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PREMIX: A FORTRAN Program for Modeling Steady Laminar One-Dimensional Premixed Flames

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

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ABSTRACT

This report documents a Fortran computer program that 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. After stating the appropriate governing equations and boundary conditions, we discuss the finite difference discretization and the Newton method for solving the boundary value problem. Global convergence of this algorithm is aided by invoking time integration procedures when the Newton method has convergence difficulties. The program runs in conjunction with preprocessors for the chemical reaction mechanism and 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.

CONTENTS

LIST OF FIGURES

NOMENCLATURE

		CGS Units
A	Cross-sectional area of the stream tube encompassing the flame	cm^2
A	Pre-exponential factor in an Arrhenius rate expression	---
c_p	Specific heat at constant pressure of gas mixture	ergs / (g K)
c_{pk}	Specific heat at constant pressure of the kth species	ergs / (g K)
$\mathcal{D}_{kj}$	Binary diffusion coefficient of species k in species j	cm^2 / sec
D_{km}	Mixture-averaged diffusion coefficient of the kth species	cm^2 / sec
$D_{k,j}$	Multicomponent diffusion coefficient of the species k in species j	cm^2 / sec
D_k^T	Thermal diffusion coefficient of the kth species	cm^2 / sec
E_A	Activation energy in an Arrhenius rate expression	ergs / mole
h_k	Specific enthalpy of the kth species	ergs / 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	g / sec
p	Pressure	dynes / cm^2
R	Universal gas constant	ergs / (mole K)
t	Time	sec
T	Temperature	K
u	Velocity of the fluid mixture	cm / sec
V_c	Correction velocity	cm / sec
V_k	Diffusion velocity of the kth species	cm / sec
$_k$	Ordinary diffusion velocity of the kth species	cm / sec
W_k	Molecular weight of kth species	g / mole
$_k$	Thermal diffusion velocity of kth species	cm / sec
$\overline{W}$	Mean molecular weight of a mixture	g / mole
x	Spatial coordinate	cm
X_k	Mole fraction of the kth species	---
Y_k	Mass fraction of the kth species	---

		CGS Units
GREEK		
β	Temperature exponent in the rate constant	---
γ	User-specified parameter for solution curvature resolution	---
δ	User-specified parameter for solution gradient resolution	---
ε_k	Inlet mass fraction of the *k*th species	---
λ	Thermal conductivity of the gas mixture	ergs / (cm K sec)
$\lambda^{(n)}$	Damping parameter for the *n*th iterate in the solution algorithm	---
ρ	Mass density	g / cm^3
ϕ	Solution vector	---
$\dot{\omega}_k$	Production rate of the *k*th species from gas-phase reactions	$mole / (cm^2 sec)$
Θ_k	Thermal diffusion ratio for mixture-averaged formula	---

PREMIX: A FORTRAN PROGRAM FOR MODELING STEADY LAMINAR ONE-DIMENSIONAL PREMIXED FLAMES[†]

I. 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 our first use of flame modeling to interpret experimental observations and to understand combustion chemistry and pollution formation can be found in Miller, et al.[1-3]

The earliest efforts at solving premixed flame problems with realistic chemical kinetics made use of shooting techniques (e.g. Hirschfelder, et al.[4]). However, as the kinetics becomes more complex the shooting methods are not useable. Spalding[5] 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.[6] Wilde[7] and Kendall and Kelly[8] introduced the idea of solving the steady-state problem directly by finite-difference boundary-value-problem techniques. Our approach 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.

The first section of this report presents the conservation equations and associated boundary conditions that are solved in each of the flame configurations we consider. The next section describes the numerical method used to solve these boundary value problems; it is a combination of a Newton's method and time integration. Then we explain how to use the program itself, which is designed to be run in conjunction with two preprocessors. The first is CHEMKIN-III Gas-phase Interpreter,[9] which processes the chemical reaction mechanism, and the second is the Transport Property[10] preprocessor. After describing how these packages work together, we describe the Keyword input needed to define and solve a particular flame problem. Finally, we present and discuss two example problems.

II. PREMIXED FLAME EQUATIONS

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

Continuity:
$$\dot{M} = \rho u A \tag{1}$$

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

Species:
$$\dot{M}\frac{dY_k}{dx} + \frac{d}{dx}\left(\rho A Y_k V_k\right) - A\dot{\omega}_k W_k = 0 \qquad (\mathrm{k} = 1,\ldots,\mathrm{K}), \tag{3}$$

Equation of State:
$$\rho = \frac{p\overline{W}}{RT}. \tag{4}$$

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 kth species (there are K species); p the pressure; u the velocity of the fluid mixture; ρ the mass density; W_k the molecular weight of the kth species; $\overline{W}$ the mean molecular weight of the mixture; R the universal gas constant; λ 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 kth species; $\dot{\omega}_k$ the molar rate of production by chemical reaction of the kth species per unit volume; h_k the specific enthalpy of the kth species; V_k the diffusion velocity of the kth 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,

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

The details of the chemical reaction equations and the thermochemical properties are found in the user's manuals for CHEMKIN-III, a program designed to evaluate these expressions. [9,11]

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.[10] 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.

Mixture-Averaged Transport Properties

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

$$V_k = \mathcal{V}_k + \mathcal{W}_k + V_c . \tag{6}$$

$_k$ is the ordinary diffusion velocity and is given in the Curtiss-Hirschfelder[12] approximation by

$$_k = -D_{km} \frac{1}{X_k} \frac{dX_k}{dx}, \tag{7}$$

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}

$$D_{km} = \frac{1 - Y_k}{\sum_{j \neq k}^{K} X_j / \mathrm{D}_{kj}} . \tag{8}$$

A non-zero thermal diffusion velocity $_k$ is included only for the low molecular weight species H, H_2, and He. The trace, light-component limit is employed in determining $_k$, i.e.,

$$_k = \frac{D_{km} \Theta_k}{X_k} \frac{1}{T} \frac{dT}{dx}, \tag{9}$$

where Θ_k is the thermal diffusion ratio.[13] The sign of Θ_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[14,15] in their extensive investigation of approximate transport models in hydrogen and methane flames.

Multicomponent Transport Properties

For the multicomponent option, the transport property evaluation follows the method described by Dixon-Lewis.[16] 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 is provided by Kee, et. al.[17] 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

$$V_k = \mathbb{V}_k + \mathbb{W}_k. \tag{10}$$

Now, the ordinary diffusion velocity term becomes:

$$_k = \frac{1}{X_k \overline{W}} \sum_{j \neq k}^{K} W_j D_{k,j} \mathbf{d_j}, \tag{11}$$

where $\overline{M}$ 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:

$$_k = -\frac{D_k^T}{\rho Y_k}\frac{1}{T}\nabla T, \tag{12}$$

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

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.[12] 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.[18] 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 the following section.

III. 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 section. 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 a time integration. 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.

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

$$\dot{M}\frac{dT}{dx}\Big|_j \approx \dot{M}_j \left|\frac{T_j - T_{j-1}}{x_j - x_{j-1}}\right|, \tag{13}$$

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

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

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,

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

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.

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

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:

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

and

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

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 $\left(Y_k = X_k W_k / \overline{W}\right)$. After the diffusion velocities are computed at all the mesh midpoints, the correction velocity V_c is computed at the midpoints from

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

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

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

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.

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

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

and

$$T_1 - T_b = 0, \tag{22}$$

where $\varepsilon_{k,1}$ is the inlet reactant fraction of the *k*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.,

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

and

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

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 the previous section.

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 Fig. 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). 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.

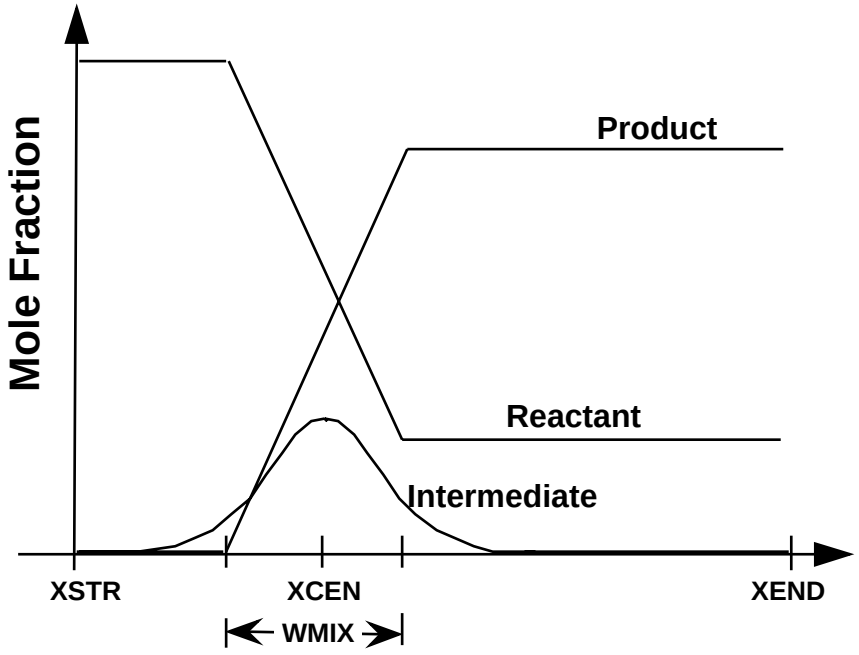

Figure 1. The general form of the starting estimate.

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.

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.

Modified Damped Newton's Method

The PREMIX code uses the modular solver routine known as TWOPNT[19] 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 ϕ. When any arbitrary ϕ 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 ϕ that satisfies

$$F(\phi) = 0. \tag{25}$$

In our case the vector ϕ is composed as follows:

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

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 the Jacobian section that follows. The ordering of the *F* vector corresponds to the order of the ϕ 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

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

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

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

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

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

Of course, the inverse Jacobian matrix in Eq. (28) is not computed; instead a system of linear equations $J^{(n)}\Delta\phi^{(n)} = F\left(\phi^{(n)}\right)$ 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[20] for accepting $\phi^{(n+1)}$ is that the undamped steps decrease in magnitude,

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

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 Newton iteration is considered to be converged when the solution correction vector $\Delta\phi$ satisfies

$$|\Delta\phi| \le \max\left(A, R\times|\phi|\right). \tag{31}$$

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 developed in a later section.

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.[21] Specifically, we evaluate a one-sided finite difference formula,

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

where

$$\delta = r \times \phi_j + a. \tag{33}$$

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 ϕ_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 ϕ 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 vectorϕ, 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.,

$$\frac{d\dot{M}}{dx} = 0. \tag{34}$$

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

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

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

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

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

$$T_{j_f} - T_f = 0. \tag{37}$$

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

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

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.[22] 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

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

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

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

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 δ and γ 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 ϕ 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.

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[6]). 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 size of the time step and number of time steps to be taken are specified by the user.

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

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

and

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

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

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

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 ϕ 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.

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,[23] Brown, et al.,[24] and Saito and Scriven[25]). 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.[3]). Coffee and Heimerl[15] 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.,[26] 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),

$$F(\phi;\alpha)=0. \tag{44}$$

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

$$\frac{\partial F}{\partial \phi}\frac{\partial \phi}{\partial \alpha}+\frac{\partial F}{\partial \alpha}=0\,. \tag{45}$$

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.

$$\frac{\alpha_i}{Y_k}\frac{\partial Y_k}{\partial \alpha_i} \tag{46}$$

or

$$\frac{\alpha_i}{T}\frac{\partial T}{\partial \alpha_i} \tag{47}$$

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.,

$$\frac{\alpha_i}{X_k}\frac{\partial X_k}{\partial \alpha_i} = \frac{\alpha_i}{Y_k}\frac{\partial Y_k}{\partial \alpha_i} - \alpha_i \overline{W} \sum_{j=1}^{K} \frac{1}{W_j}\frac{\partial Y_k}{\partial \alpha_i} \tag{48}$$

where X_k are the mole fractions and $\overline{W}$ 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

$$\frac{\alpha_i}{Y_k^{\max}}\frac{\partial Y_k}{\partial \alpha_i}, \tag{49}$$

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.

IV. PROGRAM STRUCTURE

PREMIX reads input from the user, defines the governing equations, makes calls to the boundary value solver, and prints solutions for the flame problem. This section contains a step-by-step description of the tasks required by the user to run a PREMIX problem. In addition to input directly from the user, PREMIX depends on data and subroutines from the CHEMKIN-III[9] and TRANSPORT[10] packages. Therefore, to solve a flame problem the user must first execute two preprocessor programs that have access to thermodynamic and transport-property databases. Figure 2 shows the relationships between these various components.

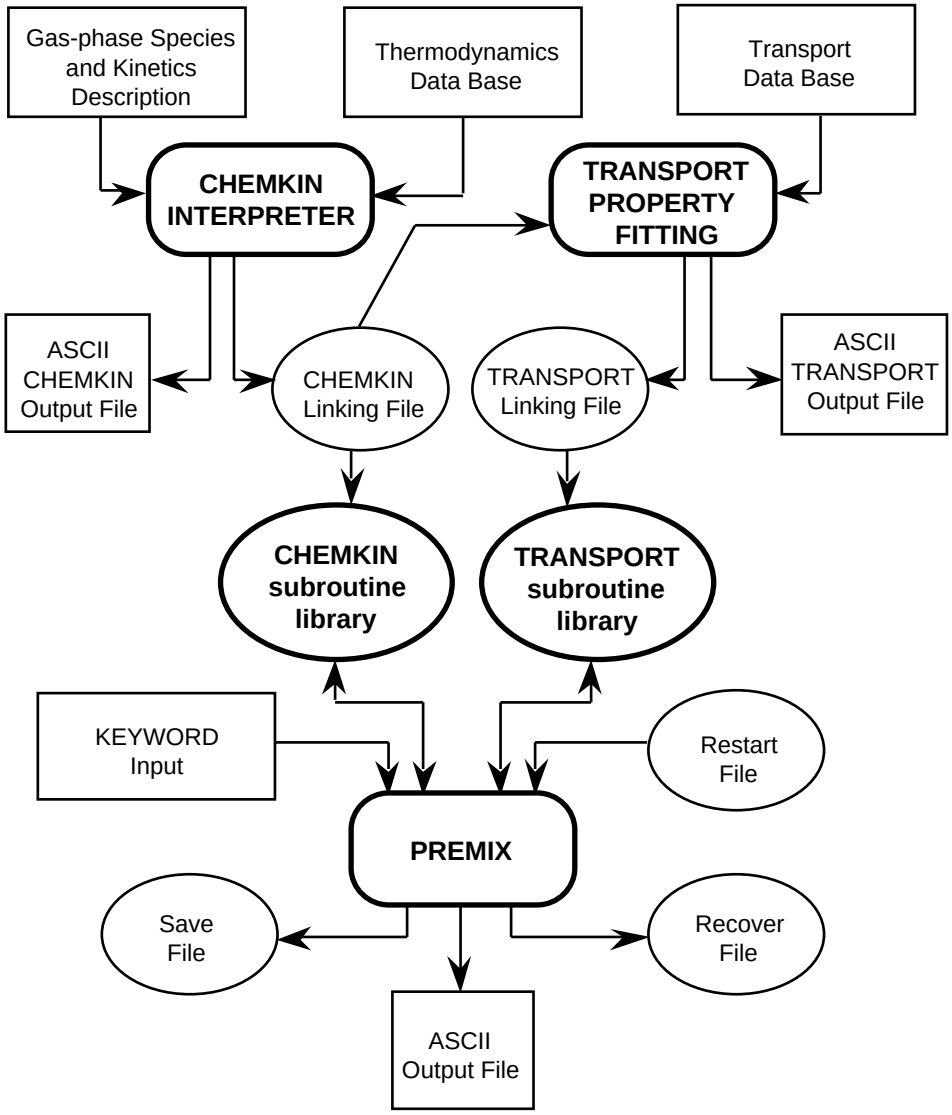

Figure 2. Relationship of the PREMIX Program to the CHEMKIN and TRANSPORT Preprocessors, and to the Associated Input and Output files.

The first step is to execute the CHEMKIN Interpreter, 'chem.exe'. The CHEMKIN Interpreter first reads (Unit 5) 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 data base, '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.exe', 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.exe'. It needs input from a transport property data base, 'tran.dat' and from the CHEMKIN subroutine library. Its purpose 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 subroutine library, which will evaluate mixture properties during the course of the flame computation.

PREMIX makes appropriate calls to the CHEMKIN and the TRANSPORT subroutine 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.

The input that defines a particular flame and the parameters needed to solve it are read by the flame program in a Keyword format from Unit 5. 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, e.g., 'rest.bin'. The flame program produces printed output on Unit 6 and it saves the solution in a binary Save File, e.g., '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'.

User-Supplied Program

PREMIX is written as a subroutine that is called from a driver program that opens all appropriate files, allocates the working storage, and calls the flame program through its subroutine interface. Although an example driver routine is provided with the PREMIX code, the user may choose to write his or her own routines to serve this function. Figure 3 shows an example of the main driver program.

```
PROGRAM PRDRIV
C*****precision > double
      IMPLICIT DOUBLE PRECISION (A-H,O-Z), INTEGER (I-N)
C*****END precision > double
C*****precision > single
C      IMPLICIT REAL (A-H,O-Z), INTEGER (I-N)
C*****END precision > single
      PARAMETER (LENLWK=100, LENIWK=5000, LENRWK=200000, LENCWK=100,
     1           LENSYM=16, LIN=5, LOUT=6, LRIN=14, LROUT=15,
     2           LRCVR=16, LINCK=25, LINMC=35, NMAX=65, ZERO=0.0)
C          LENLWK allocates the logical working space
C          LENIWK allocates the integer working space
C          LENRWK allocates the real working space
C          LENCWK allocates the character working space
C          LENSYM is the length of a character string
C          LIN is the unit from which user input is read
C          LOUT is the unit to which printed output is written
C          LRIN is the unit from which the restart file is read
C          LROUT is the unit to which the save file is written
C          LRCVR is the unit to which the scratch save file is written
C          LINCK is unit from which the Chemkin binary file is read
C          LINTP is unit from which the Transport binary file is read
C          NMAX is the total number of grid points allowed
      DIMENSION IWORK(LENIWK), RWORK(LENRWK)
      CHARACTER CWORK(LENCWK)*(LENSYM)
      LOGICAL LWORK(LENLWK)
      EXTERNAL CKTIME
      TSTART = CKTIME(ZERO)
C
      OPEN(LRIN,FORM='UNFORMATTED',STATUS='UNKNOWN',FILE='./rest.bin')
      OPEN(LROUT,FORM='UNFORMATTED',STATUS='UNKNOWN',FILE='./save.bin')
      OPEN(LRCVR,FORM='UNFORMATTED',STATUS='UNKNOWN',FILE='./recov.bin')
      OPEN(LINCK,STATUS='UNKNOWN',FORM='FORMATTED',FILE='./chem.asc')
      OPEN(LINMC,STATUS='UNKNOWN',FORM='FORMATTED', FILE='./tran.asc')
C
      CALL PREMIX (NMAX, LIN, LOUT, LINCK, LINMC, LRIN, LROUT, LRCVR,
     1             LENLWK, LWORK, LENIWK, IWORK, LENRWK, RWORK, LENCWK,
     2             CWORK)
      TEND = CKTIME (TSTART)
      IF (TEND .GT. 60.) THEN
         WRITE (LOUT, '(A,1PE15.2)') ' Total CPUtime (min): ',TEND/60.
      ELSE
          WRITE (LOUT, '(A,1PE15.2)') ' Total CPUtime (sec): ',TEND
      ENDIF
      CLOSE(LRIN)
      CLOSE(LROUT)
      CLOSE(LRCVR)
      CLOSE(LINCK)
      CLOSE(LINMC)
      STOP
      END
```

Figure 3. Example of the user-supplied main program to call the flame program.

In Figure 3, the logical, integer, and real working space is allocated with the parameters LENLWK, LENIWK, and LENRWK. The first thing the flame program does is to check to make sure that the user has provided enough space for the given problem. The first output from the program will report how much space was allocated and how much was required. If too little space is provided, the program

terminates at this point. If too much space was provided, it can be reduced by the user for the next problem. The variable NMAX sets the maximum number of mesh points that are permitted. A larger value of NMAX results in a larger requirement of working space for PREMIX. Also, larger reaction mechanisms require more working space than smaller ones, so the user may often want to change these parameters.

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 Fig. 4. 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 Fig. 4. 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.

```
      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 4. Example of a user function to pass the local flame streamtube area divided by the burner area to the PREMIX program.

Format of Save, Restart, and Recover Files

The Save File is a binary file that is written with the lines of FORTRAN shown in Figure 5. A Recover File is also written for intermediate solutions (e.g. at the end of time-stepping and before attempting a Newton iteration). The Recover File can be used as a restart file to recover where PREMIX left off, in the event that some problem occurs in the middle of the program execution. The Save and Recover Files contain up to five sets of records: CHEMKIN link file information, TRANSPORT link file information, solution variables, reaction sensitivity, and enthalpy sensitivity. Each set of records begins with a `CHARACTER*16` variable that identifies the records that follow as either 'CKLINK,' 'MCLINK', 'SOLUTION,' 'SENSITIVITY,' or 'HSENSITIVITY,' data. The header and chemistry records are only written once to Save and Recover Files. Only the latest solution will be written to the Recover File, while more than one solution may be sequentially written to the Save File (when the user invokes the CNTN Keyword).

The Chemistry data is written by the CKSAVE routine. The subroutine CKSAVE writes a list of pointers used internally in CHEMKIN libraries followed by the CHEMKIN storage arrays. It is not necessary for the user to know what is contained in this procedure. Instead, the user can read this information in from the binary file by first using the CHEMKIN subroutine, CKPNT, followed by an unformatted read of the ICKWRK, RCKWRK, and CCKWRK arrays. An example of how this is done is shown in Figure 6. The sizes of the integer, real, and character arrays are LENICK, LENRCK, and LENCCK, respectively. These values are included in the pointer list and are returned in the CKPNT subroutine call (See Fig. 6). Similarly for TRANSPORT, a call to the transport library routine MCSAVE writes the transport property data to the Save and Recover Files. For the TRANSPORT storage arrays, the size of the integer and real arrays are LENIMC, LENRMC, respectively. Again, this information can be read from the Save or Recover File using the TRANSPORT subroutine, MCPNT, followed by an unformatted read of the IMCWRK and RMCWRK arrays, as shown in Fig. 6.

```
C  Write CHEMKIN and TRANSPORT work arrays to binary file.
C
C  ICKWRK(*) -  integer array, CHEMKIN workspace
C  RCKWRK(*) -  real array, CHEMKIN workspace
C  CCKWRK(*) -  character-string array, CHEMKIN workspace
C  IMCWRK(*) -  integer array, TRANSPORT workspace
C  RMCWRK(*) -  real array, TRANSPORT workspace
C  LOUT      -  integer scalar, formatted output file unit number
C  LSAVE     -  integer scalar, binary output file unit number
C
      WRITE (LSAVE) 'CKLINK          '
      CALL CKSAVE (LOUT, LSAVE, ICKWRK, RCKWRK, CCKWRK)
C
      WRITE (LSAVE) 'MCLINK          '
      CALL MCSAVE (LOUT, LSAVE, IMCWRK, RMCWRK)
C
C  WRITE TO LSAVE WHEN SOLUTION IS COMPLETE
C
      WRITE (LSAVE) 'SOLUTION'
      WRITE (LSAVE) NATJ, JJ, P, S(NM, 1)
      WRITE (LSAVE) (X(J), J = 1, JJ)
      WRITE (LSAVE) ((S(N, J), N = 1, NATJ), J = 1, JJ)
C
C  Write the header for sensitivity, when sensitivities are requested.
      WRITE (LSAVE) 'SENSITIVITY'
C    write out the sensitivities
      DO 1000 IND = 1, II
         WRITE (LSAVE) IND, ((SN(N, J), N=1,NATJ), J=1,JJ)
1000  CONTINUE
C
      WRITE (LSAVE) 'HSENSITIVITY'
C    write out the sensitivities
      DO 2000 IND = 1, KK
         WRITE (LSAVE) IND, ((SN(N, J), N=1,NATJ), J=1,JJ)
2000  CONTINUE
```

Figure 5. Lines of FORTRAN used to write the Save and Recover Files.

The writing of solution variables begins with index or problem-size information. NATJ is the total number of solution variables in the problem (see Eq. (26)), JJ is the total number of grid points in the solution, P is the pressure in units of dynes/cm^2, and S(NM,1) is the inlet mass flow rate in units of g/sec.

The next record contains the grid information, where X is in cm. The grid locations are then followed by the solution vector at each grid point. The elements of the solution vector at each point J are in the order indicated by Eq. (26).

After the solution information, the sensitivity data is written only when the user has requested this information in the PREMIX input. Two types of sensitivity information may be requested: solution sensitivity to reaction parameters and solution sensitivity to species' enthalpies. In the sensitivity printout records, the values SN(N,J) are the sensitivity coefficients for each solution variable N at grid point J with respect to the parameter whose index is IND. In the case of reaction sensitivities, the parameters are the pre-exponential 'A' factors in the reaction rate coefficients and the index IND refers to the reaction number. In the case of enthalpy sensitivities, the parameters are the species' enthalpy values and the index IND refers to the species number.

```
C  Read the data file.
C  Keep track of number of solutions found on save file:
      NSOL = 0
1050  CONTINUE
      READ (LS, END = 2000, ERR = 2000) ICHR
      IF (ICHR .EQ. 'CKLINK') THEN
         CALL CKPNT (LS, LOUT, NPOINT, VERS, PREC, LENICK, LENRCK, LENCCK, IERR)
         READ (LS, ERR=2000, END=2000) (ICKWRK(L), L = 1, LENICK)
         READ (LS, ERR=2000, END=2000) (RCKWRK(L), L = 1, LENRCK)
         READ (LS, ERR=2000, END=2000) (CCKWRK(L), L = 1, LENCCK)
      ELSEIF (ICHR .EQ. 'MCLINK') THEN
         CALL MCPNT (LS, LOUT, NPOINT, VERS, PREC, LENIMC, LENRMC, IERR)
         READ (LS, ERR=2000, END=2000) (IMCWRK(L), L = 1, LENIMC)
         READ (LS, ERR=2000, END=2000) (RMCWRK(L), L = 1, LENRMC)
      ELSEIF (ICHR .EQ. 'SOLUTION') THEN
         READ (LS, END = 2000, ERR = 2000) NATJ, JJ, P, FLRT
         READ (LS, END = 2000, ERR = 2000) (X(J), J = 1, JJ)
         READ (LS, END = 2000, ERR = 2000)
     &        ((S(N, J), N = 1, NATJ), J = 1, JJ)
         NSOL = NSOL + 1
      ELSEIF (ICHR .EQ. 'SENSITIVITY') THEN
         DO 1080 I = 1, II
            READ (LS, END = 2000, ERR = 2000)
     &            IS, ((SN(N, J,IS), N=1,NATJ), J=1,JJ)
1080     CONTINUE
      ELSEIF (ICHR .EQ. 'HSENSITIVITY') THEN
         DO 1090 K = 1, KK
            READ (LREST, END = 2000, ERR = 2000)
     &            KS, ((SN(N, J,KS), N=1,NATJ), J=1,JJ)
1090     CONTINUE
      ELSE
         WRITE (LOUT, *)
     &     'FATAL ERROR, SOLUTION FILE FORMAT INVALID'
         KERR = .TRUE.
         RETURN
      ENDIF
      GO TO 1050
2000  CONTINUE
      IF (NSOL .LT. 1) THEN
         WRITE (LOUT, *) ' Error reading solution file...'
         KERR = .TRUE.
      ENDIF
```

Figure 6. Example of lines of FORTRAN that could be used to read the Save, Recover and Restart Files.

V. PROGRAM INPUT AND OUTPUT

The PREMIX program's input is in a Keyword format. On each input line ("card") 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 code, 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.

Keyword Descriptions

Problem Type

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 of 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 of 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 of 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 of ENRG must be specified.

Restart—can be changed.

Solution Method Options

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: $|\Delta\phi| \le \max(\text{ATOL}, \text{RTOL} \times |\phi|)$. Typically ATOL should be smaller than the maximum mass fraction of any species of interest.

Default—1.E-9

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: $|\Delta\phi| \le \max(\text{ATOL}, \text{RTOL} \times |\phi|)$. 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

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 criteria typically does not need to be as stringent as for the Newton iteration on the boundary value problem itself.

Default—1.E-9

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 criteria typically does not need to be as stringent as for the Newton iteration on the boundary value problem itself.

Default—1.E-4

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

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

Restart—can be changed.

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 [19]).

Default—20

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 [19]).

Default—50

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 [19]).

Default—2.2

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 [19]).

Units—seconds

Default—1.E-10

Restart—can be changed.

DTMX—Maximum time step allowed in TWOPNT's time stepping algorithm (refer to TMAX in the TWOPNT manual [19]).

Units—seconds

Default—1.E-4

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 [19]).

Default—20

Restart—can be changed.

Grid Parameters

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

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.

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

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

Restart—can be changed.

XSTR—The beginning of the computational interval.

Units—cm

Default—0.0

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)

XEND—The end of the computational interval.

Units—cm

Default—XEND is a required input.

Restart—can be changed to a larger value.

WMIX—An estimated width of the flame zone.

Units—cm

Default—WMIX = 0.5*(XEND-XSTR)

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 [19]).

Default— - 1.0E-3

Restart—can be changed.

Flame Definition

PRES—The pressure of the flame.

Units—atmospheres

Default—none

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^2-sec

Default—FLRT is a required input.

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_2H_2 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 of mole fractions, depending in MASS or MOLE.

Default—required input.

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_2. Any given species can participate simultaneously as a reactant, intermediate, or product.

Units—either mass of mole fractions, depending in MASS or MOLE.

Default—0.0

PROD—Mass or mole fraction values of the estimated final values of the flame products. One of these PROD inputs must appear for each product species. For example, "PROD H2O 0.5" estimates the fraction of H_2O 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.

Units—either mass of mole fractions, depending in MASS or MOLE.

Default—0.0

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. Up to NMAX (x, T) pairs may be input. 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.

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 the code 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).

Transport Options

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 tranport 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.

Sensitivity Options

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.

Miscellaneous

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 Fortran Unit 14.

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.

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

JJRG—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

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

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.

NTOT—Maximum number of grid points allowed for this job. This number must be less than or equal to NMAX, specified in the PREMIX driver program.

Default—NTOT=NMAX

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

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.

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

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.

VI. SAMPLE PREMIX PROBLEMS

We show two example problems in this section. 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.

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.[3] 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 4.63×10^{-3} gm/cm^2-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, whichuses 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, the code 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,[19] 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. (1) and (2). 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^3, and, in this case, the species are reported in mole fractions.

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
```

CHEMKIN Output for the Hydrogen-Oxygen Flame Example

```
 CHEMKIN-III GAS-PHASE MECHANISM INTERPRETER:
 DOUBLE PRECISION Vers. 6.8 97/03/11
 Copyright 1995, Sandia Corporation.
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```

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

SPECIES CONSIDERED	PHASE	CHARGE	MOLECULAR WEIGHT	TEMPERATURE LOW	TEMPERATURE HIGH	ELEMENT COUNT 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

REACTIONS CONSIDERED			(k = A T**b exp(-E/RT)) 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. 1.0 CHEMKIN linkfile chem.asc written.

WORKING SPACE REQUIREMENTS ARE
   INTEGER:      575
   REAL:         399
   CHARACTER:     12
Total CPUtime (sec):        1.13E+00
```

TRANSPORT Output for the Hydrogen-Oxygen Flame Example

```
 TRANFIT: CHEMKIN-III Transport property fitting code,
 DOUBLE PRECISION Vers. 3.9 97/03/01
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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
Total CPUtime (sec):        5.68E-01
```

PREMIX Code Output for the Hydrogen-Oxygen Flame Example

```
PREMIX: CHEMKIN-III One-dimensional steady premixed laminar flame code,
DOUBLE PRECISION Vers. 3.12 97/10/29
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               WORKING SPACE REQUIREMENTS
                PROVIDED        REQUIRED
LOGICAL              100              76
INTEGER             5000            1550
REAL               71000           70088
CHARACTER            100              32


         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 3.27 OF FEBRUARY 1997 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.

                    LOG10   LOG10
            TASK   NORM F  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   0.0312  4.014E+02  1.595E+02  2.903E-05  2.664E-01  9.109E-02  4.856E-04
 4   0.0469  4.152E+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   0.1562  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   0.0312  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   0.1562  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):        1.28E+01
```

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 the code 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 CH_4 mole fraction at the left boundary is 5.103E-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 5.0E-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, the code 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 can be seen by comparing the independently computed adiabatic flame temperature with the hot-boundary temperature. In this case, the adiabatic flame temperature is 2231K and the burned gas temperature in the flame is 2009K. Therefore, it is clear that another mesh point should be placed near the hot boundary so that the boundary condition is actually imposed far 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.

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.
HO2+HO2=H2O2+O2               2.0E12       0.         0.
H2O2+M=OH+OH+M                1.3E17       0.     45500.
H2O2+H=HO2+H2                 1.6E12       0.      3800.
H2O2+OH=H2O+HO2               1.0E13       0.      1800.
END
```

PREMIX Code Output for the Methain-Air Flame Example

```
 PREMIX: CHEMKIN-III One-dimensional steady premixed laminar flame code,
 DOUBLE PRECISION Vers. 3.12 97/10/29
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               WORKING SPACE REQUIREMENTS
                PROVIDED        REQUIRED
 LOGICAL             200              94
 INTEGER           15000            3513
 REAL            1600000          225835
 CHARACTER           200              57

          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
          WMIX      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 priting
        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 contiuation run will follow
        CNTN
        END

TWOPNT:  DOUBLE PRECISION (TWO POINT BOUNDARY VALUE PROBLEM) SOLVER,
         VERSION 3.27 OF FEBRUARY 1997 BY DR. JOSEPH F. GRCAR.

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   LOG10
             TASK  NORM F  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 3.27 OF FEBRUARY 1997 BY DR. JOSEPH F. GRCAR.

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.
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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

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




          KEYWORD INPUT

          /
          /      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

TWOPNT:  DOUBLE PRECISION (TWO POINT BOUNDARY VALUE PROBLEM) SOLVER,
          VERSION 3.27 OF FEBRUARY 1997 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
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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

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TWOPNT:  DOUBLE PRECISION (TWO POINT BOUNDARY VALUE PROBLEM) SOLVER,
         VERSION 3.27 OF FEBRUARY 1997 BY DR. JOSEPH F. GRCAR.

TWOPNT:  INITIAL GUESS:
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	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

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 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.

                    LOG10   LOG10
              TASK  NORM F  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   0.0862  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
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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	0.0862	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	0.0862	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	0.0862	1.004E-01	6.852E-01
10	0.0900	1.158E-01	6.841E-01

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 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.




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




         KEYWORD INPUT

         /
         /      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

TWOPNT:  DOUBLE PRECISION (TWO POINT BOUNDARY VALUE PROBLEM) SOLVER,
         VERSION 3.27 OF FEBRUARY 1997 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   0.0862  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
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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	0.0862	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	0.0862	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	0.0862	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	2.303E-27
2	-0.5000	2.980E+02	4.338E+01	1.130E-03	9.496E-02	6.116E-07	6.560E-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	0.0862	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	-6.733E-25	1.981E-09	1.773E-08	3.187E-06
2	-0.5000	4.201E-38	4.917E-08	-2.815E-22	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	0.0862	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	-2.052E-20	2.637E-19	1.985E-12	4.967E-11
2	-0.5000	1.046E-16	1.899E-01	-4.127E-18	5.405E-17	6.252E-10	1.575E-08
3	0.0000	2.216E-13	1.881E-01	7.322E-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	0.0862	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	0.0862	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

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 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 3.27 OF FEBRUARY 1997 BY DR. JOSEPH F. GRCAR.

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  2.303E-27
  2  -0.5000  2.980E+02  4.338E+01  1.130E-03  9.496E-02  6.116E-07  6.560E-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   0.0862  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 -6.733E-25  1.981E-09  1.773E-08  3.187E-06
  2  -0.5000  4.201E-38  4.917E-08 -2.815E-22  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   0.0862  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
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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	-2.052E-20	2.637E-19	1.985E-12	4.967E-11
2	-0.5000	1.046E-16	1.899E-01	-4.127E-18	5.405E-17	6.252E-10	1.575E-08
3	0.0000	2.216E-13	1.881E-01	7.322E-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	0.0862	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	0.0862	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	-2.855E-27
2	-0.5000	2.981E+02	4.103E+01	1.130E-03	9.498E-02	1.617E-07	-7.691E-25
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	0.0862	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	0.7812	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	-2.162E-42	1.991E-11	6.879E-26	3.314E-10	4.357E-09	2.443E-06
2	-0.5000	-3.842E-40	7.937E-09	2.719E-23	1.302E-07	1.301E-06	1.928E-04
3	0.0000	3.502E-33	7.030E-07	2.341E-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	4.590E-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	0.0862	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	0.7812	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	-6.092E-21	6.201E-21	1.777E-12	1.370E-11
2	-0.5000	2.034E-17	1.900E-01	-1.161E-18	1.202E-18	5.295E-10	4.109E-09
3	0.0000	2.522E-14	1.891E-01	1.651E-19	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	0.0862	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	0.7812	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   0.0862  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   0.7812  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.
Total CPUtime (min):        2.00E+00
```

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APPENDIX A. Example Script for Running CHEMKIN, TRANSPORT, and PREMIX

```
#!/bin/sh
# to execute:  sh premix.sh myrun &
# nqs batch mode:  qsub -q queuename -lt time(seconds) premix.sh

sh 1> ${1}.log 2>&1 << ENDSH    # shell run output is "myrun.log"

set -x

cat << EOF > makefile

F77    = f77
Fbug   = -check_bounds -g -O0 -trapuv
Fdef   =
Fopt   = -O3
FFLAGS = $(Fdef)

chem.exe:   ckdriv.o cktime.o ckinterp.o cklib.o
       $(F77) $(FFLAGS) ckdriv.o cktime.o ckinterp.o cklib.o     -o chem.exe

tran.exe:    mcdriv.o cktime.o tranfit.o cklib.o xerror.o
       $(F77) $(FFLAGS) mcdriv.o cktime.o tranfit.o cklib.o xerror.o    -o tran.exe

premix.exe:  prdriv.o cktime.o premix.o cklib.o tranlib.o twopnt.o   refine.o math.o
mach.o
       $(F77) $(FFLAGS) prdriv.o cktime.o premix.o cklib.o tranlib.o twopnt.o \
                        refine.o math.o mach.o   -o premix.exe

EOF

#
#************************************
#   Compile and link executables
#************************************
#
touch makefile
make chem.exe
make tran.exe
make premix.exe
#
#************************************
#   Run gas-phase Chemkin interpreter
#     the input file is 'chem.inp'
#     the output file is 'chem.out'
#************************************
#
chem.exe <chem.inp >chem.out
#
#************************************
#   Run Transport fitting routine
#     the output file is 'tran.out'
#************************************
#
tran.exe >tran.out
#
#************************************
#   Run PREMIX
#************************************
#
rm premix.out save.bin recov.bin;
premix.exe <premix.inp >premix.out
```

```
ENDSH
```