-05	9.970E-04	9.970E-05	9.970E-05
5	0.1800	1.905E-02	7.122E-02	9.526E-05	9.526E-04	9.526E-05	9.526E-05
6	0.2400	1.724E-02	6.174E-02	8.618E-05	8.618E-04	8.618E-05	8.618E-05
7	0.3000	1.476E-02	5.225E-02	7.382E-05	7.382E-04	7.382E-05	7.382E-05

	X	H2O	N2
1	0.0000	6.805E-02	6.402E-01
2	0.0500	7.603E-02	6.358E-01
3	0.0600	7.765E-02	6.352E-01
4	0.1200	8.768E-02	6.345E-01
5	0.1800	9.835E-02	6.381E-01
6	0.2400	1.098E-01	6.454E-01
7	0.3000	1.219E-01	6.554E-01

TWOPNT: SOLVE THE PROBLEM.

	LOG10 TASK	LOG10 NORM F	LOG10 COND J	REMARK
START	1.74			
SEARCH		7.61		GOING OUT OF BOUNDS



EVOLVE -1.08 3.43 100 TIME STEPS, 5.0E-07 LAST STRIDE  
SEARCH -8.33 7.07 21 SEARCH STEPS

TWOPNT: FINAL SOLUTION:

	X	T	V	RHO	CH4	CH3	CH2
1	0.0000	2.980E+02	3.549E+01	1.127E-03	9.339E-02	2.053E-05	7.004E-12
2	0.0500	4.000E+02	4.800E+01	8.333E-04	8.372E-02	1.631E-04	5.457E-11
3	0.0600	7.660E+02	9.222E+01	4.337E-04	7.703E-02	5.786E-04	7.821E-08
4	0.1200	2.046E+03	2.522E+02	1.586E-04	1.961E-04	1.726E-04	1.016E-05
5	0.1800	2.095E+03	2.564E+02	1.560E-04	6.822E-07	1.120E-06	8.105E-08
6	0.2400	2.132E+03	2.602E+02	1.537E-04	2.998E-09	6.850E-09	5.451E-10
7	0.3000	2.164E+03	2.641E+02	1.515E-04	2.998E-09	6.850E-09	5.451E-10

	X	CH	CH2O	HCO	CO2	CO	H2
1	0.0000	1.804E-16	1.312E-05	2.581E-10	3.086E-04	4.064E-04	2.201E-03
2	0.0500	9.925E-16	1.423E-04	2.778E-09	3.341E-03	3.480E-03	6.596E-03
3	0.0600	5.409E-11	2.715E-04	7.461E-07	6.138E-03	5.818E-03	7.953E-03
4	0.1200	1.506E-06	5.651E-05	1.365E-05	5.483E-02	3.654E-02	1.609E-02
5	0.1800	1.444E-08	4.138E-07	1.413E-07	6.379E-02	2.902E-02	1.374E-02
6	0.2400	1.029E-10	2.764E-09	3.998E-08	6.646E-02	2.674E-02	1.270E-02
7	0.3000	1.029E-10	2.764E-09	3.998E-08	6.646E-02	2.674E-02	1.270E-02

	X	H	O2	O	OH	HO2	H2O2
1	0.0000	9.970E-08	1.878E-01	9.841E-09	2.345E-07	5.693E-06	1.850E-05
2	0.0500	2.264E-07	1.730E-01	5.729E-08	1.387E-06	4.860E-05	1.589E-04
3	0.0600	7.400E-05	1.622E-01	8.880E-06	6.457E-05	1.680E-04	1.760E-04
4	0.1200	9.938E-03	2.657E-02	4.887E-03	1.071E-02	7.695E-06	1.717E-06
5	0.1800	7.531E-03	1.978E-02	3.989E-03	1.042E-02	5.188E-06	1.168E-06
6	0.2400	6.006E-03	1.743E-02	3.208E-03	9.802E-03	4.402E-06	8.417E-07
7	0.3000	6.006E-03	1.743E-02	3.208E-03	9.802E-03	4.402E-06	8.417E-07

	X	H2O	N2
1	0.0000	2.977E-03	7.129E-01
2	0.0500	2.304E-02	7.063E-01
3	0.0600	3.578E-02	7.037E-01
4	0.1200	1.502E-01	6.898E-01
5	0.1800	1.574E-01	6.943E-01
6	0.2400	1.615E-01	6.961E-01
7	0.3000	1.615E-01	6.961E-01

TWOPNT: SUCCESS. PROBLEM SOLVED.

FLDRIV: FINISHED FIXED TEMPERATURE, ADDING ENERGY EQUATION

TWOPNT: DOUBLE PRECISION (TWO POINT BOUNDARY VALUE PROBLEM) SOLVER,  
VERSION 3.30 OF APRIL 1998 BY DR. JOSEPH F. GRGAR.

TWOPNT: INITIAL GUESS:

	X	T	V	RHO	CH4	CH3	CH2
1	0.0000	2.980E+02	3.549E+01	1.127E-03	9.339E-02	2.053E-05	7.004E-12
2	0.0500	4.000E+02	4.800E+01	8.333E-04	8.372E-02	1.631E-04	5.457E-11
3	0.0600	7.660E+02	9.222E+01	4.337E-04	7.703E-02	5.786E-04	7.821E-08
4	0.1200	2.046E+03	2.522E+02	1.586E-04	1.961E-04	1.726E-04	1.016E-05
5	0.1800	2.095E+03	2.564E+02	1.560E-04	6.822E-07	1.120E-06	8.105E-08
6	0.2400	2.132E+03	2.602E+02	1.537E-04	2.998E-09	6.850E-09	5.451E-10
7	0.3000	2.164E+03	2.641E+02	1.515E-04	2.998E-09	6.850E-09	5.451E-10

	X	CH	CH2O	HCO	CO2	CO	H2
1	0.0000	1.804E-16	1.312E-05	2.581E-10	3.086E-04	4.064E-04	2.201E-03
2	0.0500	9.925E-16	1.423E-04	2.778E-09	3.341E-03	3.480E-03	6.596E-03
3	0.0600	5.409E-11	2.715E-04	7.461E-07	6.138E-03	5.818E-03	7.953E-03
4	0.1200	1.506E-06	5.651E-05	1.365E-05	5.483E-02	3.654E-02	1.609E-02
5	0.1800	1.444E-08	4.138E-07	1.413E-07	6.379E-02	2.902E-02	1.374E-02
6	0.2400	1.029E-10	2.764E-09	3.998E-08	6.646E-02	2.674E-02	1.270E-02
7	0.3000	1.029E-10	2.764E-09	3.998E-08	6.646E-02	2.674E-02	1.270E-02

	X	H	O2	O	OH	HO2	H2O2
1	0.0000	9.970E-08	1.878E-01	9.841E-09	2.345E-07	5.693E-06	1.850E-05
2	0.0500	2.264E-07	1.730E-01	5.729E-08	1.387E-06	4.860E-05	1.589E-04
3	0.0600	7.400E-05	1.622E-01	8.880E-06	6.457E-05	1.680E-04	1.760E-04
4	0.1200	9.938E-03	2.657E-02	4.887E-03	1.071E-02	7.695E-06	1.717E-06
5	0.1800	7.531E-03	1.978E-02	3.989E-03	1.042E-02	5.188E-06	1.168E-06
6	0.2400	6.006E-03	1.743E-02	3.208E-03	9.802E-03	4.402E-06	8.417E-07
7	0.3000	6.006E-03	1.743E-02	3.208E-03	9.802E-03	4.402E-06	8.417E-07

	X	H2O	N2
1	0.0000	2.977E-03	7.129E-01
2	0.0500	2.304E-02	7.063E-01
3	0.0600	3.578E-02	7.037E-01
4	0.1200	1.502E-01	6.898E-01
5	0.1800	1.574E-01	6.943E-01
6	0.2400	1.615E-01	6.961E-01
7	0.3000	1.615E-01	6.961E-01

TWOPNT: SOLVE THE PROBLEM.

TASK	LOG10 NORM F	LOG10 COND J	REMARK
START	3.03		7 GRID POINTS
SEARCH	-3.71	10.99	17 SEARCH STEPS
REFINE	3.50		1.00 AND 1.00 RATIOS, 10 GRID POINTS
SEARCH		10.85	GOING OUT OF BOUNDS
EVOLVE	1.12	9.61	200 TIME STEPS, 2.0E-06 LAST STRIDE
SEARCH	-4.11	11.02	16 SEARCH STEPS
REFINE	3.53		1.00 AND 1.00 RATIOS, 13 GRID POINTS
SEARCH	-1.87	11.41	12 SEARCH STEPS
REFINE	3.44		0.99 AND 1.00 RATIOS, 17 GRID POINTS
SEARCH	-3.51	11.75	18 SEARCH STEPS
REFINE	3.40		0.83 AND 1.00 RATIOS, 19 GRID POINTS
SEARCH	-1.47	11.91	15 SEARCH STEPS
REFINE			0.56 AND 0.62 RATIOS

TWOPNT: FINAL SOLUTION:

	X	T	V	RHO	CH4	CH3	CH2
1	0.0000	2.980E+02	4.181E+01	1.126E-03	9.396E-02	2.424E-05	7.681E-15
2	0.0500	4.000E+02	5.663E+01	8.317E-04	8.751E-02	2.222E-04	6.901E-14
3	0.0550	4.471E+02	6.345E+01	7.423E-04	8.475E-02	3.218E-04	4.556E-12
4	0.0600	5.187E+02	7.382E+01	6.380E-04	8.061E-02	4.806E-04	1.115E-10
5	0.0675	6.784E+02	9.704E+01	4.853E-04	7.129E-02	8.904E-04	6.976E-09
6	0.0750	9.023E+02	1.298E+02	3.627E-04	5.740E-02	1.805E-03	2.621E-07
7	0.0825	1.177E+03	1.705E+02	2.763E-04	3.802E-02	3.651E-03	4.553E-06
8	0.0900	1.464E+03	2.131E+02	2.210E-04	1.594E-02	4.761E-03	3.595E-05
9	0.0938	1.580E+03	2.304E+02	2.044E-04	8.058E-03	3.729E-03	5.614E-05
10	0.0975	1.667E+03	2.432E+02	1.937E-04	3.292E-03	2.091E-03	5.226E-05
11	0.1013	1.722E+03	2.512E+02	1.875E-04	1.099E-03	8.401E-04	2.904E-05
12	0.1050	1.756E+03	2.559E+02	1.841E-04	2.853E-04	2.429E-04	1.029E-05
13	0.1125	1.796E+03	2.610E+02	1.805E-04	2.944E-05	2.747E-05	1.375E-06
14	0.1200	1.827E+03	2.646E+02	1.780E-04	2.298E-06	2.371E-06	1.310E-07
15	0.1350	1.872E+03	2.702E+02	1.743E-04	7.864E-08	9.426E-08	5.702E-09
16	0.1500	1.907E+03	2.745E+02	1.716E-04	2.318E-09	3.215E-09	2.077E-10
17	0.1800	1.956E+03	2.807E+02	1.678E-04	2.992E-11	4.874E-11	3.340E-12
18	0.2400	2.009E+03	2.877E+02	1.637E-04	2.146E-13	4.098E-13	2.956E-14
19	0.3000	2.009E+03	2.877E+02	1.637E-04	2.146E-13	4.098E-13	2.956E-14

	X	CH	CH2O	HCO	CO2	CO	H2
1	0.0000	2.332E-23	3.033E-06	8.932E-14	5.890E-05	2.716E-04	3.141E-03
2	0.0500	1.468E-22	3.812E-05	1.114E-12	7.390E-04	2.687E-03	1.052E-02
3	0.0550	6.621E-19	6.002E-05	4.796E-11	1.169E-03	3.926E-03	1.200E-02
4	0.0600	3.544E-16	9.891E-05	7.643E-10	1.943E-03	5.928E-03	1.363E-02
5	0.0675	3.757E-13	2.019E-04	3.729E-08	4.035E-03	1.079E-02	1.623E-02
6	0.0750	1.162E-10	3.820E-04	1.358E-06	7.690E-03	1.843E-02	1.893E-02
7	0.0825	9.673E-09	6.883E-04	1.575E-05	1.343E-02	2.936E-02	2.160E-02
8	0.0900	3.350E-07	9.076E-04	5.895E-05	2.153E-02	4.271E-02	2.336E-02
9	0.0938	1.084E-06	8.110E-04	7.887E-05	2.619E-02	4.770E-02	2.276E-02
10	0.0975	1.884E-06	5.672E-04	7.616E-05	3.112E-02	5.013E-02	2.103E-02
11	0.1013	1.696E-06	2.906E-04	4.943E-05	3.605E-02	4.958E-02	1.868E-02
12	0.1050	8.526E-07	1.021E-04	2.046E-05	4.072E-02	4.707E-02	1.648E-02
13	0.1125	1.584E-07	1.303E-05	3.117E-06	4.864E-02	4.057E-02	1.395E-02
14	0.1200	1.780E-08	1.153E-06	4.053E-07	5.453E-02	3.539E-02	1.303E-02
15	0.1350	8.590E-10	4.428E-08	1.056E-07	6.132E-02	2.935E-02	1.271E-02
16	0.1500	3.290E-11	1.670E-09	7.276E-08	6.503E-02	2.606E-02	1.249E-02
17	0.1800	5.413E-13	2.044E-10	4.920E-08	6.815E-02	2.330E-02	1.185E-02
18	0.2400	4.911E-15	1.512E-10	3.207E-08	7.031E-02	2.145E-02	1.090E-02
19	0.3000	4.911E-15	1.512E-10	3.207E-08	7.031E-02	2.145E-02	1.090E-02

	X	H	O2	O	OH	HO2	H2O2
1	0.0000	4.156E-11	1.887E-01	1.101E-13	3.271E-10	3.775E-07	8.696E-07
2	0.0500	1.037E-10	1.811E-01	7.344E-13	2.219E-09	3.723E-06	8.627E-06
3	0.0550	9.877E-09	1.776E-01	8.494E-11	5.163E-08	1.181E-05	1.229E-05
4	0.0600	2.726E-07	1.722E-01	2.033E-09	3.693E-07	2.893E-05	1.779E-05
5	0.0675	7.843E-06	1.594E-01	8.232E-08	4.372E-06	8.092E-05	2.812E-05
6	0.0750	9.578E-05	1.400E-01	2.617E-06	3.664E-05	1.313E-04	3.106E-05
7	0.0825	5.331E-04	1.132E-01	3.195E-05	1.813E-04	1.249E-04	2.083E-05
8	0.0900	1.962E-03	8.063E-02	2.021E-04	8.011E-04	7.611E-05	6.050E-06
9	0.0938	3.263E-03	6.549E-02	4.738E-04	1.586E-03	5.232E-05	2.815E-06
10	0.0975	4.764E-03	5.256E-02	1.016E-03	2.779E-03	3.378E-05	2.099E-06
11	0.1013	6.125E-03	4.269E-02	1.841E-03	4.200E-03	2.177E-05	2.486E-06
12	0.1050	7.138E-03	3.575E-02	2.688E-03	5.485E-03	1.521E-05	3.085E-06
13	0.1125	8.126E-03	2.839E-02	3.598E-03	6.972E-03	1.071E-05	3.638E-06
14	0.1200	8.346E-03	2.467E-02	3.850E-03	7.628E-03	8.932E-06	3.499E-06
15	0.1350	7.874E-03	2.140E-02	3.673E-03	7.965E-03	7.362E-06	2.774E-06
16	0.1500	7.203E-03	1.956E-02	3.383E-03	8.012E-03	6.469E-06	2.215E-06
17	0.1800	5.997E-03	1.752E-02	2.875E-03	7.868E-03	5.468E-06	1.557E-06
18	0.2400	4.687E-03	1.550E-02	2.312E-03	7.545E-03	4.513E-06	1.027E-06
19	0.3000	4.687E-03	1.550E-02	2.312E-03	7.545E-03	4.513E-06	1.027E-06

	X	H2O	N2
1	0.0000	1.403E-03	7.124E-01
2	0.0500	1.254E-02	7.047E-01
3	0.0550	1.754E-02	7.026E-01
4	0.0600	2.496E-02	7.001E-01
5	0.0675	4.105E-02	6.959E-01
6	0.0750	6.325E-02	6.918E-01
7	0.0825	9.089E-02	6.883E-01
8	0.0900	1.209E-01	6.861E-01
9	0.0938	1.338E-01	6.859E-01
10	0.0975	1.442E-01	6.863E-01
11	0.1013	1.515E-01	6.870E-01
12	0.1050	1.561E-01	6.879E-01
13	0.1125	1.599E-01	6.898E-01
14	0.1200	1.611E-01	6.914E-01
15	0.1350	1.620E-01	6.937E-01
16	0.1500	1.630E-01	6.952E-01
17	0.1800	1.654E-01	6.970E-01
18	0.2400	1.688E-01	6.985E-01
19	0.3000	1.688E-01	6.985E-01

TWOPNT: SUCCESS. PROBLEM SOLVED.

////////////////////////////////// CONTINUING TO NEW PROBLEM //////////////////////////////////  
 ////////////////////////////////// CONTINUING TO NEW PROBLEM //////////////////////////////////  
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 ////////////////////////////////// CONTINUING TO NEW PROBLEM //////////////////////////////////  
 ////////////////////////////////// CONTINUING TO NEW PROBLEM //////////////////////////////////

KEYWORD INPUT

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/
/   This is the second continuation. The mesh adaptation is more
/   stringent, and th computational comain is expanded. Yet another
/   continuation will follow after this one.
/
GRAD  0.5
CURV  0.7
XSTR  -0.5
XEND  8.0
CNTN
END

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TWOPNT: DOUBLE PRECISION (TWO POINT BOUNDARY VALUE PROBLEM) SOLVER,  
VERSION 3.30 OF APRIL 1998 BY DR. JOSEPH F. GRCAR.

TWOPNT: INITIAL GUESS:

	X	T	V	RHO	CH4	CH3	CH2
1	-0.5000	2.980E+02	4.181E+01	1.126E-03	9.396E-02	2.424E-05	7.681E-15
2	0.0000	2.980E+02	4.181E+01	1.126E-03	9.396E-02	2.424E-05	7.681E-15
3	0.0500	4.000E+02	5.663E+01	8.317E-04	8.751E-02	2.222E-04	6.901E-14
4	0.0550	4.471E+02	6.345E+01	7.423E-04	8.475E-02	3.218E-04	4.556E-12
5	0.0600	5.187E+02	7.382E+01	6.380E-04	8.061E-02	4.806E-04	1.115E-10
6	0.0675	6.784E+02	9.704E+01	4.853E-04	7.129E-02	8.904E-04	6.976E-09
7	0.0750	9.023E+02	1.298E+02	3.627E-04	5.740E-02	1.805E-03	2.621E-07
8	0.0825	1.177E+03	1.705E+02	2.763E-04	3.802E-02	3.651E-03	4.553E-06
9	0.0900	1.464E+03	2.131E+02	2.210E-04	1.594E-02	4.761E-03	3.595E-05
10	0.0938	1.580E+03	2.304E+02	2.044E-04	8.058E-03	3.729E-03	5.614E-05
11	0.0975	1.667E+03	2.432E+02	1.937E-04	3.292E-03	2.091E-03	5.226E-05
12	0.1013	1.722E+03	2.512E+02	1.875E-04	1.099E-03	8.401E-04	2.904E-05
13	0.1050	1.756E+03	2.559E+02	1.841E-04	2.853E-04	2.429E-04	1.029E-05
14	0.1125	1.796E+03	2.610E+02	1.805E-04	2.944E-05	2.747E-05	1.375E-06
15	0.1200	1.827E+03	2.646E+02	1.780E-04	2.298E-06	2.371E-06	1.310E-07
16	0.1350	1.872E+03	2.702E+02	1.743E-04	7.864E-08	9.426E-08	5.702E-09
17	0.1500	1.907E+03	2.745E+02	1.716E-04	2.318E-09	3.215E-09	2.077E-10
18	0.1800	1.956E+03	2.807E+02	1.678E-04	2.992E-11	4.874E-11	3.340E-12
19	0.2400	2.009E+03	2.877E+02	1.637E-04	2.146E-13	4.098E-13	2.956E-14
20	0.3000	2.009E+03	2.877E+02	1.637E-04	2.146E-13	4.098E-13	2.956E-14
21	8.0000	2.009E+03	2.877E+02	1.637E-04	2.146E-13	4.098E-13	2.956E-14

	X	CH	CH2O	HCO	CO2	CO	H2
1	-0.5000	2.332E-23	3.033E-06	8.932E-14	5.890E-05	2.716E-04	3.141E-03
2	0.0000	2.332E-23	3.033E-06	8.932E-14	5.890E-05	2.716E-04	3.141E-03
3	0.0500	1.468E-22	3.812E-05	1.114E-12	7.390E-04	2.687E-03	1.052E-02
4	0.0550	6.621E-19	6.002E-05	4.796E-11	1.169E-03	3.926E-03	1.200E-02
5	0.0600	3.544E-16	9.891E-05	7.643E-10	1.943E-03	5.928E-03	1.363E-02
6	0.0675	3.757E-13	2.019E-04	3.729E-08	4.035E-03	1.079E-02	1.623E-02
7	0.0750	1.162E-10	3.820E-04	1.358E-06	7.690E-03	1.843E-02	1.893E-02
8	0.0825	9.673E-09	6.883E-04	1.575E-05	1.343E-02	2.936E-02	2.160E-02
9	0.0900	3.350E-07	9.076E-04	5.895E-05	2.153E-02	4.271E-02	2.336E-02
10	0.0938	1.084E-06	8.110E-04	7.887E-05	2.619E-02	4.770E-02	2.276E-02
11	0.0975	1.884E-06	5.672E-04	7.616E-05	3.112E-02	5.013E-02	2.103E-02
12	0.1013	1.696E-06	2.906E-04	4.943E-05	3.605E-02	4.958E-02	1.868E-02
13	0.1050	8.526E-07	1.021E-04	2.046E-05	4.072E-02	4.707E-02	1.648E-02
14	0.1125	1.584E-07	1.303E-05	3.117E-06	4.864E-02	4.057E-02	1.395E-02
15	0.1200	1.780E-08	1.153E-06	4.053E-07	5.453E-02	3.539E-02	1.303E-02
16	0.1350	8.590E-10	4.428E-08	1.056E-07	6.132E-02	2.935E-02	1.271E-02
17	0.1500	3.290E-11	1.670E-09	7.276E-08	6.503E-02	2.606E-02	1.249E-02
18	0.1800	5.413E-13	2.044E-10	4.920E-08	6.815E-02	2.330E-02	1.185E-02
19	0.2400	4.911E-15	1.512E-10	3.207E-08	7.031E-02	2.145E-02	1.090E-02
20	0.3000	4.911E-15	1.512E-10	3.207E-08	7.031E-02	2.145E-02	1.090E-02
21	8.0000	4.911E-15	1.512E-10	3.207E-08	7.031E-02	2.145E-02	1.090E-02

	X	H	O2	O	OH	HO2	H2O2
1	-0.5000	4.156E-11	1.887E-01	1.101E-13	3.271E-10	3.775E-07	8.696E-07
2	0.0000	4.156E-11	1.887E-01	1.101E-13	3.271E-10	3.775E-07	8.696E-07
3	0.0500	1.037E-10	1.811E-01	7.344E-13	2.219E-09	3.723E-06	8.627E-06
4	0.0550	9.877E-09	1.776E-01	8.494E-11	5.163E-08	1.181E-05	1.229E-05
5	0.0600	2.726E-07	1.722E-01	2.033E-09	3.693E-07	2.893E-05	1.779E-05
6	0.0675	7.843E-06	1.594E-01	8.232E-08	4.372E-06	8.092E-05	2.812E-05
7	0.0750	9.578E-05	1.400E-01	2.617E-06	3.664E-05	1.313E-04	3.106E-05
8	0.0825	5.331E-04	1.132E-01	3.195E-05	1.813E-04	1.249E-04	2.083E-05
9	0.0900	1.962E-03	8.063E-02	2.021E-04	8.011E-04	7.611E-05	6.050E-06
10	0.0938	3.263E-03	6.549E-02	4.738E-04	1.586E-03	5.232E-05	2.815E-06
11	0.0975	4.764E-03	5.256E-02	1.016E-03	2.779E-03	3.378E-05	2.099E-06
12	0.1013	6.125E-03	4.269E-02	1.841E-03	4.200E-03	2.177E-05	2.486E-06
13	0.1050	7.138E-03	3.575E-02	2.688E-03	5.485E-03	1.521E-05	3.085E-06
14	0.1125	8.126E-03	2.839E-02	3.598E-03	6.972E-03	1.071E-05	3.638E-06
15	0.1200	8.346E-03	2.467E-02	3.850E-03	7.628E-03	8.932E-06	3.499E-06
16	0.1350	7.874E-03	2.140E-02	3.673E-03	7.965E-03	7.362E-06	2.774E-06
17	0.1500	7.203E-03	1.956E-02	3.383E-03	8.012E-03	6.469E-06	2.215E-06
18	0.1800	5.997E-03	1.752E-02	2.875E-03	7.868E-03	5.468E-06	1.557E-06
19	0.2400	4.687E-03	1.550E-02	2.312E-03	7.545E-03	4.513E-06	1.027E-06
20	0.3000	4.687E-03	1.550E-02	2.312E-03	7.545E-03	4.513E-06	1.027E-06
21	8.0000	4.687E-03	1.550E-02	2.312E-03	7.545E-03	4.513E-06	1.027E-06

	X	H2O	N2
1	-0.5000	1.403E-03	7.124E-01
2	0.0000	1.403E-03	7.124E-01
3	0.0500	1.254E-02	7.047E-01
4	0.0550	1.754E-02	7.026E-01
5	0.0600	2.496E-02	7.001E-01
6	0.0675	4.105E-02	6.959E-01
7	0.0750	6.325E-02	6.918E-01
8	0.0825	9.089E-02	6.883E-01
9	0.0900	1.209E-01	6.861E-01
10	0.0938	1.338E-01	6.859E-01
11	0.0975	1.442E-01	6.863E-01
12	0.1013	1.515E-01	6.870E-01
13	0.1050	1.561E-01	6.879E-01
14	0.1125	1.599E-01	6.898E-01
15	0.1200	1.611E-01	6.914E-01
16	0.1350	1.620E-01	6.937E-01
17	0.1500	1.630E-01	6.952E-01
18	0.1800	1.654E-01	6.970E-01
19	0.2400	1.688E-01	6.985E-01
20	0.3000	1.688E-01	6.985E-01
21	8.0000	1.688E-01	6.985E-01

TWOPNT: SOLVE THE PROBLEM.

TASK	LOG10 NORM F	LOG10 COND J	REMARK
START	-2.50		
SEARCH	-5.49	9.15	6 SEARCH STEPS

TWOPNT: FINAL SOLUTION:

	X	T	V	RHO	CH4	CH3	CH2
1	-0.5000	2.980E+02	4.168E+01	1.130E-03	9.497E-02	4.373E-07	2.414E-20
2	0.0000	2.980E+02	4.190E+01	1.124E-03	9.318E-02	4.098E-05	2.212E-18
3	0.0500	4.000E+02	5.672E+01	8.304E-04	8.684E-02	2.297E-04	7.252E-14
4	0.0550	4.471E+02	6.354E+01	7.412E-04	8.410E-02	3.252E-04	4.784E-12
5	0.0600	5.187E+02	7.392E+01	6.371E-04	7.999E-02	4.778E-04	1.163E-10
6	0.0675	6.784E+02	9.717E+01	4.847E-04	7.074E-02	8.750E-04	7.225E-09
7	0.0750	9.023E+02	1.300E+02	3.623E-04	5.692E-02	1.778E-03	2.683E-07
8	0.0825	1.177E+03	1.707E+02	2.760E-04	3.763E-02	3.613E-03	4.619E-06
9	0.0900	1.464E+03	2.133E+02	2.208E-04	1.570E-02	4.703E-03	3.617E-05
10	0.0938	1.580E+03	2.306E+02	2.042E-04	7.909E-03	3.673E-03	5.608E-05
11	0.0975	1.667E+03	2.434E+02	1.935E-04	3.222E-03	2.055E-03	5.189E-05
12	0.1013	1.722E+03	2.514E+02	1.873E-04	1.074E-03	8.253E-04	2.876E-05
13	0.1050	1.756E+03	2.561E+02	1.839E-04	2.788E-04	2.392E-04	1.021E-05
14	0.1125	1.796E+03	2.612E+02	1.803E-04	2.885E-05	2.719E-05	1.370E-06
15	0.1200	1.827E+03	2.648E+02	1.778E-04	2.263E-06	2.360E-06	1.313E-07
16	0.1350	1.872E+03	2.704E+02	1.742E-04	7.803E-08	9.456E-08	5.756E-09
17	0.1500	1.907E+03	2.747E+02	1.714E-04	2.327E-09	3.261E-09	2.117E-10
18	0.1800	1.956E+03	2.808E+02	1.677E-04	3.080E-11	5.054E-11	3.472E-12
19	0.2400	2.009E+03	2.874E+02	1.639E-04	2.436E-13	4.632E-13	3.309E-14
20	0.3000	2.009E+03	2.865E+02	1.644E-04	2.092E-15	4.172E-15	3.228E-16
21	8.0000	2.009E+03	2.865E+02	1.644E-04	2.092E-15	4.172E-15	3.228E-16

	X	CH	CH2O	HCO	CO2	CO	H2
1	-0.5000	-3.629E-29	3.985E-08	1.099E-18	7.957E-07	4.799E-06	1.873E-04
2	0.0000	-2.201E-27	5.385E-06	1.473E-16	1.060E-04	4.868E-04	5.118E-03
3	0.0500	1.657E-22	3.987E-05	1.185E-12	7.832E-04	2.887E-03	1.192E-02
4	0.0550	7.297E-19	6.141E-05	5.102E-11	1.212E-03	4.120E-03	1.329E-02
5	0.0600	3.894E-16	9.969E-05	8.095E-10	1.983E-03	6.113E-03	1.480E-02
6	0.0675	4.085E-13	2.011E-04	3.914E-08	4.071E-03	1.095E-02	1.721E-02
7	0.0750	1.239E-10	3.790E-04	1.402E-06	7.718E-03	1.856E-02	1.970E-02
8	0.0825	1.013E-08	6.829E-04	1.605E-05	1.345E-02	2.945E-02	2.218E-02
9	0.0900	3.453E-07	8.969E-04	5.931E-05	2.152E-02	4.270E-02	2.375E-02
10	0.0938	1.105E-06	7.984E-04	7.868E-05	2.616E-02	4.762E-02	2.306E-02
11	0.0975	1.902E-06	5.558E-04	7.532E-05	3.105E-02	4.998E-02	2.126E-02
12	0.1013	1.702E-06	2.837E-04	4.855E-05	3.595E-02	4.938E-02	1.887E-02
13	0.1050	8.556E-07	9.952E-05	2.004E-05	4.059E-02	4.686E-02	1.666E-02
14	0.1125	1.594E-07	1.274E-05	3.056E-06	4.845E-02	4.041E-02	1.411E-02
15	0.1200	1.801E-08	1.133E-06	4.006E-07	5.429E-02	3.526E-02	1.319E-02
16	0.1350	8.741E-10	4.389E-08	1.050E-07	6.106E-02	2.925E-02	1.284E-02
17	0.1500	3.374E-11	1.675E-09	7.202E-08	6.478E-02	2.594E-02	1.257E-02
18	0.1800	5.630E-13	2.022E-10	4.766E-08	6.804E-02	2.305E-02	1.180E-02
19	0.2400	5.346E-15	1.362E-10	2.744E-08	7.103E-02	2.042E-02	1.029E-02
20	0.3000	8.133E-17	1.046E-10	1.839E-08	7.364E-02	1.810E-02	8.909E-03
21	8.0000	8.133E-17	1.046E-10	1.839E-08	7.364E-02	1.810E-02	8.909E-03

	X	H	O2	O	OH	HO2	H2O2
1	-0.5000	3.862E-15	1.900E-01	1.882E-16	4.266E-14	7.168E-10	1.587E-08
2	0.0000	6.979E-14	1.878E-01	1.218E-14	2.822E-12	7.255E-08	1.617E-06
3	0.0500	1.127E-10	1.802E-01	7.497E-13	2.244E-09	3.697E-06	9.591E-06
4	0.0550	1.033E-08	1.768E-01	8.968E-11	5.340E-08	1.206E-05	1.338E-05
5	0.0600	2.863E-07	1.714E-01	2.167E-09	3.859E-07	2.975E-05	1.906E-05
6	0.0675	8.207E-06	1.586E-01	8.727E-08	4.590E-06	8.313E-05	2.965E-05
7	0.0750	9.930E-05	1.392E-01	2.732E-06	3.790E-05	1.328E-04	3.232E-05
8	0.0825	5.483E-04	1.123E-01	3.288E-05	1.847E-04	1.246E-04	2.148E-05
9	0.0900	2.002E-03	7.987E-02	2.061E-04	8.104E-04	7.528E-05	6.206E-06
10	0.0938	3.313E-03	6.480E-02	4.801E-04	1.600E-03	5.161E-05	2.871E-06
11	0.0975	4.816E-03	5.196E-02	1.022E-03	2.795E-03	3.329E-05	2.124E-06
12	0.1013	6.173E-03	4.218E-02	1.839E-03	4.212E-03	2.150E-05	2.500E-06
13	0.1050	7.181E-03	3.529E-02	2.671E-03	5.490E-03	1.506E-05	3.090E-06
14	0.1125	8.153E-03	2.800E-02	3.559E-03	6.965E-03	1.063E-05	3.630E-06
15	0.1200	8.359E-03	2.431E-02	3.803E-03	7.614E-03	8.855E-06	3.487E-06
16	0.1350	7.858E-03	2.107E-02	3.619E-03	7.940E-03	7.292E-06	2.757E-06
17	0.1500	7.155E-03	1.926E-02	3.323E-03	7.974E-03	6.403E-06	2.195E-06
18	0.1800	5.863E-03	1.724E-02	2.793E-03	7.786E-03	5.400E-06	1.526E-06
19	0.2400	4.188E-03	1.502E-02	2.091E-03	7.212E-03	4.351E-06	9.396E-07
20	0.3000	3.126E-03	1.337E-02	1.582E-03	6.327E-03	3.794E-06	7.263E-07
21	8.0000	3.126E-03	1.337E-02	1.582E-03	6.327E-03	3.794E-06	7.263E-07

	X	H2O	N2
1	-0.5000	2.702E-05	7.149E-01
2	0.0000	2.536E-03	7.107E-01
3	0.0500	1.370E-02	7.033E-01
4	0.0550	1.873E-02	7.013E-01
5	0.0600	2.618E-02	6.989E-01
6	0.0675	4.234E-02	6.949E-01
7	0.0750	6.464E-02	6.908E-01
8	0.0825	9.238E-02	6.873E-01
9	0.0900	1.224E-01	6.852E-01
10	0.0938	1.353E-01	6.851E-01
11	0.0975	1.457E-01	6.854E-01
12	0.1013	1.529E-01	6.862E-01
13	0.1050	1.575E-01	6.871E-01
14	0.1125	1.613E-01	6.890E-01
15	0.1200	1.625E-01	6.907E-01
16	0.1350	1.634E-01	6.930E-01
17	0.1500	1.644E-01	6.946E-01
18	0.1800	1.668E-01	6.966E-01
19	0.2400	1.705E-01	6.992E-01
20	0.3000	1.735E-01	7.015E-01
21	8.0000	1.735E-01	7.015E-01

TWOPNT: SUCCESS. PROBLEM SOLVED.

FLDRIV: FINISHED FIXED TEMPERATURE, ADDING ENERGY EQUATION

TWOPNT: DOUBLE PRECISION (TWO POINT BOUNDARY VALUE PROBLEM) SOLVER,  
VERSION 3.30 OF APRIL 1998 BY DR. JOSEPH F. GRCAR.

TWOPNT: INITIAL GUESS:

	X	T	V	RHO	CH4	CH3	CH2
1	-0.5000	2.980E+02	4.168E+01	1.130E-03	9.497E-02	4.373E-07	2.414E-20
2	0.0000	2.980E+02	4.190E+01	1.124E-03	9.318E-02	4.098E-05	2.212E-18
3	0.0500	4.000E+02	5.672E+01	8.304E-04	8.684E-02	2.297E-04	7.252E-14
4	0.0550	4.471E+02	6.354E+01	7.412E-04	8.410E-02	3.252E-04	4.784E-12
5	0.0600	5.187E+02	7.392E+01	6.371E-04	7.999E-02	4.778E-04	1.163E-10
6	0.0675	6.784E+02	9.717E+01	4.847E-04	7.074E-02	8.750E-04	7.225E-09
7	0.0750	9.023E+02	1.300E+02	3.623E-04	5.692E-02	1.778E-03	2.683E-07
8	0.0825	1.177E+03	1.707E+02	2.760E-04	3.763E-02	3.613E-03	4.619E-06
9	0.0900	1.464E+03	2.133E+02	2.208E-04	1.570E-02	4.703E-03	3.617E-05
10	0.0938	1.580E+03	2.306E+02	2.042E-04	7.909E-03	3.673E-03	5.608E-05
11	0.0975	1.667E+03	2.434E+02	1.935E-04	3.222E-03	2.055E-03	5.189E-05
12	0.1013	1.722E+03	2.514E+02	1.873E-04	1.074E-03	8.253E-04	2.876E-05
13	0.1050	1.756E+03	2.561E+02	1.839E-04	2.788E-04	2.392E-04	1.021E-05
14	0.1125	1.796E+03	2.612E+02	1.803E-04	2.885E-05	2.719E-05	1.370E-06
15	0.1200	1.827E+03	2.648E+02	1.778E-04	2.263E-06	2.360E-06	1.313E-07
16	0.1350	1.872E+03	2.704E+02	1.742E-04	7.803E-08	9.456E-08	5.756E-09
17	0.1500	1.907E+03	2.747E+02	1.714E-04	2.327E-09	3.261E-09	2.117E-10
18	0.1800	1.956E+03	2.808E+02	1.677E-04	3.080E-11	5.054E-11	3.472E-12
19	0.2400	2.009E+03	2.874E+02	1.639E-04	2.436E-13	4.632E-13	3.309E-14
20	0.3000	2.009E+03	2.865E+02	1.644E-04	2.092E-15	4.172E-15	3.228E-16
21	8.0000	2.009E+03	2.865E+02	1.644E-04	2.092E-15	4.172E-15	3.228E-16

	X	CH	CH2O	HCO	CO2	CO	H2
1	-0.5000	-3.629E-29	3.985E-08	1.099E-18	7.957E-07	4.799E-06	1.873E-04
2	0.0000	-2.201E-27	5.385E-06	1.473E-16	1.060E-04	4.868E-04	5.118E-03
3	0.0500	1.657E-22	3.987E-05	1.185E-12	7.832E-04	2.887E-03	1.192E-02
4	0.0550	7.297E-19	6.141E-05	5.102E-11	1.212E-03	4.120E-03	1.329E-02
5	0.0600	3.894E-16	9.969E-05	8.095E-10	1.983E-03	6.113E-03	1.480E-02
6	0.0675	4.085E-13	2.011E-04	3.914E-08	4.071E-03	1.095E-02	1.721E-02
7	0.0750	1.239E-10	3.790E-04	1.402E-06	7.718E-03	1.856E-02	1.970E-02
8	0.0825	1.013E-08	6.829E-04	1.605E-05	1.345E-02	2.945E-02	2.218E-02
9	0.0900	3.453E-07	8.969E-04	5.931E-05	2.152E-02	4.270E-02	2.375E-02
10	0.0938	1.105E-06	7.984E-04	7.868E-05	2.616E-02	4.762E-02	2.306E-02
11	0.0975	1.902E-06	5.558E-04	7.532E-05	3.105E-02	4.998E-02	2.126E-02
12	0.1013	1.702E-06	2.837E-04	4.855E-05	3.595E-02	4.938E-02	1.887E-02
13	0.1050	8.556E-07	9.952E-05	2.004E-05	4.059E-02	4.686E-02	1.666E-02
14	0.1125	1.594E-07	1.274E-05	3.056E-06	4.845E-02	4.041E-02	1.411E-02
15	0.1200	1.801E-08	1.133E-06	4.006E-07	5.429E-02	3.526E-02	1.319E-02
16	0.1350	8.741E-10	4.389E-08	1.050E-07	6.106E-02	2.925E-02	1.284E-02
17	0.1500	3.374E-11	1.675E-09	7.202E-08	6.478E-02	2.594E-02	1.257E-02
18	0.1800	5.630E-13	2.022E-10	4.766E-08	6.804E-02	2.305E-02	1.180E-02

19	0.2400	5.346E-15	1.362E-10	2.744E-08	7.103E-02	2.042E-02	1.029E-02
20	0.3000	8.133E-17	1.046E-10	1.839E-08	7.364E-02	1.810E-02	8.909E-03
21	8.0000	8.133E-17	1.046E-10	1.839E-08	7.364E-02	1.810E-02	8.909E-03

	X	H	O2	O	OH	HO2	H2O2
1	-0.5000	3.862E-15	1.900E-01	1.882E-16	4.266E-14	7.168E-10	1.587E-08
2	0.0000	6.979E-14	1.878E-01	1.218E-14	2.822E-12	7.255E-08	1.617E-06
3	0.0500	1.127E-10	1.802E-01	7.497E-13	2.244E-09	3.697E-06	9.591E-06
4	0.0550	1.033E-08	1.768E-01	8.968E-11	5.340E-08	1.206E-05	1.338E-05
5	0.0600	2.863E-07	1.714E-01	2.167E-09	3.859E-07	2.975E-05	1.906E-05
6	0.0675	8.207E-06	1.586E-01	8.727E-08	4.590E-06	8.313E-05	2.965E-05
7	0.0750	9.930E-05	1.392E-01	2.732E-06	3.790E-05	1.328E-04	3.232E-05
8	0.0825	5.483E-04	1.123E-01	3.288E-05	1.847E-04	1.246E-04	2.148E-05
9	0.0900	2.002E-03	7.987E-02	2.061E-04	8.104E-04	7.528E-05	6.206E-06
10	0.0938	3.313E-03	6.480E-02	4.801E-04	1.600E-03	5.161E-05	2.871E-06
11	0.0975	4.816E-03	5.196E-02	1.022E-03	2.795E-03	3.329E-05	2.124E-06
12	0.1013	6.173E-03	4.218E-02	1.839E-03	4.212E-03	2.150E-05	2.500E-06
13	0.1050	7.181E-03	3.529E-02	2.671E-03	5.490E-03	1.506E-05	3.090E-06
14	0.1125	8.153E-03	2.800E-02	3.559E-03	6.965E-03	1.063E-05	3.630E-06
15	0.1200	8.359E-03	2.431E-02	3.803E-03	7.614E-03	8.855E-06	3.487E-06
16	0.1350	7.858E-03	2.107E-02	3.619E-03	7.940E-03	7.292E-06	2.757E-06
17	0.1500	7.155E-03	1.926E-02	3.323E-03	7.974E-03	6.403E-06	2.195E-06
18	0.1800	5.863E-03	1.724E-02	2.793E-03	7.786E-03	5.400E-06	1.526E-06
19	0.2400	4.188E-03	1.502E-02	2.091E-03	7.212E-03	4.351E-06	9.396E-07
20	0.3000	3.126E-03	1.337E-02	1.582E-03	6.327E-03	3.794E-06	7.263E-07
21	8.0000	3.126E-03	1.337E-02	1.582E-03	6.327E-03	3.794E-06	7.263E-07

	X	H2O	N2
1	-0.5000	2.702E-05	7.149E-01
2	0.0000	2.536E-03	7.107E-01
3	0.0500	1.370E-02	7.033E-01
4	0.0550	1.873E-02	7.013E-01
5	0.0600	2.618E-02	6.989E-01
6	0.0675	4.234E-02	6.949E-01
7	0.0750	6.464E-02	6.908E-01
8	0.0825	9.238E-02	6.873E-01
9	0.0900	1.224E-01	6.852E-01
10	0.0938	1.353E-01	6.851E-01
11	0.0975	1.457E-01	6.854E-01
12	0.1013	1.529E-01	6.862E-01
13	0.1050	1.575E-01	6.871E-01
14	0.1125	1.613E-01	6.890E-01
15	0.1200	1.625E-01	6.907E-01
16	0.1350	1.634E-01	6.930E-01
17	0.1500	1.644E-01	6.946E-01
18	0.1800	1.668E-01	6.966E-01
19	0.2400	1.705E-01	6.992E-01
20	0.3000	1.735E-01	7.015E-01
21	8.0000	1.735E-01	7.015E-01

TWOPNT: SOLVE THE PROBLEM.

TASK	LOG10 NORM F	LOG10 COND J	REMARK
START	1.52		21 GRID POINTS
SEARCH	-1.60	13.22	9 SEARCH STEPS
REFINE	2.69		0.51 AND 0.62 RATIOS, 22 GRID POINTS
SEARCH	-1.81	13.34	8 SEARCH STEPS
REFINE			0.50 AND 0.57 RATIOS

TWOPNT: FINAL SOLUTION:



	X	T	V	RHO	CH4	CH3	CH2
1	-0.5000	2.980E+02	4.337E+01	1.130E-03	9.497E-02	4.092E-07	1.603E-20
2	0.0000	3.170E+02	4.637E+01	1.057E-03	9.346E-02	3.890E-05	1.490E-18
3	0.0500	4.000E+02	5.897E+01	8.309E-04	8.815E-02	2.208E-04	3.565E-14
4	0.0550	4.400E+02	6.501E+01	7.537E-04	8.580E-02	3.152E-04	2.113E-12
5	0.0600	5.028E+02	7.449E+01	6.579E-04	8.217E-02	4.693E-04	4.856E-11
6	0.0675	6.483E+02	9.654E+01	5.076E-04	7.373E-02	8.667E-04	3.173E-09
7	0.0750	8.610E+02	1.290E+02	3.799E-04	6.078E-02	1.717E-03	1.426E-07
8	0.0825	1.133E+03	1.709E+02	2.867E-04	4.212E-02	3.582E-03	2.838E-06
9	0.0863	1.280E+03	1.937E+02	2.530E-04	3.105E-02	4.610E-03	1.079E-05
10	0.0900	1.425E+03	2.162E+02	2.266E-04	1.991E-02	5.104E-03	2.988E-05
11	0.0938	1.555E+03	2.364E+02	2.073E-04	1.059E-02	4.418E-03	5.557E-05
12	0.0975	1.656E+03	2.519E+02	1.945E-04	4.526E-03	2.745E-03	6.160E-05
13	0.1013	1.722E+03	2.621E+02	1.870E-04	1.554E-03	1.190E-03	3.912E-05
14	0.1050	1.762E+03	2.680E+02	1.829E-04	4.074E-04	3.590E-04	1.501E-05
15	0.1125	1.806E+03	2.738E+02	1.790E-04	4.117E-05	4.015E-05	2.031E-06
16	0.1200	1.837E+03	2.777E+02	1.765E-04	3.112E-06	3.366E-06	1.897E-07
17	0.1350	1.883E+03	2.835E+02	1.728E-04	1.028E-07	1.295E-07	8.019E-09
18	0.1500	1.919E+03	2.881E+02	1.701E-04	2.942E-09	4.293E-09	2.841E-10
19	0.1800	1.968E+03	2.945E+02	1.664E-04	3.750E-11	6.420E-11	4.498E-12
20	0.2400	2.026E+03	3.020E+02	1.623E-04	2.845E-13	5.677E-13	4.147E-14
21	0.3000	2.065E+03	3.069E+02	1.597E-04	2.119E-15	4.768E-15	4.066E-16
22	8.0000	2.065E+03	3.069E+02	1.597E-04	2.119E-15	4.768E-15	4.066E-16

	X	CH	CH2O	HCO	CO2	CO	H2
1	-0.5000	2.312E-31	3.283E-08	4.381E-19	5.494E-07	3.736E-06	1.787E-04
2	0.0000	1.426E-29	4.483E-06	5.934E-17	7.412E-05	3.849E-04	4.965E-03
3	0.0500	5.265E-23	3.364E-05	5.141E-13	5.563E-04	2.321E-03	1.171E-02
4	0.0550	1.403E-19	5.269E-05	2.137E-11	8.750E-04	3.359E-03	1.311E-02
5	0.0600	7.626E-17	8.777E-05	3.307E-10	1.470E-03	5.089E-03	1.468E-02
6	0.0675	9.865E-14	1.846E-04	1.654E-08	3.146E-03	9.447E-03	1.726E-02
7	0.0750	4.243E-11	3.588E-04	7.435E-07	6.200E-03	1.656E-02	1.997E-02
8	0.0825	4.172E-09	6.631E-04	1.114E-05	1.117E-02	2.710E-02	2.271E-02
9	0.0863	3.666E-08	8.346E-04	2.856E-05	1.456E-02	3.356E-02	2.387E-02
10	0.0900	2.225E-07	9.409E-04	5.437E-05	1.859E-02	4.039E-02	2.456E-02
11	0.0938	8.786E-07	8.949E-04	7.966E-05	2.316E-02	4.645E-02	2.430E-02
12	0.0975	1.910E-06	6.757E-04	8.561E-05	2.807E-02	5.021E-02	2.280E-02
13	0.1013	2.078E-06	3.759E-04	6.210E-05	3.308E-02	5.072E-02	2.039E-02
14	0.1050	1.186E-06	1.413E-04	2.813E-05	3.790E-02	4.871E-02	1.792E-02
15	0.1125	2.347E-07	1.843E-05	4.444E-06	4.622E-02	4.209E-02	1.486E-02
16	0.1200	2.639E-08	1.606E-06	5.318E-07	5.245E-02	3.663E-02	1.372E-02
17	0.1350	1.247E-09	5.985E-08	1.148E-07	5.961E-02	3.025E-02	1.332E-02
18	0.1500	4.652E-11	2.143E-09	7.646E-08	6.351E-02	2.678E-02	1.306E-02
19	0.1800	7.508E-13	2.197E-10	5.072E-08	6.687E-02	2.380E-02	1.229E-02
20	0.2400	6.924E-15	1.464E-10	2.924E-08	6.985E-02	2.120E-02	1.074E-02
21	0.3000	1.213E-16	1.144E-10	1.834E-08	7.209E-02	1.924E-02	9.378E-03
22	8.0000	1.213E-16	1.144E-10	1.834E-08	7.209E-02	1.924E-02	9.378E-03

	X	H	O2	O	OH	HO2	H2O2
1	-0.5000	1.191E-14	1.900E-01	1.110E-18	1.897E-14	5.794E-10	1.050E-08
2	0.0000	2.179E-13	1.881E-01	7.323E-17	1.275E-12	5.956E-08	1.087E-06
3	0.0500	8.153E-11	1.819E-01	2.915E-13	1.163E-09	2.721E-06	6.555E-06
4	0.0550	4.388E-09	1.790E-01	3.349E-11	2.701E-08	8.676E-06	9.317E-06
5	0.0600	1.257E-07	1.744E-01	8.228E-10	1.928E-07	2.163E-05	1.369E-05
6	0.0675	4.198E-06	1.631E-01	3.563E-08	2.375E-06	6.477E-05	2.284E-05
7	0.0750	6.223E-05	1.453E-01	1.341E-06	2.363E-05	1.228E-04	2.806E-05
8	0.0825	3.912E-04	1.198E-01	1.985E-05	1.264E-04	1.306E-04	2.069E-05
9	0.0863	8.733E-04	1.044E-01	6.136E-05	2.984E-04	1.134E-04	1.412E-05
10	0.0900	1.698E-03	8.788E-02	1.585E-04	6.537E-04	8.738E-05	7.520E-06
11	0.0938	2.956E-03	7.153E-02	3.788E-04	1.340E-03	6.087E-05	3.354E-06
12	0.0975	4.528E-03	5.709E-02	8.478E-04	2.471E-03	3.930E-05	2.059E-06
13	0.1013	6.061E-03	4.576E-02	1.648E-03	3.945E-03	2.473E-05	2.254E-06
14	0.1050	7.256E-03	3.769E-02	2.570E-03	5.382E-03	1.650E-05	2.849E-06
15	0.1125	8.476E-03	2.920E-02	3.671E-03	7.137E-03	1.102E-05	3.556E-06
16	0.1200	8.784E-03	2.505E-02	4.004E-03	7.907E-03	9.025E-06	3.488E-06
17	0.1350	8.309E-03	2.158E-02	3.840E-03	8.288E-03	7.383E-06	2.777E-06
18	0.1500	7.586E-03	1.969E-02	3.533E-03	8.334E-03	6.474E-06	2.214E-06
19	0.1800	6.233E-03	1.763E-02	2.976E-03	8.148E-03	5.465E-06	1.542E-06
20	0.2400	4.467E-03	1.541E-02	2.242E-03	7.602E-03	4.402E-06	9.411E-07
21	0.3000	3.302E-03	1.384E-02	1.735E-03	7.009E-03	3.678E-06	6.358E-07
22	8.0000	3.302E-03	1.384E-02	1.735E-03	7.009E-03	3.678E-06	6.358E-07

	X	H2O	N2
1	-0.5000	2.150E-05	7.149E-01
2	0.0000	2.036E-03	7.109E-01
3	0.0500	1.114E-02	7.040E-01
4	0.0550	1.542E-02	7.020E-01
5	0.0600	2.198E-02	6.996E-01
6	0.0675	3.678E-02	6.954E-01
7	0.0750	5.797E-02	6.909E-01
8	0.0825	8.528E-02	6.868E-01
9	0.0863	1.004E-01	6.852E-01
10	0.0900	1.158E-01	6.841E-01
11	0.0938	1.301E-01	6.836E-01
12	0.0975	1.421E-01	6.838E-01
13	0.1013	1.508E-01	6.844E-01
14	0.1050	1.564E-01	6.852E-01
15	0.1125	1.610E-01	6.872E-01
16	0.1200	1.625E-01	6.889E-01
17	0.1350	1.634E-01	6.914E-01
18	0.1500	1.645E-01	6.930E-01
19	0.1800	1.669E-01	6.951E-01
20	0.2400	1.707E-01	6.978E-01
21	0.3000	1.735E-01	6.999E-01
22	8.0000	1.735E-01	6.999E-01

TWOPNT: SUCCESS. PROBLEM SOLVED.

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////////// CONTINUING TO NEW PROBLEM //////////
////////// CONTINUING TO NEW PROBLEM //////////
////////// CONTINUING TO NEW PROBLEM //////////
////////// CONTINUING TO NEW PROBLEM //////////
////////// CONTINUING TO NEW PROBLEM //////////

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KEYWORD INPUT

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/
/   This is the third and final continuation. The mesh adaptation
/   is more stringent, and th computational domain is again expanded.
/
GRAD  0.2
CURV  0.5
XEND  10.0
XSTR  -2.0
END

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TWOPNT: DOUBLE PRECISION (TWO POINT BOUNDARY VALUE PROBLEM) SOLVER,  
VERSION 3.30 OF APRIL 1998 BY DR. JOSEPH F. GRCAR.

TWOPNT: INITIAL GUESS:

	X	T	V	RHO	CH4	CH3	CH2
1	-2.0000	2.980E+02	4.337E+01	1.130E-03	9.497E-02	4.092E-07	1.603E-20
2	-0.5000	2.980E+02	4.337E+01	1.130E-03	9.497E-02	4.092E-07	1.603E-20
3	0.0000	3.170E+02	4.637E+01	1.057E-03	9.346E-02	3.890E-05	1.490E-18
4	0.0500	4.000E+02	5.897E+01	8.309E-04	8.815E-02	2.208E-04	3.565E-14
5	0.0550	4.400E+02	6.501E+01	7.537E-04	8.580E-02	3.152E-04	2.113E-12
6	0.0600	5.028E+02	7.449E+01	6.579E-04	8.217E-02	4.693E-04	4.856E-11
7	0.0675	6.483E+02	9.654E+01	5.076E-04	7.373E-02	8.667E-04	3.173E-09
8	0.0750	8.610E+02	1.290E+02	3.799E-04	6.078E-02	1.717E-03	1.426E-07
9	0.0825	1.133E+03	1.709E+02	2.867E-04	4.212E-02	3.582E-03	2.838E-06
10	0.0863	1.280E+03	1.937E+02	2.530E-04	3.105E-02	4.610E-03	1.079E-05
11	0.0900	1.425E+03	2.162E+02	2.266E-04	1.991E-02	5.104E-03	2.988E-05
12	0.0938	1.555E+03	2.364E+02	2.073E-04	1.059E-02	4.418E-03	5.557E-05
13	0.0975	1.656E+03	2.519E+02	1.945E-04	4.526E-03	2.745E-03	6.160E-05
14	0.1013	1.722E+03	2.621E+02	1.870E-04	1.554E-03	1.190E-03	3.912E-05
15	0.1050	1.762E+03	2.680E+02	1.829E-04	4.074E-04	3.590E-04	1.501E-05
16	0.1125	1.806E+03	2.738E+02	1.790E-04	4.117E-05	4.015E-05	2.031E-06
17	0.1200	1.837E+03	2.777E+02	1.765E-04	3.112E-06	3.366E-06	1.897E-07
18	0.1350	1.883E+03	2.835E+02	1.728E-04	1.028E-07	1.295E-07	8.019E-09
19	0.1500	1.919E+03	2.881E+02	1.701E-04	2.942E-09	4.293E-09	2.841E-10
20	0.1800	1.968E+03	2.945E+02	1.664E-04	3.750E-11	6.420E-11	4.498E-12
21	0.2400	2.026E+03	3.020E+02	1.623E-04	2.845E-13	5.677E-13	4.147E-14
22	0.3000	2.065E+03	3.069E+02	1.597E-04	2.119E-15	4.768E-15	4.066E-16
23	8.0000	2.065E+03	3.069E+02	1.597E-04	2.119E-15	4.768E-15	4.066E-16
24	10.0000	2.065E+03	3.069E+02	1.597E-04	2.119E-15	4.768E-15	4.066E-16

	X	CH	CH2O	HCO	CO2	CO	H2
1	-2.0000	2.312E-31	3.283E-08	4.381E-19	5.494E-07	3.736E-06	1.787E-04
2	-0.5000	2.312E-31	3.283E-08	4.381E-19	5.494E-07	3.736E-06	1.787E-04
3	0.0000	1.426E-29	4.483E-06	5.934E-17	7.412E-05	3.849E-04	4.965E-03
4	0.0500	5.265E-23	3.364E-05	5.141E-13	5.563E-04	2.321E-03	1.171E-02
5	0.0550	1.403E-19	5.269E-05	2.137E-11	8.750E-04	3.359E-03	1.311E-02
6	0.0600	7.626E-17	8.777E-05	3.307E-10	1.470E-03	5.089E-03	1.468E-02
7	0.0675	9.865E-14	1.846E-04	1.654E-08	3.146E-03	9.447E-03	1.726E-02
8	0.0750	4.243E-11	3.588E-04	7.435E-07	6.200E-03	1.656E-02	1.997E-02
9	0.0825	4.172E-09	6.631E-04	1.114E-05	1.117E-02	2.710E-02	2.271E-02
10	0.0863	3.666E-08	8.346E-04	2.856E-05	1.456E-02	3.356E-02	2.387E-02
11	0.0900	2.225E-07	9.409E-04	5.437E-05	1.859E-02	4.039E-02	2.456E-02
12	0.0938	8.786E-07	8.949E-04	7.966E-05	2.316E-02	4.645E-02	2.430E-02
13	0.0975	1.910E-06	6.757E-04	8.561E-05	2.807E-02	5.021E-02	2.280E-02
14	0.1013	2.078E-06	3.759E-04	6.210E-05	3.308E-02	5.072E-02	2.039E-02
15	0.1050	1.186E-06	1.413E-04	2.813E-05	3.790E-02	4.871E-02	1.792E-02
16	0.1125	2.347E-07	1.843E-05	4.444E-06	4.622E-02	4.209E-02	1.486E-02
17	0.1200	2.639E-08	1.606E-06	5.318E-07	5.245E-02	3.663E-02	1.372E-02
18	0.1350	1.247E-09	5.985E-08	1.148E-07	5.961E-02	3.025E-02	1.332E-02
19	0.1500	4.652E-11	2.143E-09	7.646E-08	6.351E-02	2.678E-02	1.306E-02
20	0.1800	7.508E-13	2.197E-10	5.072E-08	6.687E-02	2.380E-02	1.229E-02
21	0.2400	6.924E-15	1.464E-10	2.924E-08	6.985E-02	2.120E-02	1.074E-02
22	0.3000	1.213E-16	1.144E-10	1.834E-08	7.209E-02	1.924E-02	9.378E-03
23	8.0000	1.213E-16	1.144E-10	1.834E-08	7.209E-02	1.924E-02	9.378E-03
24	10.0000	1.213E-16	1.144E-10	1.834E-08	7.209E-02	1.924E-02	9.378E-03

	X	H	O2	O	OH	HO2	H2O2
1	-2.0000	1.191E-14	1.900E-01	1.110E-18	1.897E-14	5.794E-10	1.050E-08
2	-0.5000	1.191E-14	1.900E-01	1.110E-18	1.897E-14	5.794E-10	1.050E-08
3	0.0000	2.179E-13	1.881E-01	7.323E-17	1.275E-12	5.956E-08	1.087E-06
4	0.0500	8.153E-11	1.819E-01	2.915E-13	1.163E-09	2.721E-06	6.555E-06
5	0.0550	4.388E-09	1.790E-01	3.349E-11	2.701E-08	8.676E-06	9.317E-06
6	0.0600	1.257E-07	1.744E-01	8.228E-10	1.928E-07	2.163E-05	1.369E-05
7	0.0675	4.198E-06	1.631E-01	3.563E-08	2.375E-06	6.477E-05	2.284E-05
8	0.0750	6.223E-05	1.453E-01	1.341E-06	2.363E-05	1.228E-04	2.806E-05
9	0.0825	3.912E-04	1.198E-01	1.985E-05	1.264E-04	1.306E-04	2.069E-05
10	0.0863	8.733E-04	1.044E-01	6.136E-05	2.984E-04	1.134E-04	1.412E-05
11	0.0900	1.698E-03	8.788E-02	1.585E-04	6.537E-04	8.738E-05	7.520E-06
12	0.0938	2.956E-03	7.153E-02	3.788E-04	1.340E-03	6.087E-05	3.354E-06
13	0.0975	4.528E-03	5.709E-02	8.478E-04	2.471E-03	3.930E-05	2.059E-06
14	0.1013	6.061E-03	4.576E-02	1.648E-03	3.945E-03	2.473E-05	2.254E-06
15	0.1050	7.256E-03	3.769E-02	2.570E-03	5.382E-03	1.650E-05	2.849E-06
16	0.1125	8.476E-03	2.920E-02	3.671E-03	7.137E-03	1.102E-05	3.556E-06
17	0.1200	8.784E-03	2.505E-02	4.004E-03	7.907E-03	9.025E-06	3.488E-06
18	0.1350	8.309E-03	2.158E-02	3.840E-03	8.288E-03	7.383E-06	2.777E-06
19	0.1500	7.586E-03	1.969E-02	3.533E-03	8.334E-03	6.474E-06	2.214E-06
20	0.1800	6.233E-03	1.763E-02	2.976E-03	8.148E-03	5.465E-06	1.542E-06
21	0.2400	4.467E-03	1.541E-02	2.242E-03	7.602E-03	4.402E-06	9.411E-07
22	0.3000	3.302E-03	1.384E-02	1.735E-03	7.009E-03	3.678E-06	6.358E-07
23	8.0000	3.302E-03	1.384E-02	1.735E-03	7.009E-03	3.678E-06	6.358E-07
24	10.0000	3.302E-03	1.384E-02	1.735E-03	7.009E-03	3.678E-06	6.358E-07

	X	H2O	N2
1	-2.0000	2.150E-05	7.149E-01
2	-0.5000	2.150E-05	7.149E-01
3	0.0000	2.036E-03	7.109E-01
4	0.0500	1.114E-02	7.040E-01
5	0.0550	1.542E-02	7.020E-01
6	0.0600	2.198E-02	6.996E-01
7	0.0675	3.678E-02	6.954E-01
8	0.0750	5.797E-02	6.909E-01
9	0.0825	8.528E-02	6.868E-01
10	0.0863	1.004E-01	6.852E-01
11	0.0900	1.158E-01	6.841E-01
12	0.0938	1.301E-01	6.836E-01
13	0.0975	1.421E-01	6.838E-01
14	0.1013	1.508E-01	6.844E-01
15	0.1050	1.564E-01	6.852E-01
16	0.1125	1.610E-01	6.872E-01
17	0.1200	1.625E-01	6.889E-01
18	0.1350	1.634E-01	6.914E-01
19	0.1500	1.645E-01	6.930E-01
20	0.1800	1.669E-01	6.951E-01
21	0.2400	1.707E-01	6.978E-01
22	0.3000	1.735E-01	6.999E-01
23	8.0000	1.735E-01	6.999E-01
24	10.0000	1.735E-01	6.999E-01

TWOPNT: SOLVE THE PROBLEM.

TASK	LOG10 NORM F	LOG10 COND J	REMARK
START	-2.57		
SEARCH	-5.11	9.56	21 SEARCH STEPS

TWOPNT: FINAL SOLUTION:

	X	T	V	RHO	CH4	CH3	CH2
1	-2.0000	2.980E+02	4.336E+01	1.130E-03	9.500E-02	2.099E-09	2.305E-27
2	-0.5000	2.980E+02	4.338E+01	1.130E-03	9.496E-02	6.116E-07	6.564E-25
3	0.0000	3.170E+02	4.637E+01	1.057E-03	9.344E-02	3.906E-05	1.496E-18
4	0.0500	4.000E+02	5.898E+01	8.309E-04	8.814E-02	2.208E-04	3.567E-14
5	0.0550	4.400E+02	6.502E+01	7.537E-04	8.579E-02	3.151E-04	2.115E-12
6	0.0600	5.028E+02	7.449E+01	6.578E-04	8.216E-02	4.690E-04	4.861E-11
7	0.0675	6.483E+02	9.654E+01	5.076E-04	7.372E-02	8.660E-04	3.176E-09
8	0.0750	8.610E+02	1.290E+02	3.799E-04	6.077E-02	1.716E-03	1.428E-07
9	0.0825	1.133E+03	1.709E+02	2.867E-04	4.212E-02	3.581E-03	2.840E-06
10	0.0863	1.280E+03	1.937E+02	2.530E-04	3.104E-02	4.609E-03	1.080E-05
11	0.0900	1.425E+03	2.162E+02	2.266E-04	1.991E-02	5.103E-03	2.990E-05
12	0.0938	1.555E+03	2.364E+02	2.073E-04	1.059E-02	4.416E-03	5.558E-05
13	0.0975	1.656E+03	2.520E+02	1.945E-04	4.523E-03	2.744E-03	6.160E-05
14	0.1013	1.722E+03	2.621E+02	1.870E-04	1.552E-03	1.190E-03	3.912E-05
15	0.1050	1.762E+03	2.680E+02	1.829E-04	4.071E-04	3.589E-04	1.501E-05
16	0.1125	1.806E+03	2.738E+02	1.790E-04	4.114E-05	4.014E-05	2.032E-06
17	0.1200	1.837E+03	2.777E+02	1.765E-04	3.110E-06	3.366E-06	1.898E-07
18	0.1350	1.883E+03	2.836E+02	1.728E-04	1.027E-07	1.295E-07	8.022E-09
19	0.1500	1.919E+03	2.881E+02	1.701E-04	2.940E-09	4.294E-09	2.843E-10
20	0.1800	1.968E+03	2.946E+02	1.664E-04	3.748E-11	6.422E-11	4.501E-12
21	0.2400	2.026E+03	3.020E+02	1.623E-04	2.845E-13	5.680E-13	4.151E-14
22	0.3000	2.065E+03	3.069E+02	1.597E-04	2.120E-15	4.773E-15	4.072E-16
23	8.0000	2.065E+03	3.029E+02	1.618E-04	6.240E-18	1.658E-17	3.125E-18
24	10.0000	2.065E+03	3.029E+02	1.618E-04	6.240E-18	1.658E-17	3.125E-18

	X	CH	CH2O	HCO	CO2	CO	H2
1	-2.0000	2.236E-40	1.167E-10	5.214E-26	1.981E-09	1.773E-08	3.187E-06
2	-0.5000	4.201E-38	4.917E-08	2.180E-23	8.229E-07	5.595E-06	2.657E-04
3	0.0000	1.444E-29	4.497E-06	5.954E-17	7.438E-05	3.868E-04	5.039E-03
4	0.0500	5.289E-23	3.365E-05	5.146E-13	5.566E-04	2.323E-03	1.176E-02
5	0.0550	1.408E-19	5.269E-05	2.140E-11	8.752E-04	3.361E-03	1.316E-02
6	0.0600	7.652E-17	8.775E-05	3.312E-10	1.470E-03	5.091E-03	1.473E-02
7	0.0675	9.895E-14	1.846E-04	1.657E-08	3.146E-03	9.449E-03	1.730E-02
8	0.0750	4.253E-11	3.587E-04	7.444E-07	6.200E-03	1.657E-02	2.001E-02
9	0.0825	4.179E-09	6.630E-04	1.115E-05	1.117E-02	2.710E-02	2.274E-02
10	0.0863	3.672E-08	8.344E-04	2.858E-05	1.456E-02	3.356E-02	2.389E-02
11	0.0900	2.228E-07	9.406E-04	5.439E-05	1.859E-02	4.039E-02	2.458E-02
12	0.0938	8.795E-07	8.945E-04	7.967E-05	2.316E-02	4.646E-02	2.432E-02
13	0.0975	1.912E-06	6.753E-04	8.560E-05	2.807E-02	5.021E-02	2.282E-02
14	0.1013	2.080E-06	3.755E-04	6.207E-05	3.308E-02	5.072E-02	2.040E-02
15	0.1050	1.187E-06	1.412E-04	2.811E-05	3.790E-02	4.871E-02	1.793E-02
16	0.1125	2.348E-07	1.841E-05	4.441E-06	4.622E-02	4.209E-02	1.487E-02
17	0.1200	2.642E-08	1.604E-06	5.316E-07	5.244E-02	3.663E-02	1.373E-02
18	0.1350	1.248E-09	5.981E-08	1.148E-07	5.960E-02	3.025E-02	1.333E-02
19	0.1500	4.658E-11	2.142E-09	7.651E-08	6.350E-02	2.678E-02	1.307E-02
20	0.1800	7.519E-13	2.199E-10	5.076E-08	6.686E-02	2.381E-02	1.230E-02
21	0.2400	6.936E-15	1.466E-10	2.927E-08	6.983E-02	2.121E-02	1.075E-02
22	0.3000	1.215E-16	1.145E-10	1.835E-08	7.207E-02	1.924E-02	9.387E-03
23	8.0000	1.123E-18	1.492E-11	8.746E-10	8.536E-02	7.187E-03	3.243E-03
24	10.0000	1.123E-18	1.492E-11	8.746E-10	8.536E-02	7.187E-03	3.243E-03

	X	H	O2	O	OH	HO2	H2O2
1	-2.0000	1.924E-18	1.900E-01	9.953E-20	2.638E-19	1.985E-12	4.967E-11
2	-0.5000	1.046E-16	1.899E-01	2.001E-17	5.407E-17	6.252E-10	1.575E-08
3	0.0000	2.216E-13	1.881E-01	7.324E-17	1.275E-12	5.947E-08	1.094E-06
4	0.0500	8.188E-11	1.819E-01	2.927E-13	1.164E-09	2.725E-06	6.571E-06
5	0.0550	4.401E-09	1.790E-01	3.361E-11	2.705E-08	8.688E-06	9.337E-06
6	0.0600	1.260E-07	1.744E-01	8.254E-10	1.931E-07	2.166E-05	1.371E-05
7	0.0675	4.207E-06	1.631E-01	3.571E-08	2.379E-06	6.484E-05	2.287E-05
8	0.0750	6.232E-05	1.453E-01	1.344E-06	2.366E-05	1.229E-04	2.809E-05
9	0.0825	3.917E-04	1.198E-01	1.988E-05	1.265E-04	1.306E-04	2.071E-05
10	0.0863	8.741E-04	1.044E-01	6.141E-05	2.985E-04	1.133E-04	1.413E-05
11	0.0900	1.700E-03	8.785E-02	1.586E-04	6.539E-04	8.735E-05	7.525E-06
12	0.0938	2.958E-03	7.150E-02	3.790E-04	1.340E-03	6.084E-05	3.356E-06
13	0.0975	4.531E-03	5.706E-02	8.480E-04	2.472E-03	3.927E-05	2.060E-06
14	0.1013	6.065E-03	4.574E-02	1.648E-03	3.945E-03	2.471E-05	2.255E-06
15	0.1050	7.259E-03	3.767E-02	2.569E-03	5.382E-03	1.650E-05	2.849E-06
16	0.1125	8.480E-03	2.917E-02	3.670E-03	7.136E-03	1.101E-05	3.556E-06
17	0.1200	8.787E-03	2.502E-02	4.002E-03	7.907E-03	9.019E-06	3.488E-06
18	0.1350	8.313E-03	2.155E-02	3.838E-03	8.287E-03	7.378E-06	2.777E-06
19	0.1500	7.589E-03	1.967E-02	3.531E-03	8.333E-03	6.469E-06	2.213E-06
20	0.1800	6.236E-03	1.761E-02	2.974E-03	8.147E-03	5.460E-06	1.541E-06
21	0.2400	4.469E-03	1.539E-02	2.241E-03	7.601E-03	4.398E-06	9.408E-07
22	0.3000	3.304E-03	1.382E-02	1.733E-03	7.008E-03	3.674E-06	6.355E-07

23	8.0000	4.062E-04	5.811E-03	2.345E-04	2.668E-03	9.229E-07	9.364E-08
24	10.0000	4.062E-04	5.811E-03	2.345E-04	2.668E-03	9.229E-07	9.364E-08

	X	H2O	N2
1	-2.0000	1.103E-07	7.150E-01
2	-0.5000	3.220E-05	7.148E-01
3	0.0000	2.047E-03	7.109E-01
4	0.0500	1.115E-02	7.039E-01
5	0.0550	1.543E-02	7.020E-01
6	0.0600	2.200E-02	6.996E-01
7	0.0675	3.680E-02	6.953E-01
8	0.0750	5.800E-02	6.908E-01
9	0.0825	8.531E-02	6.868E-01
10	0.0863	1.005E-01	6.852E-01
11	0.0900	1.159E-01	6.841E-01
12	0.0938	1.302E-01	6.836E-01
13	0.0975	1.421E-01	6.837E-01
14	0.1013	1.508E-01	6.843E-01
15	0.1050	1.564E-01	6.852E-01
16	0.1125	1.611E-01	6.872E-01
17	0.1200	1.626E-01	6.889E-01
18	0.1350	1.635E-01	6.913E-01
19	0.1500	1.645E-01	6.930E-01
20	0.1800	1.670E-01	6.951E-01
21	0.2400	1.707E-01	6.977E-01
22	0.3000	1.736E-01	6.998E-01
23	8.0000	1.859E-01	7.092E-01
24	10.0000	1.859E-01	7.092E-01

TWOPNT: SUCCESS. PROBLEM SOLVED.

FLDRIV: FINISHED FIXED TEMPERATURE, ADDING ENERGY EQUATION

TWOPNT: DOUBLE PRECISION (TWO POINT BOUNDARY VALUE PROBLEM) SOLVER,  
VERSION 3.30 OF APRIL 1998 BY DR. JOSEPH F. GRGAR.

TWOPNT: INITIAL GUESS:

	X	T	V	RHO	CH4	CH3	CH2
1	-2.0000	2.980E+02	4.336E+01	1.130E-03	9.500E-02	2.099E-09	2.305E-27
2	-0.5000	2.980E+02	4.338E+01	1.130E-03	9.496E-02	6.116E-07	6.564E-25
3	0.0000	3.170E+02	4.637E+01	1.057E-03	9.344E-02	3.906E-05	1.496E-18
4	0.0500	4.000E+02	5.898E+01	8.309E-04	8.814E-02	2.208E-04	3.567E-14
5	0.0550	4.400E+02	6.502E+01	7.537E-04	8.579E-02	3.151E-04	2.115E-12
6	0.0600	5.028E+02	7.449E+01	6.578E-04	8.216E-02	4.690E-04	4.861E-11
7	0.0675	6.483E+02	9.654E+01	5.076E-04	7.372E-02	8.660E-04	3.176E-09
8	0.0750	8.610E+02	1.290E+02	3.799E-04	6.077E-02	1.716E-03	1.428E-07
9	0.0825	1.133E+03	1.709E+02	2.867E-04	4.212E-02	3.581E-03	2.840E-06
10	0.0863	1.280E+03	1.937E+02	2.530E-04	3.104E-02	4.609E-03	1.080E-05
11	0.0900	1.425E+03	2.162E+02	2.266E-04	1.991E-02	5.103E-03	2.990E-05
12	0.0938	1.555E+03	2.364E+02	2.073E-04	1.059E-02	4.416E-03	5.558E-05
13	0.0975	1.656E+03	2.520E+02	1.945E-04	4.523E-03	2.744E-03	6.160E-05
14	0.1013	1.722E+03	2.621E+02	1.870E-04	1.552E-03	1.190E-03	3.912E-05
15	0.1050	1.762E+03	2.680E+02	1.829E-04	4.071E-04	3.589E-04	1.501E-05
16	0.1125	1.806E+03	2.738E+02	1.790E-04	4.114E-05	4.014E-05	2.032E-06
17	0.1200	1.837E+03	2.777E+02	1.765E-04	3.110E-06	3.366E-06	1.898E-07
18	0.1350	1.883E+03	2.836E+02	1.728E-04	1.027E-07	1.295E-07	8.022E-09
19	0.1500	1.919E+03	2.881E+02	1.701E-04	2.940E-09	4.294E-09	2.843E-10
20	0.1800	1.968E+03	2.946E+02	1.664E-04	3.748E-11	6.422E-11	4.501E-12
21	0.2400	2.026E+03	3.020E+02	1.623E-04	2.845E-13	5.680E-13	4.151E-14
22	0.3000	2.065E+03	3.069E+02	1.597E-04	2.120E-15	4.773E-15	4.072E-16
23	8.0000	2.065E+03	3.029E+02	1.618E-04	6.240E-18	1.658E-17	3.125E-18
24	10.0000	2.065E+03	3.029E+02	1.618E-04	6.240E-18	1.658E-17	3.125E-18

	X	CH	CH2O	HCO	CO2	CO	H2
1	-2.0000	2.236E-40	1.167E-10	5.214E-26	1.981E-09	1.773E-08	3.187E-06
2	-0.5000	4.201E-38	4.917E-08	2.180E-23	8.229E-07	5.595E-06	2.657E-04
3	0.0000	1.444E-29	4.497E-06	5.954E-17	7.438E-05	3.868E-04	5.039E-03
4	0.0500	5.289E-23	3.365E-05	5.146E-13	5.566E-04	2.323E-03	1.176E-02
5	0.0550	1.408E-19	5.269E-05	2.140E-11	8.752E-04	3.361E-03	1.316E-02
6	0.0600	7.652E-17	8.775E-05	3.312E-10	1.470E-03	5.091E-03	1.473E-02
7	0.0675	9.895E-14	1.846E-04	1.657E-08	3.146E-03	9.449E-03	1.730E-02
8	0.0750	4.253E-11	3.587E-04	7.444E-07	6.200E-03	1.657E-02	2.001E-02
9	0.0825	4.179E-09	6.630E-04	1.115E-05	1.117E-02	2.710E-02	2.274E-02
10	0.0863	3.672E-08	8.344E-04	2.858E-05	1.456E-02	3.356E-02	2.389E-02
11	0.0900	2.228E-07	9.406E-04	5.439E-05	1.859E-02	4.039E-02	2.458E-02
12	0.0938	8.795E-07	8.945E-04	7.967E-05	2.316E-02	4.646E-02	2.432E-02
13	0.0975	1.912E-06	6.753E-04	8.560E-05	2.807E-02	5.021E-02	2.282E-02
14	0.1013	2.080E-06	3.755E-04	6.207E-05	3.308E-02	5.072E-02	2.040E-02
15	0.1050	1.187E-06	1.412E-04	2.811E-05	3.790E-02	4.871E-02	1.793E-02
16	0.1125	2.348E-07	1.841E-05	4.441E-06	4.622E-02	4.209E-02	1.487E-02
17	0.1200	2.642E-08	1.604E-06	5.316E-07	5.244E-02	3.663E-02	1.373E-02
18	0.1350	1.248E-09	5.981E-08	1.148E-07	5.960E-02	3.025E-02	1.333E-02
19	0.1500	4.658E-11	2.142E-09	7.651E-08	6.350E-02	2.678E-02	1.307E-02
20	0.1800	7.519E-13	2.199E-10	5.076E-08	6.686E-02	2.381E-02	1.230E-02
21	0.2400	6.936E-15	1.466E-10	2.927E-08	6.983E-02	2.121E-02	1.075E-02
22	0.3000	1.215E-16	1.145E-10	1.835E-08	7.207E-02	1.924E-02	9.387E-03
23	8.0000	1.123E-18	1.492E-11	8.746E-10	8.536E-02	7.187E-03	3.243E-03
24	10.0000	1.123E-18	1.492E-11	8.746E-10	8.536E-02	7.187E-03	3.243E-03

	X	H	O2	O	OH	HO2	H2O2
1	-2.0000	1.924E-18	1.900E-01	9.953E-20	2.638E-19	1.985E-12	4.967E-11
2	-0.5000	1.046E-16	1.899E-01	2.001E-17	5.407E-17	6.252E-10	1.575E-08
3	0.0000	2.216E-13	1.881E-01	7.324E-17	1.275E-12	5.947E-08	1.094E-06
4	0.0500	8.188E-11	1.819E-01	2.927E-13	1.164E-09	2.725E-06	6.571E-06
5	0.0550	4.401E-09	1.790E-01	3.361E-11	2.705E-08	8.688E-06	9.337E-06
6	0.0600	1.260E-07	1.744E-01	8.254E-10	1.931E-07	2.166E-05	1.371E-05
7	0.0675	4.207E-06	1.631E-01	3.571E-08	2.379E-06	6.484E-05	2.287E-05
8	0.0750	6.232E-05	1.453E-01	1.344E-06	2.366E-05	1.229E-04	2.809E-05
9	0.0825	3.917E-04	1.198E-01	1.988E-05	1.265E-04	1.306E-04	2.071E-05
10	0.0863	8.741E-04	1.044E-01	6.141E-05	2.985E-04	1.133E-04	1.413E-05
11	0.0900	1.700E-03	8.785E-02	1.586E-04	6.539E-04	8.735E-05	7.525E-06
12	0.0938	2.958E-03	7.150E-02	3.790E-04	1.340E-03	6.084E-05	3.356E-06
13	0.0975	4.531E-03	5.706E-02	8.480E-04	2.472E-03	3.927E-05	2.060E-06
14	0.1013	6.065E-03	4.574E-02	1.648E-03	3.945E-03	2.471E-05	2.255E-06
15	0.1050	7.259E-03	3.767E-02	2.569E-03	5.382E-03	1.650E-05	2.849E-06
16	0.1125	8.480E-03	2.917E-02	3.670E-03	7.136E-03	1.101E-05	3.556E-06
17	0.1200	8.787E-03	2.502E-02	4.002E-03	7.907E-03	9.019E-06	3.488E-06
18	0.1350	8.313E-03	2.155E-02	3.838E-03	8.287E-03	7.378E-06	2.777E-06
19	0.1500	7.589E-03	1.967E-02	3.531E-03	8.333E-03	6.469E-06	2.213E-06
20	0.1800	6.236E-03	1.761E-02	2.974E-03	8.147E-03	5.460E-06	1.541E-06
21	0.2400	4.469E-03	1.539E-02	2.241E-03	7.601E-03	4.398E-06	9.408E-07
22	0.3000	3.304E-03	1.382E-02	1.733E-03	7.008E-03	3.674E-06	6.355E-07
23	8.0000	4.062E-04	5.811E-03	2.345E-04	2.668E-03	9.229E-07	9.364E-08
24	10.0000	4.062E-04	5.811E-03	2.345E-04	2.668E-03	9.229E-07	9.364E-08

	X	H2O	N2
1	-2.0000	1.103E-07	7.150E-01
2	-0.5000	3.220E-05	7.148E-01
3	0.0000	2.047E-03	7.109E-01
4	0.0500	1.115E-02	7.039E-01
5	0.0550	1.543E-02	7.020E-01
6	0.0600	2.200E-02	6.996E-01
7	0.0675	3.680E-02	6.953E-01
8	0.0750	5.800E-02	6.908E-01
9	0.0825	8.531E-02	6.868E-01
10	0.0863	1.005E-01	6.852E-01
11	0.0900	1.159E-01	6.841E-01
12	0.0938	1.302E-01	6.836E-01
13	0.0975	1.421E-01	6.837E-01
14	0.1013	1.508E-01	6.843E-01
15	0.1050	1.564E-01	6.852E-01
16	0.1125	1.611E-01	6.872E-01
17	0.1200	1.626E-01	6.889E-01
18	0.1350	1.635E-01	6.913E-01
19	0.1500	1.645E-01	6.930E-01
20	0.1800	1.670E-01	6.951E-01
21	0.2400	1.707E-01	6.977E-01
22	0.3000	1.736E-01	6.998E-01
23	8.0000	1.859E-01	7.092E-01
24	10.0000	1.859E-01	7.092E-01

TWOPNT: SOLVE THE PROBLEM.

TASK	LOG10 NORM F	LOG10 COND J	REMARK
START	0.05		24 GRID POINTS
SEARCH	-1.96	13.88	6 SEARCH STEPS
REFINE	3.38		0.50 AND 0.57 RATIOS, 37 GRID POINTS
SEARCH	-1.51	14.27	15 SEARCH STEPS
REFINE	3.38		0.34 AND 0.34 RATIOS, 50 GRID POINTS
SEARCH	-1.37	14.35	12 SEARCH STEPS
REFINE	3.33		0.29 AND 0.28 RATIOS, 54 GRID POINTS
SEARCH	-1.51	14.33	8 SEARCH STEPS
REFINE	2.01		0.25 AND 0.22 RATIOS, 55 GRID POINTS
SEARCH	-1.18	14.33	5 SEARCH STEPS
REFINE	1.80		0.21 AND 0.22 RATIOS, 56 GRID POINTS
SEARCH	-1.70	14.33	4 SEARCH STEPS
REFINE			0.20 AND 0.22 RATIOS

TWOPNT: FINAL SOLUTION:

	X	T	V	RHO	CH4	CH3	CH2
1	-2.0000	2.980E+02	4.101E+01	1.130E-03	9.500E-02	5.867E-10	3.148E-28
2	-0.5000	2.981E+02	4.103E+01	1.130E-03	9.498E-02	1.617E-07	8.452E-26
3	0.0000	3.029E+02	4.183E+01	1.108E-03	9.437E-02	9.963E-06	5.655E-21
4	0.0250	3.139E+02	4.346E+01	1.066E-03	9.351E-02	3.353E-05	9.096E-18
5	0.0375	3.366E+02	4.672E+01	9.920E-04	9.202E-02	8.275E-05	7.170E-16
6	0.0500	4.000E+02	5.577E+01	8.311E-04	8.822E-02	2.238E-04	1.034E-13
7	0.0550	4.523E+02	6.323E+01	7.330E-04	8.521E-02	3.453E-04	2.821E-12
8	0.0600	5.303E+02	7.437E+01	6.232E-04	8.077E-02	5.349E-04	6.759E-11
9	0.0638	6.094E+02	8.571E+01	5.408E-04	7.626E-02	7.435E-04	8.896E-10
10	0.0656	6.566E+02	9.249E+01	5.011E-04	7.354E-02	8.836E-04	3.440E-09
11	0.0675	7.091E+02	1.000E+02	4.633E-04	7.047E-02	1.059E-03	1.144E-08
12	0.0694	7.666E+02	1.083E+02	4.278E-04	6.703E-02	1.281E-03	3.447E-08
13	0.0713	8.290E+02	1.173E+02	3.950E-04	6.320E-02	1.565E-03	9.639E-08
14	0.0750	9.661E+02	1.372E+02	3.378E-04	5.433E-02	2.352E-03	5.335E-07
15	0.0769	1.040E+03	1.479E+02	3.134E-04	4.929E-02	2.860E-03	1.225E-06
16	0.0787	1.116E+03	1.590E+02	2.915E-04	4.385E-02	3.430E-03	2.633E-06
17	0.0806	1.193E+03	1.703E+02	2.721E-04	3.810E-02	4.022E-03	5.346E-06
18	0.0825	1.271E+03	1.817E+02	2.550E-04	3.215E-02	4.567E-03	1.019E-05
19	0.0844	1.348E+03	1.930E+02	2.401E-04	2.619E-02	4.973E-03	1.805E-05
20	0.0863	1.423E+03	2.040E+02	2.272E-04	2.046E-02	5.138E-03	2.930E-05
21	0.0872	1.458E+03	2.092E+02	2.216E-04	1.778E-02	5.100E-03	3.586E-05



22	0.0881	1.493E+03	2.142E+02	2.163E-04	1.526E-02	4.976E-03	4.271E-05
23	0.0891	1.525E+03	2.190E+02	2.116E-04	1.292E-02	4.765E-03	4.938E-05
24	0.0900	1.556E+03	2.236E+02	2.073E-04	1.079E-02	4.473E-03	5.532E-05
25	0.0909	1.586E+03	2.278E+02	2.034E-04	8.882E-03	4.112E-03	5.996E-05
26	0.0919	1.613E+03	2.318E+02	2.000E-04	7.204E-03	3.697E-03	6.279E-05
27	0.0928	1.637E+03	2.354E+02	1.969E-04	5.756E-03	3.248E-03	6.347E-05
28	0.0938	1.660E+03	2.386E+02	1.942E-04	4.531E-03	2.787E-03	6.191E-05
29	0.0947	1.680E+03	2.416E+02	1.919E-04	3.513E-03	2.336E-03	5.827E-05
30	0.0956	1.698E+03	2.441E+02	1.898E-04	2.685E-03	1.912E-03	5.294E-05
31	0.0966	1.714E+03	2.464E+02	1.881E-04	2.023E-03	1.529E-03	4.649E-05
32	0.0975	1.727E+03	2.483E+02	1.866E-04	1.503E-03	1.197E-03	3.951E-05
33	0.0984	1.739E+03	2.500E+02	1.854E-04	1.103E-03	9.169E-04	3.257E-05
34	0.0994	1.750E+03	2.515E+02	1.843E-04	7.991E-04	6.893E-04	2.610E-05
35	0.1003	1.759E+03	2.527E+02	1.834E-04	5.723E-04	5.091E-04	2.039E-05
36	0.1013	1.767E+03	2.538E+02	1.826E-04	4.054E-04	3.700E-04	1.556E-05
37	0.1022	1.774E+03	2.548E+02	1.819E-04	2.839E-04	2.649E-04	1.163E-05
38	0.1031	1.781E+03	2.556E+02	1.813E-04	1.962E-04	1.868E-04	8.527E-06
39	0.1050	1.792E+03	2.571E+02	1.803E-04	9.488E-05	9.287E-05	4.490E-06
40	0.1069	1.802E+03	2.583E+02	1.794E-04	4.446E-05	4.461E-05	2.258E-06
41	0.1087	1.811E+03	2.594E+02	1.787E-04	1.948E-05	2.007E-05	1.058E-06
42	0.1125	1.827E+03	2.613E+02	1.774E-04	3.984E-06	4.306E-06	2.394E-07
43	0.1200	1.855E+03	2.645E+02	1.752E-04	2.973E-07	3.500E-07	2.077E-08
44	0.1350	1.897E+03	2.696E+02	1.719E-04	9.929E-09	1.338E-08	8.536E-10
45	0.1500	1.930E+03	2.736E+02	1.694E-04	2.885E-10	4.440E-10	2.991E-11
46	0.1800	1.977E+03	2.794E+02	1.659E-04	4.281E-12	7.605E-12	5.381E-13
47	0.2100	2.010E+03	2.836E+02	1.634E-04	7.289E-14	1.457E-13	1.071E-14
48	0.2400	2.036E+03	2.868E+02	1.616E-04	1.245E-15	2.800E-15	2.676E-16
49	0.3000	2.072E+03	2.911E+02	1.592E-04	2.625E-17	1.493E-16	6.687E-17
50	0.5406	2.131E+03	2.981E+02	1.555E-04	2.006E-17	1.217E-16	5.058E-17
51	0.7813	2.162E+03	3.018E+02	1.536E-04	2.159E-17	1.104E-16	3.957E-17
52	1.2625	2.191E+03	3.052E+02	1.519E-04	2.222E-17	9.403E-17	2.860E-17
53	2.2250	2.213E+03	3.078E+02	1.506E-04	2.196E-17	7.780E-17	2.031E-17
54	4.1500	2.228E+03	3.095E+02	1.498E-04	2.135E-17	6.635E-17	1.550E-17
55	8.0000	2.234E+03	3.103E+02	1.494E-04	2.095E-17	6.093E-17	1.346E-17
56	10.0000	2.234E+03	3.103E+02	1.494E-04	2.095E-17	6.093E-17	1.346E-17

	X	CH	CH2O	HCO	CO2	CO	H2
1	-2.0000	3.026E-43	1.991E-11	3.969E-26	3.314E-10	4.357E-09	2.443E-06
2	-0.5000	5.362E-41	7.937E-09	1.568E-23	1.302E-07	1.301E-06	1.928E-04
3	0.0000	3.502E-33	7.030E-07	2.342E-19	1.137E-05	8.670E-05	3.527E-03
4	0.0250	4.865E-29	3.074E-06	3.179E-16	4.928E-05	3.071E-04	5.904E-03
5	0.0375	4.591E-26	9.629E-06	1.972E-14	1.535E-04	7.962E-04	8.135E-03
6	0.0500	2.904E-22	3.334E-05	1.440E-12	5.320E-04	2.274E-03	1.142E-02
7	0.0550	2.212E-19	5.763E-05	2.541E-11	9.244E-04	3.590E-03	1.308E-02
8	0.0600	9.401E-17	9.990E-05	4.205E-10	1.617E-03	5.682E-03	1.488E-02
9	0.0638	9.940E-15	1.490E-04	4.788E-09	2.436E-03	7.943E-03	1.629E-02
10	0.0656	1.063E-13	1.814E-04	1.791E-08	2.981E-03	9.358E-03	1.701E-02
11	0.0675	7.843E-13	2.201E-04	5.904E-08	3.635E-03	1.099E-02	1.774E-02
12	0.0694	4.660E-12	2.662E-04	1.790E-07	4.412E-03	1.286E-02	1.847E-02
13	0.0713	2.368E-11	3.208E-04	5.027E-07	5.323E-03	1.496E-02	1.919E-02
14	0.0750	3.266E-10	4.584E-04	2.721E-06	7.565E-03	1.992E-02	2.064E-02
15	0.0769	1.174E-09	5.431E-04	5.675E-06	8.918E-03	2.277E-02	2.135E-02
16	0.0787	3.823E-09	6.368E-04	1.056E-05	1.044E-02	2.587E-02	2.203E-02
17	0.0806	1.162E-08	7.341E-04	1.779E-05	1.214E-02	2.919E-02	2.268E-02
18	0.0825	3.303E-08	8.260E-04	2.755E-05	1.401E-02	3.270E-02	2.326E-02
19	0.0844	8.715E-08	9.007E-04	3.963E-05	1.605E-02	3.629E-02	2.371E-02
20	0.0863	2.099E-07	9.454E-04	5.331E-05	1.825E-02	3.987E-02	2.399E-02
21	0.0872	3.135E-07	9.528E-04	6.031E-05	1.941E-02	4.158E-02	2.404E-02
22	0.0881	4.536E-07	9.489E-04	6.709E-05	2.059E-02	4.321E-02	2.402E-02
23	0.0891	6.345E-07	9.331E-04	7.334E-05	2.181E-02	4.474E-02	2.393E-02
24	0.0900	8.560E-07	9.052E-04	7.871E-05	2.305E-02	4.614E-02	2.376E-02
25	0.0909	1.111E-06	8.656E-04	8.284E-05	2.431E-02	4.739E-02	2.350E-02
26	0.0919	1.384E-06	8.150E-04	8.541E-05	2.559E-02	4.846E-02	2.317E-02
27	0.0928	1.652E-06	7.545E-04	8.612E-05	2.689E-02	4.933E-02	2.277E-02
28	0.0938	1.887E-06	6.860E-04	8.482E-05	2.820E-02	4.999E-02	2.229E-02
29	0.0947	2.063E-06	6.114E-04	8.146E-05	2.951E-02	5.042E-02	2.176E-02
30	0.0956	2.157E-06	5.336E-04	7.619E-05	3.083E-02	5.064E-02	2.118E-02
31	0.0966	2.161E-06	4.555E-04	6.931E-05	3.215E-02	5.064E-02	2.057E-02
32	0.0975	2.076E-06	3.799E-04	6.130E-05	3.345E-02	5.045E-02	1.995E-02
33	0.0984	1.916E-06	3.095E-04	5.269E-05	3.475E-02	5.009E-02	1.931E-02
34	0.0994	1.704E-06	2.464E-04	4.403E-05	3.603E-02	4.958E-02	1.869E-02
35	0.1003	1.464E-06	1.917E-04	3.582E-05	3.728E-02	4.895E-02	1.809E-02
36	0.1013	1.218E-06	1.460E-04	2.839E-05	3.852E-02	4.822E-02	1.752E-02
37	0.1022	9.855E-07	1.090E-04	2.196E-05	3.972E-02	4.743E-02	1.699E-02
38	0.1031	7.773E-07	7.975E-05	1.661E-05	4.089E-02	4.659E-02	1.649E-02

39	0.1050	4.594E-07	4.171E-05	9.188E-06	4.313E-02	4.485E-02	1.564E-02
40	0.1069	2.538E-07	2.073E-05	4.810E-06	4.523E-02	4.312E-02	1.496E-02
41	0.1087	1.289E-07	9.551E-06	2.357E-06	4.717E-02	4.146E-02	1.444E-02
42	0.1125	3.228E-08	2.082E-06	6.397E-07	5.058E-02	3.847E-02	1.376E-02
43	0.1200	3.082E-09	1.678E-07	1.621E-07	5.578E-02	3.387E-02	1.325E-02
44	0.1350	1.359E-10	6.363E-09	8.938E-08	6.166E-02	2.866E-02	1.300E-02
45	0.1500	4.935E-12	4.169E-10	6.754E-08	6.488E-02	2.581E-02	1.271E-02
46	0.1800	9.020E-14	1.852E-10	4.593E-08	6.776E-02	2.329E-02	1.192E-02
47	0.2100	1.879E-15	1.571E-10	3.392E-08	6.941E-02	2.186E-02	1.113E-02
48	0.2400	1.163E-16	1.388E-10	2.632E-08	7.061E-02	2.081E-02	1.043E-02
49	0.3000	6.826E-17	1.135E-10	1.767E-08	7.243E-02	1.923E-02	9.334E-03
50	0.5406	3.853E-17	7.310E-11	7.796E-09	7.607E-02	1.599E-02	7.321E-03
51	0.7813	2.462E-17	5.402E-11	4.564E-09	7.827E-02	1.400E-02	6.209E-03
52	1.2625	1.431E-17	3.831E-11	2.538E-09	8.048E-02	1.200E-02	5.162E-03
53	2.2250	8.293E-18	2.750E-11	1.465E-09	8.234E-02	1.030E-02	4.328E-03
54	4.1500	5.438E-18	2.139E-11	9.738E-10	8.358E-02	9.155E-03	3.791E-03
55	8.0000	4.372E-18	1.880E-11	7.916E-10	8.417E-02	8.613E-03	3.543E-03
56	10.0000	4.372E-18	1.880E-11	7.916E-10	8.417E-02	8.613E-03	3.543E-03

	X	H	O2	O	OH	HO2	H2O2
1	-2.0000	3.954E-19	1.900E-01	-6.871E-21	6.188E-21	1.777E-12	1.370E-11
2	-0.5000	2.034E-17	1.900E-01	-1.307E-18	1.200E-18	5.295E-10	4.109E-09
3	0.0000	2.522E-14	1.891E-01	1.347E-20	2.878E-14	3.905E-08	2.752E-07
4	0.0250	2.059E-13	1.881E-01	7.488E-17	1.031E-11	3.645E-07	9.741E-07
5	0.0375	2.147E-12	1.864E-01	4.910E-15	1.901E-10	1.335E-06	2.519E-06
6	0.0500	1.435E-10	1.820E-01	4.030E-13	3.293E-09	5.588E-06	7.121E-06
7	0.0550	5.574E-09	1.784E-01	1.513E-11	2.820E-08	1.257E-05	1.100E-05
8	0.0600	1.423E-07	1.728E-01	3.662E-10	2.006E-07	2.844E-05	1.669E-05
9	0.0638	1.506E-06	1.669E-01	5.575E-09	1.086E-06	5.199E-05	2.183E-05
10	0.0656	4.697E-06	1.632E-01	2.671E-08	2.654E-06	6.817E-05	2.429E-05
11	0.0675	1.171E-05	1.591E-01	9.869E-08	5.694E-06	8.598E-05	2.643E-05
12	0.0694	2.572E-05	1.544E-01	3.205E-07	1.113E-05	1.033E-04	2.797E-05
13	0.0713	5.108E-05	1.491E-01	9.262E-07	2.006E-05	1.180E-04	2.868E-05
14	0.0750	1.512E-04	1.370E-01	4.747E-06	5.197E-05	1.345E-04	2.730E-05
15	0.0769	2.481E-04	1.301E-01	1.000E-05	8.220E-05	1.363E-04	2.528E-05
16	0.0787	3.866E-04	1.227E-01	1.916E-05	1.268E-04	1.334E-04	2.247E-05
17	0.0806	5.801E-04	1.148E-01	3.433E-05	1.927E-04	1.264E-04	1.905E-05
18	0.0825	8.440E-04	1.065E-01	5.848E-05	2.905E-04	1.160E-04	1.528E-05
19	0.0844	1.195E-03	9.787E-02	9.592E-05	4.339E-04	1.031E-04	1.148E-05
20	0.0863	1.648E-03	8.914E-02	1.528E-04	6.403E-04	8.902E-05	8.016E-06
21	0.0872	1.916E-03	8.481E-02	1.918E-04	7.745E-04	8.194E-05	6.545E-06
22	0.0881	2.211E-03	8.052E-02	2.396E-04	9.322E-04	7.495E-05	5.280E-06
23	0.0891	2.532E-03	7.631E-02	2.982E-04	1.116E-03	6.816E-05	4.235E-06
24	0.0900	2.877E-03	7.221E-02	3.697E-04	1.327E-03	6.165E-05	3.413E-06
25	0.0909	3.241E-03	6.823E-02	4.566E-04	1.567E-03	5.549E-05	2.800E-06
26	0.0919	3.621E-03	6.442E-02	5.613E-04	1.837E-03	4.972E-05	2.373E-06
27	0.0928	4.010E-03	6.078E-02	6.862E-04	2.135E-03	4.439E-05	2.104E-06
28	0.0938	4.403E-03	5.734E-02	8.326E-04	2.460E-03	3.951E-05	1.960E-06
29	0.0947	4.792E-03	5.411E-02	1.001E-03	2.807E-03	3.509E-05	1.915E-06
30	0.0956	5.172E-03	5.109E-02	1.190E-03	3.172E-03	3.115E-05	1.942E-06
31	0.0966	5.537E-03	4.830E-02	1.398E-03	3.548E-03	2.766E-05	2.022E-06
32	0.0975	5.884E-03	4.573E-02	1.619E-03	3.928E-03	2.462E-05	2.138E-06
33	0.0984	6.209E-03	4.338E-02	1.848E-03	4.306E-03	2.201E-05	2.276E-06
34	0.0994	6.511E-03	4.124E-02	2.079E-03	4.674E-03	1.980E-05	2.427E-06
35	0.1003	6.787E-03	3.930E-02	2.306E-03	5.027E-03	1.794E-05	2.581E-06
36	0.1013	7.038E-03	3.754E-02	2.523E-03	5.360E-03	1.639E-05	2.733E-06
37	0.1022	7.264E-03	3.596E-02	2.725E-03	5.670E-03	1.511E-05	2.876E-06
38	0.1031	7.466E-03	3.454E-02	2.911E-03	5.954E-03	1.406E-05	3.006E-06
39	0.1050	7.803E-03	3.211E-02	3.226E-03	6.446E-03	1.249E-05	3.219E-06
40	0.1069	8.060E-03	3.015E-02	3.468E-03	6.844E-03	1.139E-05	3.364E-06
41	0.1087	8.249E-03	2.854E-02	3.646E-03	7.162E-03	1.058E-05	3.445E-06
42	0.1125	8.460E-03	2.617E-02	3.849E-03	7.602E-03	9.483E-06	3.454E-06
43	0.1200	8.458E-03	2.337E-02	3.915E-03	8.025E-03	8.224E-06	3.170E-06
44	0.1350	7.844E-03	2.066E-02	3.655E-03	8.224E-03	6.936E-06	2.492E-06
45	0.1500	7.120E-03	1.905E-02	3.345E-03	8.213E-03	6.159E-06	1.999E-06
46	0.1800	5.847E-03	1.717E-02	2.818E-03	7.998E-03	5.246E-06	1.411E-06
47	0.2100	4.888E-03	1.588E-02	2.415E-03	7.724E-03	4.633E-06	1.068E-06
48	0.2400	4.170E-03	1.489E-02	2.106E-03	7.445E-03	4.174E-06	8.492E-07
49	0.3000	3.225E-03	1.347E-02	1.685E-03	6.949E-03	3.540E-06	6.006E-07
50	0.5406	1.895E-03	1.094E-02	1.053E-03	5.879E-03	2.467E-06	3.085E-07
51	0.7813	1.335E-03	9.510E-03	7.680E-04	5.199E-03	1.901E-06	2.037E-07
52	1.2625	9.096E-04	8.134E-03	5.415E-04	4.503E-03	1.399E-06	1.313E-07
53	2.2250	6.346E-04	7.012E-03	3.892E-04	3.909E-03	1.032E-06	8.813E-08
54	4.1500	4.857E-04	6.274E-03	3.043E-04	3.509E-03	8.182E-07	6.597E-08
55	8.0000	4.241E-04	5.927E-03	2.685E-04	3.319E-03	7.264E-07	5.706E-08

56 10.0000 4.241E-04 5.927E-03 2.685E-04 3.319E-03 7.264E-07 5.706E-08

	X	H2O	N2
1	-2.0000	3.088E-08	7.150E-01
2	-0.5000	8.528E-06	7.149E-01
3	0.0000	5.255E-04	7.124E-01
4	0.0250	1.752E-03	7.103E-01
5	0.0375	4.266E-03	7.081E-01
6	0.0500	1.118E-02	7.041E-01
7	0.0550	1.675E-02	7.017E-01
8	0.0600	2.486E-02	6.988E-01
9	0.0638	3.289E-02	6.963E-01
10	0.0656	3.762E-02	6.951E-01
11	0.0675	4.283E-02	6.939E-01
12	0.0694	4.851E-02	6.926E-01
13	0.0713	5.465E-02	6.914E-01
14	0.0750	6.818E-02	6.892E-01
15	0.0769	7.548E-02	6.882E-01
16	0.0787	8.309E-02	6.873E-01
17	0.0806	9.095E-02	6.864E-01
18	0.0825	9.894E-02	6.857E-01
19	0.0844	1.070E-01	6.852E-01
20	0.0863	1.148E-01	6.847E-01
21	0.0872	1.187E-01	6.846E-01
22	0.0881	1.224E-01	6.845E-01
23	0.0891	1.260E-01	6.844E-01
24	0.0900	1.295E-01	6.844E-01
25	0.0909	1.328E-01	6.844E-01
26	0.0919	1.359E-01	6.845E-01
27	0.0928	1.389E-01	6.846E-01
28	0.0938	1.416E-01	6.847E-01
29	0.0947	1.441E-01	6.849E-01
30	0.0956	1.464E-01	6.851E-01
31	0.0966	1.484E-01	6.853E-01
32	0.0975	1.503E-01	6.855E-01
33	0.0984	1.520E-01	6.857E-01
34	0.0994	1.534E-01	6.859E-01
35	0.1003	1.547E-01	6.862E-01
36	0.1013	1.558E-01	6.864E-01
37	0.1022	1.568E-01	6.867E-01
38	0.1031	1.577E-01	6.870E-01
39	0.1050	1.590E-01	6.875E-01
40	0.1069	1.601E-01	6.880E-01
41	0.1087	1.608E-01	6.885E-01
42	0.1125	1.617E-01	6.894E-01
43	0.1200	1.624E-01	6.909E-01
44	0.1350	1.632E-01	6.931E-01
45	0.1500	1.643E-01	6.945E-01
46	0.1800	1.668E-01	6.964E-01
47	0.2100	1.689E-01	6.977E-01
48	0.2400	1.707E-01	6.988E-01
49	0.3000	1.733E-01	7.004E-01
50	0.5406	1.776E-01	7.033E-01
51	0.7813	1.798E-01	7.049E-01
52	1.2625	1.819E-01	7.064E-01
53	2.2250	1.835E-01	7.076E-01
54	4.1500	1.846E-01	7.083E-01
55	8.0000	1.850E-01	7.087E-01
56	10.0000	1.850E-01	7.087E-01

TWOPNT: SUCCESS. PROBLEM SOLVED.

## 8. REFERENCES

1. R. J. Kee, J. F. Grcar, M. D. Smooke, and J. A. Miller, "A Fortran Program for Modeling Steady Laminar One-Dimensional Premixed Flames" Sandia National Laboratories Report SAND85-8240 (1985).
2. J. A. Miller, R. E. Mitchell, M. D. Smooke, and R. J. Kee, in Proceedings of the Nineteenth Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, PA, p. 181 (1982).
3. J. A. Miller, M. D. Smooke, R. M. Green, and R. J. Kee, Combustion Science and Technology 34: 149 (1983).
4. J. A. Miller, M. C. Branch, W. J. McLean, D. W. Chandler, M. D. Smooke, and R. J. Kee, in Proceedings of the Twentieth Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, PA, p. 673 (1985).
5. J. O. Hirschfelder, C. F. Curtiss, and D. E. Campbell, in Proceedings of the Nineteenth Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, PA, p. 190 (1953).
6. B. Spalding, Philos. Trans. R. Soc. London 249A: 1 (1967).
7. N. Peters and J. Warnatz, (Friedr. Vieweg & Sohn, Wiesbaden, 1982).
8. K. A. Wilde, Combustion and Flame 18: 43 (1972).
9. R. M. Kendall and J. T. Kelly, "Premixed One-Dimensional Flame (PROF) Code User's Manual" EPA Report EPA-600/7-78-172a (1978).
10. C. F. Curtiss and J. O. Hirschfelder, Journal of Chemical Physics 17: 550 (1949).
11. S. Chapman and T. G. Cowling, The Mathematical Theory of Non-Uniform Gases Cambridge University Press, Cambridge (1970).
12. T. P. Coffee and J. M. Heimerl, Combustion and Flame 43: 273 (1981).
13. T. P. Coffee and J. M. Heimerl, Combustion Science and Technology 34: 31 (1983).
14. G. Dixon-Lewis, Proceedings of the Royal Society A. 304: 111 (1968).
15. R. J. Kee and J. A. Miller, "A Structured Approach to the Computational Modeling of Chemical Kinetics and Molecular Transport in Flowing Systems" Sandia National Laboratories Report SAND86-8841 (1986).
16. M. D. Smooke, J. A. Miller, and R. J. Kee, Combustion Science and Technology 34: 79 (1983).
17. P. Deuflhard, Numerical Mathematics 22: 289 (1974).
18. A. R. Curtis, M. J. Powell, and J. K. Reid, J. Inst. of Math. Appl. 13: 117 (1974).
19. M. D. Smooke and R. M. M. Mattheij, Appl. Numer. Math. 1: 463 (1985).
20. W. E. Stewart and J. P. Sørensen, in Proceedings of the 4th International / 6th European Symposium on Chemical Reactor Engineering, Dechema, Frankfurt (1976).
21. R. A. Brown, L. E. Scriven, and W. J. Silliman, in Nonlinear Problems in Dynamics, edited by P. Holmes (SIAM, Philadelphia, 1980), Vol. p. 289.
22. H. Saito and L. E. Scriven, Journal of Computational Physics 42: 53 (1981).

23. Y. Reuven, M. D. Smooke, and H. Rabitz, "Sensitivity Analysis of Boundary Value Problems: Application to Nonlinear Reaction-Diffusion Systems" Yale University Mechanical Engineering Department Report ME-104-85 (1985).