Computer Lab & Introduction to Chemkin

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Contents of the chapter

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- Example 1: Chemical and phase equilibrium – propane/air equilibrium
- Exercise: CO2-CO/O2 equilibrium
- Example 2: constant-volume methane combustion

CHEMKIN is a proprietary software tool for solving complex chemical kinetics problems. It is used worldwide in the combustion, chemical processing, microelectronics and automotive industries, and also in atmospheric science.

Also allows coupled simulation with CFD and chemical kinetics.

Very powerful post-processing tool boxes.

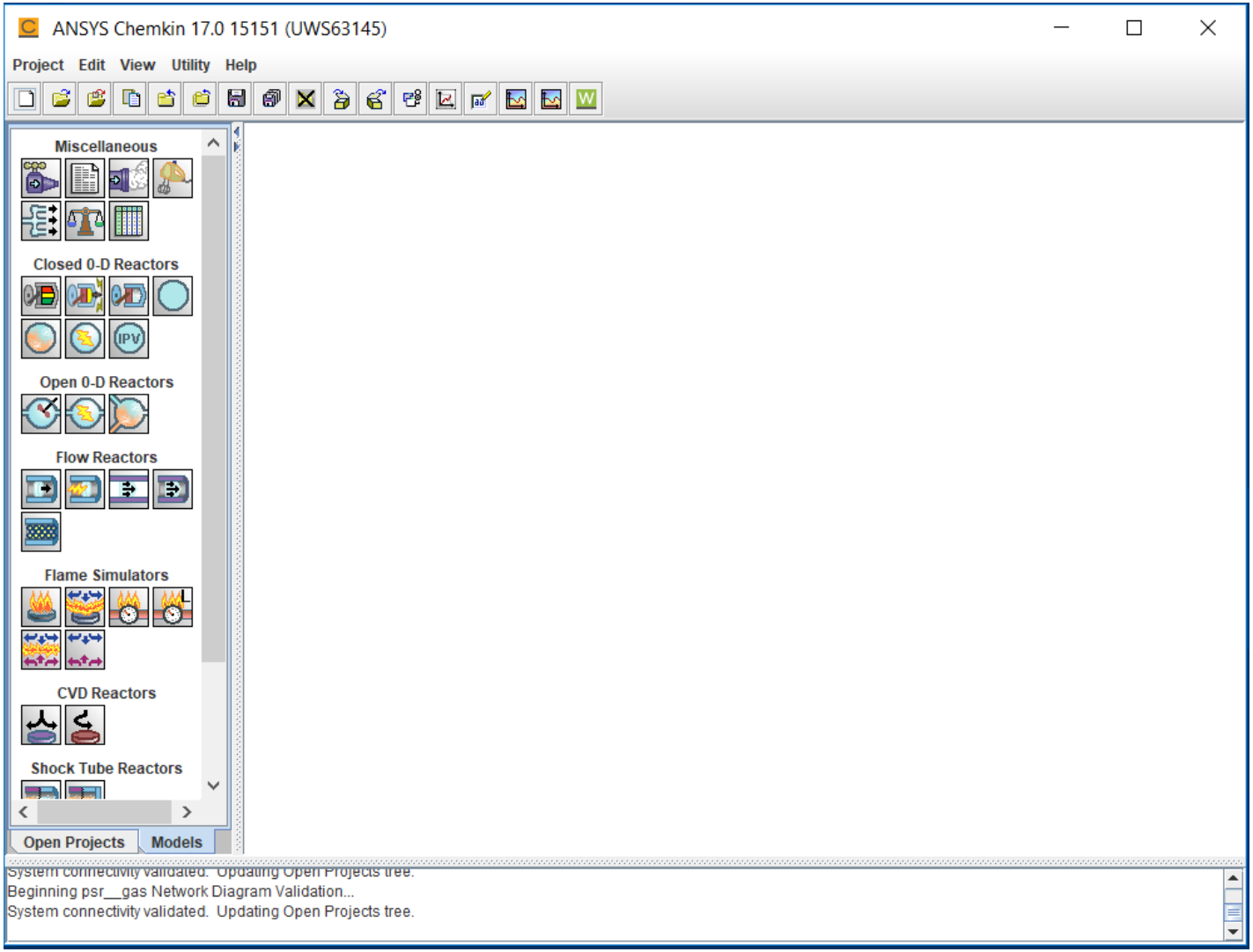
The new features of Chemkin 4 and later versions

- JAVA based user interface
- The operation interface is no longer based on the calculation modules. Instead, it is based on reactor models
- Brand new post-process functions
- Graphic project view
- New parametric study functions
- Particle tracing modules
- Part of Ansys family

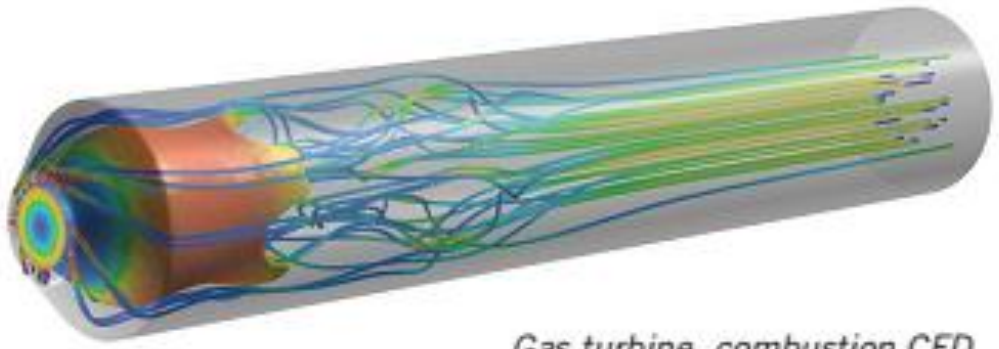
Chemkin 17.0

New icon

Interface



- Detailed chemical kinetic mechanism coupled with CFD
- Now available by ANSYS Fluent



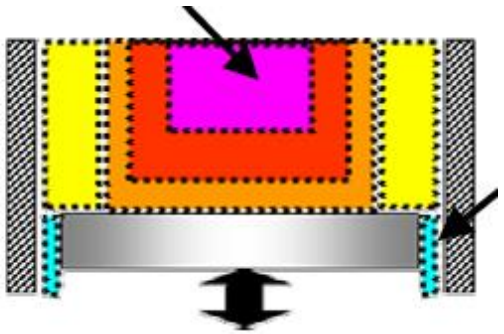
Gas turbine combustion CFD using FLUENT® and CHEMKIN-CFD

Example applications

Internal combustion engine multi-zone models

- To understand the CO and HC formation at different locations in the combustion chamber
- To understand how the in-cylinder conditions can affect firing
- To accurately simulate pollutants formation

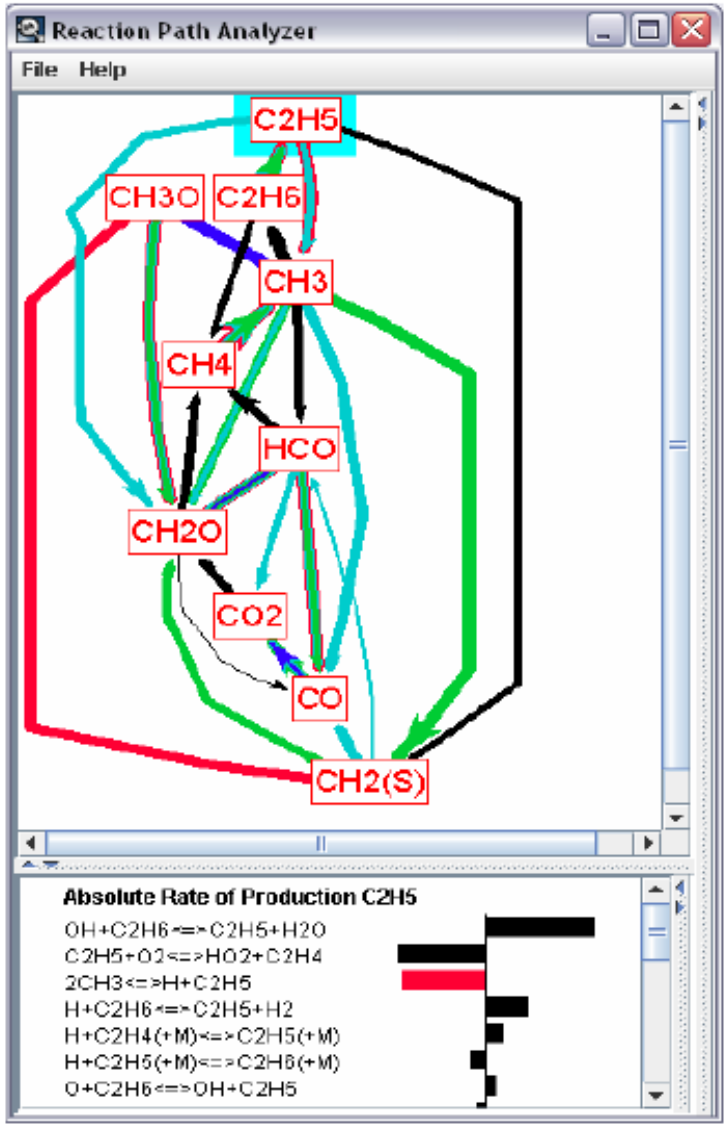
Central high temperature zone, firing



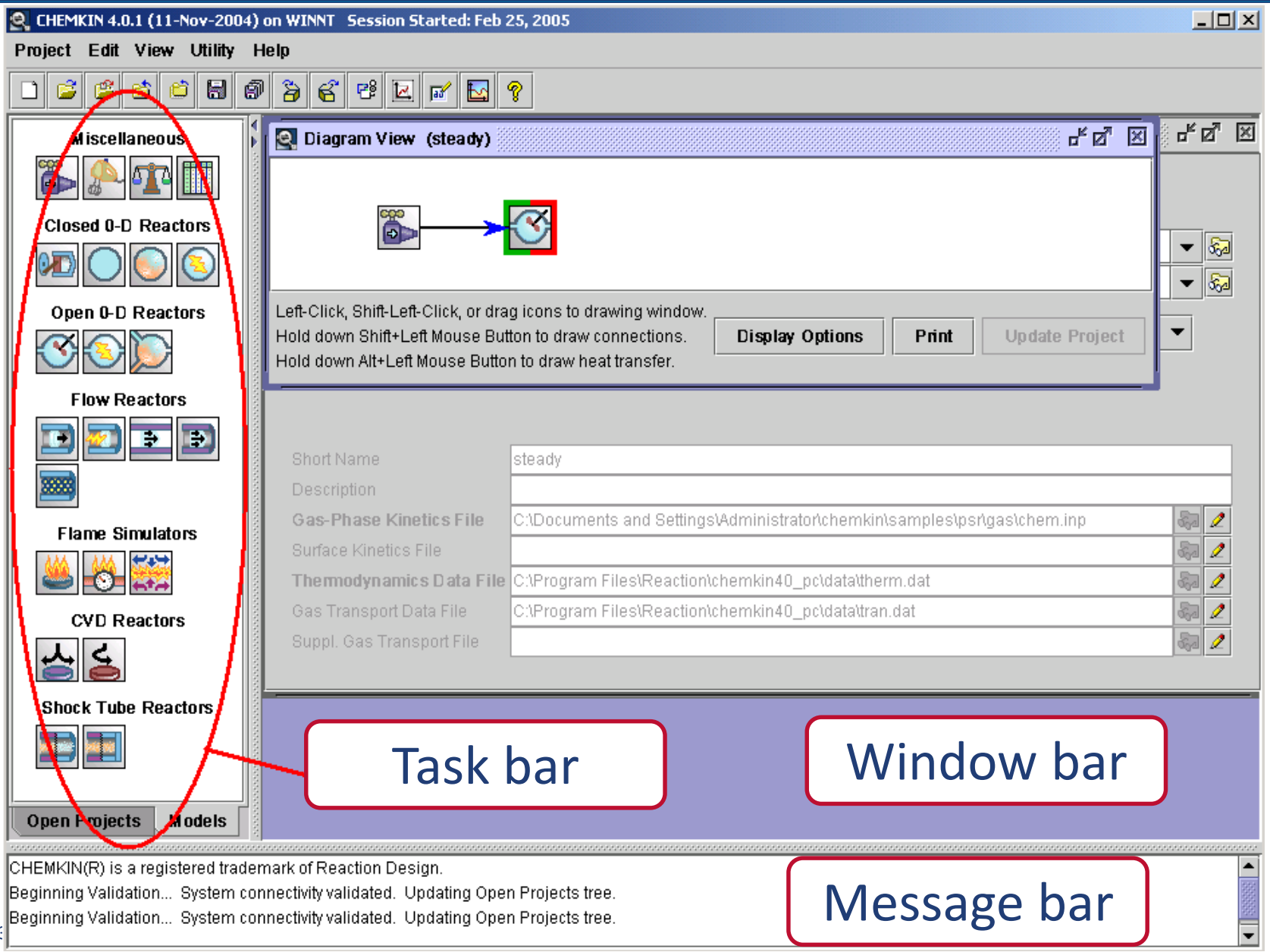
Crevice low temperature zone, CO and ash formation

Reaction path analyser

- A useful tool to simplify reaction mechanism
- Identify main reactions and species
- Check potential chemical reaction mechanisms
- Can be used together with sensitivity analysis
- Available for all the reactors

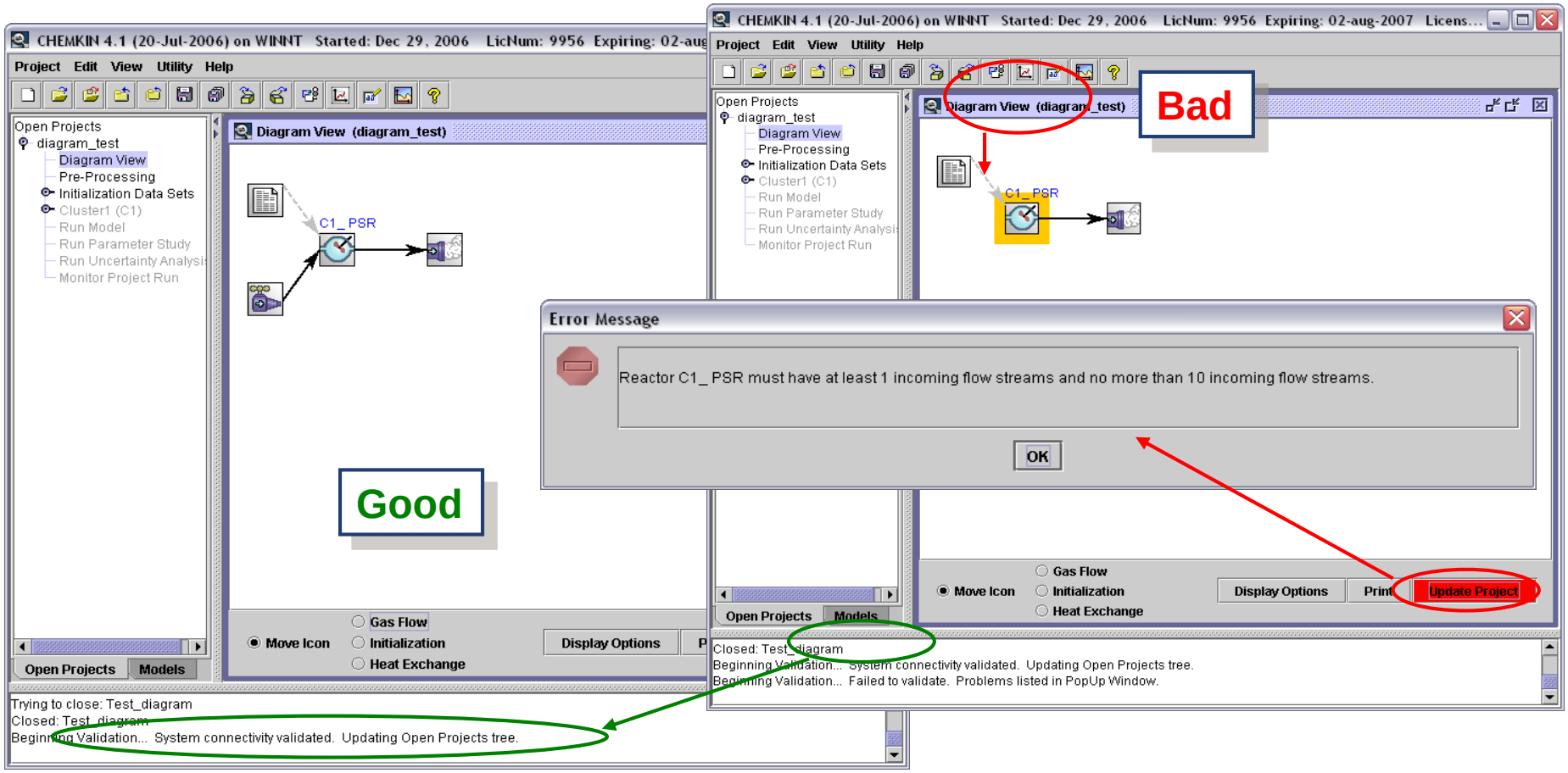


Chemkin user interface

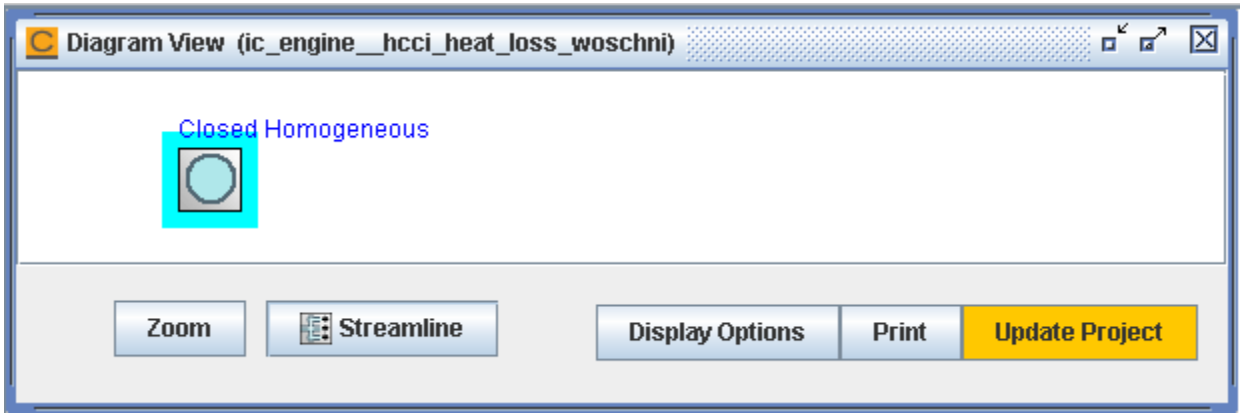


Chemkin user interface

Note: a reactor needs an input and an output

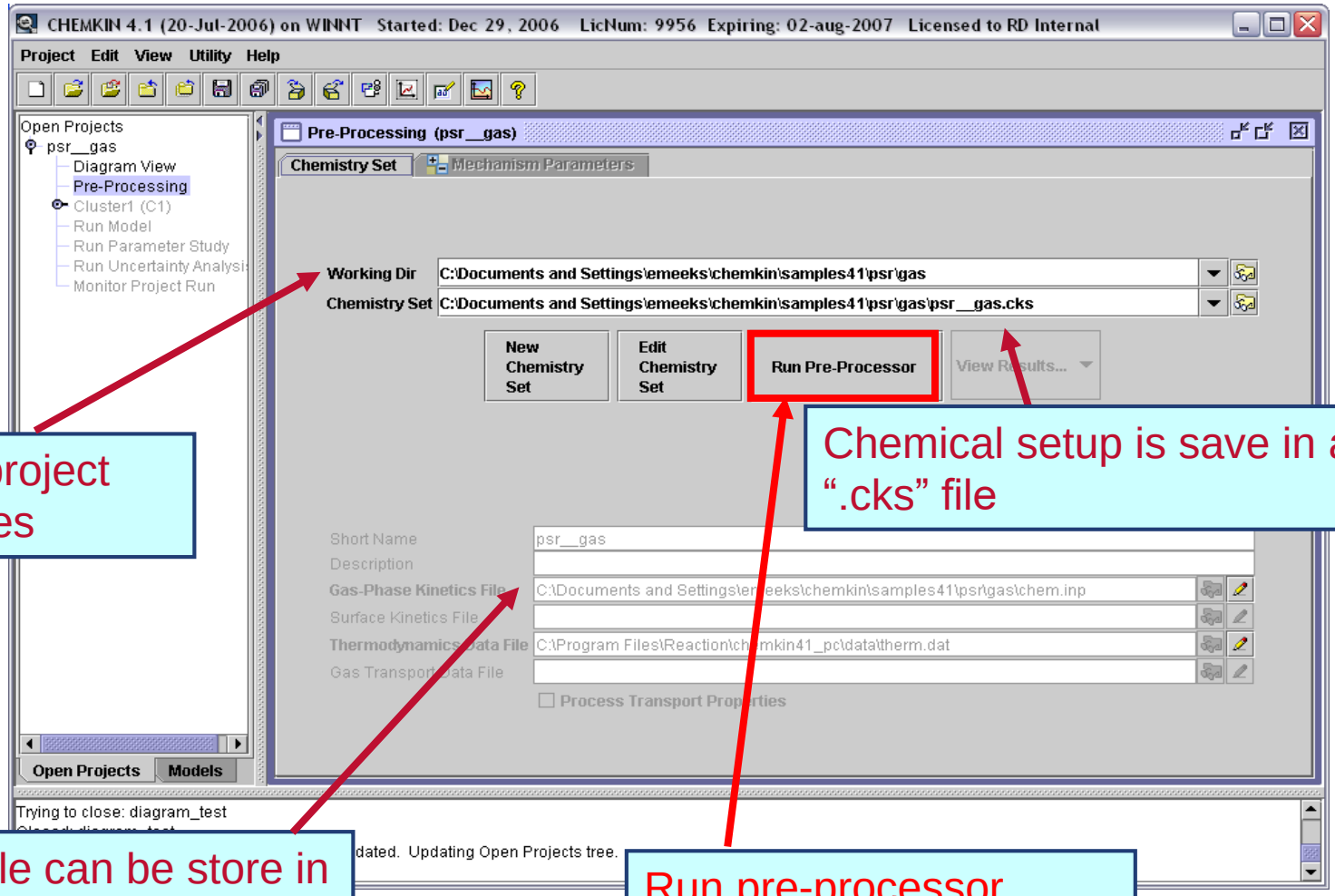


Zero-D IC engine model



Zero-D constant volume reactor model

Pre-processing



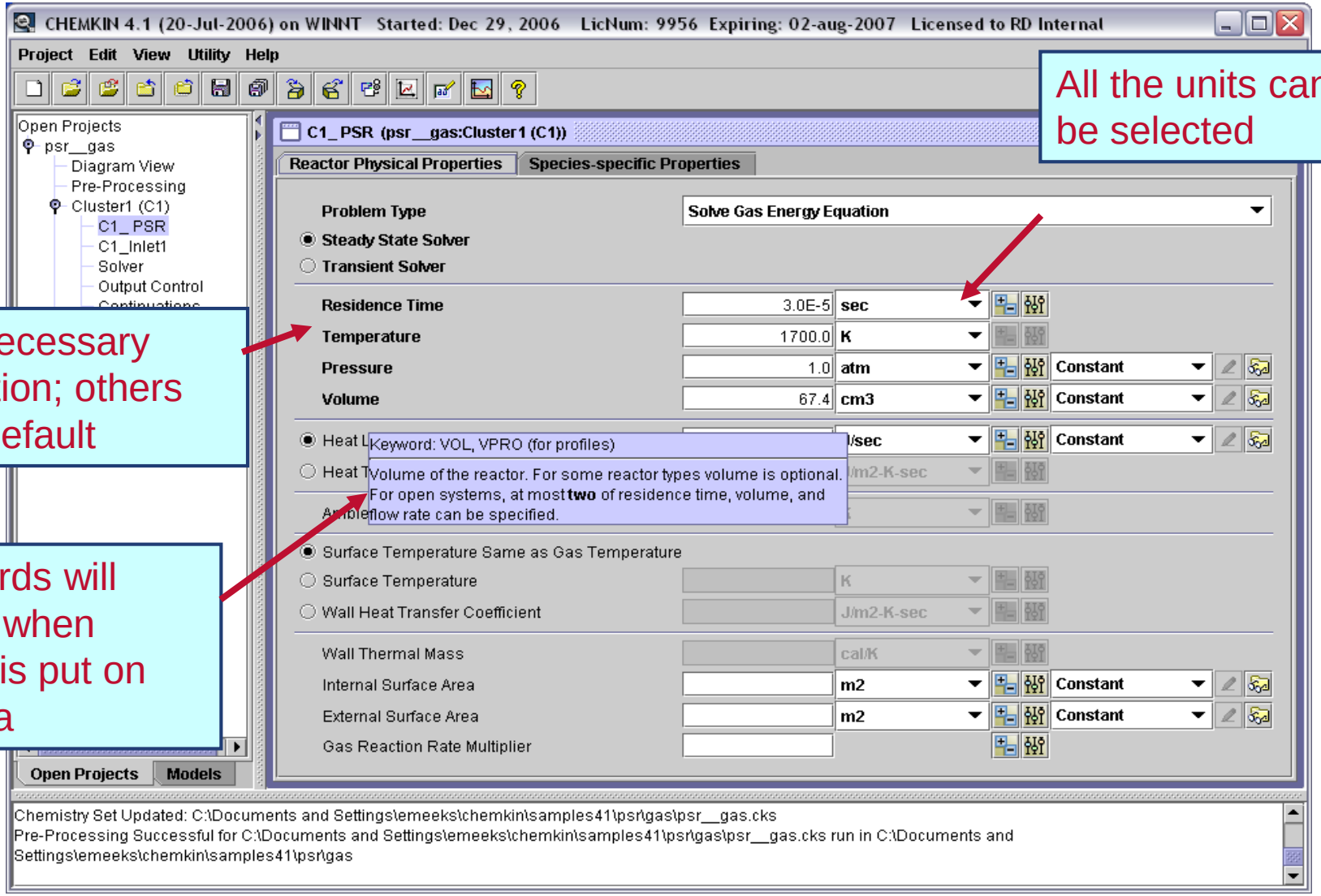
Location of a project input/output files

Chemical setup is save in a ".cks" file

Kinetics file can be store in a different location

Run pre-processor before you move on.

Reaction setup

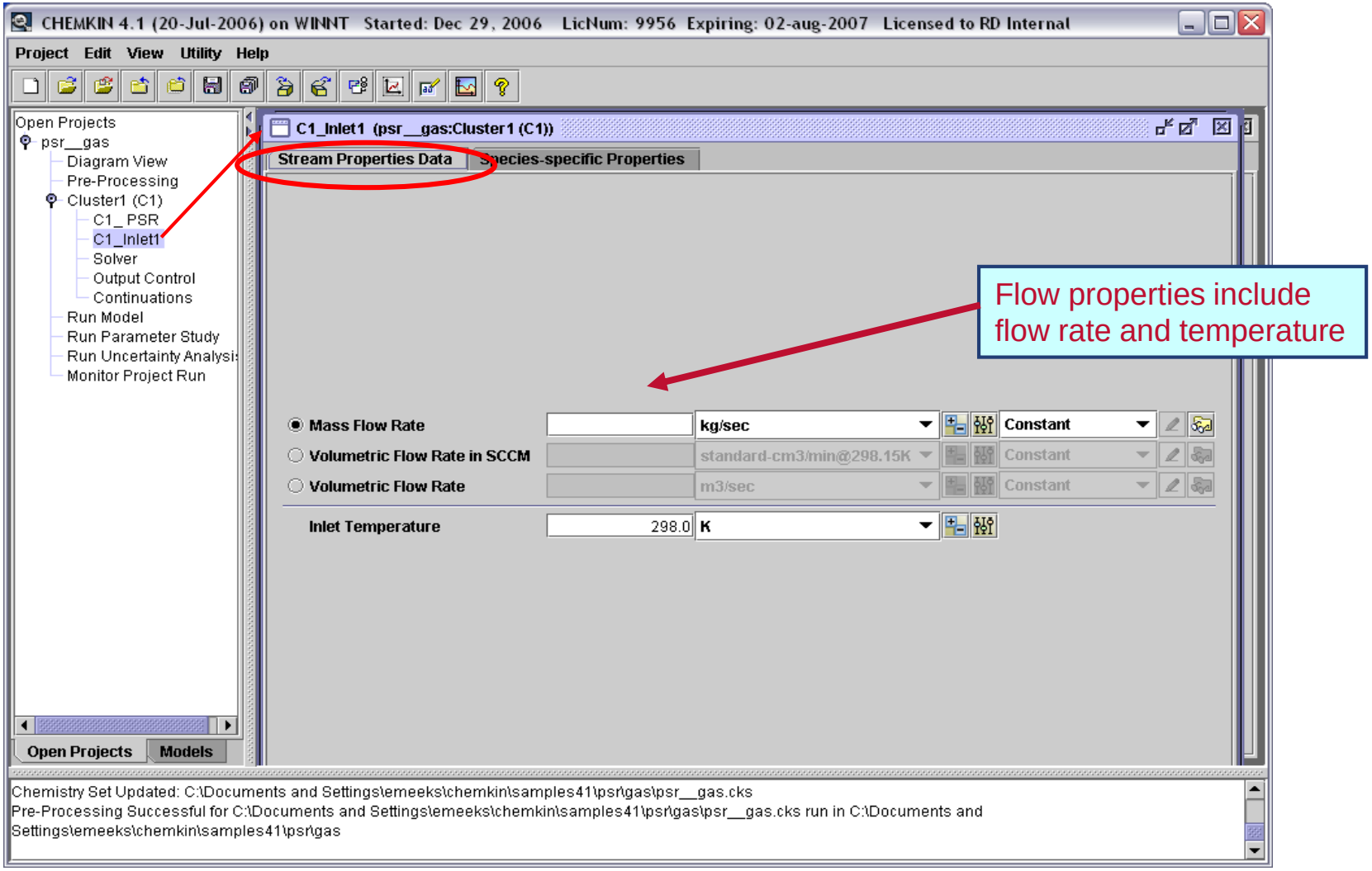


All the units can be selected

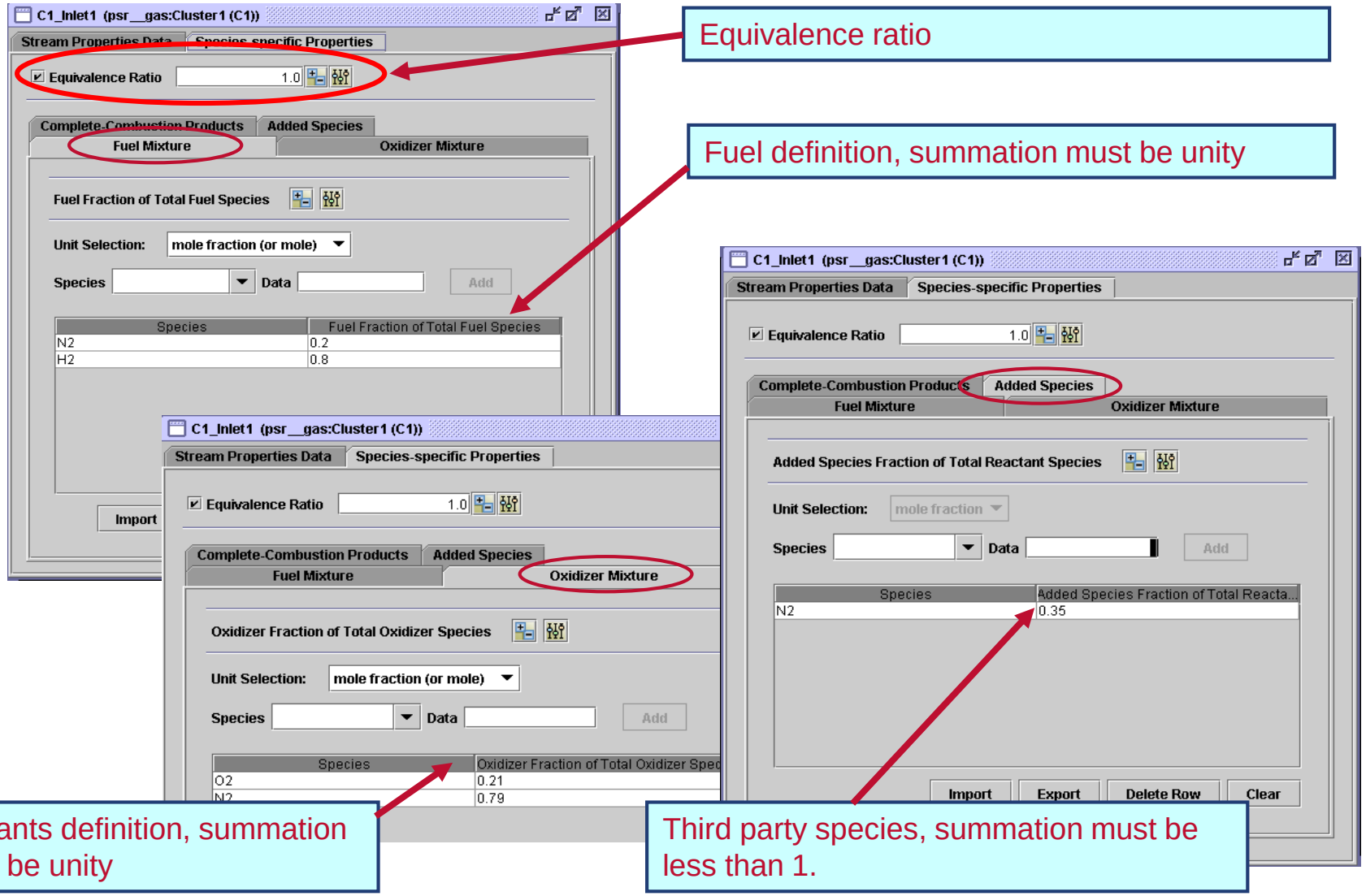
Setup necessary information; others will be default

Key words will appear when mouse is put on the area

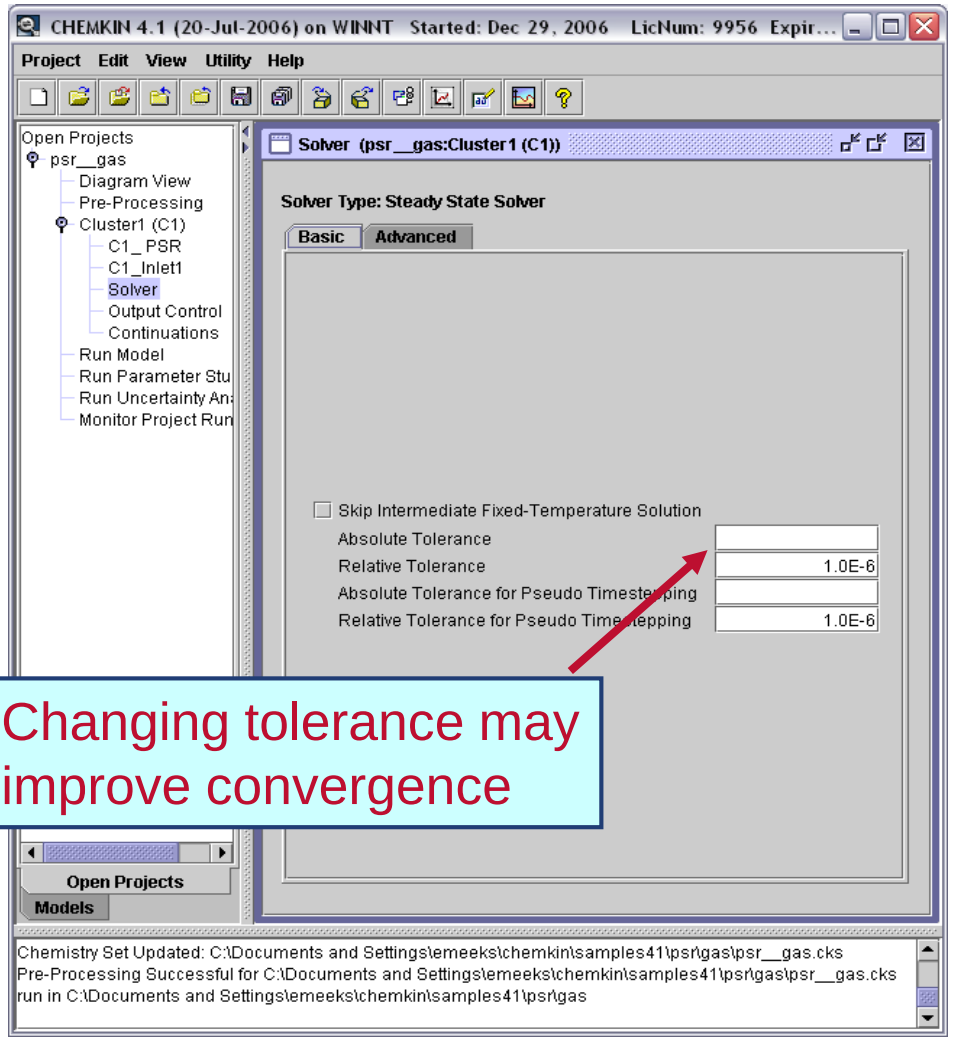
Flow parameters and reactants setting



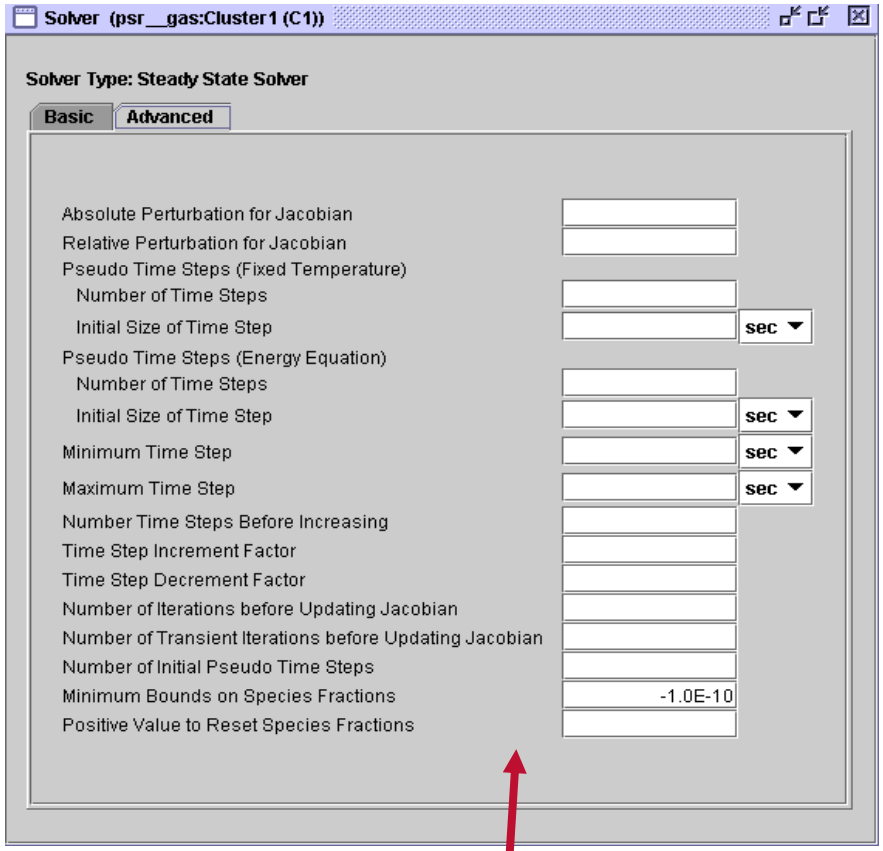
Oxidants/reactants setup



Solver setup: usually leave as default

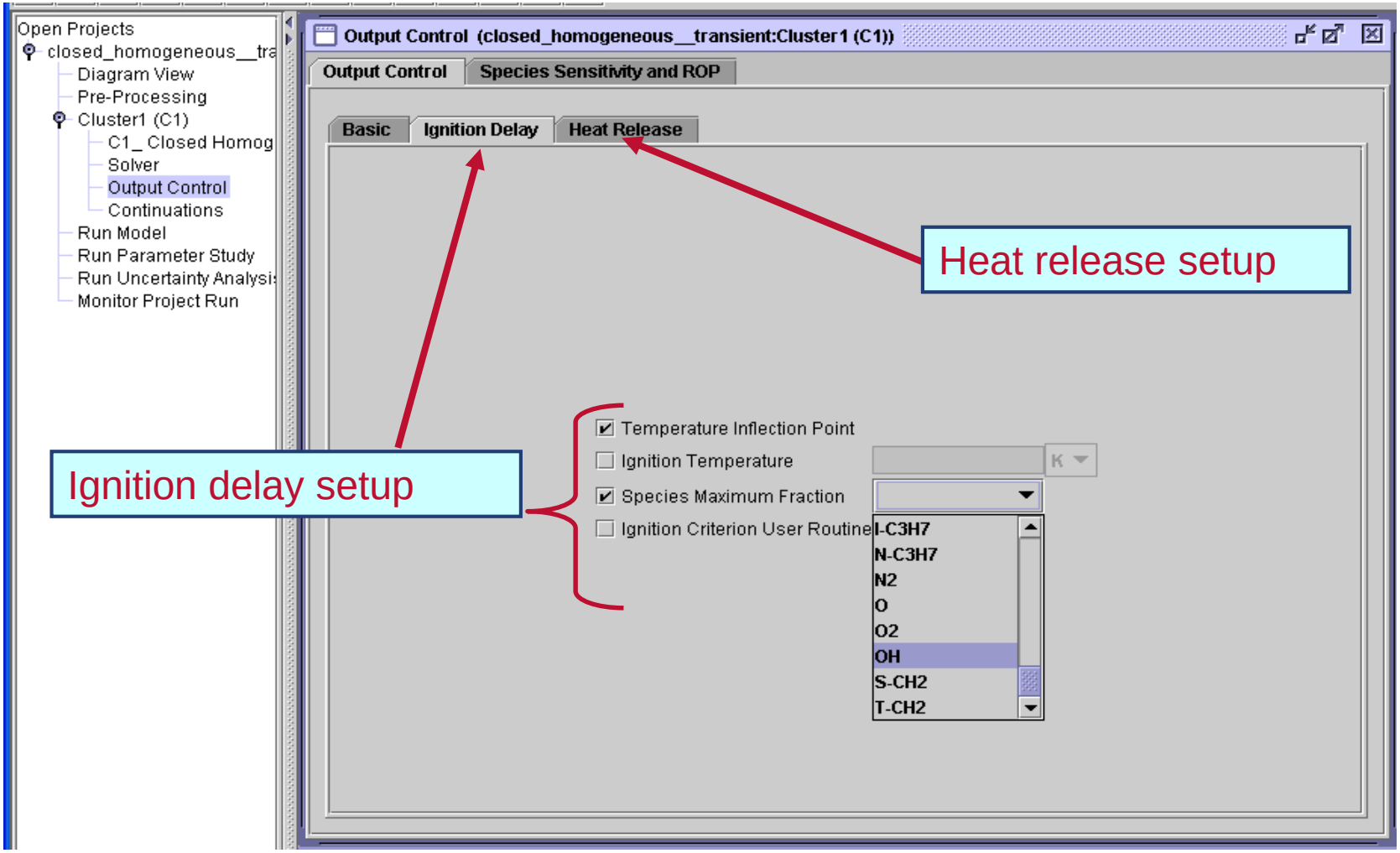


Changing tolerance may improve convergence

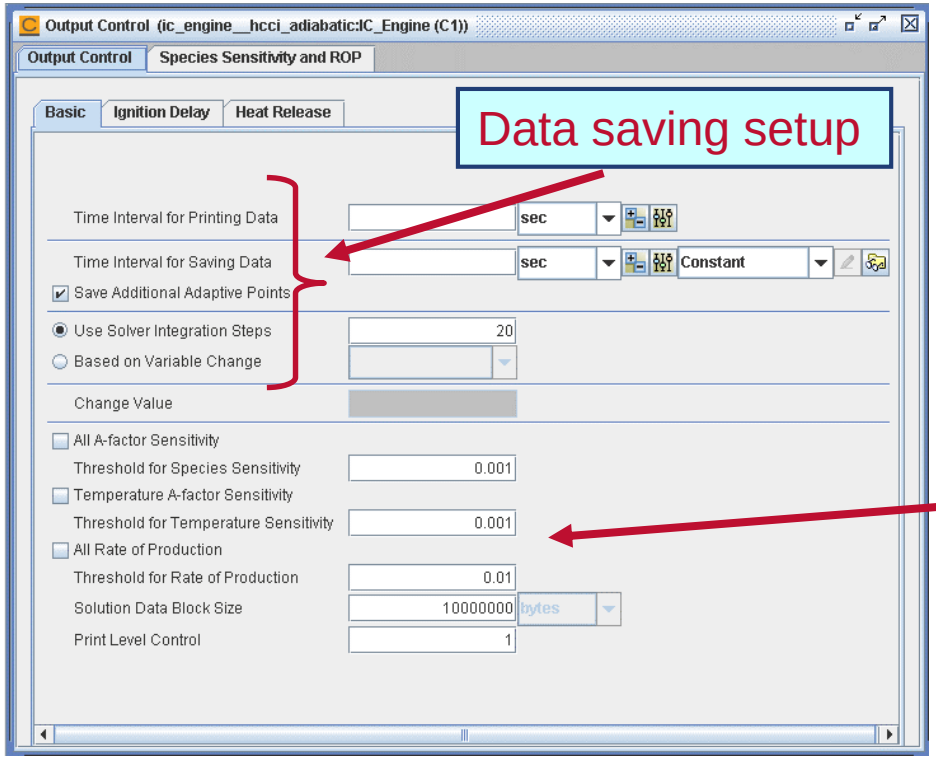


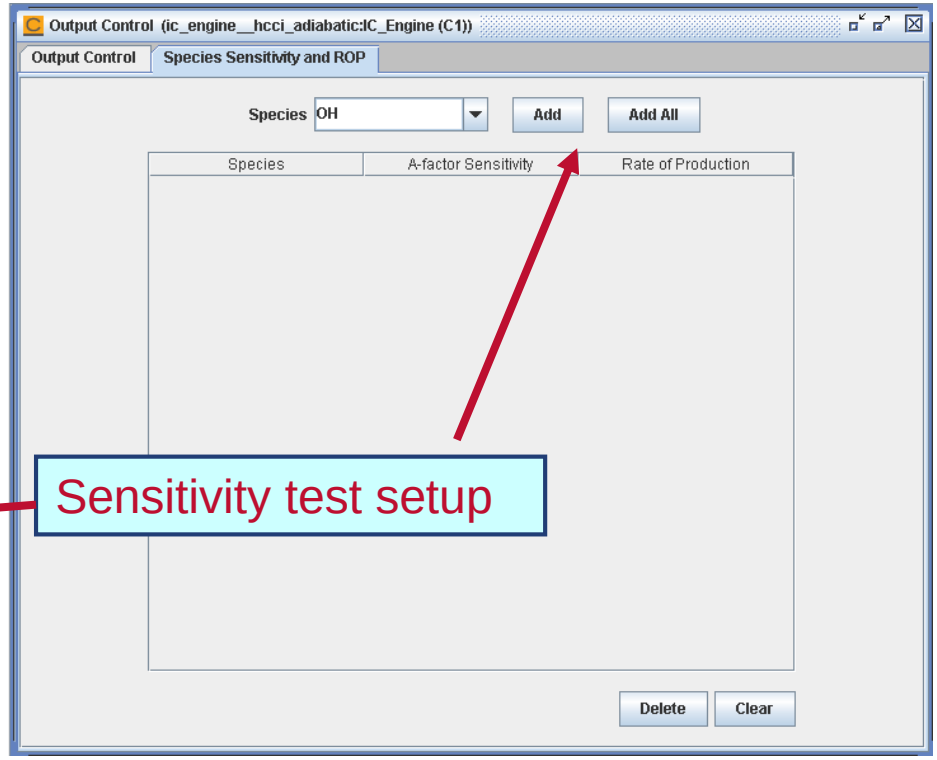
Details can be found in manual

Output control setup



Output setup



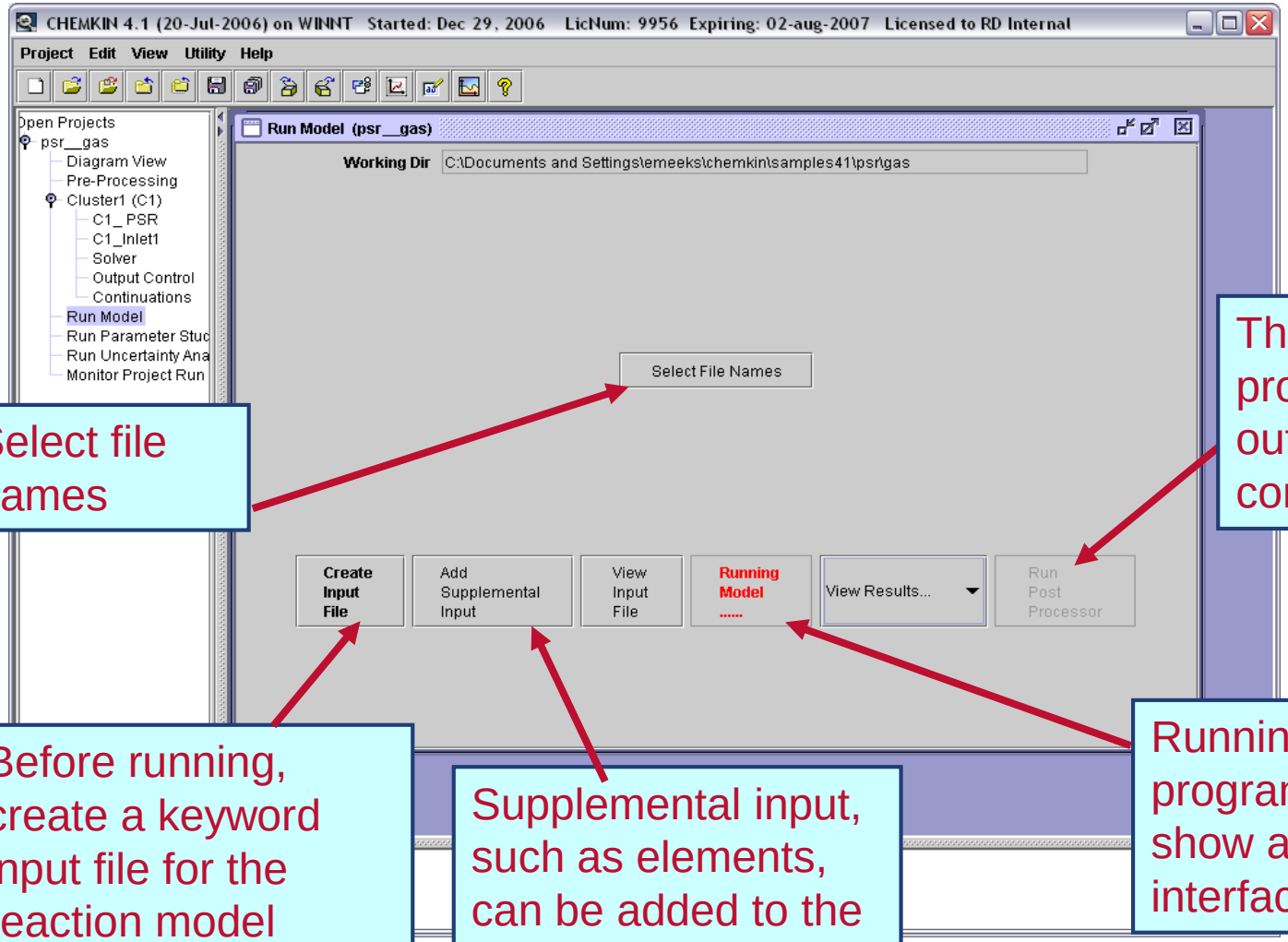


Sensitivity： How much the results rely on a parameter Km

$$E_{i,m} = \frac{\partial C_i}{\partial K_m}$$

$$K_m = A$$

Running setup



Select file names

The post-process programme will pop out when running completed.

Before running, create a keyword input file for the reaction model

Supplemental input, such as elements, can be added to the input files

Running programme; also show a monitoring interface

Chemkin Chemical setup

Chemical is setup by 2 or more files

- Thermodynamic data file (necessary)
- Gas phase kinetics file (necessary)
- Gas transport data file (optional, sometimes necessary)
- Surface kinetics data file (optional)

Thermodynamic data file

- the data is the constants in the polynomials that calculate substances' heat capacities, enthalpies and entropies

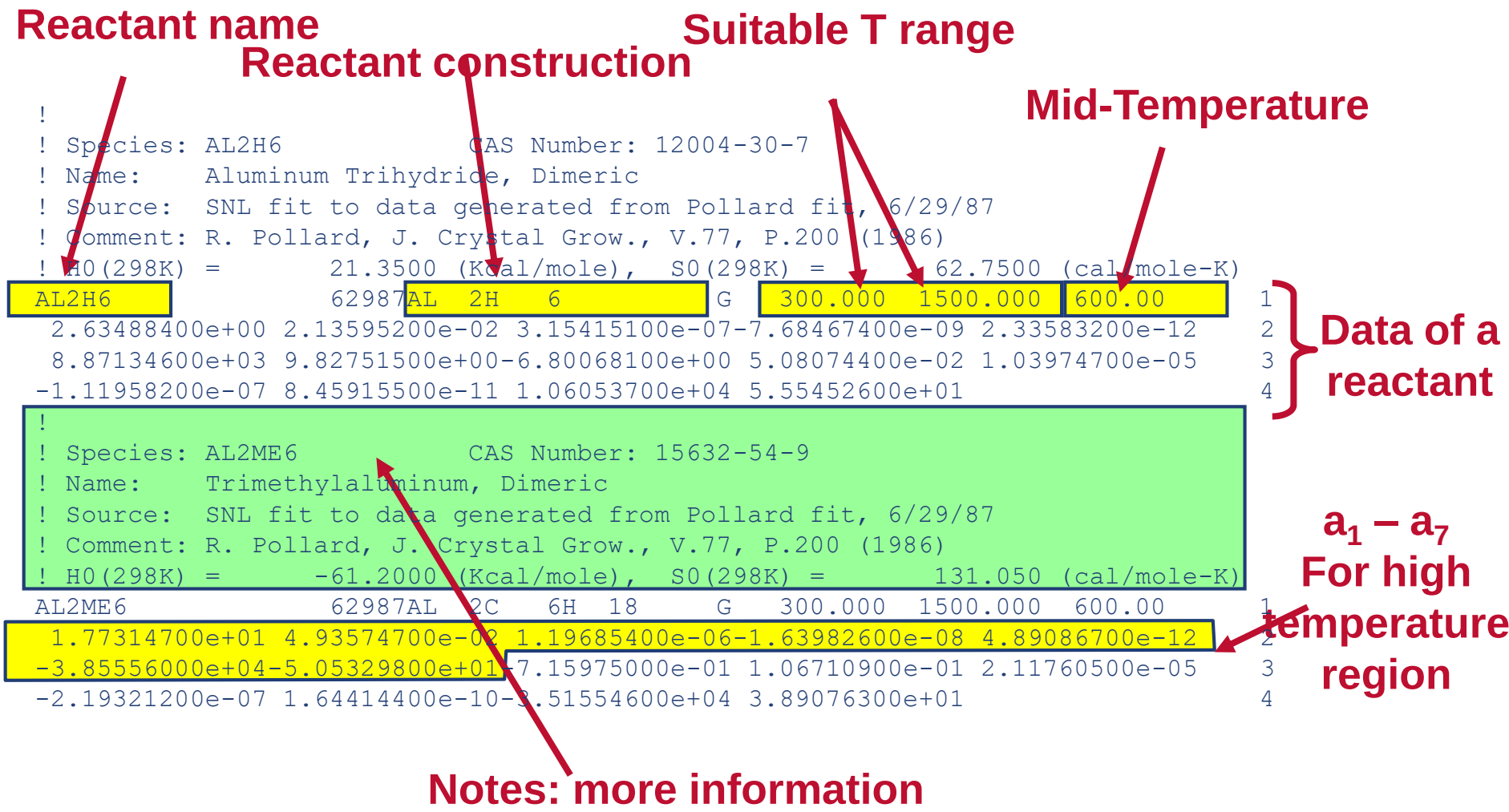
$$\frac{c_p^0}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\frac{H^0}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T}$$

$$\frac{S^0}{R} = a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + \frac{a_7}{T}$$

- Fixed format following NASA format, flexible to include new substances
- Include all the elements in the reactions
- In the reaction mechanism files, users can include more thermodynamic data

Example of thermodynamics data




```
!
! Species: AL2H6              CAS Number: 12004-30-7
! Name:    Aluminum Trihydride, Dimeric
! Source:  SNL fit to data generated from Pollard fit, 6/29/87
! Comment: R. Pollard, J. Crystal Grow., V.77, P.200 (1986)
! H0(298K) =       21.3500 (Kcal/mole),  S0(298K) =       62.7500 (cal/mole-K)
AL2H6            62987AL  2H   6          G   300.000  1500.000  600.00      1
 2.63488400e+00 2.13595200e-02 3.15415100e-07-7.68467400e-09 2.33583200e-12    2
 8.87134600e+03 9.82751500e+00-6.80068100e+00 5.08074400e-02 1.03974700e-05    3
-1.11958200e-07 8.45915500e-11 1.06053700e+04 5.55452600e+01                  4
!
! Species: AL2ME6             CAS Number: 15632-54-9
! Name:    Trimethylaluminum, Dimeric
! Source:  SNL fit to data generated from Pollard fit, 6/29/87
! Comment: R. Pollard, J. Crystal Grow., V.77, P.200 (1986)
! H0(298K) =      -61.2000 (Kcal/mole),  S0(298K) =      131.050 (cal/mole-K)
AL2ME6           62987AL  2C   6H  18     G   300.000  1500.000  600.00      1
 1.77314700e+01 4.93574700e-02 1.19685400e-06-1.63982600e-08 4.89086700e-12    2
-3.85556000e+04-5.05329800e+01 7.15975000e-01 1.06710900e-01 2.11760500e-05    3
-2.19321200e-07 1.64414400e-10-3.51554600e+04 3.89076300e+01                  4
```

Gas phase kinetics example

```
ELEMENTS H   O   N  END
SPECIES  H2 H O2 O OH HO2 H2O2 H2O N N2 NO END
REACTIONS
   H2+O2=2OH                          0.170E+14  0.00  47780
   OH+H2=H2O+H                        0.117E+10  1.30   3626 ! D-L&W
   O+OH=O2+H                          0.400E+15 -0.50      0 ! JAM 1986
   O+H2=OH+H                          0.506E+05  2.67   6290 ! KLEMM,ET AL
   H+O2+M=HO2+M                       0.361E+18 -0.72      0 ! DIXON-LEWIS
       H2O/18.6/  H2/2.86/  N2/1.26/
   OH+HO2=H2O+O2                      0.750E+13  0.00      0 ! D-L
   H+HO2=2OH                          0.140E+15  0.00   1073 ! D-L
   O+HO2=O2+OH                        0.140E+14  0.00   1073 ! D-L
   2OH=O+H2O                          0.600E+09  1.30      0 ! COHEN-WEST.
   ……
END
```

Reactants must be included in the thermodynamic data

Reactions

Parameters: A, B, E

- **H_2/air flame**
- **3 elements**
- **11 reactants**
- **23 reactions**

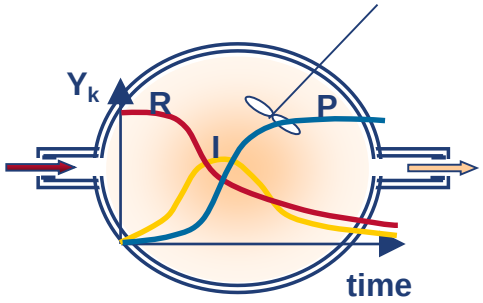
Reaction constants

Following Arrhenius formula

- Corrected Arrhenius formula we have 3 parameters

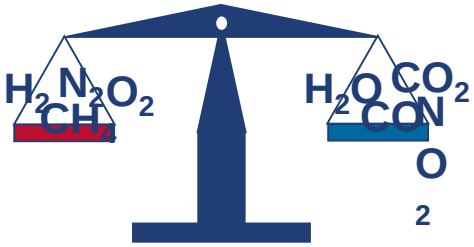
$$k_{fi} = A_i T^{B_i} \exp\left(\frac{-E_i}{R_c T}\right)$$

- E has a unit of Calories/mole (default)
  - You can select another unit for all or one of the reactions
  - kcal/mole, Joule/mole, Kelvin, or eV

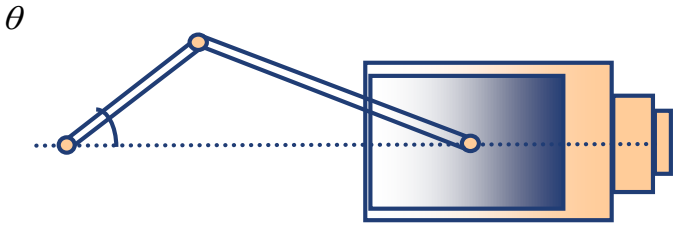


Perfect stirred reactor PSR

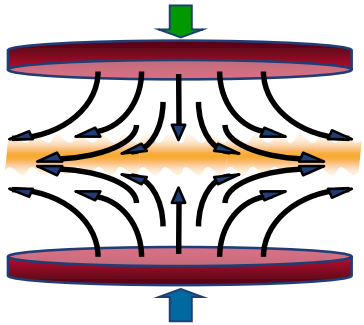
Plug Flow Reactor



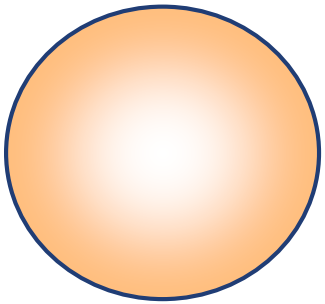
Chemical and phase equilibrium calculations



Internal combustion engines

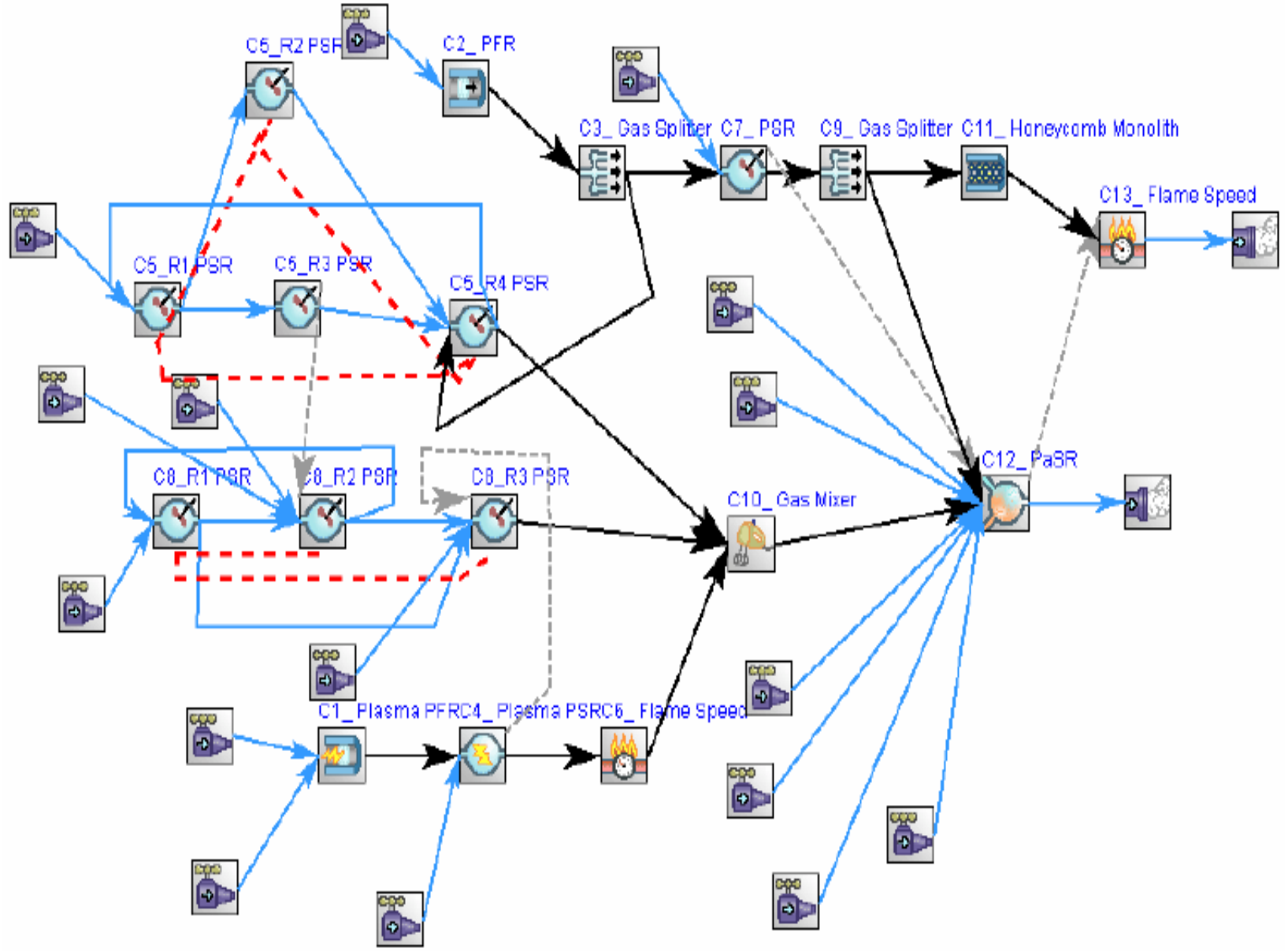


Flame simulators

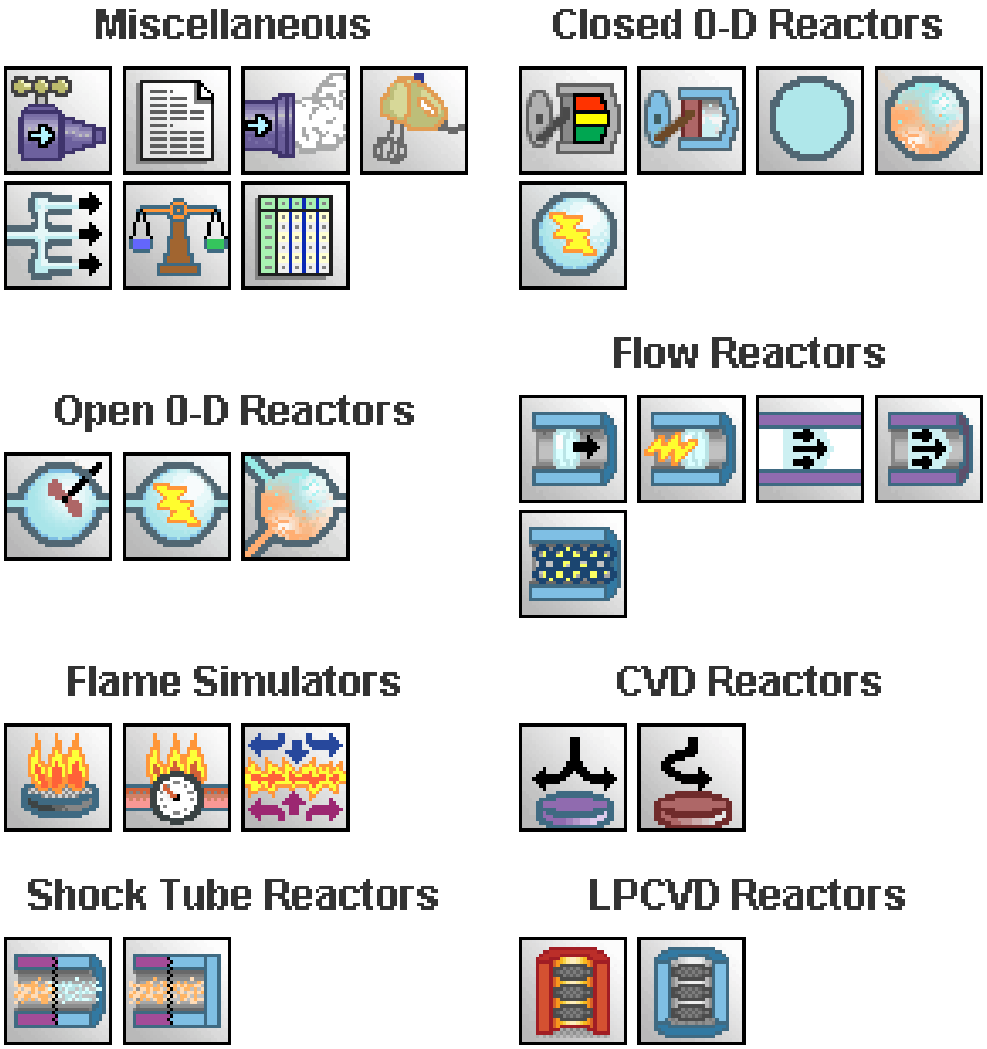


Closed homogeneous batch reactor

Chemkin model example

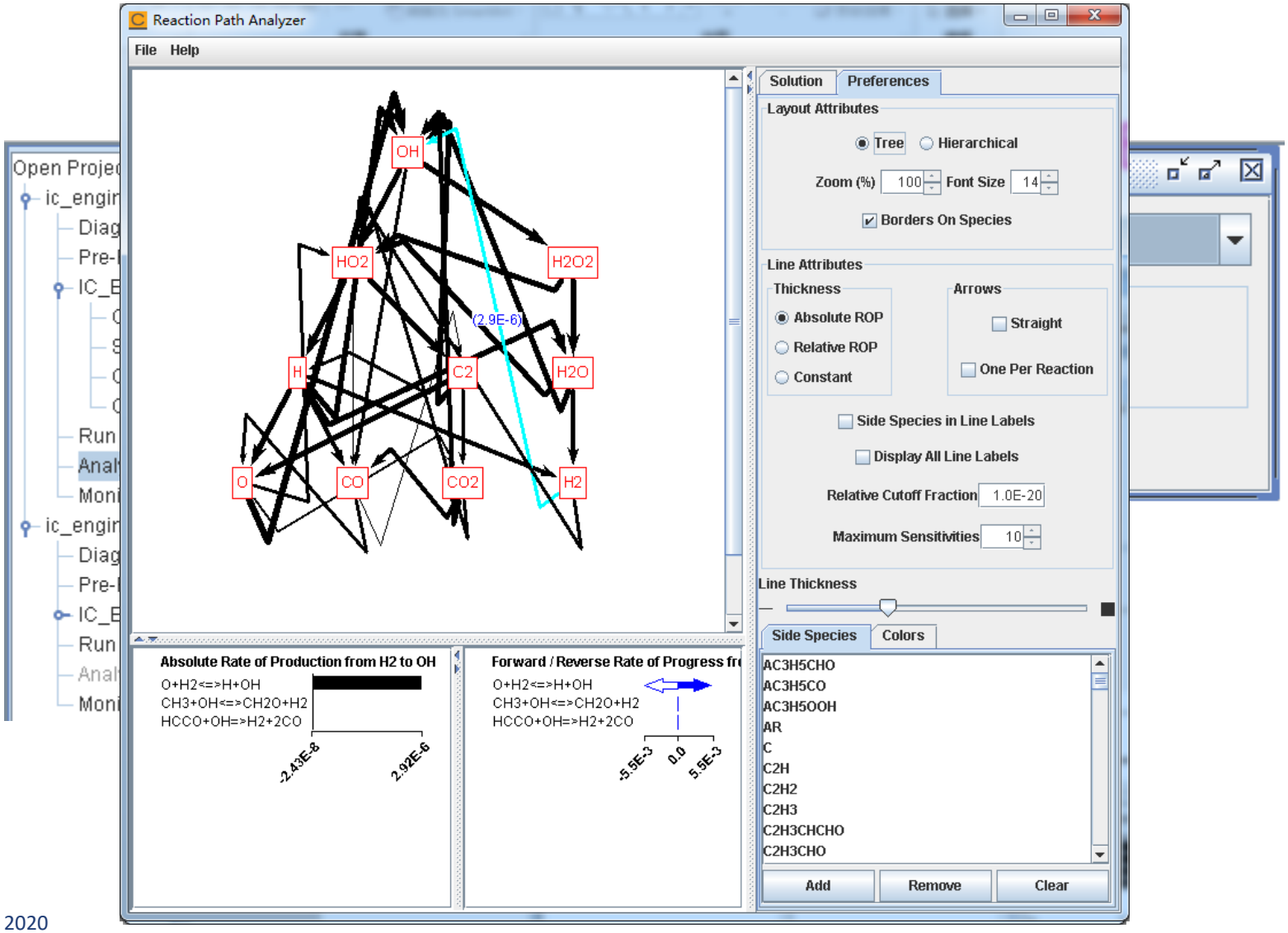


Chemkin Models

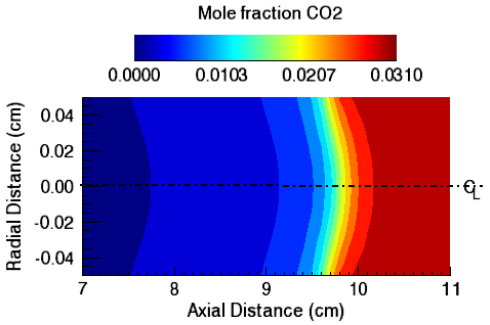


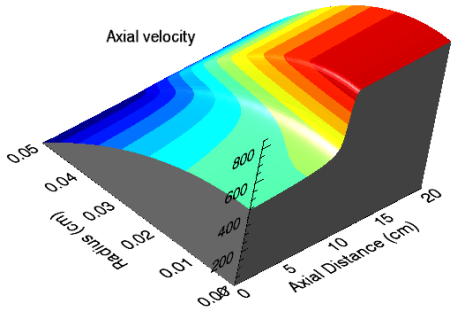
Chemkin post-process

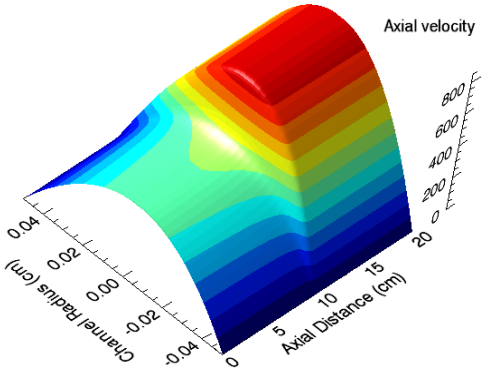
Reaction path analysis and other visualisation options



3-D contour plot

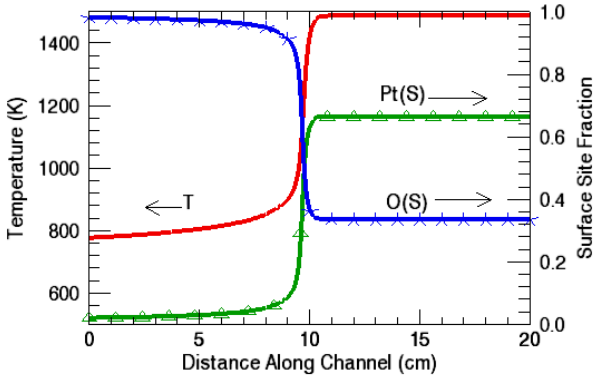


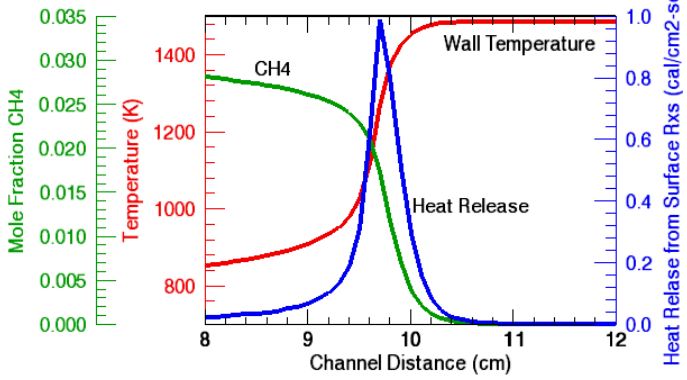




- Symmetric coordinates

- Multi Y axis



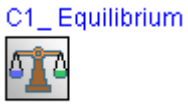


Example 1

Adiabatic flame temperature of H2 – O2 combustion, equilibrium

This example presents the use of a gas-phase equilibrium calculation to determine the adiabatic flame temperature for the hydrogen/air system. In a real system which includes heat losses, chemical kinetic and/or mass transport limitations, the flame temperature is likely to be lower than the adiabatic flame temperature.

In this project, we are using Equilibrium model for the calculation.



Chemistry set using chem.inp as the Gas-phase kinetics file

ELEMENTS H O N END

SPECIES H2 H O2 O OH HO2 H2O N2 H2O2 END

Thermodyamic data use ...\data\therm.dat

Example 1

Adiabatic flame temperature of H2 – O2 combustion, equilibrium

Hydrogen/Air reaction

The chemistry sets used to describe the combustion of hydrogen in air are provided for the purposes of illustration only. These are slight variations of early work done at Sandia National Laboratories, and are out-of-date. The gas-phase kinetics input files are relatively simple. They generally contain 3 elements H, O and N or Ar, and 9 gas phase species: H2, H, O2, O, OH, H2O, HO2, H2O2 and N2 or Ar, with about 18-20 reactions. Nitrogen is generally present as N2 only, where it does not participate in any chemical reactions (i.e., NO formation is not included). Pressure dependencies for reaction rates are not explicitly treated, although there are enhanced collision efficiencies for some reactions.

Example 1

Adiabatic flame temperature of H2 – O2 combustion, equilibrium

Further setup

Reactor physical properties

Problem type: constant pressure enthalpy

Calculate species composition

Initial condition: temperature 300K, pressure 1 atm, estimated equilibrium temperature 2000K

Reaction in mole fraction

H2 - 2

N2 - 3.76

O2 - 1

Continuations

Insert 2 new runs, set temperature 400 and 500 K

Run the model

Example 1

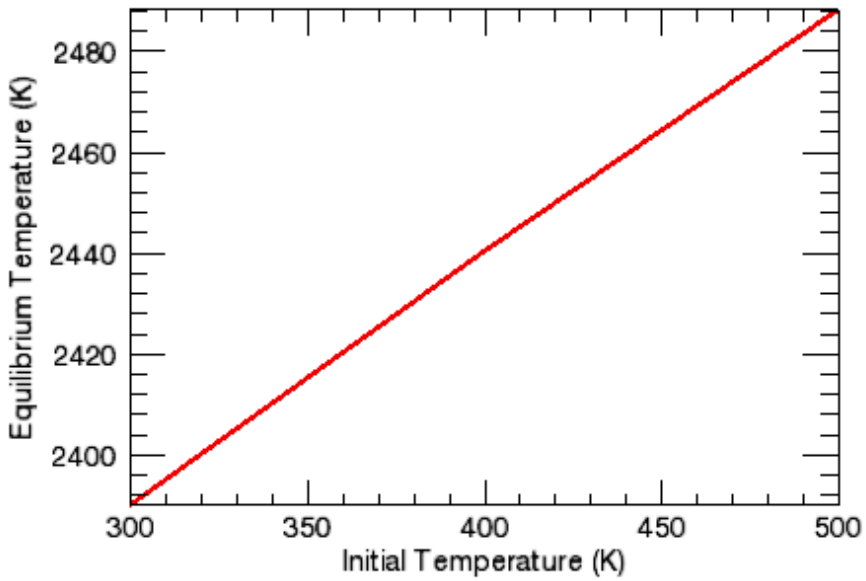
Adiabatic flame temperature of H2 – O2 combustion, equilibrium

Analyse results

Choose x as initial temperature

Choose y as equilibrium temperature

Display the results



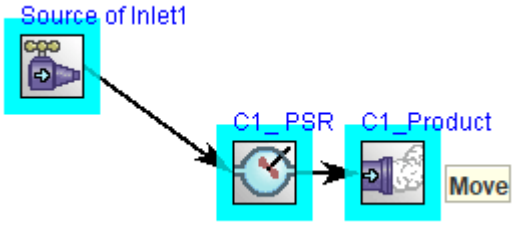
Example 2

Steady-state Gas-phase Combustion

This example presents the simulation of the steady-state combustion of a mixture of hydrogen, nitrogen, and oxygen in a perfectly-stirred reactor at atmospheric pressure.

This example uses the chemistry set of hydrogen combustion which is the same as for last example. This project demonstrates the use of equivalence ratio for specifying the starting gas mixture, as well as the use of a continuation to alter the equivalence ratio.

This project uses a Perfectly Stirred Reactor (PSR) with a gas inlet and an out.



Example 2

Steady-state Gas-phase Combustion

Detailed setup: PSR

Problem Type is first set to Solve Gas Energy Equation, and the Steady State Solver is chosen

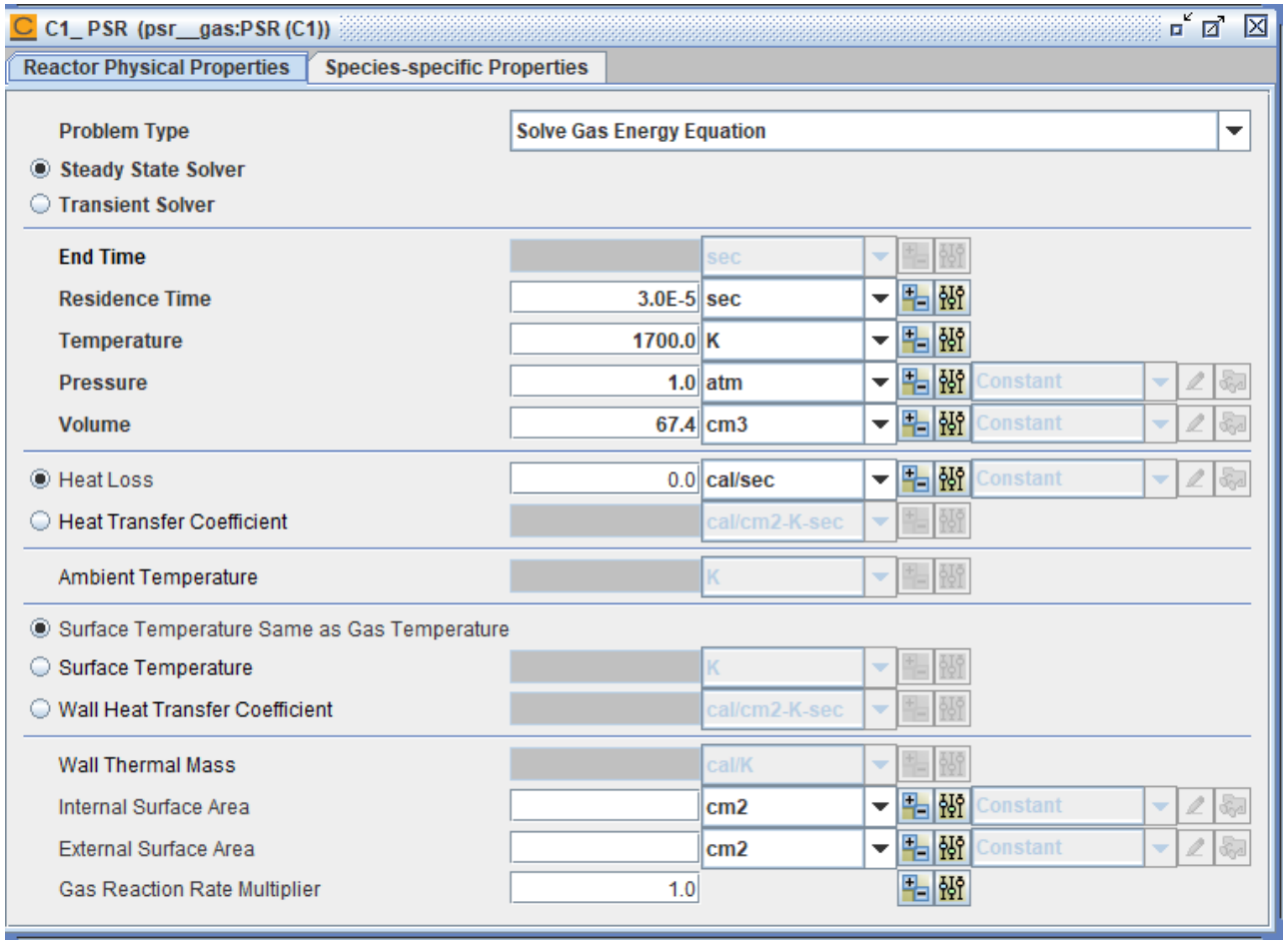
Residence time 0.03ms

Pressure 1atm

Volume 67.4cm^3

No heat losses (adiabatic)

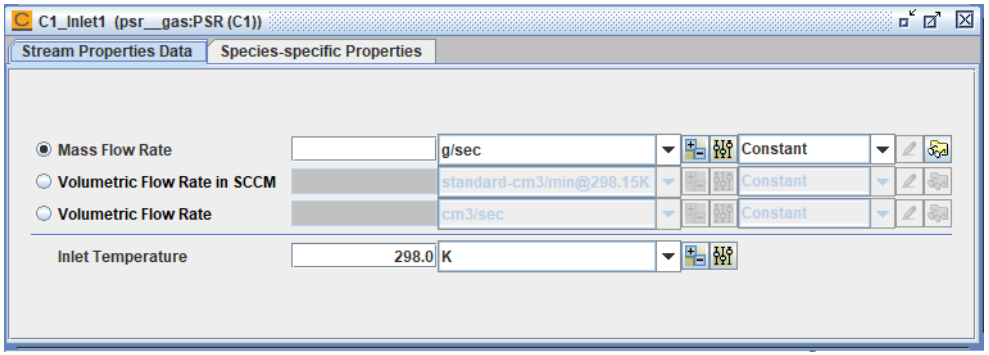
1700 K is estimated gas temperature.

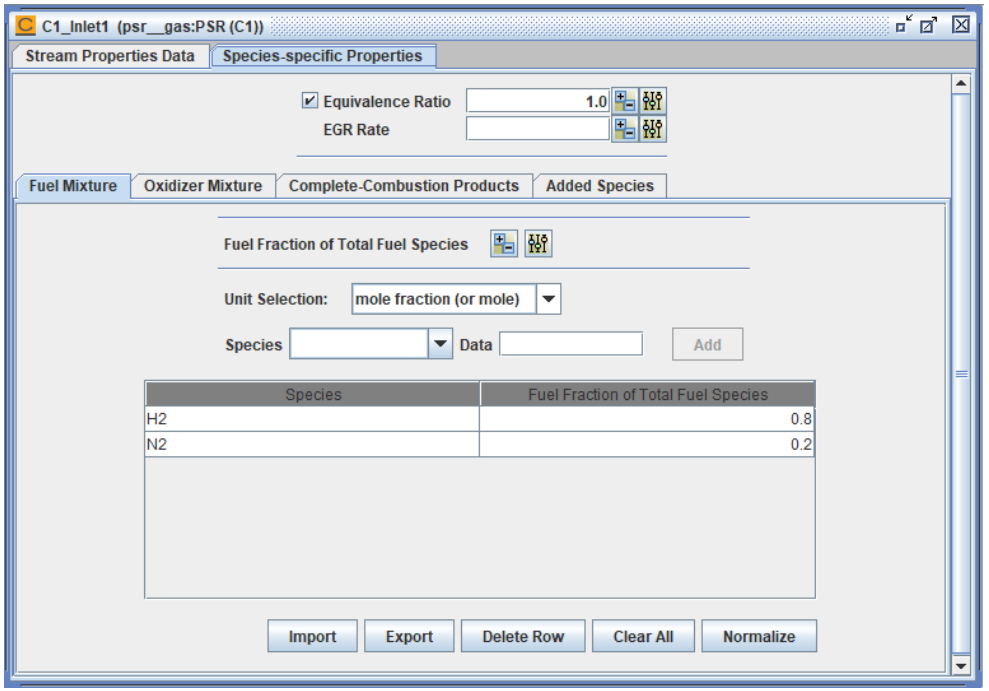


Example 2

Steady-state Gas-phase Combustion

- Detailed setup: inlet
- Temperature 298 K
- Other parameters set in the PSR (mass flow rate ..)
- Equivalence ratio: 1
- Fuel composition: 80% hydrogen and 20 nitrogen
- Oxdizer: 79% N_2 and 21% O_2
- Complete combustion products tab specifies the complete combustion products.





Example 2

Steady-state Gas-phase Combustion

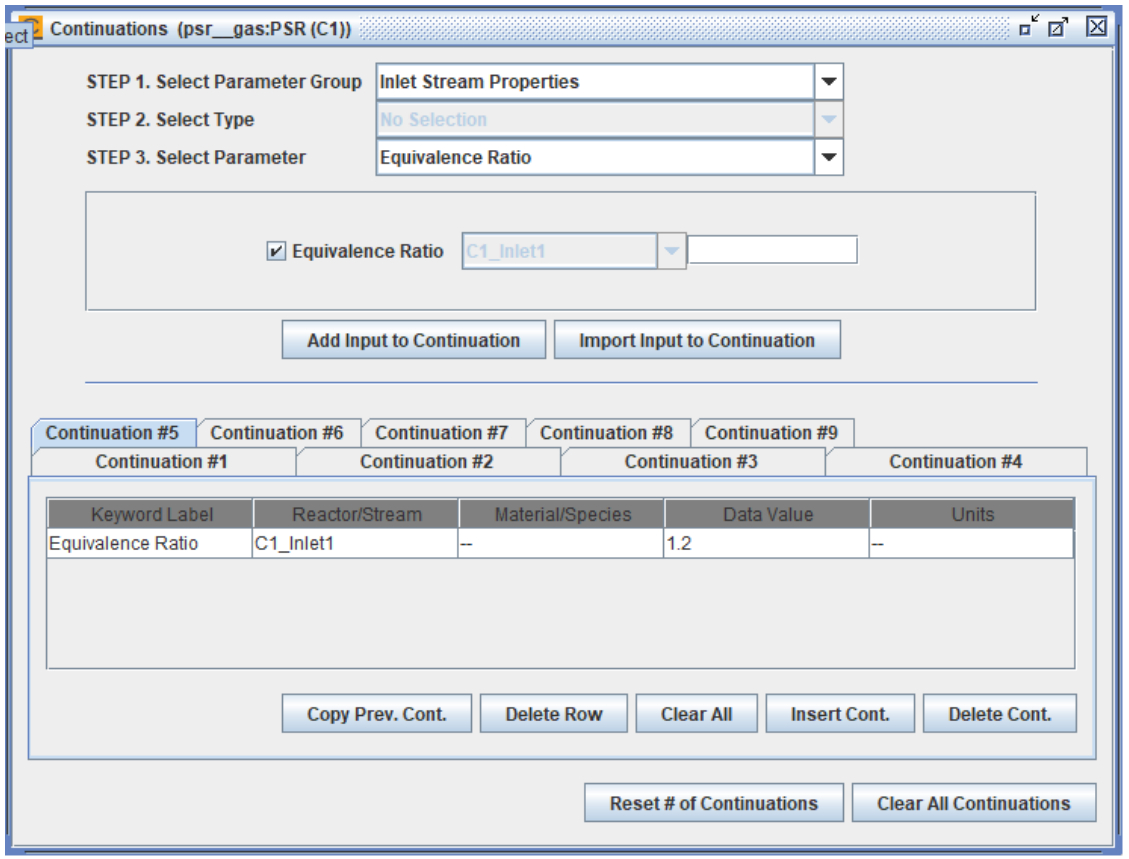
Detailed setup: Continuation

Inlet-stream properties

Equivalence ratio

From 1.05 to 1.4 in 0.05 interval.

Solve…



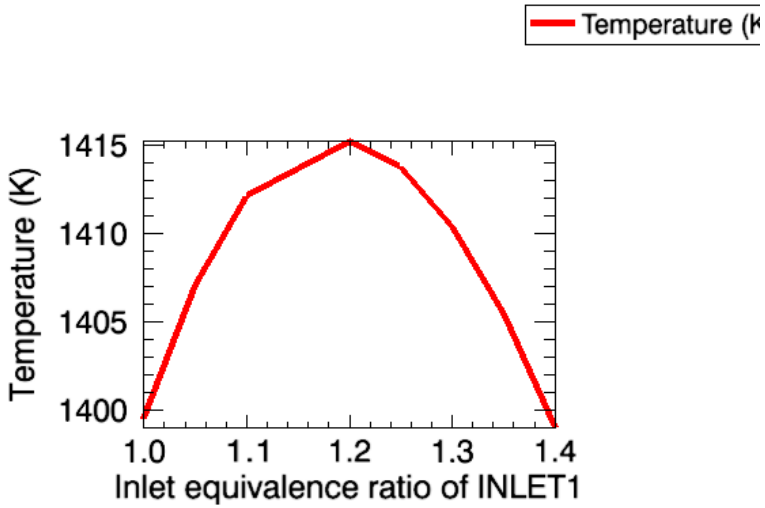
Example 2

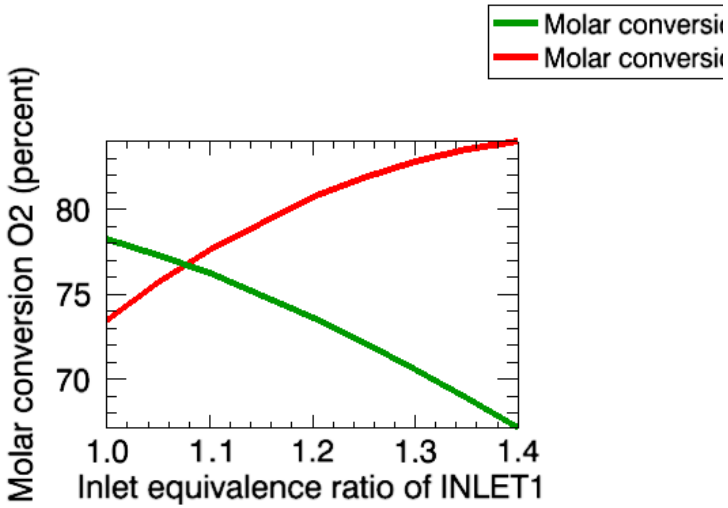
Steady-state Gas-phase Combustion

Results:

In this case, the temperature peaks at a fuel/air equivalence ratio of about 1.20.

Neither the fuel nor the oxidizer is completely consumed in this combustor, as a result of the PSR residence time.





Example 3

Ignition-delay Times for Propane Autoignition

This example presents an ignition-delay time calculation for the homogeneous, isobaric, adiabatic combustion of propane in air. The ignition times are computed using two distinct definitions. Discrepancies between results will be presented.

Propane/Air mechanism

This mechanism is the result of work at the Center for Energy Research (CER), University of California, San Diego. It consists of 46 species and 235 reactions. The elements constituting the species are N, H, C, O, Ar, and He. The thermodynamic and transport data in this chemistry set are included from the same source. All reactions are reversible, and some of the reactions include pressure-dependencies on the rate constant using the Troe formulation. Enhanced collision efficiencies are used for some reactions. The references for the reaction rate parameters as well as for thermodynamic and transport data can be obtained from the CER website.

Example 3

Ignition-delay Times for Propane Autoignition

The study of ignition delay is useful for automotive and turbine industry. It is a measure to avoid auto-ignition of premixed combustion.

There are various ways of defining the ignition time. CHEMKIN allows the user to select different ignition definition. For example, in CHEMKIN's closed homogeneous batch reactor, the ignition time can be defined to be the time during which the maximum amount of heat is released during a combustion process (as indicated by the inflection point in the temperature profile), as well as the time corresponding to the maximum of a certain species concentration chosen by the user. CHEMKIN further allows users to input a specific definition of the ignition time via the Ignition Criterion User Routine.

A closed homogeneous batch reactor is used in this example.

Chemistry set:

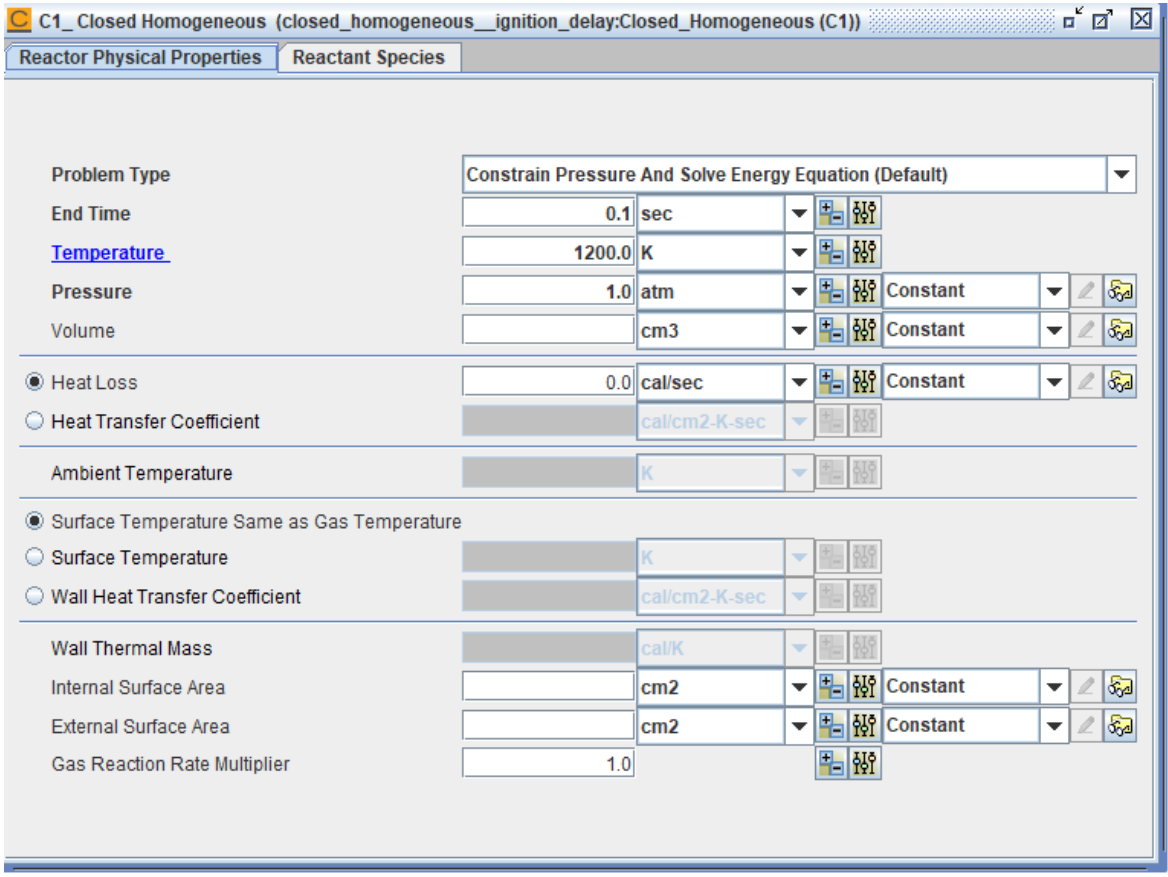
Gas-phase kinetics file: SDmech.inp

Thermodynamics data file: SDtherm.dat

Example 3

Ignition-delay Times for Propane Autoignition

- Reactor setup (isobaric)
- Problem type:
- Constrain pressure and solve energy equation
- Initial temperature: 1200K
- Pressure: 1atm
- Volume: unimportant, not specified, default 1cm^3 will be used
- End time: 0.1 sec (This needs to be large enough to allow for ignition to occur)



Example 3

Ignition-delay Times for Propane Autoignition

Further reactor setup

Reactant species

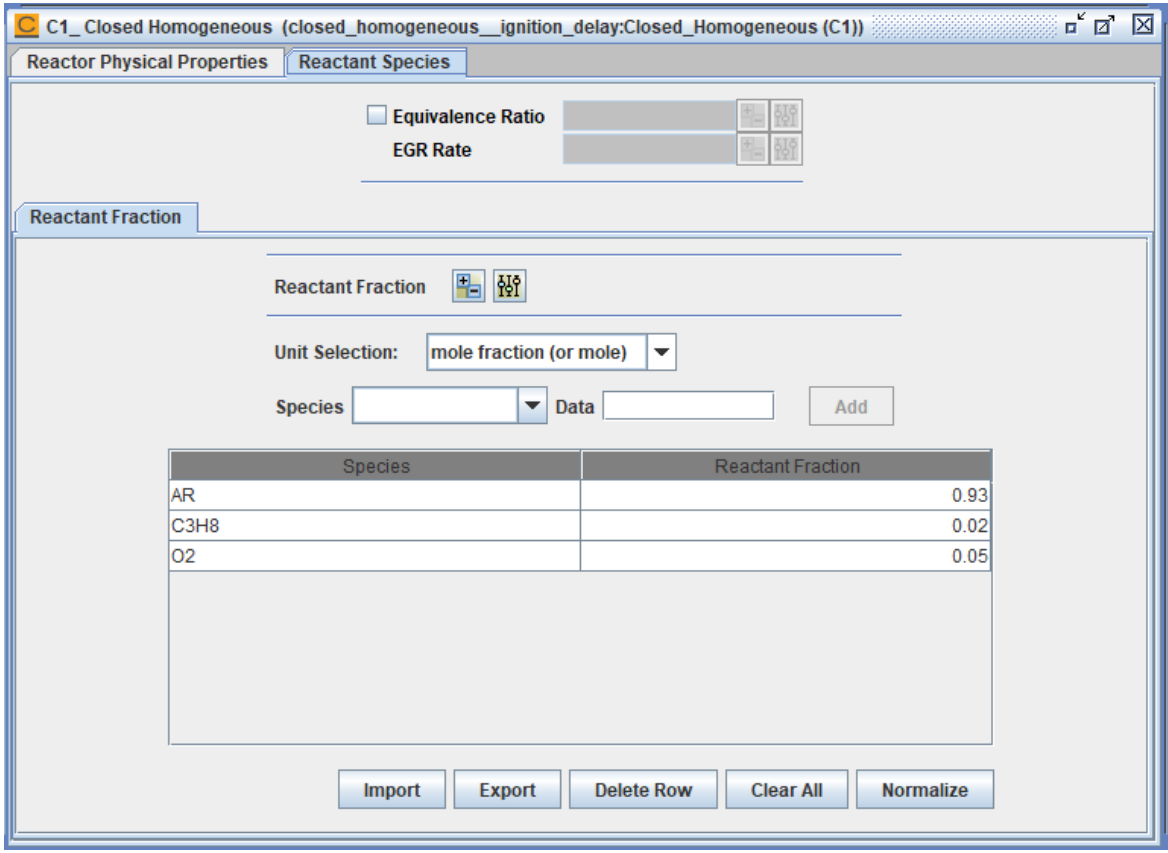
Starting gas mixture

0.02 C_3H_8

0.05 O_2

0.93 Ar

A rather diluted condition



Example 3

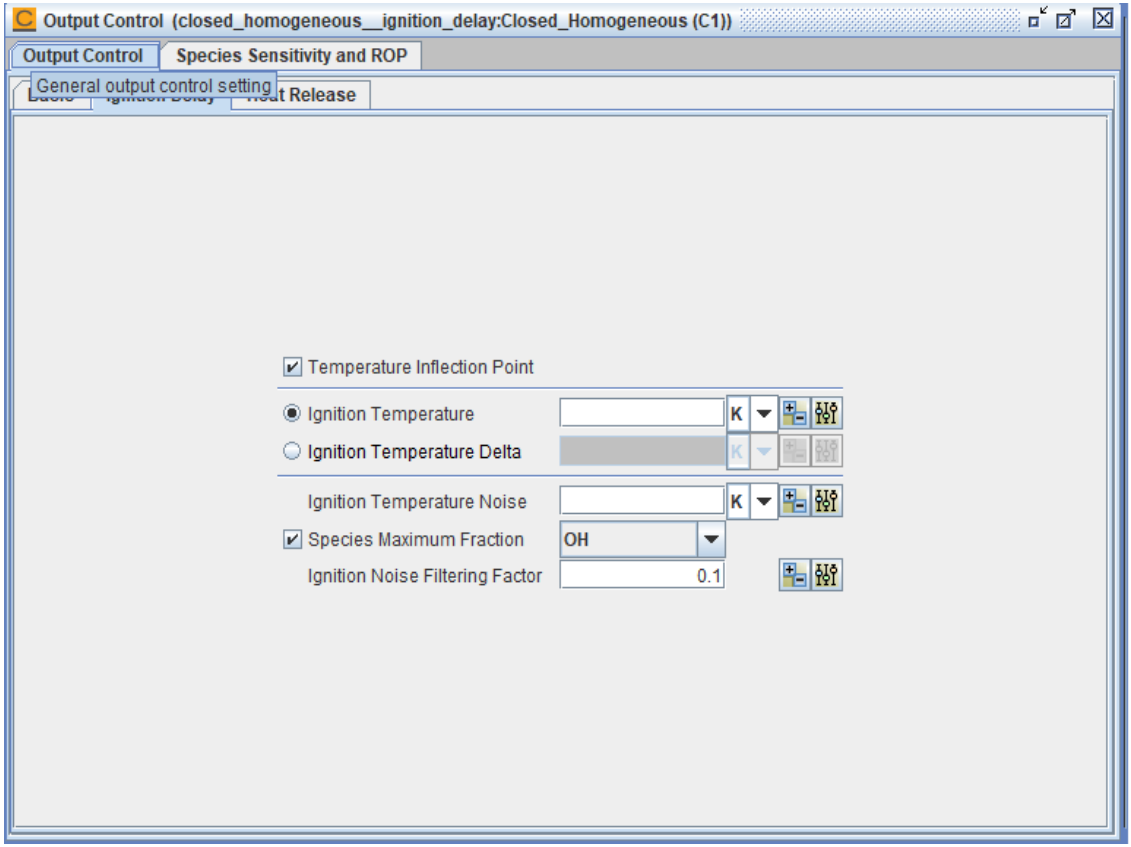
Ignition-delay Times for Propane Autoignition

Output setup

Ignition delay sub-tab

Temperature inflection point box and species Maximum Fraction box checked for computational ignition time criteria.

Species Maximum Fraction set to OH concentration (any species can be chosen), This means the ignition time will be computed based on the maximum of the OH concentration.



The ignition time will also be computed at the point where the rate of change of temperature with respect to time is the largest (Temperature Inflection Point criteria). The user can choose any or all of the definitions of ignition times provided by CHEMKIN.

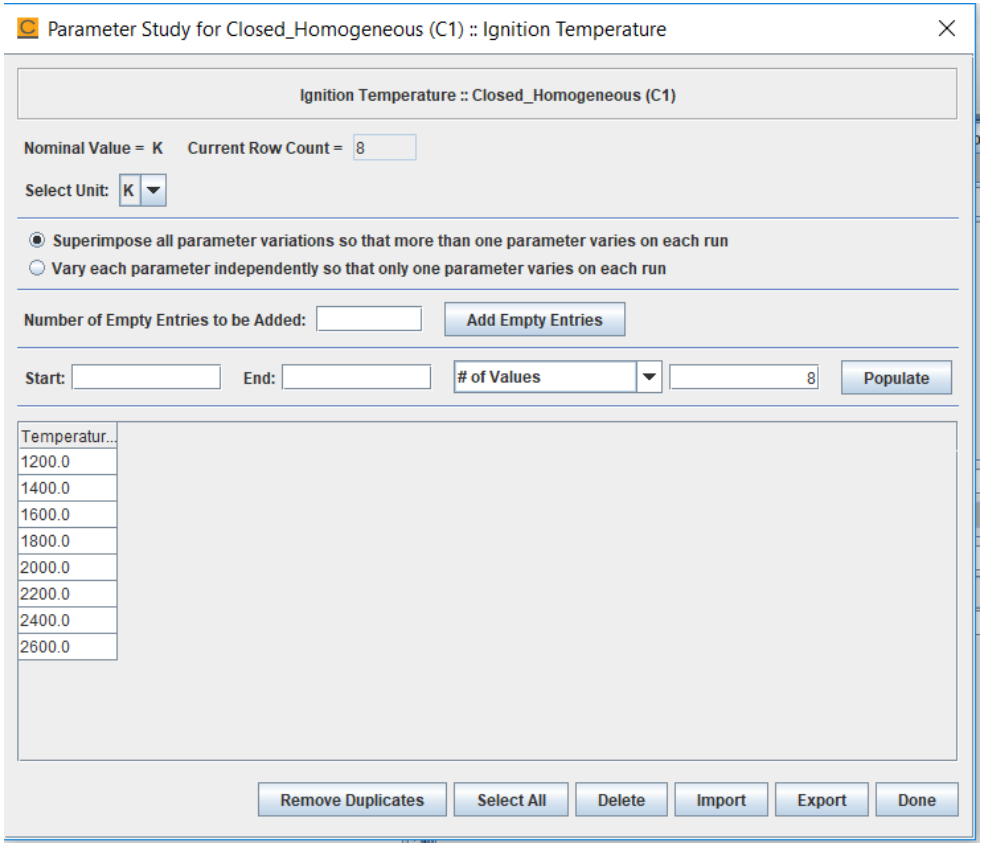
Example 3

Ignition-delay Times for Propane Autoignition

Parametric study setup

It is of interest to run the same problem, but vary the initial temperature in order to demonstrate ignition time dependence on temperature as well as its dependence on the chosen ignition time criteria. For this purpose CHEMKIN's Parameter Study Facility is used. The initial Temperature is changed over a range of 1200 - 2600 K.

This is setup in the Reactant Species tab.



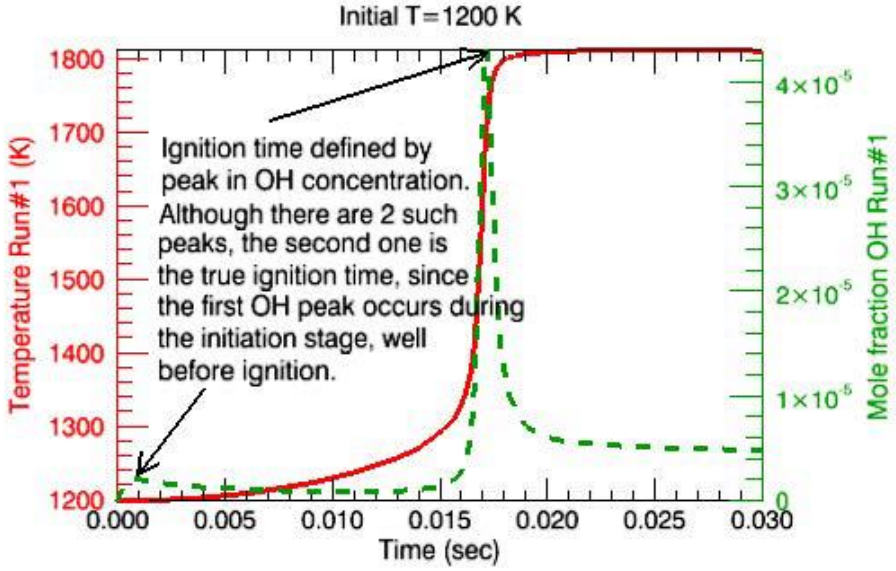
Example 3

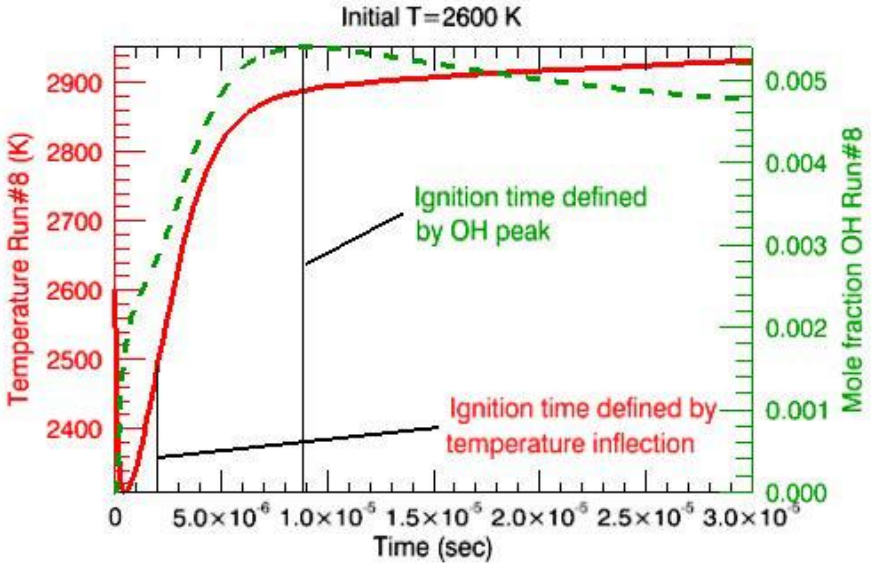
Ignition-delay Times for Propane Autoignition

Results

Table 2-6 Initial Temperatures and Ignition Times

	Ignition time [sec]	
T [K]	***T inflection***	***OH max***
1200	1.69E-02	1.71E-02
1600	1.85E-04	2.11E-04
2600	1.95E-06	9.03E-06



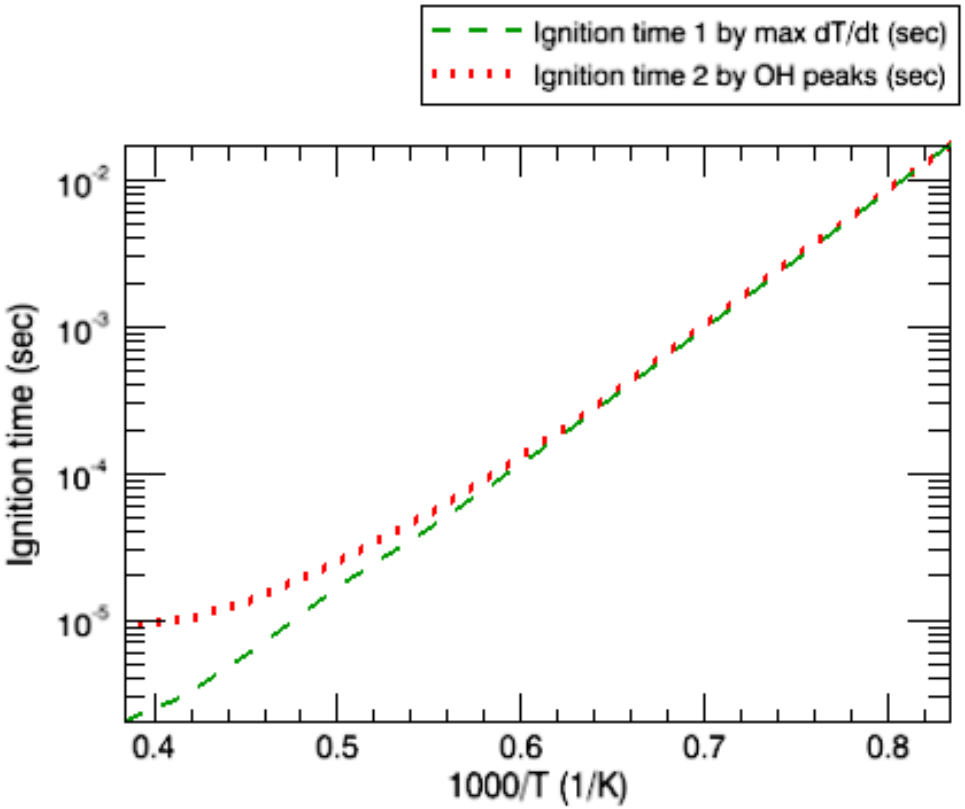


Example 3

Ignition-delay Times for Propane Autoignition

More results

difference between the two ignition time definitions



Example 4

Parameter Study: Propane/Air Flame Speed as a Function of Equivalence Ratio and Unburned Gas Temperature

This example illustrates using the Parameter Study Facility to calculate laminar flame speeds of propane-air mixtures over a wide range of equivalence ratios and unburned gas temperatures at atmospheric pressure.

The behaviour of flames in fuel-lean and fuel-rich systems at a range of unburned gas temperatures are of interest in several applications, such as engine combustion. In this example the flame speeds of propane-air mixtures are calculated for the following conditions:

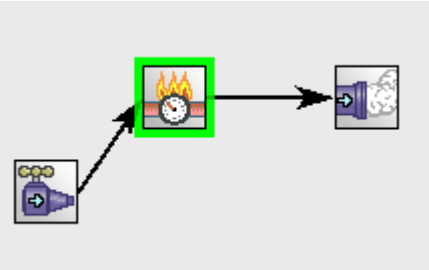
1. Equivalence ratios of 0.6 –1.4 in 0.1 interval.
2. Initial temperatures of 300 K and 700 K.
3. Pressure of 1 atm

A total of 18 parameter-study cases are run to cover the range of operating conditions.

Example 4

Parameter Study: Propane/Air Flame Speed as a Function of Equivalence Ratio and Unburned Gas Temperature

In this example, we use Premixed Laminar Flame Speed Calculation model. We also need an inlet and a product.



Pre-processing

We use a skeleton propane (C_3H_8) reaction mechanism without considering NOx formation.

Gas-phase Kinetics file: sd-chem.inp

Thermodynamics data file: sd-thermo.dat

Gas transport data file: sd-transport.dat

Example 4

Parameter Study: Propane/Air Flame Speed as a Function of Equivalence Ratio and Unburned Gas Temperature

Inlet setup

Inlet velocity: guess value 40cm/s

Fuel mixture: pure propane

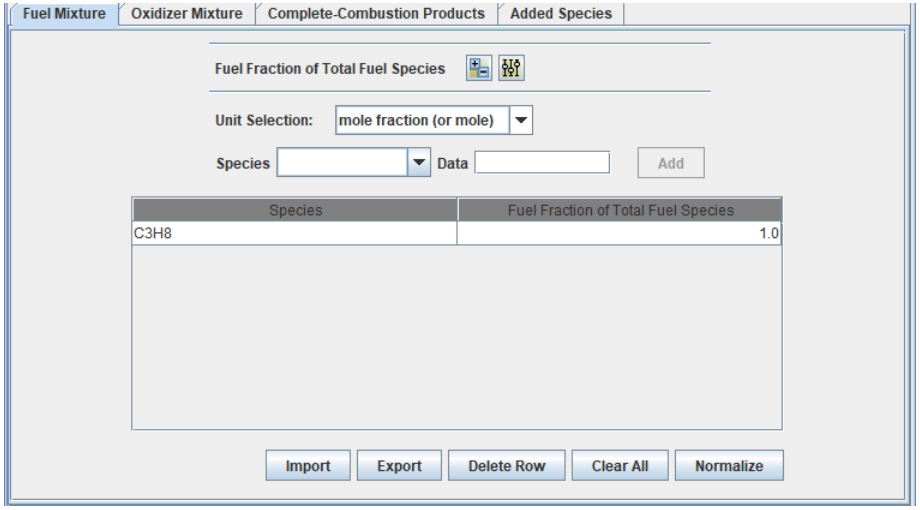
Oxidiser mixture: air (using the auto-populate Air function)

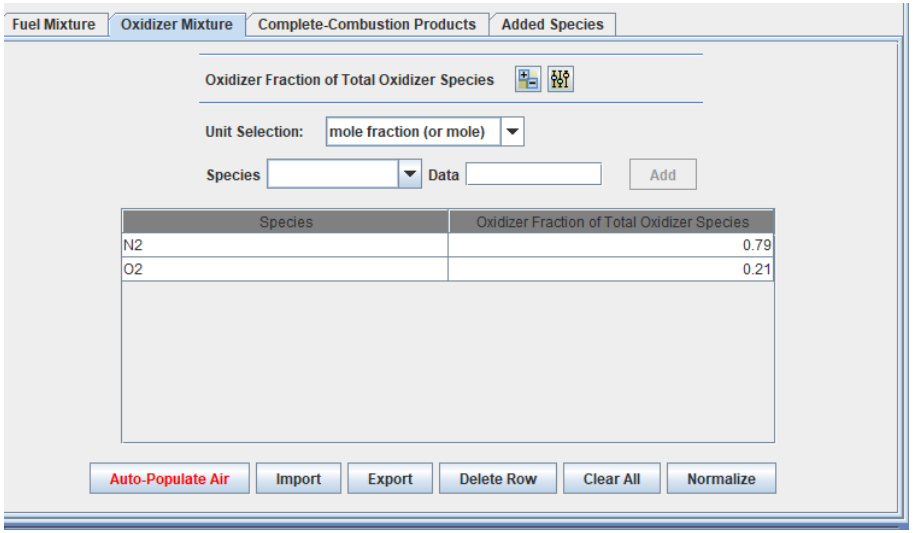
Complete-combustion products:

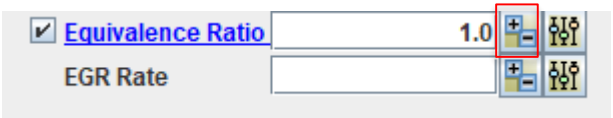
Use the auto-populate function

Equivalence ratio:1.0 but conduct

Parametric study on this







Example 4

Parameter Study: Propane/Air Flame Speed as a Function of Equivalence Ratio and Unburned Gas Temperature

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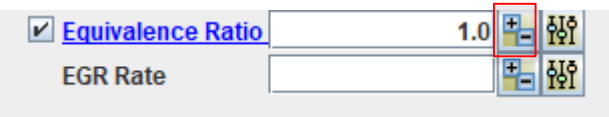
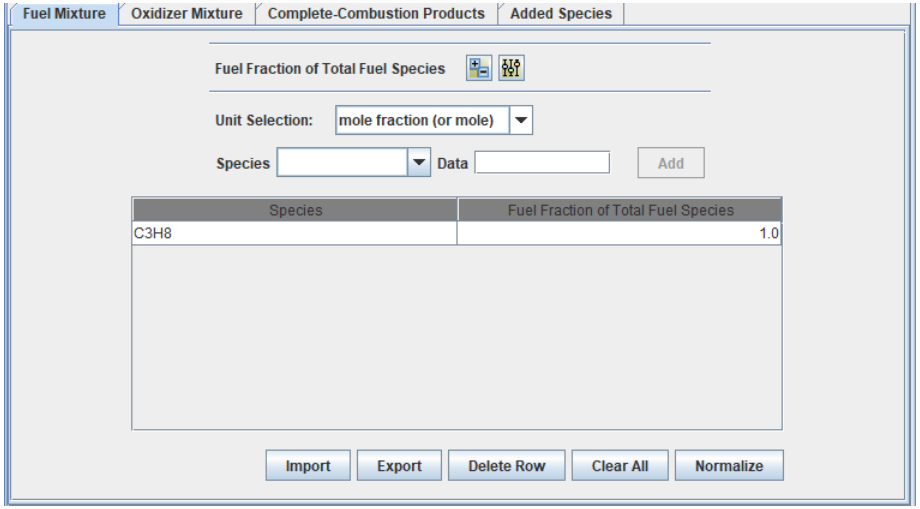
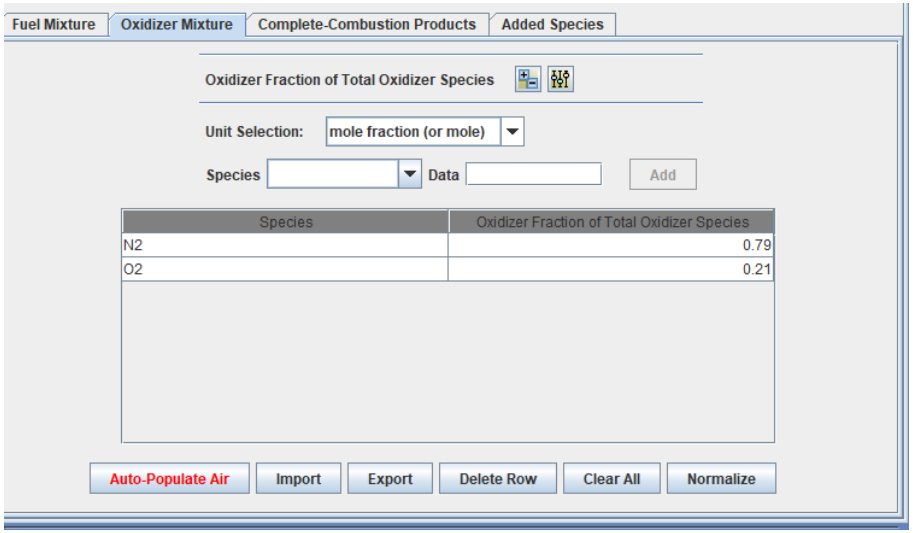
Parametric study on this



Start from 0.6 end 1.4, 9 values.

After setup parametric study, this variable becomes blue underlined.





Example 4

Parameter Study: Propane/Air Flame Speed as a Function of Equivalence Ratio and Unburned Gas Temperature

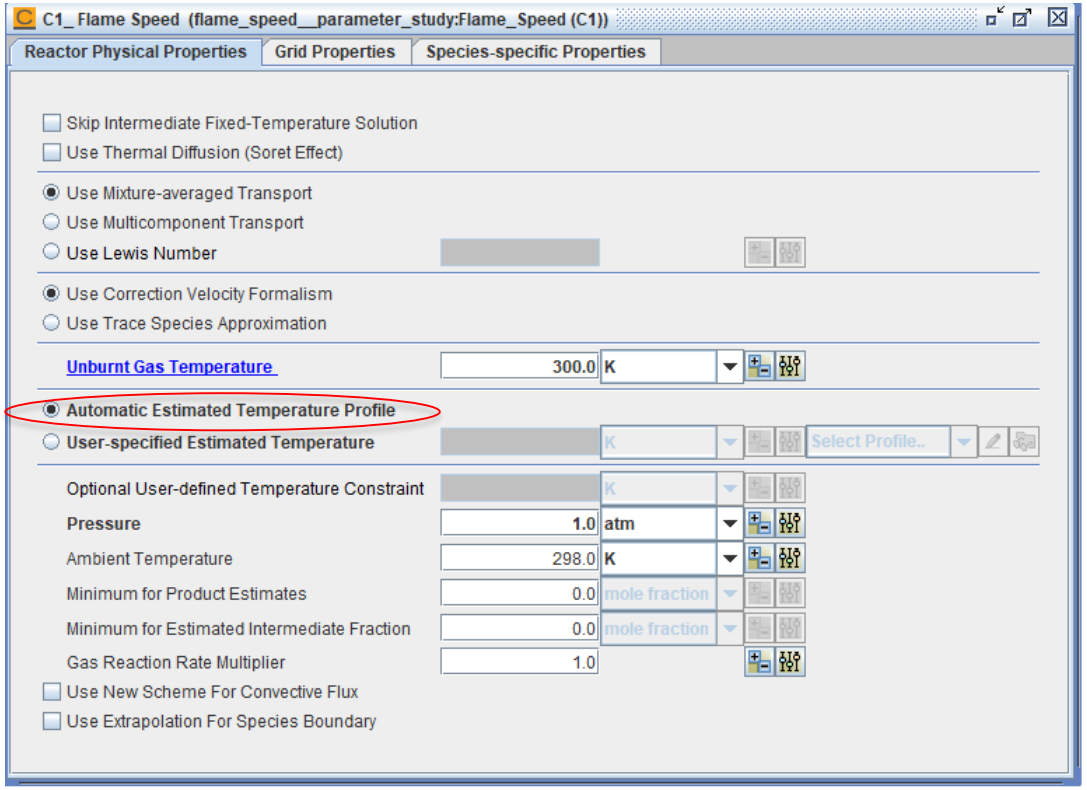
Reactor setup

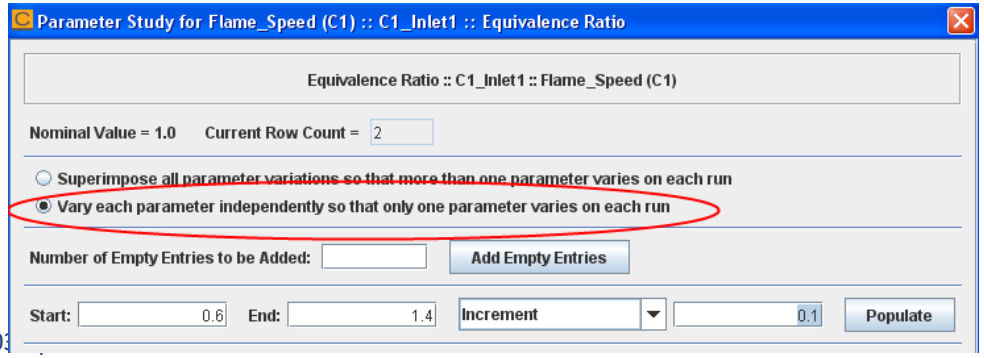
Unburned gas temperature also set for parametric study

Two values: 300K and 700K.

- To modify one of the values, double-click it.
- To delete a value, select it and press the **Delete** button.
- To add a value, press the **Populate** button.

Two parameters set, so

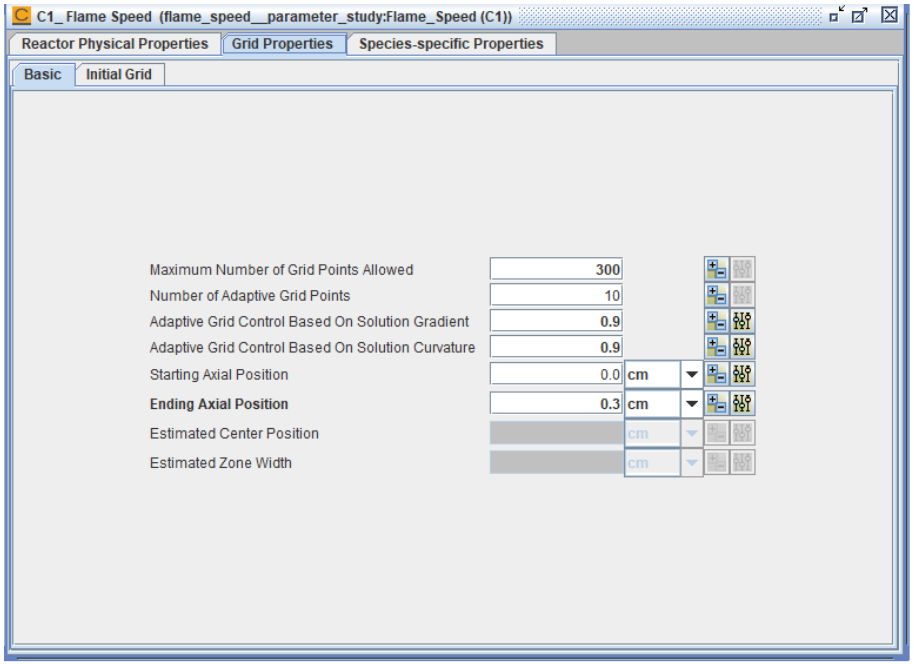


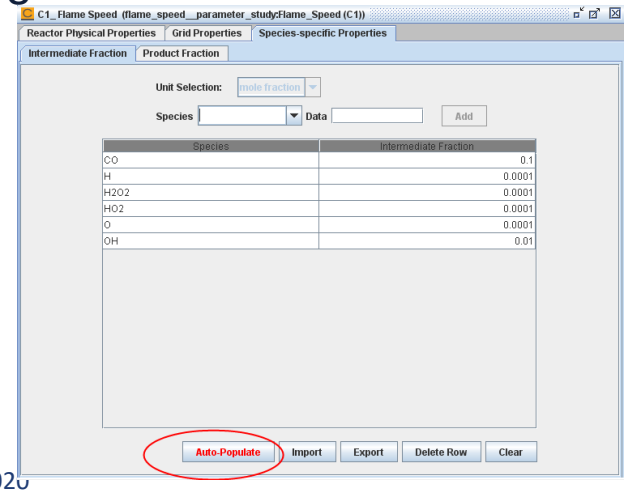


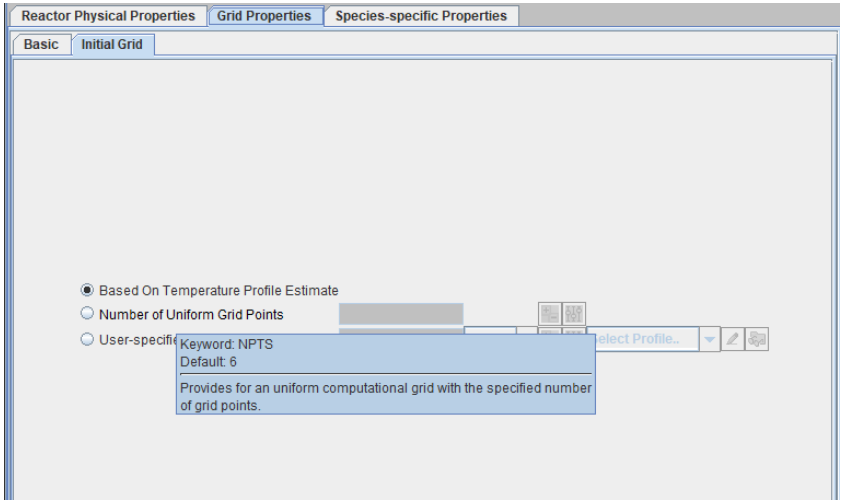
Example 4

Parameter Study: Propane/Air Flame Speed as a Function of Equivalence Ratio and Unburned Gas Temperature

- Reactor setup
- Grid properties
- A rather coarse grid is used
- Species-specific properties
- Using auto-populate function can help in convergence. If not setup, equilibrium values are calculated by Chemkin and used for the product fraction initial guesses.







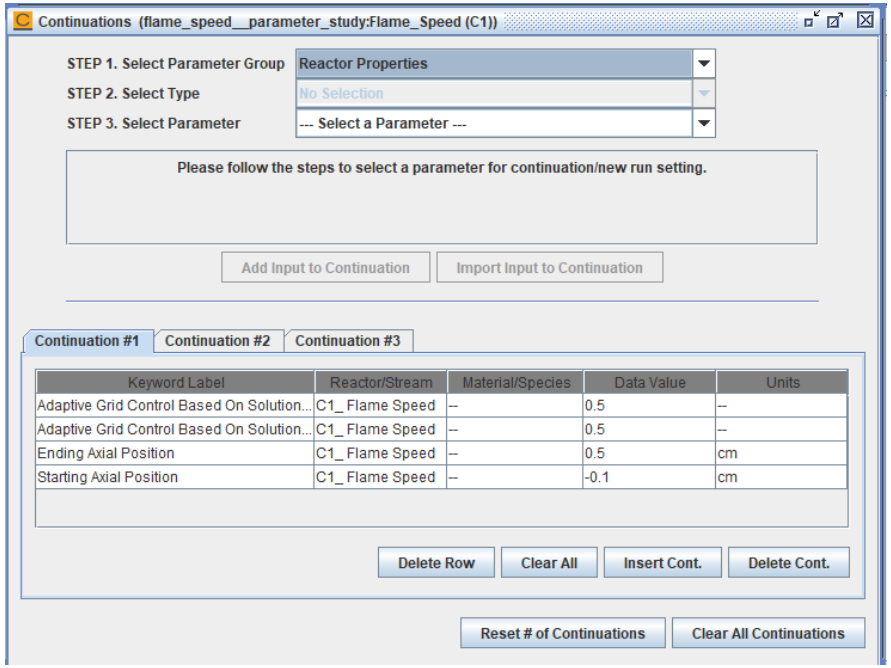
Example 4

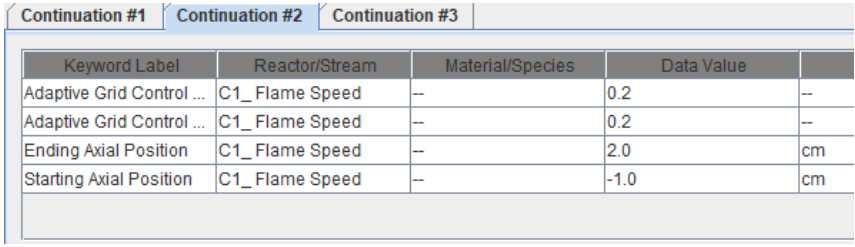
Parameter Study: Propane/Air Flame Speed as a Function of Equivalence Ratio and Unburned Gas Temperature

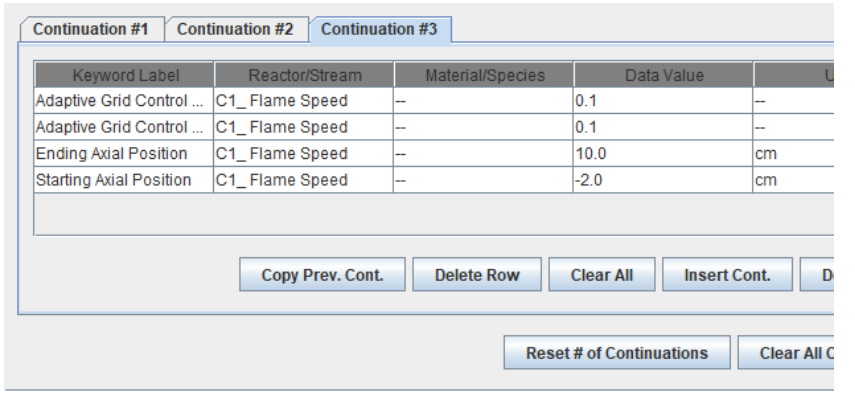
Continuation setup

The continuation is for check the effect of grid setup.

we will start the problem on a small domain and a coarse grid, and subsequently use Continuations to expand the domain and refine the grid, which improves convergence. A starting small domain of 0.3 cm is specified in the Grid Properties panel. Subsequently, in the Continuations panel, the domain is expanded to 12 cm.







Example 4

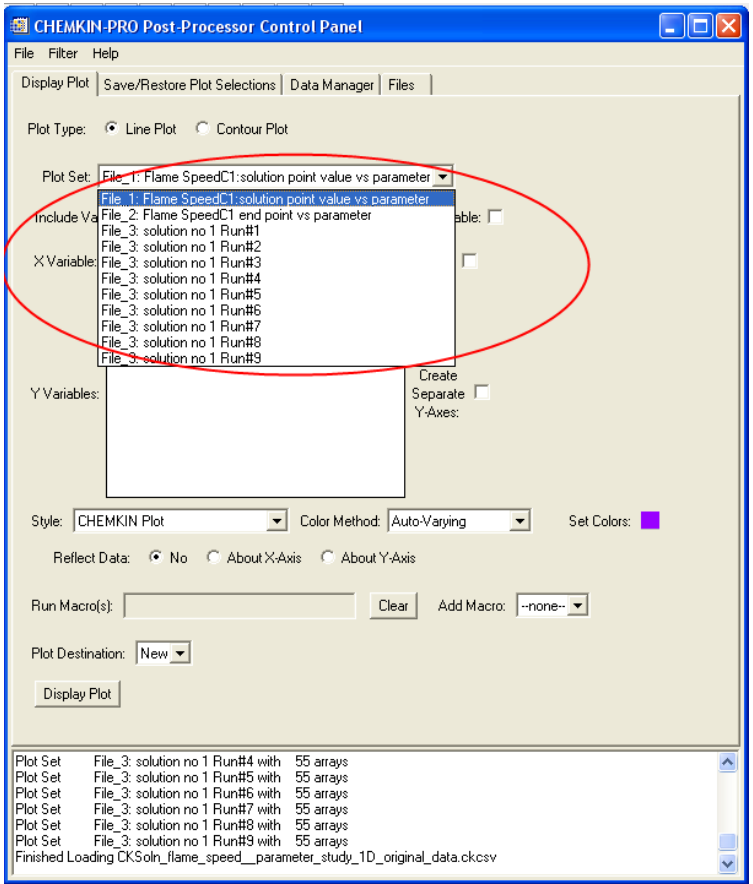
Parameter Study: Propane/Air Flame Speed as a Function of Equivalence Ratio and Unburned Gas Temperature

Results and post process

After running the parameter studies, several additional post-processing options are available. By selecting the Line plot from **Plot Type** in the Post-Processor, options appear for accessing the calculated results.

Choose line plot

The first and second options are exclusive to parameter studies.



Example 4

Parameter Study: Propane/Air Flame Speed as a Function of Equivalence Ratio and Unburned Gas Temperature

Results and post process

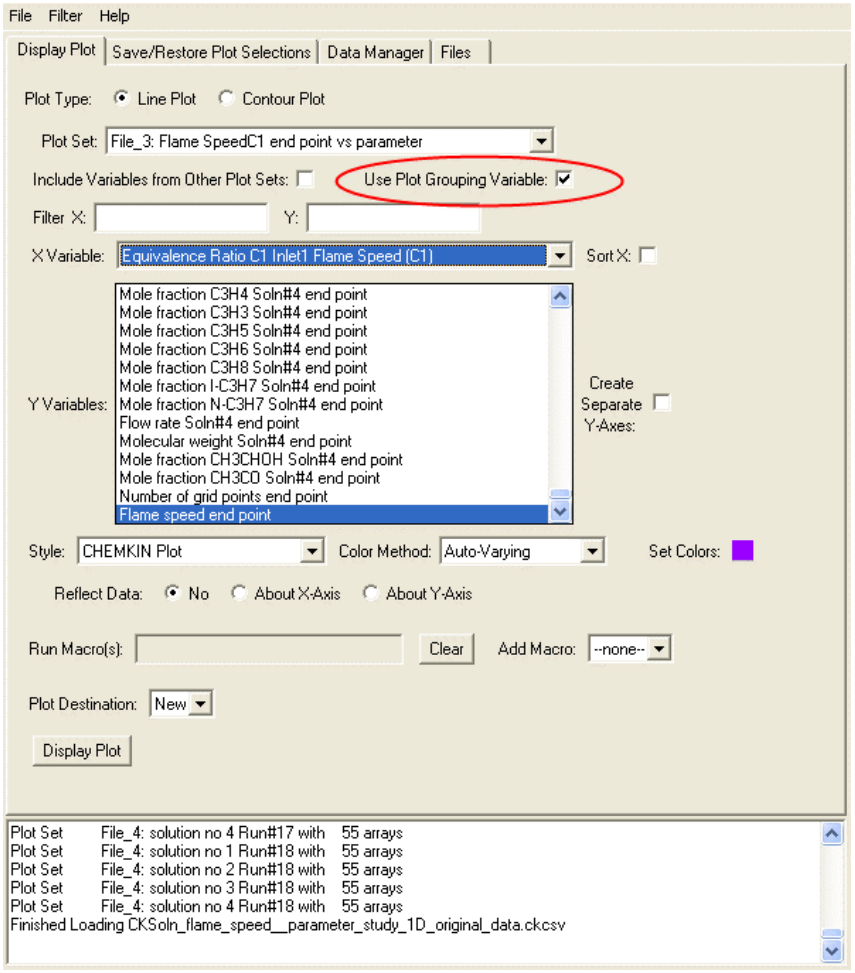
In this example, we have used parameter studies to cover a range of operating conditions, and continuations to refine and expand the grid for each parameter study. Since we have used continuations for each parameter study, there are multiple solutions available for each parameter study run. Consequently, there would be multiple flame speed values for each parameter study run. Since we have used continuations only for refining the grid, we are interested in only the flame speed value of the final continuation. To access this value in the post-processor, we can use the The second option in the **Plot Set** (under **Plot Type** as **Line plot**), i.e., Cluster1C1 end point vs parameter, and one of the values here is the **Flame Speed end point**.

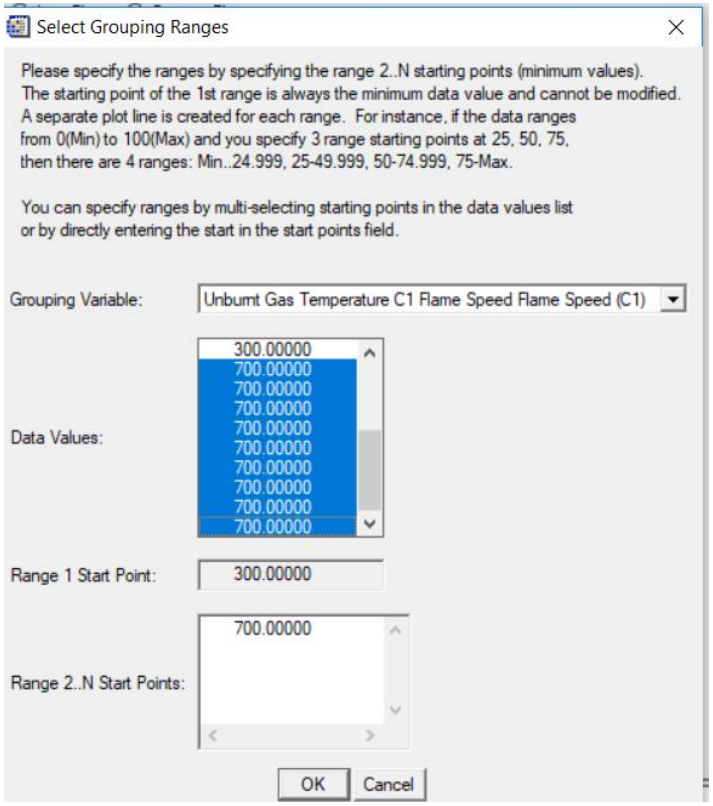
We can now plot the flame speed values as a function of equivalence ratio. Since there are two unburned gas temperatures, it would be good to separate the flame speed vs. equivalence ratio plots into two series. This is done through the **Use Plot Grouping Variable** option as shown in *Figure*, and choosing the unburned gas temperature.

Example 4

Parameter Study: Propane/Air Flame Speed as a Function of Equivalence Ratio and Unburned Gas Temperature

Results and post process





Example 4

Parameter Study: Propane/Air Flame Speed as a Function of Equivalence Ratio and Unburned Gas Temperature

Results and post process