Premix

Simulating steady, laminar, one-dimensional premixed flames

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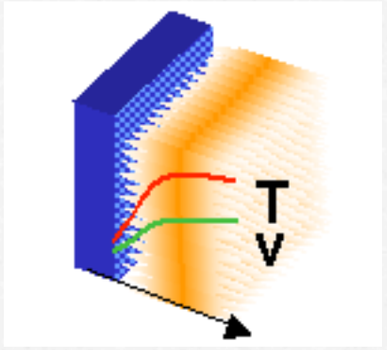
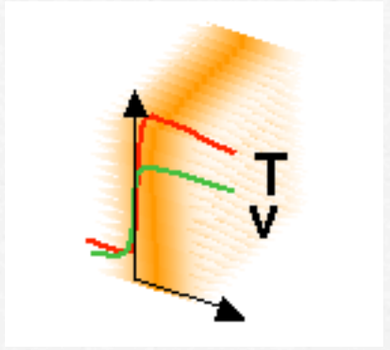
Introduction

PREMIX computes species and temperature profiles in steady-state burner-stabilized and freely propagating premixed laminar flames. PREMIX can be used to determine laminar flame speeds of combustive gas mixtures that are important for flammability studies. The Application accounts for finite-rate chemical kinetics and multicomponent molecular transport.

The PREMIX Application runs in conjunction with the GAS-PHASE KINETICS and TRANSPORT Pre-processors for processing the chemical reaction mechanism and for calculating the transport properties. TRANSPORT property formulations include the option of using multicomponent or mixtureaveraged formulas for molecular diffusion.

Introduction

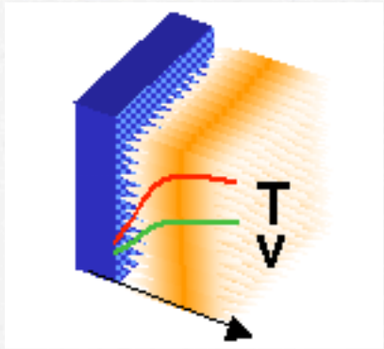




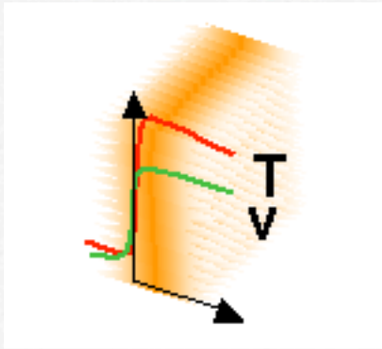
Many practical combustors, such as internal combustion engines, rely on premixed flame propagation. Moreover, burner-stabilized laminar premixed flames are often used to study chemical kinetics in a combustion environment. Such flames are effectively one-dimensional and can be made very steady, facilitating 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.

PREMIX solves the set of governing differential equations that describe the flame dynamics using implicit finite difference methods, as well as, a combination of time-dependent and steady-state methods. Furthermore, PREMIX automates coarse-to-fine grid refinement as a means to enhance the convergence properties of the steadystate 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. 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.



Introduction



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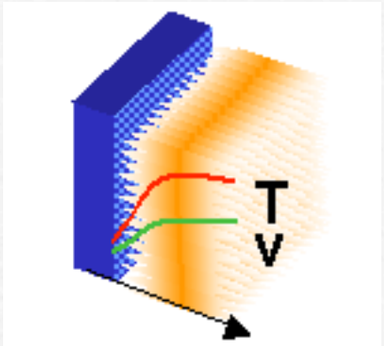
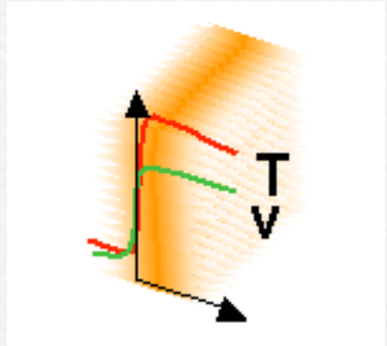
The second flame configuration that we consider is the freely propagating flame. This configuration is used to determine the characteristic flame speed of the gas mixture at specified pressure and inlet temperature. In this case there are no heat losses (by definition) and thus the temperatures should 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.

Premix Application

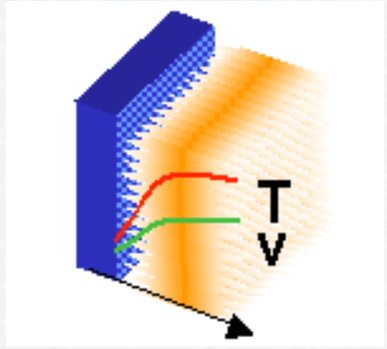
Keyword Syntax and Rules

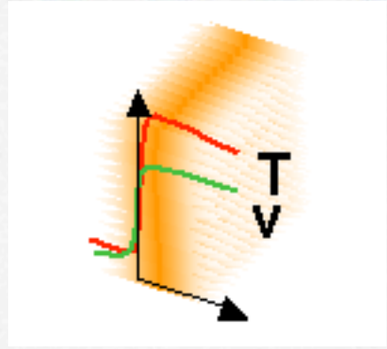


Rule	Description
1	The first character-string in the line must be a keyword; the length of the character-string depends on keyword descriptions.
2	Any further input associated with the keyword can appear anywhere after the keyword, through column 80. The specific starting column is not important, as long as there is at least one space after the keyword.
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 Application 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 GAS-PHASE KINETICS 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 occurence is implemented.
8	A "comment" line is one that has either a period (.), slash (/), or exclamation mark (!) as the first non-blank character. In addition, on any keyword line, any input that follows an exclamation mark is taken as a comment. All input lines, including comments, are printed to the output.
9	The keyword END must be the last input line.



Input File: Keywords



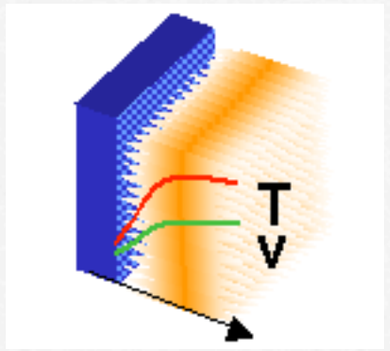


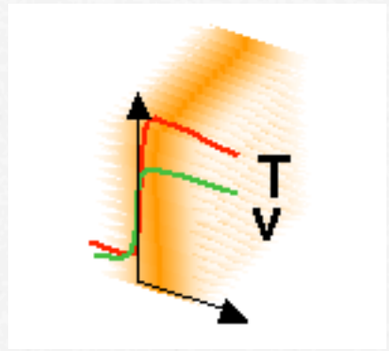
Problem Type Keywords

Keyword	*Description*
BURN	Inclusion of this keyword means that PREMIX will solve a burner-stabilized flame, with specified inlet flow rates. **Default:** none, either BURN or FREE is required. **Restart:** can be changed
FREE	Inclusion of this keyword means that PREMIX will solve freely propagating flame, thereby determining flame speed. **Default:** none, either BURN or FREE is required. **Restart:** can be changed
MOLE	All input (and output) data will be in terms of mole fractions. **Default:** none, either MOLE or MASS is required.
MASS	All input (and output) data will be in terms of mass fractions. **Default:** none, either MOLE or MASS is required.

Keyword	*Description*
TGIV	Inclusion of this keyword means that a solution will be obtained for the species equations with a user-supplied temperature profile. This input only has meaning for burner-stabilized flames. **Default:** none, either TGIV or ENRG must be specified. **Restart:** can be changed
ENRG	Inclusion of this keyword means that a solution will be obtained for the coupled energy-species equations. However, the user must still specify an initial (guessed) temperature profile. This profile is used for solving the temperature-fixed problem, whose solution serves as the first iterate for the solution of the full problem including the energy equation. **Default:** none, either TGIV or ENRG must be specified. **Restart:** can be changed
TINF	Ambient temperature needed in `FUNCTION PRQFUN`. The sample `PRQFUN` computes the gas radiation to/from the surroundings of temperature `TINF` based on the optically-thin limit model. The emissivity of the gas mixture is computed based on an empirical formula. **Unit:** K **Default:** none, optional input. **Restart:** can be changed
QFUN	Enable the user-defined heat-loss function; a sample of `FUNCTION PRQFUN` can be found in the file *premix_user_functions.f*. **Unit:** $\mathrm{ergs/sec/cm^3}$ **Default:** none, optional input. **Restart:** can be changed

Input File: Keywords





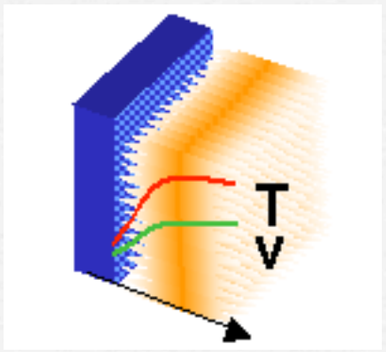
Grid Parameter Keywords

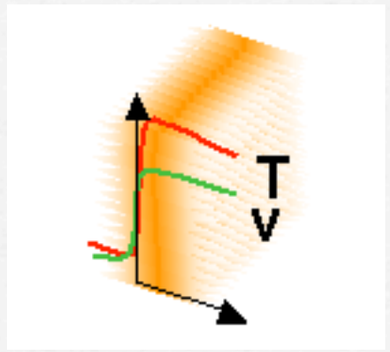
Keyword	*Description*
NPTS	The number of initial mesh points. The inclusion of NPTS will generate an equally spaced mesh of NPTS points between 0 and XEND. The user can also specify an initial nonuniform mesh using the keyword GRID, in which case the NPTS input is not needed. **Example:** NPTS 10 **Default:** 6; unless GRID keywords are included
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. **Example:** GRID 0.0 **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. **Example:** GRAD 0.2 **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. **Example:** CURV 0.7 **Default:** 0.5 **Restart:** can be changed

Keyword	*Description*
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). **Example:** SFLR -1.0E-4 **Default:** - 1.0E-3 **Restart:** can be changed
NTOT	Maximum number of grid points allowed for this job. **Example:** NTOT 200 **Default:** NTOT=maximum grid dimension set by PREMIX driver program **Restart:** cannot be changed on restart.
NADP	Maximum number of grid points that can be added at a time during grid adaptation. **Example:** NADP 2 **Default:** no limit is set **Restart:** cannot be changed on restart.

Input File: Keywords

Grid Parameter Keywords





Keyword	*Description*
XSTR	The beginning of the computational interval. For burner-stabilized flames, this is the burner location. **Example:** XSTR -0.2 **Units:** cm **Default:** 0.0 **Restart:** can be changed to a smaller value.
XCEN	An estimated value for the center of the flame. **Example:** XCEN 3.0 **Units:** cm **Default:** XCEN = 0.35*(XEND-XSTR)
XEND	The end of the computational interval. **Example:** XEND 10.0 **Units:** cm **Default:** XEND is a required input. **Restart:** can be changed to a larger value.
WMIX	An estimated width of the flame zone. **Example:** WMIX 2.0 **Units:** cm **Default:** WMIX = 0.5*(XEND-XSTR)
APRO	Use of the `APRO` keyword(s) allow the user to specify a profile as a function of distance for the stream tube area. The stream-tube area is given relative to the burner area and is therefore dimensionless. Each input provides an pair and the x coordinates must be in ascending order. Example: `APRO 0.1 1.2` assigns a relative area of 1.2 at a position 0.1 cm from the burner surface. **Example:** APRO 0.1 1.2 **Units:** cm , dimensionless **Default:** 1.0 over entire domain **Restart:** can be changed
WDIF	Including this keyword means that windward differencing is to be used on the convective terms. **Default:** WDIF **Restart:** can be changed

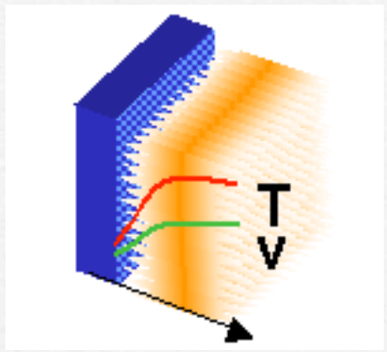
Input File: Keywords

Keyword	*Description*
PRES	The pressure of the flame. **Example:** PRES 0.5 **Units:** atm **Default:** none **Restart:** can be changed.
FLRT	The mass flow rate through the burner (divided by the burner area). For flame problems this is the initial estimate of the mass flow rate. **Example:** FLRT 10. **Units:** $\mathrm{g/cm^2 sec}$ **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 $\mathrm{C_2H_2}$ 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. **Example:** REAC C2H2 0.5 **Units:** either mass or mole fractions, depending on 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 $\mathrm{HO_2}$. Any given species can participate simultaneously as a reactant, intermediate, or product. **Example:** INTM HO2 0.001 **Units:** either mass or mole fractions, depending on MASS or MOLE. **Default:** 0.0

Flame Definition Keywords

PROD	Estimated mass or mole fractions of the flame products. For example, `PROD H2O 0.5` estimates the fraction of $\mathrm{H_2O}$ 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. If no `PROD` is given, `PROD` for each species will be its fraction of the mixture’s equilibrium composition. **Example:** PROD H2O 0.5 **Units:** either mass or mole fractions, depending in MASS or MOLE. **Default:** 0.0; if no PROD entries, then an equilibrium calculation is made.
PRMN	Minimum mass or mole fraction value applied to the estimated values of the flame products, when the (default) equilibrium is used to determine product estimates. Ignored in the case that `PROD` keywords are present. **Example:** PRMN 1.0E-10 **Units:** either mass or mole fractions, depending in MASS or MOLE. **Default:** 0.0
XIMN	Minimum mass or mole fraction value applied to intermediate species estimates, when the (default) equilibrium is used to determine product estimates. Ignored in the case that `PROD` keywords are present. In this case, the intermediate species fraction is initialized to be the average of its `PROD` and `REAC` values; or `XIMN`, if `XIMN` is greater than this average. **Example:** XIMN 1.0E-10 **Units:** either mass or 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. Example: `TEMP 0.1 1000` assigns a temperature of 1000 K at a position 0.1 cm from the burner surface. **Example:** TEMP 0.0 300. **Units:** cm, K **Default:** required input, except on a restart. **Restart:** can be changed, provided USTG is included.

Premix



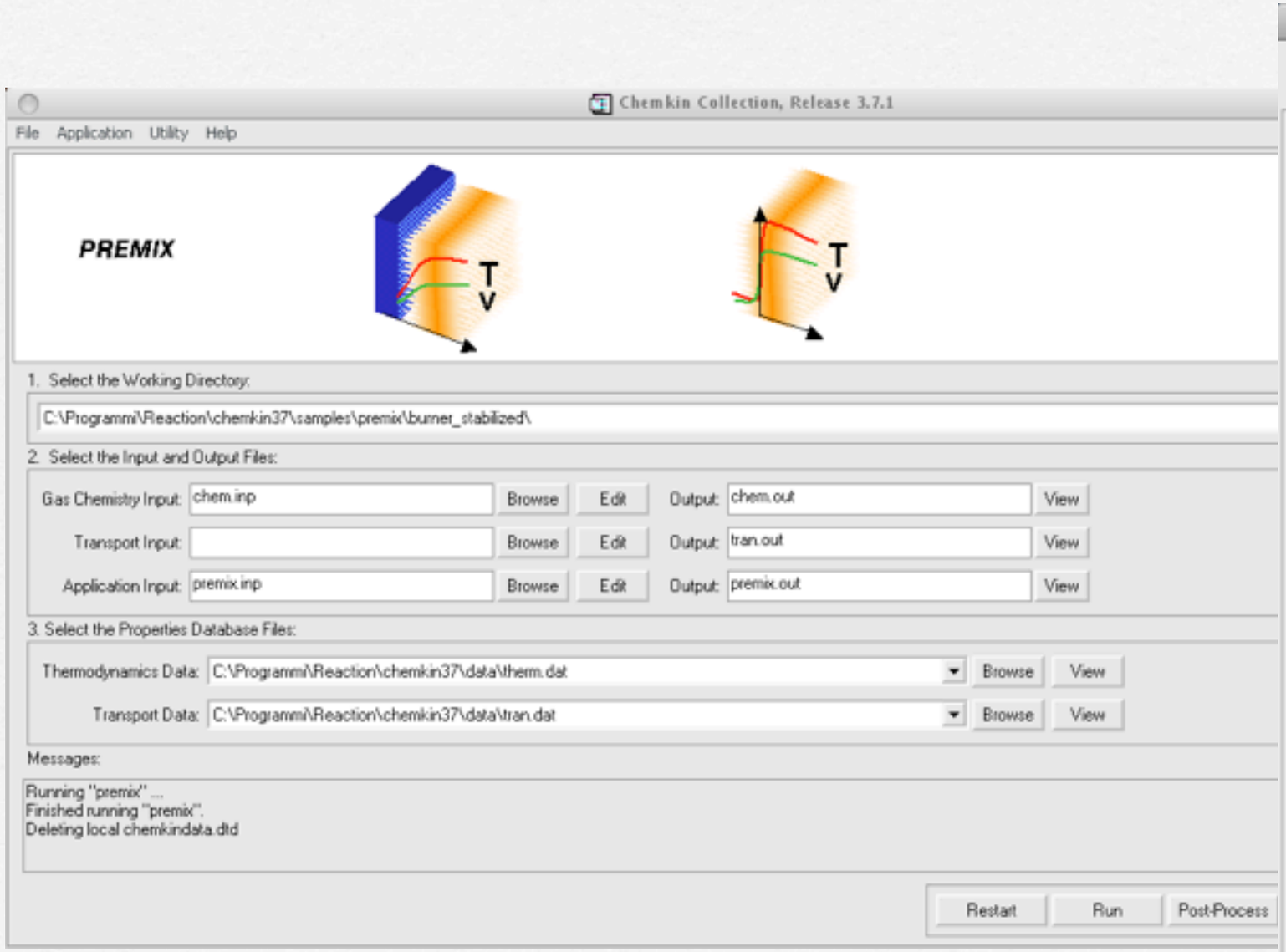
Example

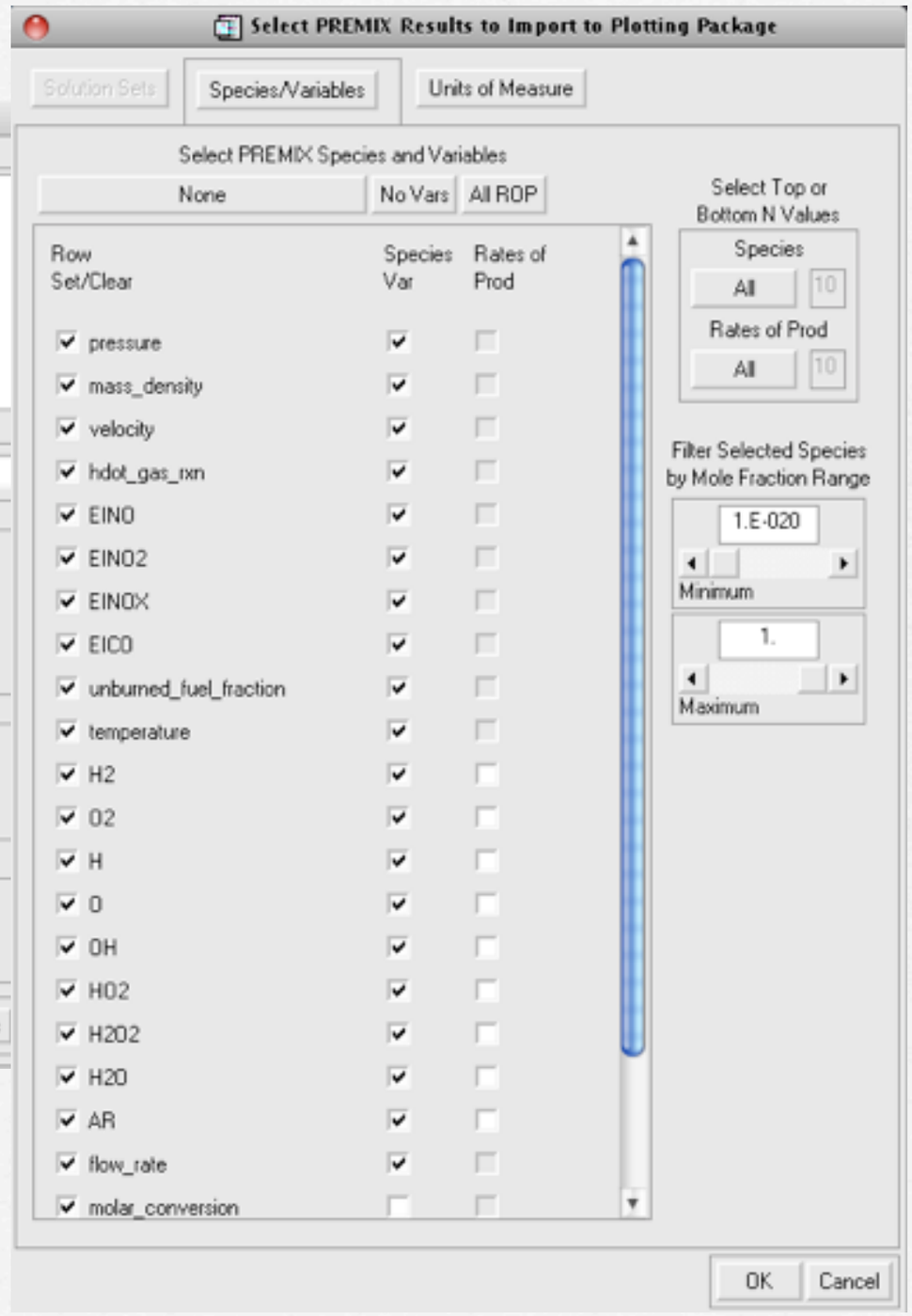
Burner-Stabilized Hydrogen-Oxygen Flame

Input File

```
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
```

Graphical Post-process

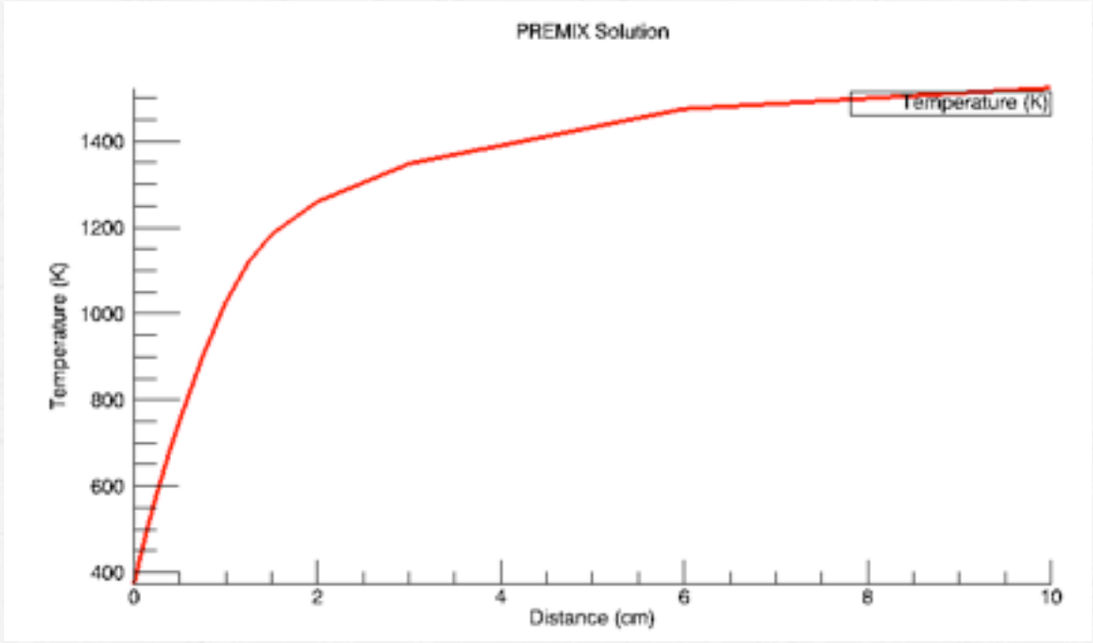




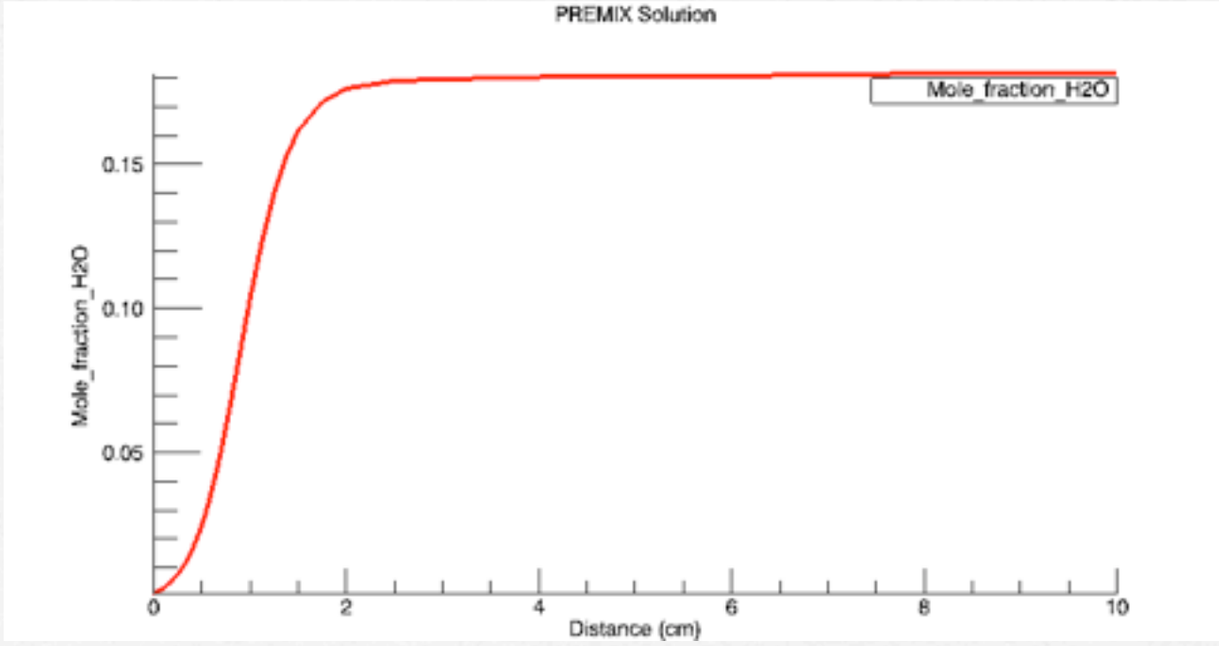
Results....

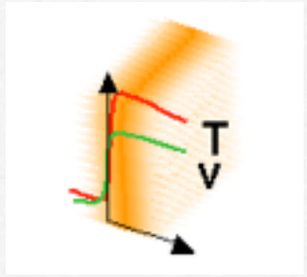
Premix

Temperature profile versus axial distance



H_2O Mole fraction profile versus axial distance





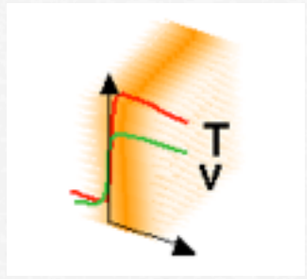
Example
Freely Propagating Stoichiometric Methane-Air Flame

Input File

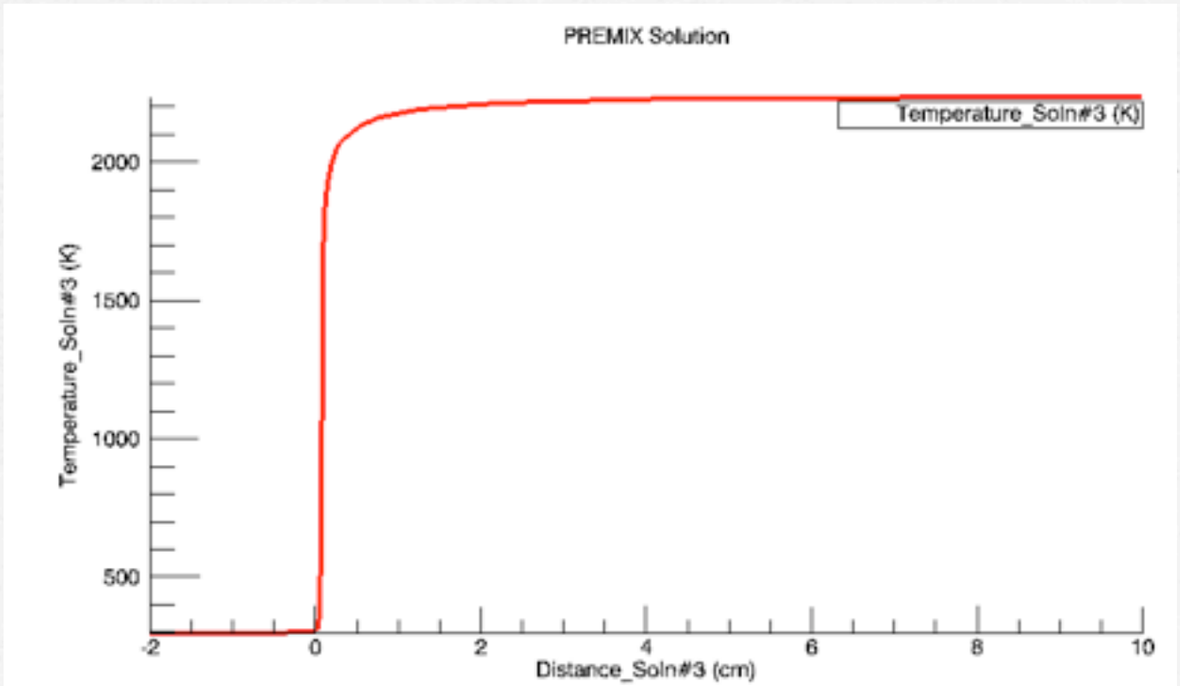
```
KEYWORD INPUT

/  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
NADP    50
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
```

Results....

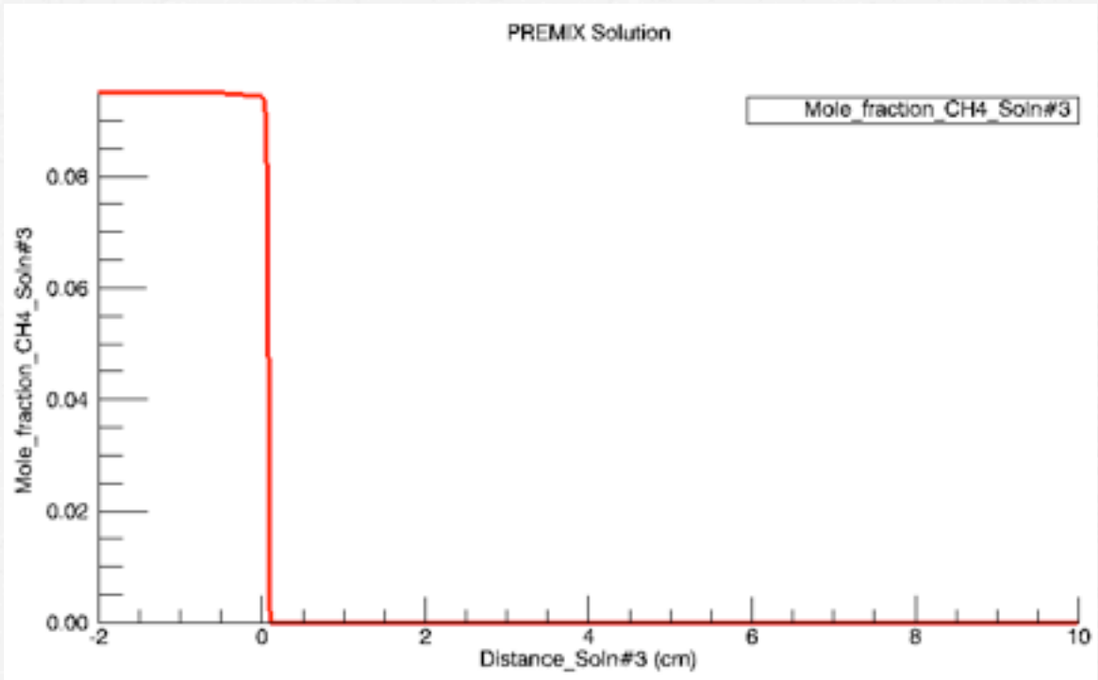
Premix



Temperature profile versus axial distance



CH_4 Mole fraction profile versus axial distance



References

1. http://www.reactiondesign.com/lobby/open/index.html (sito di riferimento CHEMKIN)
2. http://maeweb.ucsd.edu/~combustion/cermech/ (SANDIEGO mechanism)
3. http://www.me.berkeley.edu/gri-mech/ (GRI mechanism)
4. http://creckmodeling.chem.polimi.it/kinetic.html (Ranzi mechanism)