

# Computer Lab & Introduction to Chemkin

---

Dr Guohong Tian  
[g.tian@surrey.ac.uk](mailto:g.tian@surrey.ac.uk)

## Contents of the chapter

- Introduction to Chemkin
- Example 1: Chemical and phase equilibrium – propane/air equilibrium
- Exercise: CO<sub>2</sub>-CO/O<sub>2</sub> 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.

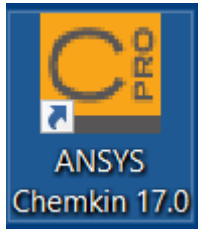
Also allows coupled simulation with CFD and chemical kinetics.

Very powerful post-processing tool boxes.



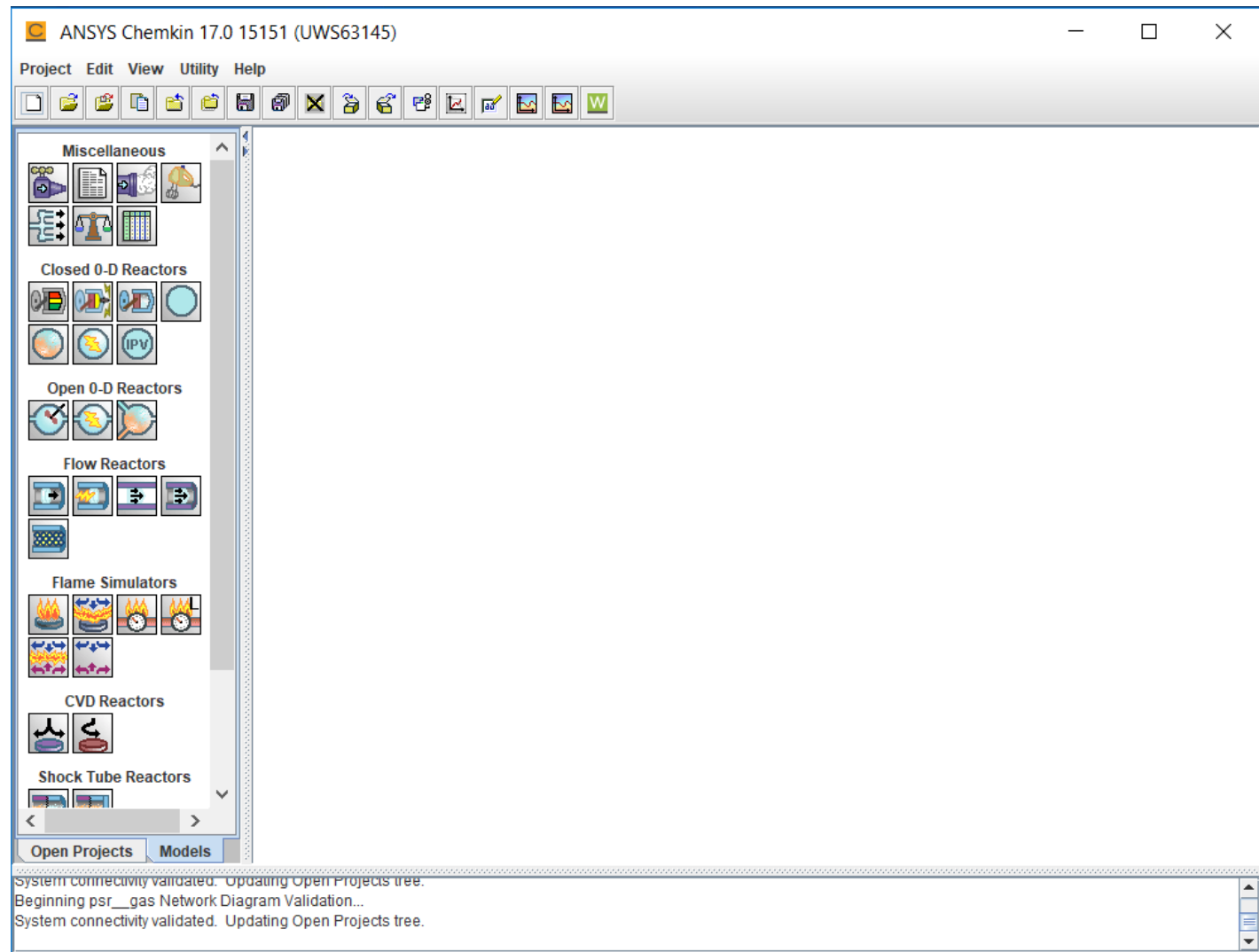
# The new features of Chemkin 4 and later versions

- 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

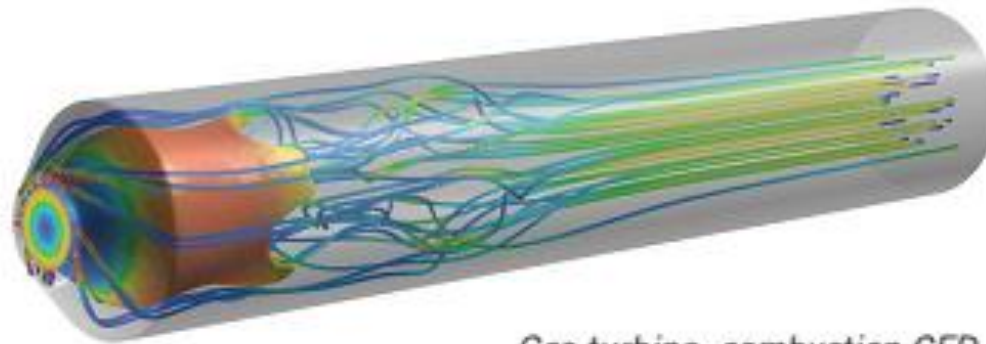


New icon

Interface



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



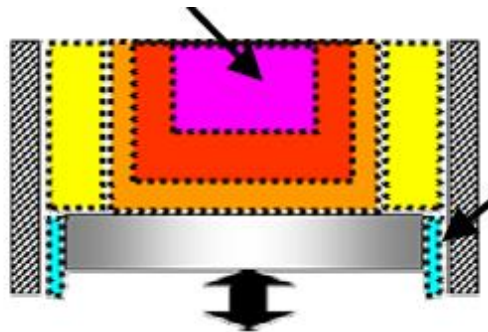
*Gas turbine combustion CFD  
using FLUENT® and CHEMKIN-CFD*

## 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

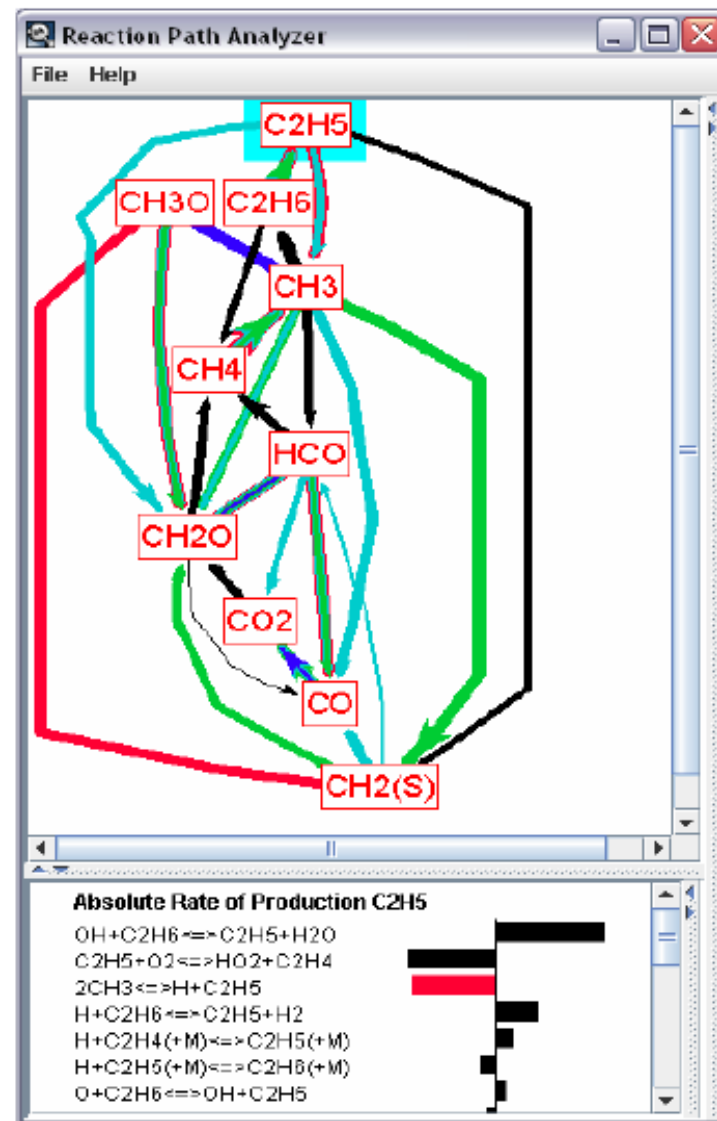
Central high temperature  
zone, firing



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 4.0.1 (11-Nov-2004) on WINNT Session Started: Feb 25, 2005

Project Edit View Utility Help

Miscellaneous  
Closed 0-D Reactors  
Open 0-D Reactors  
Flow Reactors  
Flame Simulators  
CVD Reactors  
Shock Tube Reactors

Diagram View (steady)

Left-Click, Shift-Left-Click, or drag icons to drawing window.  
Hold down Shift+Left Mouse Button to draw connections.  
Hold down Alt+Left Mouse Button to draw heat transfer.

Display Options Print Update Project

Short Name: steady  
Description:  
Gas-Phase Kinetics File: C:\Documents and Settings\Administrator\chemkin\samples\psr\gas\chem.inp  
Surface Kinetics File:  
Thermodynamics Data File: C:\Program Files\Reaction\chemkin40\_pc\data\therm.dat  
Gas Transport Data File: C:\Program Files\Reaction\chemkin40\_pc\data\tran.dat  
Suppl. Gas Transport File:

Open Projects Models

CHEMKIN(R) is a registered trademark of Reaction Design.  
Beginning Validation... System connectivity validated. Updating Open Projects tree.  
Beginning Validation... System connectivity validated. Updating Open Projects tree.

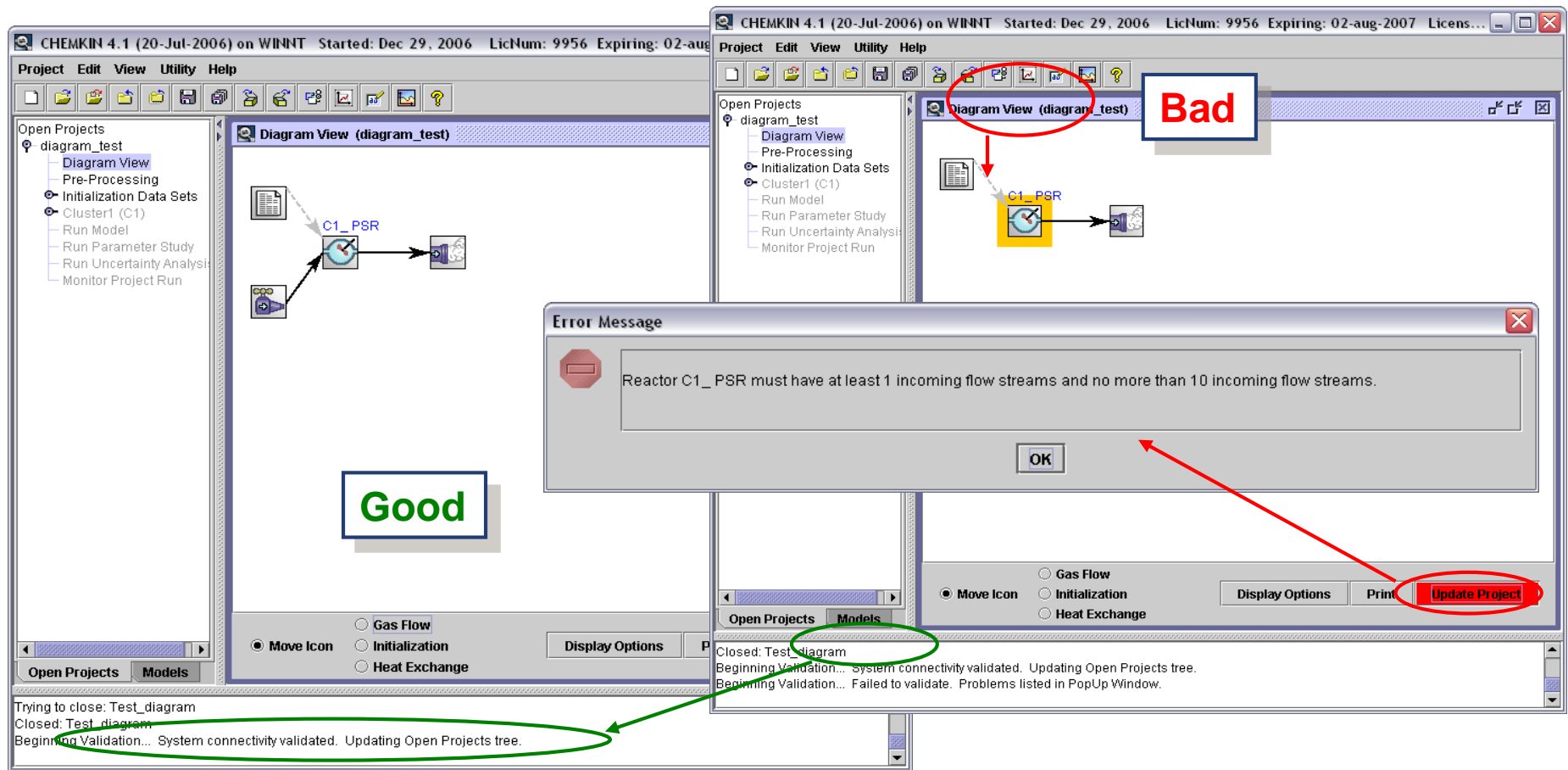
Task bar

Window bar

Message bar

# Chemkin user interface

Note: a reactor needs an input and an output



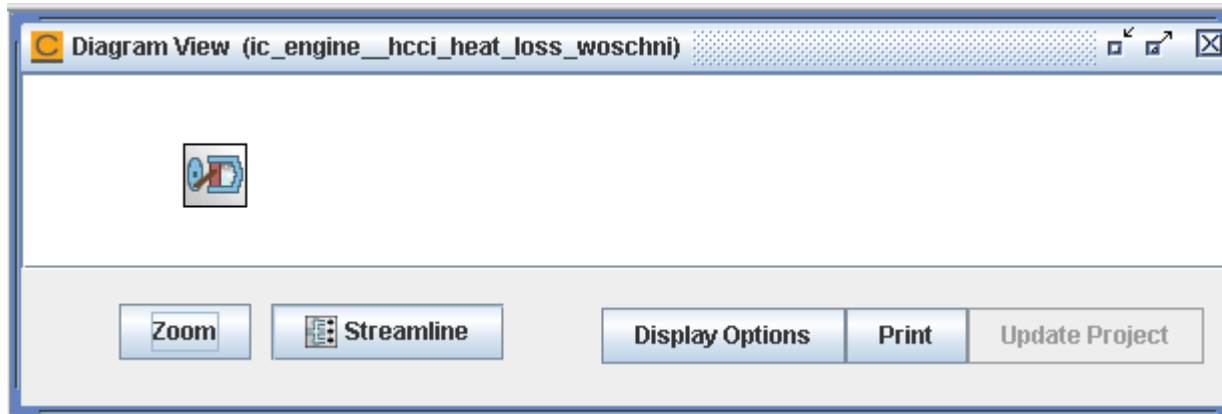
The screenshot displays the Chemkin 4.1 (20-Jul-2006) on WINNT interface. The main window shows a diagram view (diagram\_test) with a reactor labeled C1\_PSR. The reactor is highlighted with a red circle and labeled "Bad". The diagram shows a flow stream entering the reactor from the left and another flow stream exiting to the right. The reactor is labeled "C1\_PSR".

An error message dialog box is displayed, stating: "Reactor C1\_PSR must have at least 1 incoming flow streams and no more than 10 incoming flow streams." The dialog box has an "OK" button.

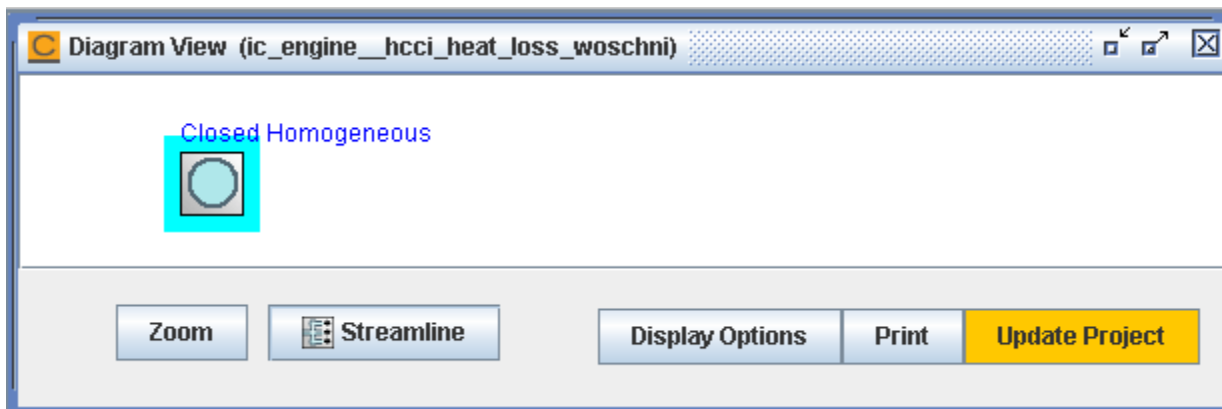
The interface also shows a "Good" label next to the reactor. The "Open Projects" list on the left includes: diagram\_test, Diagram View, Pre-Processing, Initialization Data Sets, Cluster1 (C1), Run Model, Run Parameter Study, Run Uncertainty Analysis, and Monitor Project Run.

The "Models" section at the bottom shows: ☒ Move Icon, ☐ Gas Flow, ☐ Initialization, and ☐ Heat Exchange. The "Display Options" button is visible.

The "Update Project" button is circled in red. The status bar at the bottom shows: "Trying to close: Test\_diagram", "Closed: Test\_diagram", and "Beginning Validation... System connectivity validated. Updating Open Projects tree."

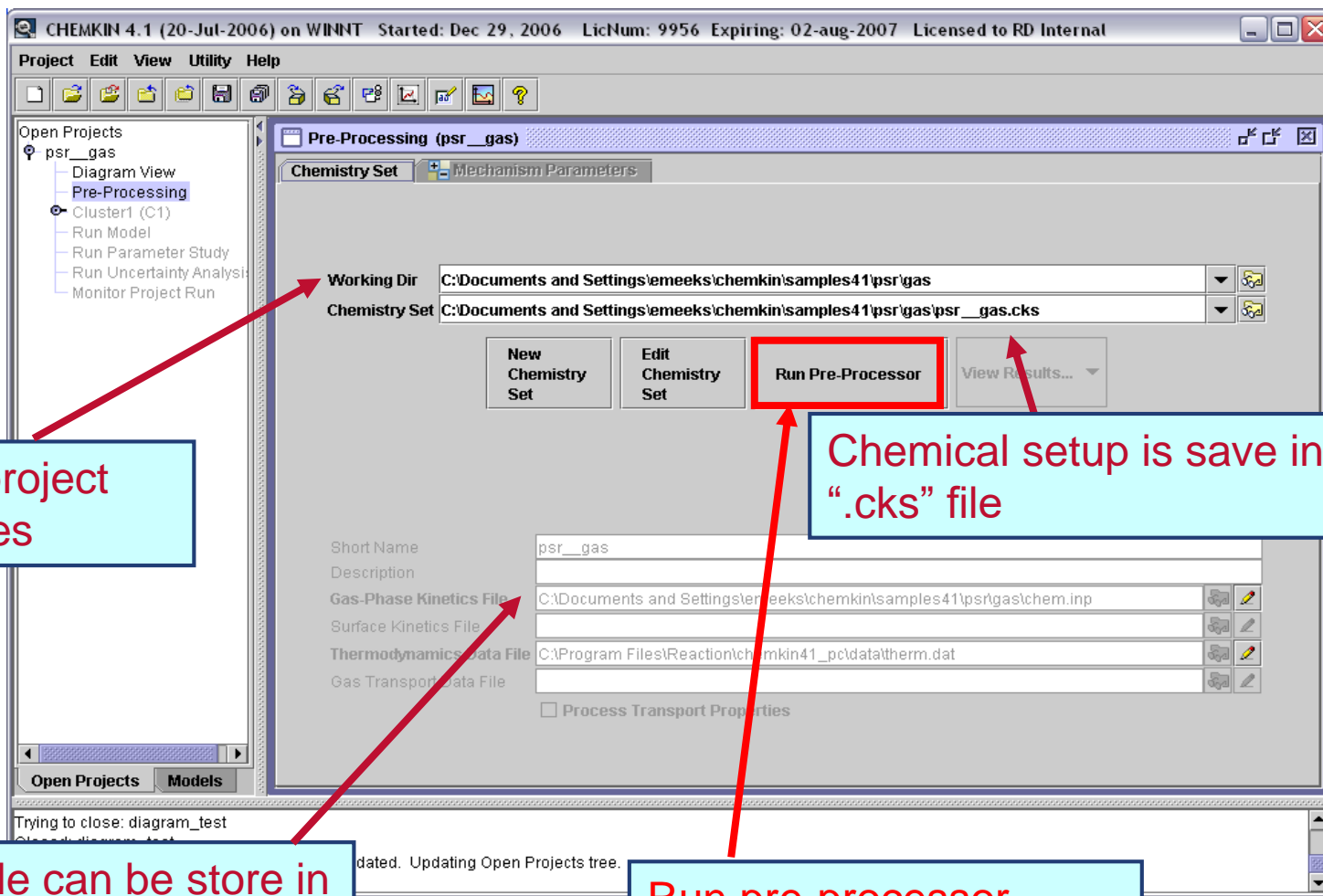


Zero-D IC engine  
model



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

CHEMKIN 4.1 (20-Jul-2006) on WINNT Started: Dec 29, 2006 LicNum: 9956 Expiring: 02-aug-2007 Licensed to RD Internal

Project Edit View Utility Help

Open Projects

- psr\_gas
  - Diagram View
  - Pre-Processing
  - Cluster1 (C1)
    - C1\_PSR
    - C1\_Inlet1
    - Solver
    - Output Control
    - Continuations

C1\_PSR (psr\_gas:Cluster1 (C1))

Reactor Physical Properties Species-specific Properties

Problem Type: Solve Gas Energy Equation

☒ Steady State Solver  
☐ Transient Solver

Residence Time: 3.0E-5 sec

Temperature: 1700.0 K

Pressure: 1.0 atm

Volume: 67.4 cm3

☒ Heat Transfer: Keyword: VOL, VPRO (for profiles) /sec

☐ Heat Transfer: Volume of the reactor. For some reactor types volume is optional. For open systems, at most two of residence time, volume, and Amle flow rate can be specified.

☒ Surface Temperature Same as Gas Temperature

☐ Surface Temperature: K

☐ Wall Heat Transfer Coefficient: J/m2-K-sec

Wall Thermal Mass: cal/K

Internal Surface Area: m2

External Surface Area: m2

Gas Reaction Rate Multiplier

Open Projects Models

Chemistry Set Updated: C:\Documents and Settings\emeeks\chemkin\samples41\psr\gas\psr\_gas.cks  
Pre-Processing Successful for C:\Documents and Settings\emeeks\chemkin\samples41\psr\gas\psr\_gas.cks run in C:\Documents and Settings\emeeks\chemkin\samples41\psr\gas

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

CHEMKIN 4.1 (20-Jul-2006) on WINNT Started: Dec 29, 2006 LicNum: 9956 Expiring: 02-aug-2007 Licensed to RD Internal

Project Edit View Utility Help

Open Projects

- psr\_gas
  - Diagram View
  - Pre-Processing
  - Cluster1 (C1)
    - C1\_PSR
    - C1\_Inlet1
    - Solver
    - Output Control
    - Continuations
  - Run Model
  - Run Parameter Study
  - Run Uncertainty Analysis
  - Monitor Project Run

C1\_Inlet1 (psr\_gas:Cluster1 (C1))

Stream Properties Data Species-specific Properties

Flow properties include flow rate and temperature

☒ Mass Flow Rate  kg/sec   Constant

☐ Volumetric Flow Rate in SCCM    Constant

☐ Volumetric Flow Rate  m3/sec   Constant

Inlet Temperature  K

Open Projects Models

Chemistry Set Updated: C:\Documents and Settings\emeeks\chemkin\samples41\psrgas\psr\_gas.cks  
Pre-Processing Successful for C:\Documents and Settings\emeeks\chemkin\samples41\psrgas\psr\_gas.cks run in C:\Documents and Settings\emeeks\chemkin\samples41\psrgas

# Oxidants/reactants setup

C1\_Inlet1 (psr\_gas:Cluster1 (C1))

Stream Properties Data Species-specific Properties

☒ Equivalence Ratio 1.0

Complete-Combustion Products Added Species

Fuel Mixture Oxidizer Mixture

Fuel Fraction of Total Fuel Species

Unit Selection: mole fraction (or mole)

Species Data Add

| Species | Fuel Fraction of Total Fuel Species |
|---------|-------------------------------------|
| N2      | 0.2                                 |
| H2      | 0.8                                 |

Equivalence ratio

Fuel definition, summation must be unity

C1\_Inlet1 (psr\_gas:Cluster1 (C1))

Stream Properties Data Species-specific Properties

☒ Equivalence Ratio 1.0

Complete-Combustion Products Added Species

Fuel Mixture Oxidizer Mixture

Oxidizer Fraction of Total Oxidizer Species

Unit Selection: mole fraction (or mole)

Species Data Add

| Species | Oxidizer Fraction of Total Oxidizer Species |
|---------|---|
| O2      | 0.21  |
| N2      | 0.79  |

Oxidants definition, summation must be unity

C1\_Inlet1 (psr\_gas:Cluster1 (C1))

Stream Properties Data Species-specific Properties

☒ Equivalence Ratio 1.0

Complete-Combustion Products Added Species

Fuel Mixture Oxidizer Mixture

Added Species Fraction of Total Reactant Species

Unit Selection: mole fraction

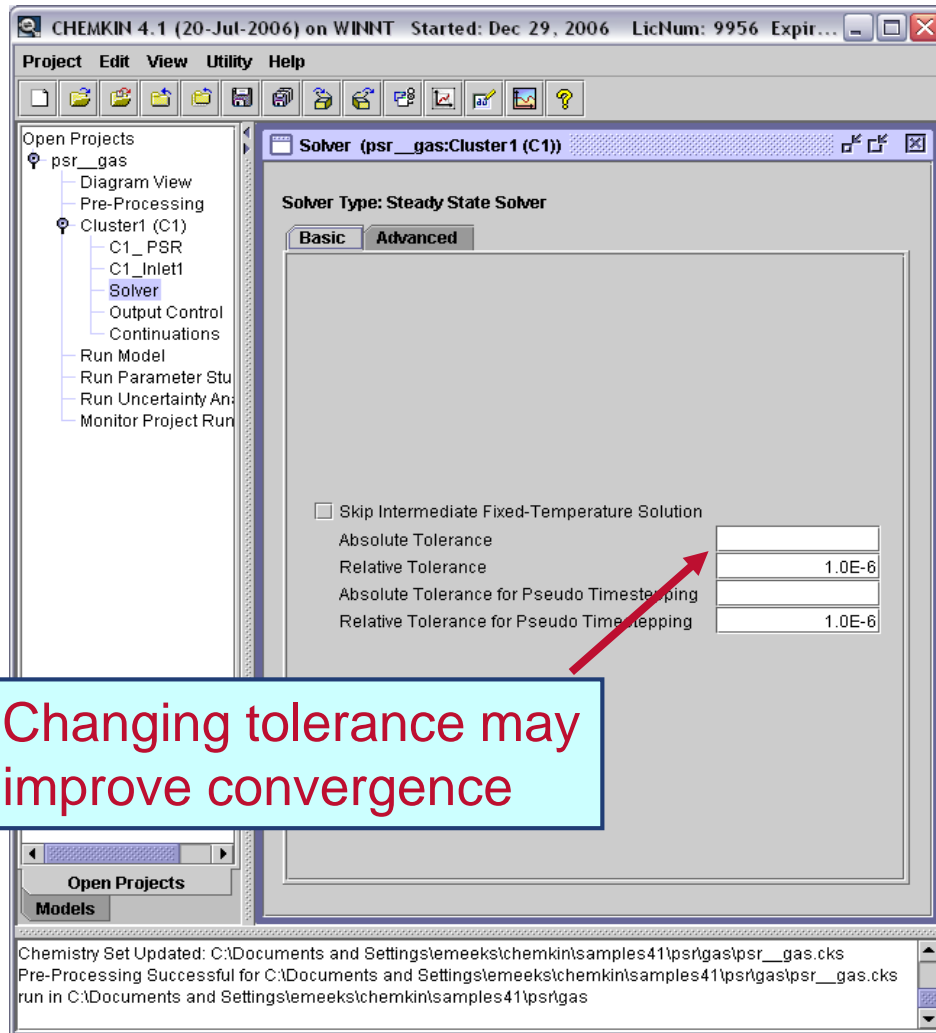
Species Data Add

| Species | Added Species Fraction of Total Reactant Species |
|---------|--|
| N2      | 0.35   |

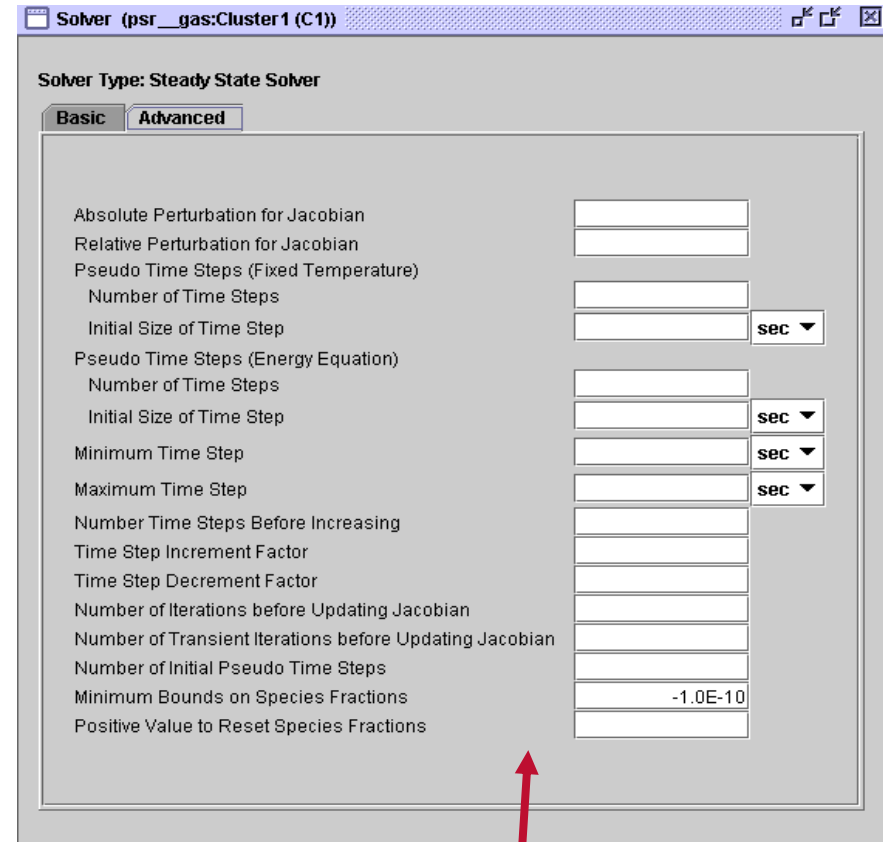
Import Export Delete Row Clear

Third party species, summation must be less than 1.

# Solver setup: usually leave as default



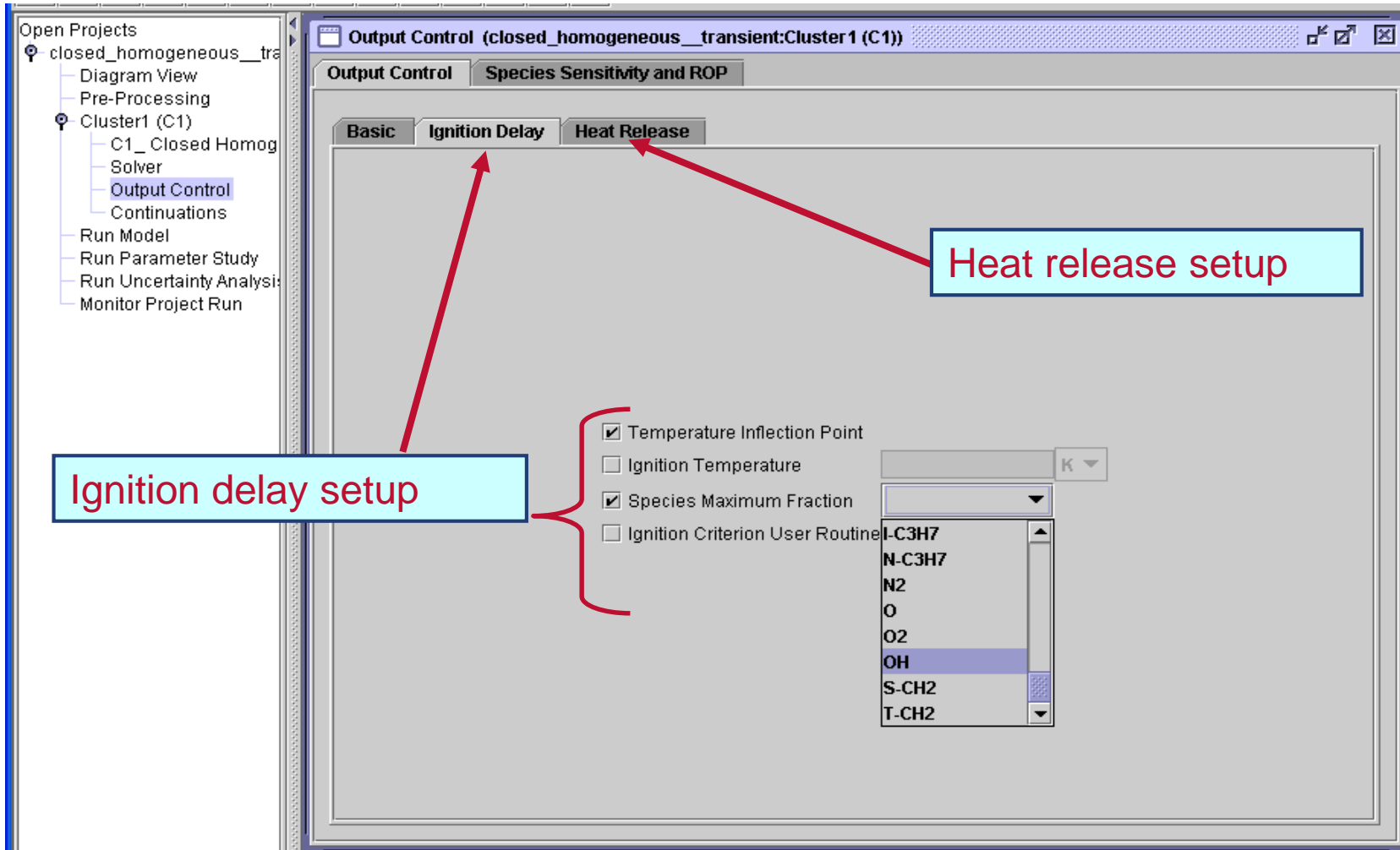
Changing tolerance may improve convergence



Details can be found in manual



# Output control setup



Open Projects

- closed\_homogeneous\_\_tra
- Diagram View
- Pre-Processing
- Cluster1 (C1)
  - C1\_ Closed Homog
  - Solver
  - Output Control
  - Continuations
- Run Model
- Run Parameter Study
- Run Uncertainty Analysis
- Monitor Project Run

Output Control (closed\_homogeneous\_\_transient:Cluster1 (C1))

Output Control Species Sensitivity and ROP

Basic Ignition Delay Heat Release

Heat release setup

Ignition delay setup

- ☒ Temperature Inflection Point
- ☐ Ignition Temperature
- ☒ Species Maximum Fraction
- ☐ Ignition Criterion User Routine

Temperature: K

Species List:

- I-C3H7
- N-C3H7
- N2
- O
- O2
- OH
- S-CH2
- T-CH2

# Output setup

Output Control (ic\_engine\_hcci\_adiabatic:IC\_Engine (C1))

Output Control Species Sensitivity and ROP

Basic Ignition Delay Heat Release

**Data saving setup**

Time Interval for Printing Data  sec

Time Interval for Saving Data  sec   Constant

☒ Save Additional Adaptive Points

☒ Use Solver Integration Steps  20

☐ Based on Variable Change

Change Value

☐ All A-factor Sensitivity

Threshold for Species Sensitivity  0.001

☐ Temperature A-factor Sensitivity

Threshold for Temperature Sensitivity  0.001

☐ All Rate of Production

Threshold for Rate of Production  0.01

Solution Data Block Size  10000000 bytes

Print Level Control  1

Output Control (ic\_engine\_hcci\_adiabatic:IC\_Engine (C1))

Output Control Species Sensitivity and ROP

Species OH

| Species | A-factor Sensitivity | Rate of Production |
|---------|----------------------|--------------------|
|         |                      |                    |

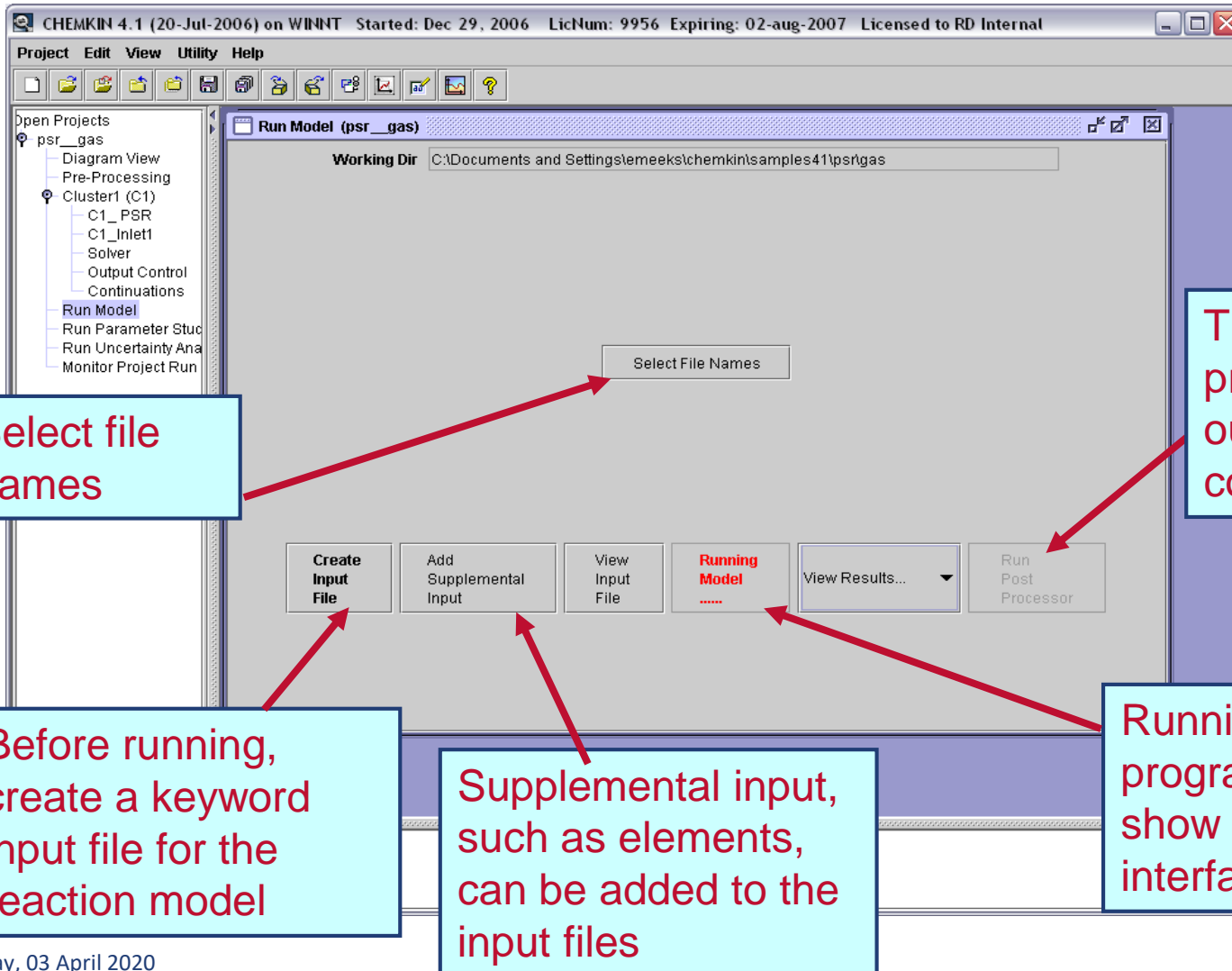
**Sensitivity test setup**

Sensitivity: How much the results rely on a parameter  $K_m$

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

$$K_m = A$$

# Running setup



The screenshot shows the CHEM-KIN 4.1 software interface. The title bar indicates it is running on WINNT, started on Dec 29, 2006, with license number 9956, expiring on 02-aug-2007, and licensed to RD Internal. The menu bar includes Project, Edit, View, Utility, and Help. The toolbar contains icons for file operations and running. The left sidebar shows a project tree for 'psr\_gas' with sub-items: Diagram View, Pre-Processing, Cluster1 (C1) (containing C1\_PSR, C1\_Inlet1, Solver, Output Control, and Continuations), Run Model (highlighted), Run Parameter Stud, Run Uncertainty Ana, and Monitor Project Run. The main window is titled 'Run Model (psr\_gas)' and shows the 'Working Dir' as 'C:\Documents and Settings\emeeks\chemkin\samples41\psr\gas'. A 'Select File Names' button is visible. Below the main window, a row of buttons includes 'Create Input File', 'Add Supplemental Input', 'View Input File', 'Running Model' (highlighted in red), 'View Results...' (with a dropdown arrow), and 'Run Post Processor'. Red arrows point from text boxes to these buttons and the 'Select File Names' button.

**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)

- 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

**Reactant name**

**Reactant construction**

**Suitable T range**

**Mid-Temperature**

```
!
! 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
2.63488400e+00 2.13595200e-02 3.15415100e-07-7.68467400e-09 2.33583200e-12
8.87134600e+03 9.82751500e+00-6.80068100e+00 5.08074400e-02 1.03974700e-05
-1.11958200e-07 8.45915500e-11 1.06053700e+04 5.55452600e+01
```

**Data of a  
reactant**

```
!
! 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
1.77314700e+01 4.93574700e-02 1.19685400e-06-1.63982600e-08 4.89086700e-12
-3.85556000e+04-5.05329800e+01-7.15975000e-01 1.06710900e-01 2.11760500e-05
-2.19321200e-07 1.64414400e-10-3.51554600e+04 3.89076300e+01
```

**$a_1 - a_7$   
For high  
temperature  
region**

**Notes: more information**

# 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
```

**Reactions**

**Parameters: A, B, E**

**Reactants must be  
included in the  
thermodynamic data**

- $\text{H}_2$ /air flame
- 3 elements
- 11 reactants
- 23 reactions

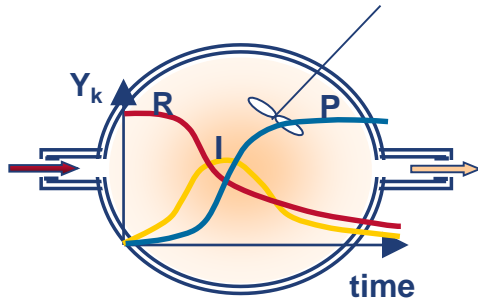
Following Arrhenius formula

- 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

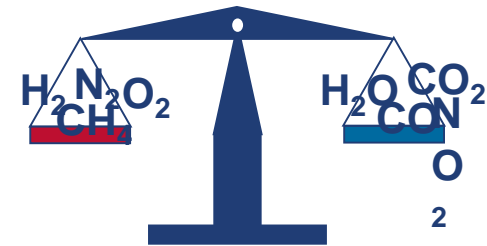




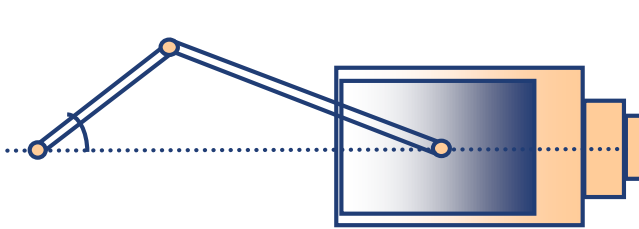
**Perfect stirred reactor  
PSR**



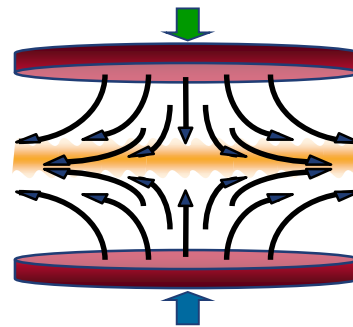
**Plug Flow Reactor**



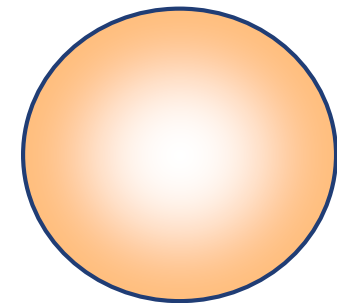
**Chemical and phase  
equilibrium  
calculations**



**Internal combustion  
engines**

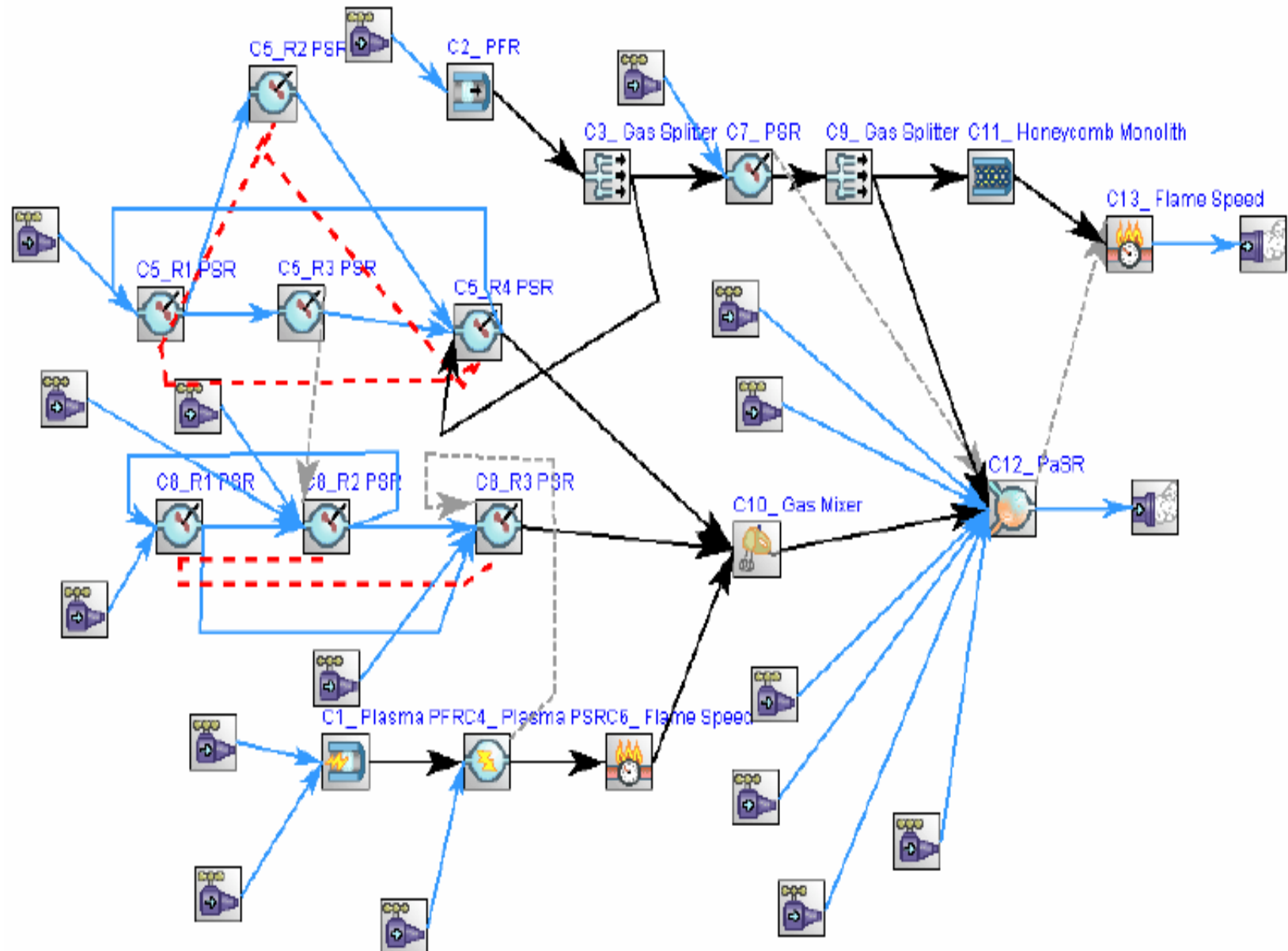


**Flame  
simulators**

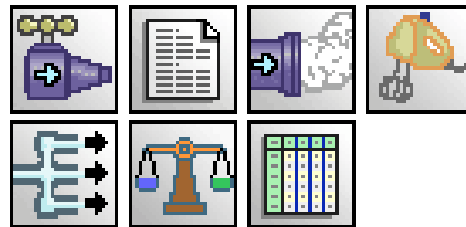


**Closed  
homogeneous  
batch reactor**

# Chemkin model example



## Miscellaneous



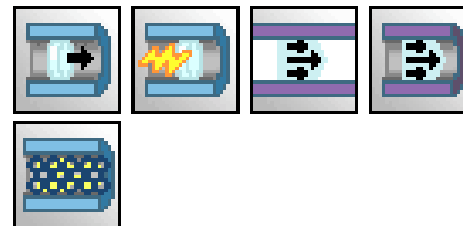
## Closed 0-D Reactors



## Open 0-D Reactors



## Flow Reactors



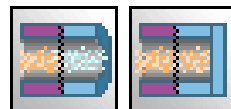
## Flame Simulators



## CVD Reactors



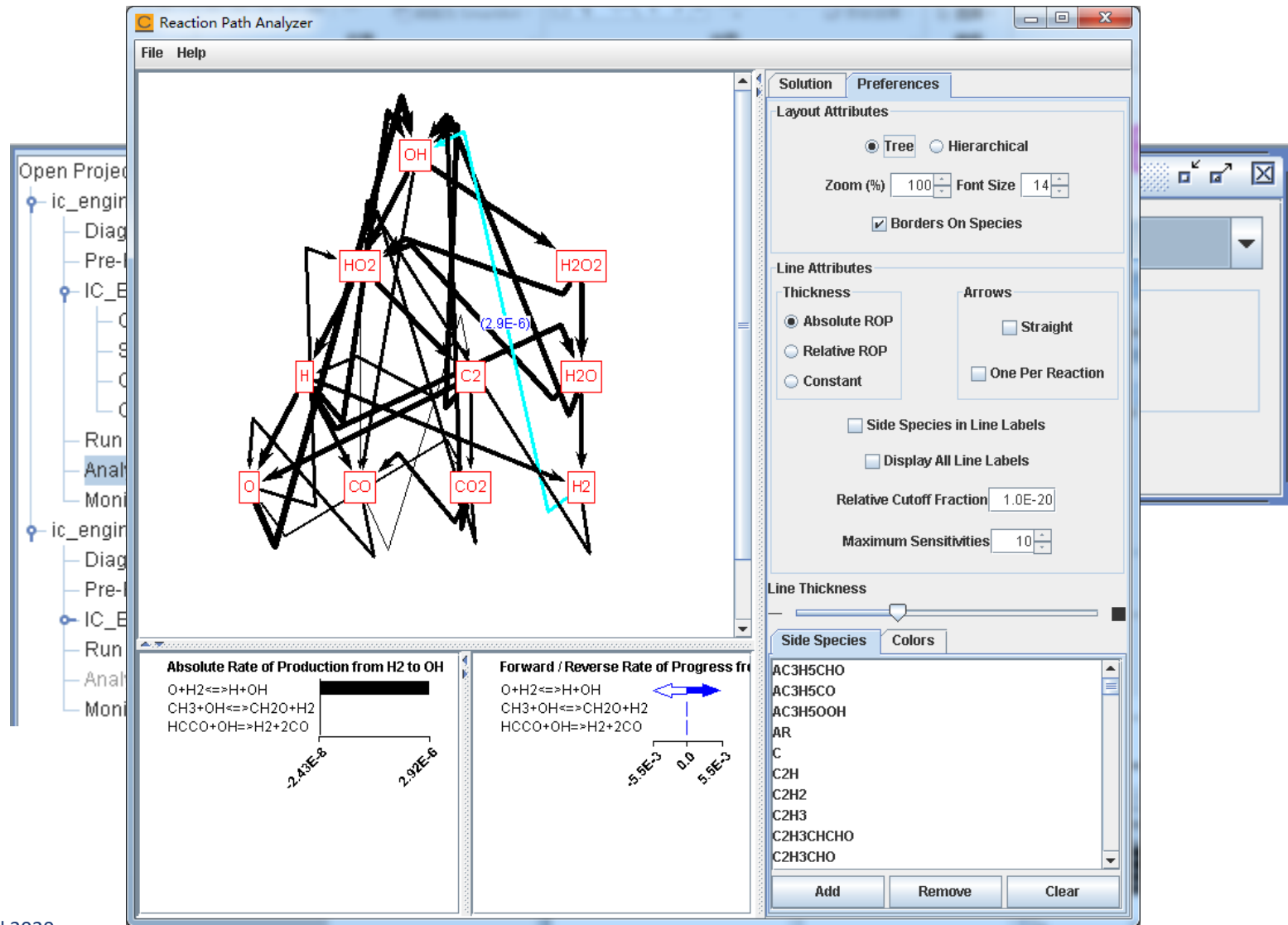
## Shock Tube Reactors



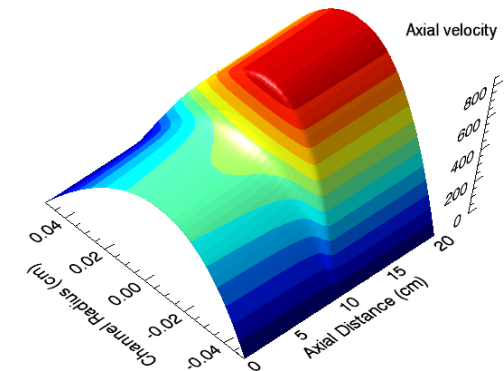
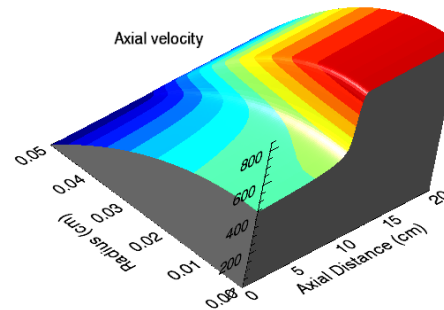
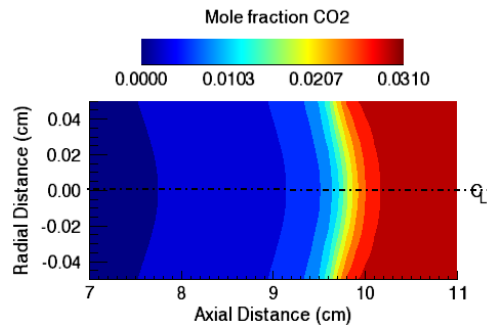
## LPCVD Reactors



## Reaction path analysis and other visualisation options

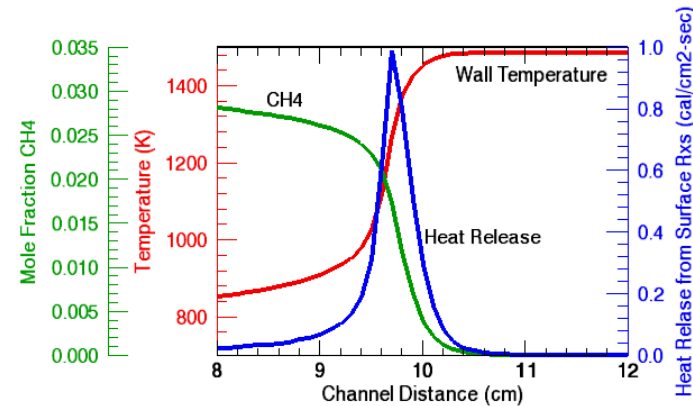
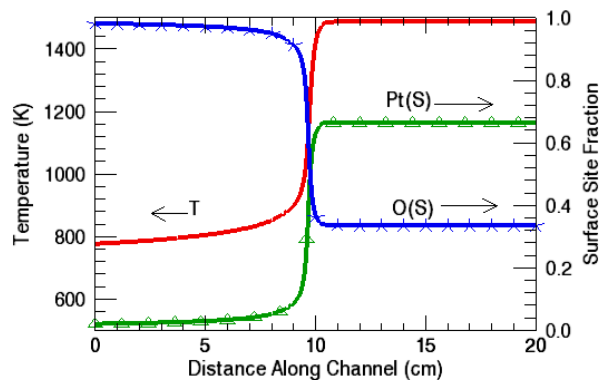


## 3-D contour plot



● Symmetric coordinates

## ● Multi Y axis



## Example 1

Adiabatic flame temperature of  $\text{H}_2 - \text{O}_2$  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.

C1\_Equilibrium



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

ELEMENTS H O N END

SPECIES  $\text{H}_2$  H  $\text{O}_2$  O OH HO $_2$   $\text{H}_2\text{O}$   $\text{N}_2$   $\text{H}_2\text{O}_2$  END

Thermodynamic data use ...\\data\\therm.dat

## Example 1

Adiabatic flame temperature of  $\text{H}_2 - \text{O}_2$  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:  $\text{H}_2$ , H,  $\text{O}_2$ , O, OH,  $\text{H}_2\text{O}$ , HO $_2$ ,  $\text{H}_2\text{O}_2$  and  $\text{N}_2$  or Ar, with about 18-20 reactions. Nitrogen is generally present as  $\text{N}_2$  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  $\text{H}_2 - \text{O}_2$  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

$\text{H}_2$  - 2

$\text{N}_2$  - 3.76

$\text{O}_2$  - 1

Continuations

Insert 2 new runs, set temperature 400 and 500 K

Run the model



## Example 1

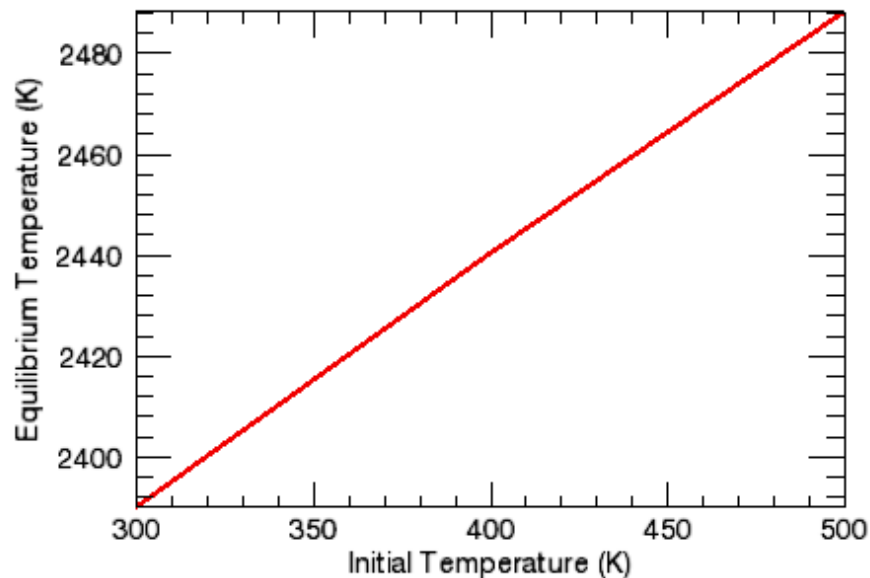
Adiabatic flame temperature of  $\text{H}_2 - \text{O}_2$  combustion, equilibrium

Analyse results

Choose x as initial temperature

Choose y as equilibrium temperature

Display the results



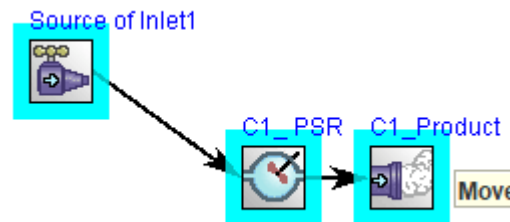
## Example 2

### 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

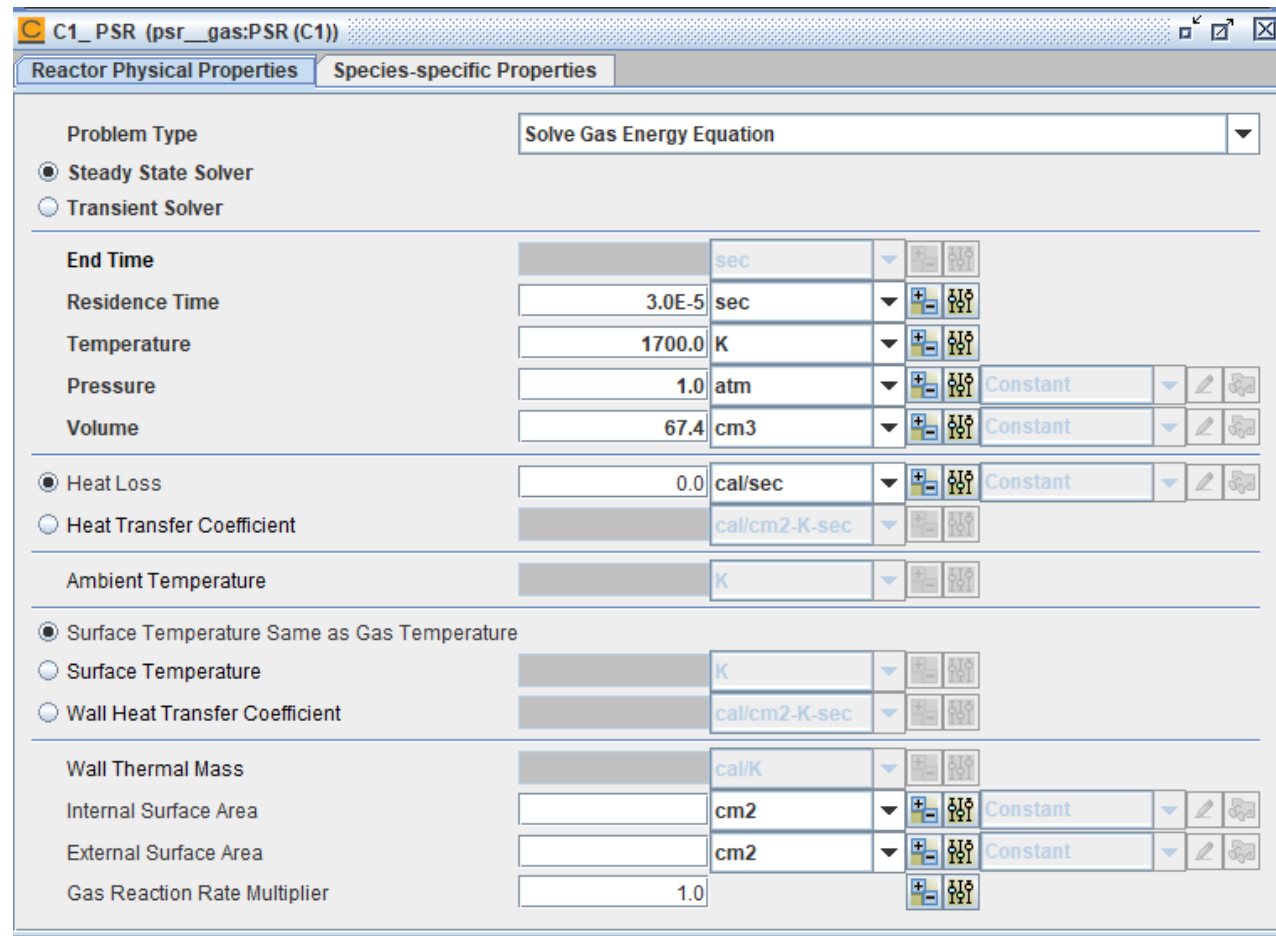
Problem Type is first set  
to Solve Gas Energy  
Equation, and the Steady  
State Solver is chosen

Residence time 0.03ms

Pressure 1atm

Volume 67.4cm<sup>3</sup>

No heat losses (adiabatic)  
1700 K is estimated gas  
temperature.



**C1\_PSR (psr\_gas:PSR (C1))**

**Reactor Physical Properties** | **Species-specific Properties**

**Problem Type**: Solve Gas Energy Equation

☒ **Steady State Solver**  
☐ **Transient Solver**

|                       |        |     |          |
|-----------------------|--------|-----|----------|
| <b>End Time</b>       |        | sec |          |
| <b>Residence Time</b> | 3.0E-5 | sec |          |
| <b>Temperature</b>    | 1700.0 | K   |          |
| <b>Pressure</b>       | 1.0    | atm | Constant |
| <b>Volume</b>         | 67.4   | cm3 | Constant |

☒ **Heat Loss**: 0.0 cal/sec  
☐ **Heat Transfer Coefficient**: cal/cm2-K-sec

**Ambient Temperature**: K

☒ **Surface Temperature Same as Gas Temperature**  
☐ **Surface Temperature**: K  
☐ **Wall Heat Transfer Coefficient**: cal/cm2-K-sec

**Wall Thermal Mass**: cal/K  
**Internal Surface Area**: cm2  
**External Surface Area**: cm2  
**Gas Reaction Rate Multiplier**: 1.0

## Example 2

### Steady-state Gas-phase Combustion

Detailed setup: inlet

Temperature 298 K

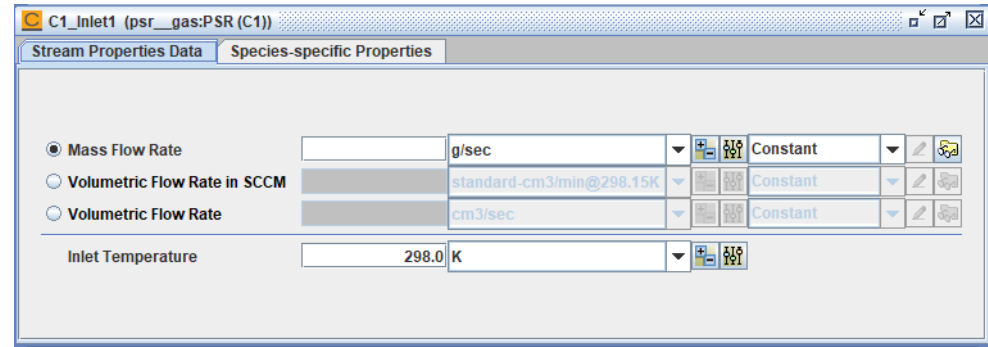
Other parameters set in the PSR  
(mass flow rate ..)

Equivalence ratio: 1

Fuel composition: 80% hydrogen  
and 20 nitrogen

Oxidizer: 79% N<sub>2</sub> and 21% O<sub>2</sub>

Complete combustion products  
tab specifies the complete  
combustion products.



C1\_Inlet1 (psr\_gas:PSR (C1))

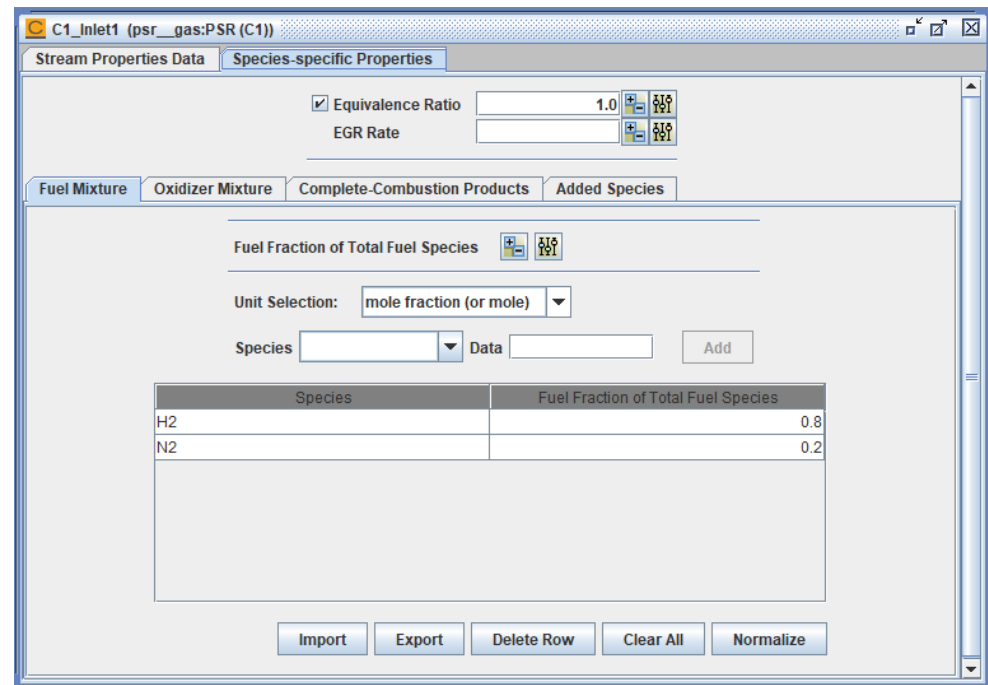
Stream Properties Data Species-specific Properties

☒ Mass Flow Rate  g/sec   Constant

☐ Volumetric Flow Rate in SCCM    Constant

☐ Volumetric Flow Rate    Constant

Inlet Temperature  K



C1\_Inlet1 (psr\_gas:PSR (C1))

Stream Properties Data Species-specific Properties

☒ Equivalence Ratio

EGR Rate

Fuel Mixture Oxidizer Mixture Complete-Combustion Products Added Species

Fuel Fraction of Total Fuel Species

Unit Selection:

Species  Data

| Species | Fuel Fraction of Total Fuel Species |
|---------|-------------------------------------|
| H2      | 0.8                                 |
| N2      | 0.2                                 |

# 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...

Continuations (psr\_gas:PSR (C1))

STEP 1. Select Parameter Group: Inlet Stream Properties

STEP 2. Select Type: No Selection

STEP 3. Select Parameter: Equivalence Ratio

☒ Equivalence Ratio C1\_Inlet1

Add Input to Continuation Import Input to Continuation

Continuation #5 Continuation #6 Continuation #7 Continuation #8 Continuation #9

Continuation #1 Continuation #2 Continuation #3 Continuation #4

| Keyword Label     | Reactor/Stream | Material/Species | Data Value | Units |
|-------------------|----------------|------------------|------------|-------|
| Equivalence Ratio | C1_Inlet1      | --               | 1.2        | --    |

Copy Prev. Cont. Delete Row Clear All Insert Cont. Delete Cont.

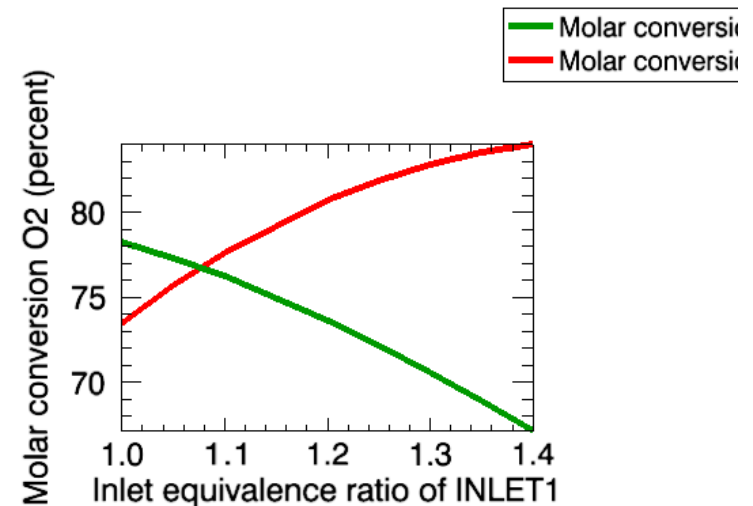
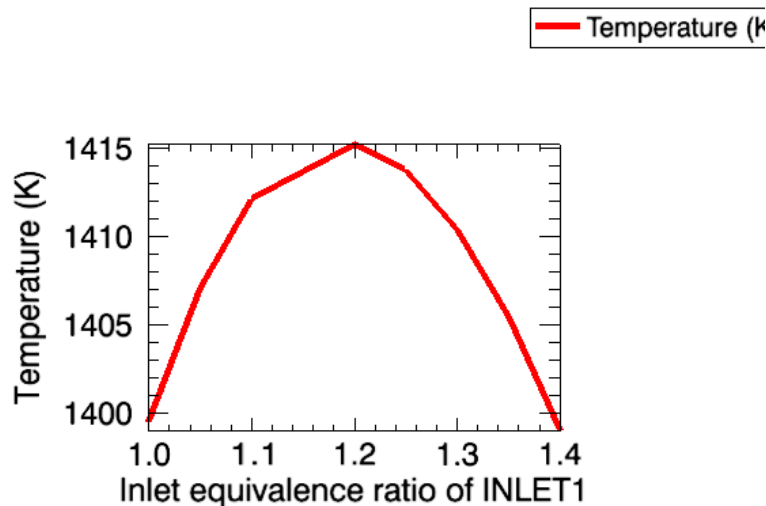
Reset # of Continuations Clear All Continuations

## 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<sup>3</sup> will be used

End time: 0.1 sec (This needs to be large enough to allow for ignition to occur)

C1\_Closed Homogeneous (closed\_homogeneous\_ignition\_delay:Closed\_Homogeneous (C1))

Reactor Physical Properties    Reactant Species

|  |  |               |          |  |
|--|--|---------------|----------|--|
| Problem Type   | Constrain Pressure And Solve Energy Equation (Default) |               |          |  |
| End Time   | 0.1  | sec           |          |  |
| Temperature  | 1200.0   | K             |          |  |
| Pressure   | 1.0  | atm           | Constant |  |
| Volume   |  | cm3           | Constant |  |
| <input checked="" type="radio"/> Heat Loss                                   | 0.0  | cal/sec       | Constant |  |
| <input type="radio"/> Heat Transfer Coefficient                              |  | cal/cm2-K-sec |          |  |
| Ambient Temperature  |  | K             |          |  |
| <input checked="" type="radio"/> Surface Temperature Same as Gas Temperature |  | K             |          |  |
| <input type="radio"/> Surface Temperature                                    |  | K             |          |  |
| <input type="radio"/> Wall Heat Transfer Coefficient                         |  | cal/cm2-K-sec |          |  |
| Wall Thermal Mass  |  | cal/K         |          |  |
| Internal Surface Area  |  | cm2           | Constant |  |
| External Surface Area  |  | cm2           | Constant |  |
| Gas Reaction Rate Multiplier   | 1.0  |               |          |  |

# Example 3

## Ignition-delay Times for Propane Autoignition

Further reactor setup

Reactant species

Starting gas mixture

0.02 C<sub>3</sub>H<sub>8</sub>

0.05 O<sub>2</sub>

0.93 Ar

A rather diluted condition

C1\_Closed Homogeneous (closed\_homogeneous\_ignition\_delay:Closed\_Homogeneous (C1))

Reactor Physical Properties    **Reactant Species**

☐ Equivalence Ratio

EGR Rate

---

**Reactant Fraction**

Reactant Fraction

Unit Selection:

Species   Data

| Species | Reactant Fraction |
|---------|-------------------|
| AR      | 0.93              |
| C3H8    | 0.02              |
| O2      | 0.05              |

## Example 3

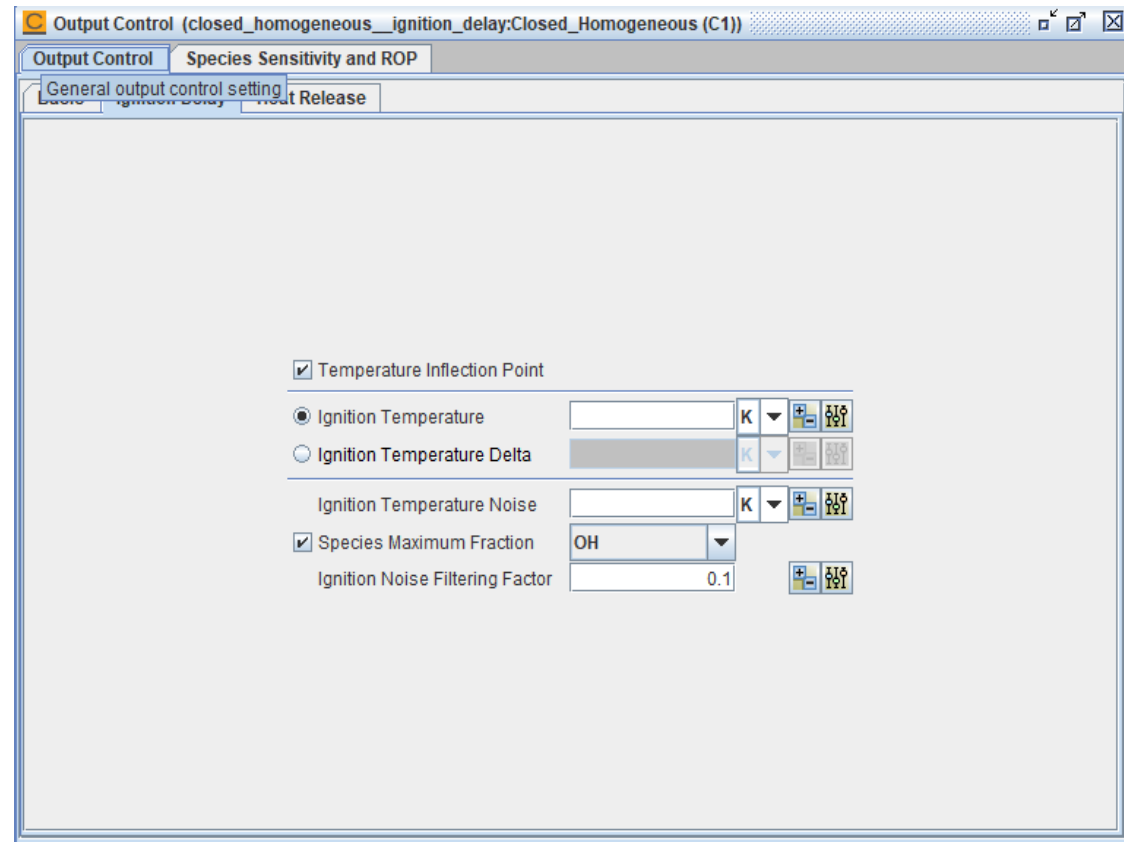
### Ignition-delay Times for Propane Autoignition

#### 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.

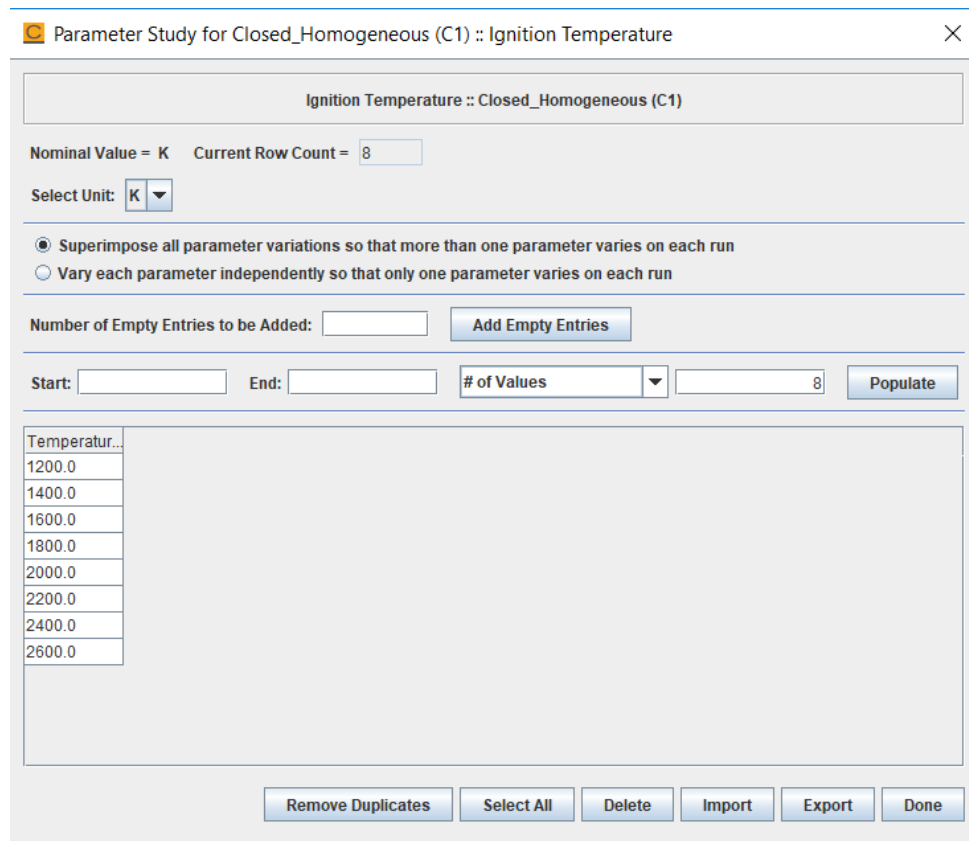
## Example 3

### 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.



Parameter Study for Closed\_Homogeneous (C1) :: Ignition Temperature

Ignition Temperature :: Closed\_Homogeneous (C1)

Nominal Value = K    Current Row Count = 8

Select Unit: K

☒ Superimpose all parameter variations so that more than one parameter varies on each run  
☐ Vary each parameter independently so that only one parameter varies on each run

Number of Empty Entries to be Added:    Add Empty Entries

Start:    End:    # of Values    8    Populate

| Temperatur... |
|---------------|
| 1200.0        |
| 1400.0        |
| 1600.0        |
| 1800.0        |
| 2000.0        |
| 2200.0        |
| 2400.0        |
| 2600.0        |

Remove Duplicates    Select All    Delete    Import    Export    Done

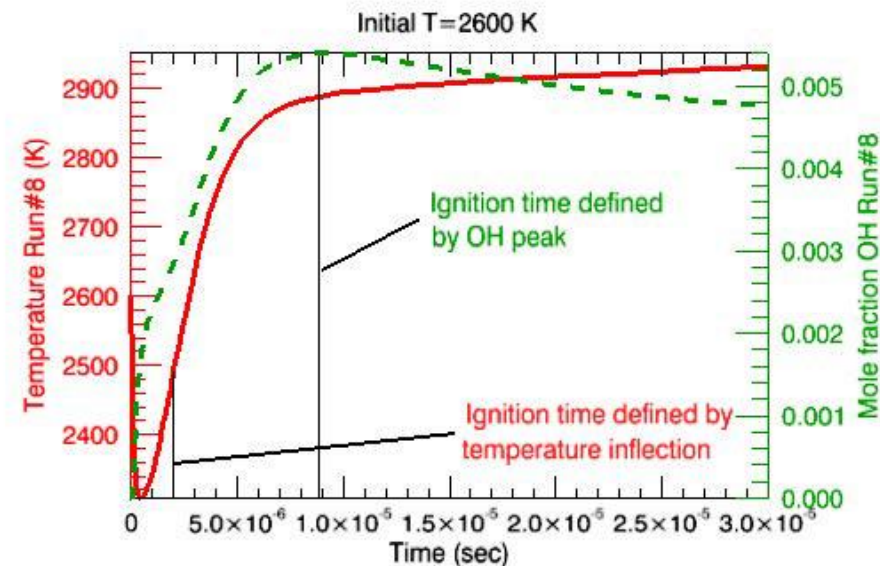
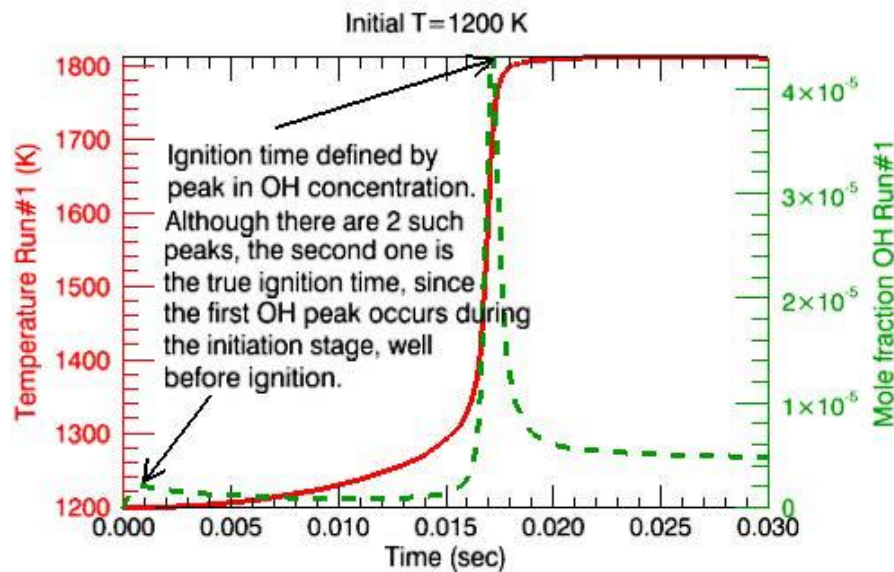
# Example 3

## Ignition-delay Times for Propane Autoignition

### Results

**Table 2-6** Initial Temperatures and Ignition Times

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

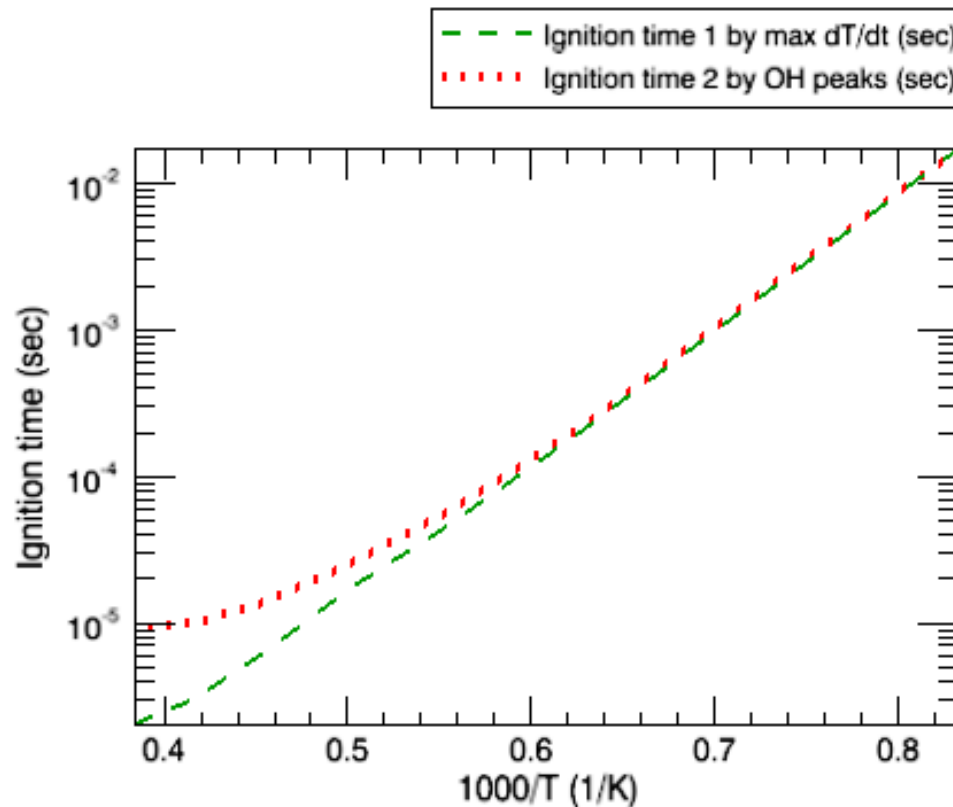


## Example 3

### 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:

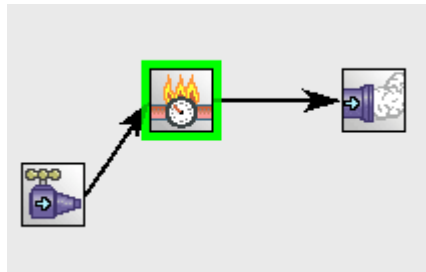
1. Equivalence ratios of 0.6 –1.4 in 0.1 interval.
2. Initial temperatures of 300 K and 700 K.
3. Pressure of 1 atm

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


☒ **Equivalence Ratio**   

**EGR Rate**   





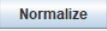
Fuel Mixture | Oxidizer Mixture | Complete-Combustion Products | Added Species

Fuel Fraction of Total Fuel Species  



Unit Selection: **mole fraction (or mole)**

Species  Data  


| Species | Fuel Fraction of Total Fuel Species |
|---------|-------------------------------------|
| C3H8    | 1.0                                 |




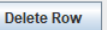

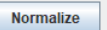
Fuel Mixture | Oxidizer Mixture | Complete-Combustion Products | Added Species

Oxidizer Fraction of Total Oxidizer Species  

Unit Selection: **mole fraction (or mole)**

Species  Data  

| Species | Oxidizer Fraction of Total Oxidizer Species |
|---------|---|
| N2      | 0.79  |
| O2      | 0.21  |

## 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

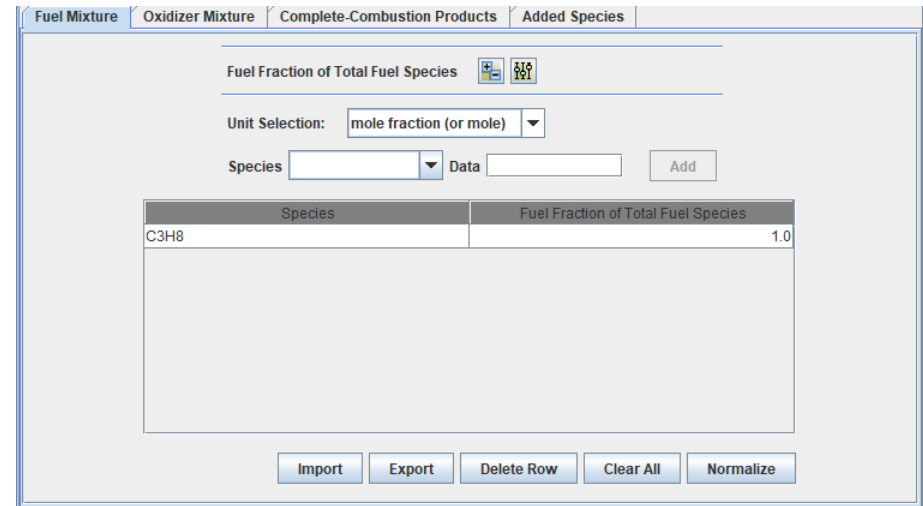


☒ Equivalence Ratio 1.0


EGR Rate

Start from 0.6 end 1.4, 9 values.

After setup parametric study, this variable becomes blue underlined.



Fuel Mixture | Oxidizer Mixture | Complete-Combustion Products | Added Species

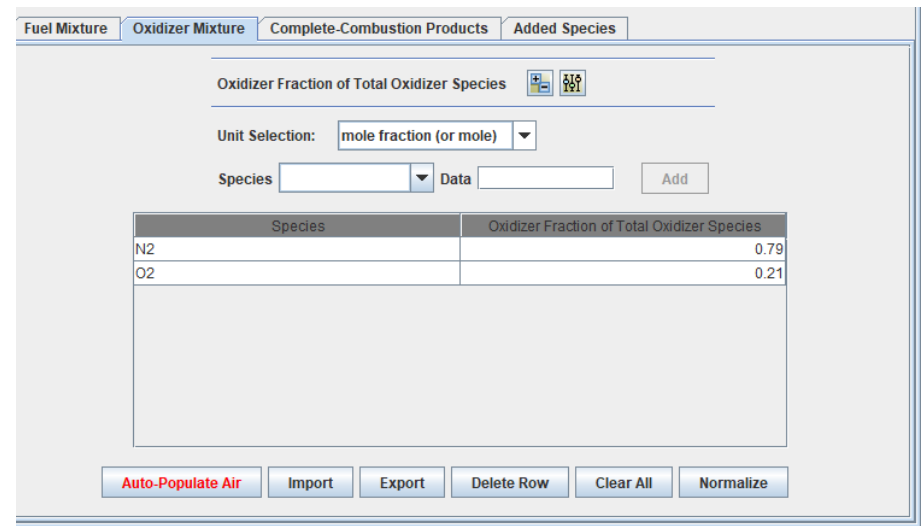
Fuel Fraction of Total Fuel Species 

Unit Selection: mole fraction (or mole)


Species  Data  Add

| Species | Fuel Fraction of Total Fuel Species |
|---------|-------------------------------------|
| C3H8    | 1.0                                 |

Import Export Delete Row Clear All Normalize



Fuel Mixture | Oxidizer Mixture | Complete-Combustion Products | Added Species

Oxidizer Fraction of Total Oxidizer Species 

Unit Selection: mole fraction (or mole)

Species  Data  Add

| Species | Oxidizer Fraction of Total Oxidizer Species |
|---------|---|
| N2      | 0.79  |
| O2      | 0.21  |

Auto-Populate Air Import Export Delete Row Clear All Normalize

## Example 4

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

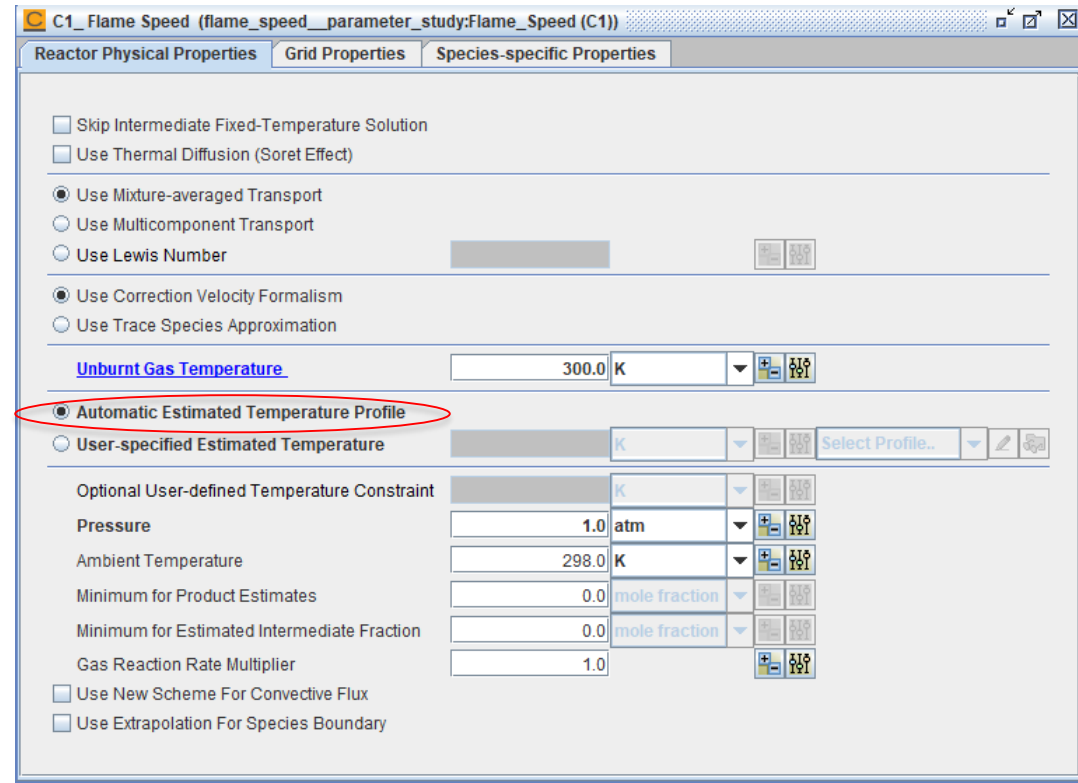
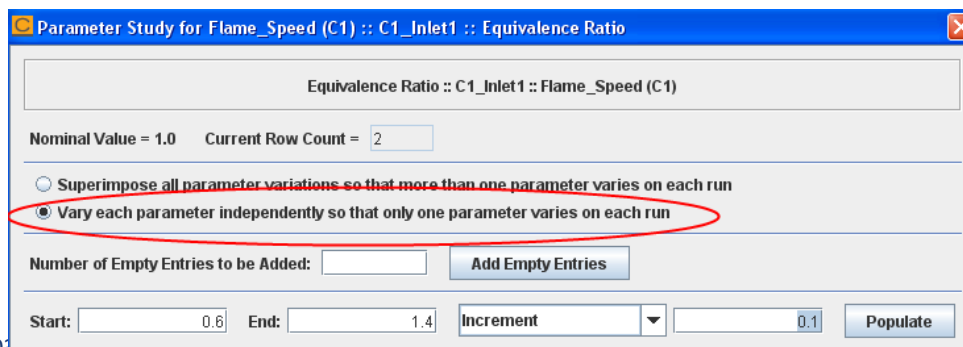
#### Reactor setup

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

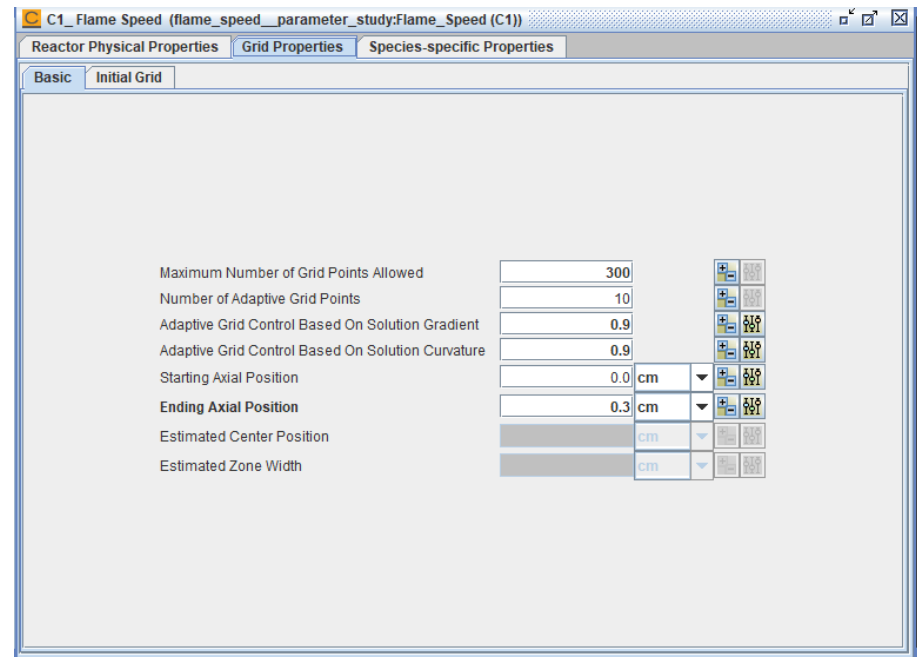
Reactor setup

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.



C1\_Flame Speed (flame\_speed\_parameter\_study:Flame\_Speed (C1))

Reactor Physical Properties | Grid Properties | Species-specific Properties

Basic | Initial Grid

Maximum Number of Grid Points Allowed: 300

Number of Adaptive Grid Points: 10

Adaptive Grid Control Based On Solution Gradient: 0.9

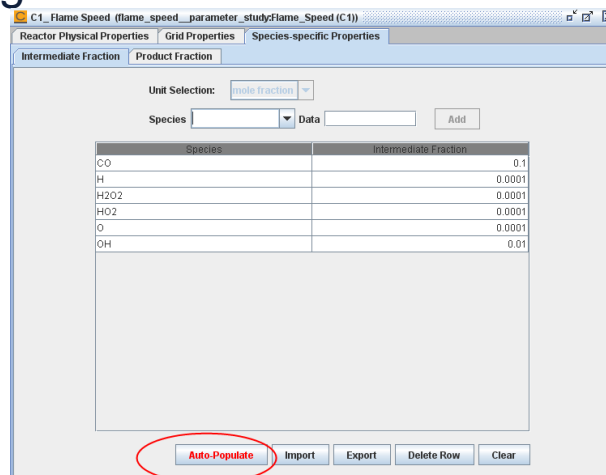
Adaptive Grid Control Based On Solution Curvature: 0.9

Starting Axial Position: 0.0 cm

Ending Axial Position: 0.3 cm

Estimated Center Position: cm

Estimated Zone Width: cm



C1\_Flame Speed (flame\_speed\_parameter\_study:Flame\_Speed (C1))

Reactor Physical Properties | Grid Properties | Species-specific Properties

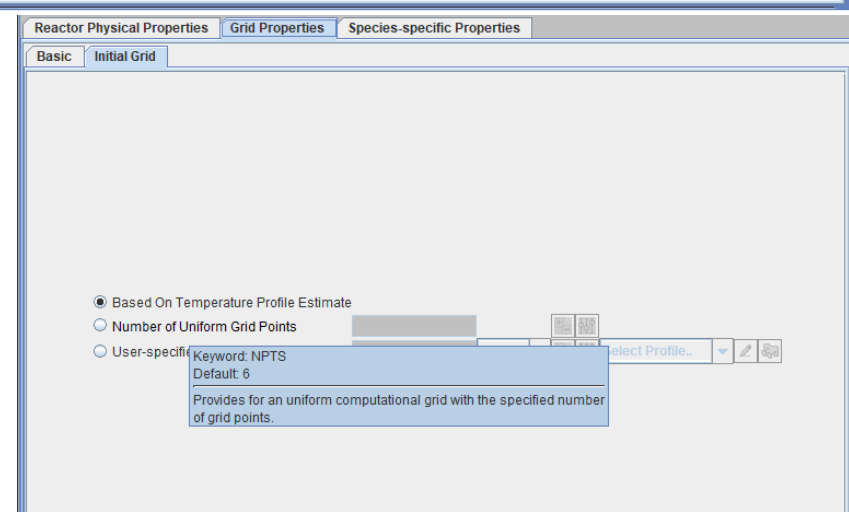
Intermediate Fraction | Product Fraction

Unit Selection: mole fraction

Species: Data Add

| Species | Intermediate Fraction |
|---------|-----------------------|
| CO      | 0.1                   |
| H       | 0.0001                |
| H2O2    | 0.0001                |
| HO2     | 0.0001                |
| O       | 0.0001                |
| OH      | 0.01                  |

Auto-Populate Import Export Delete Row Clear



Reactor Physical Properties | Grid Properties | Species-specific Properties

Basic | Initial Grid

☒ Based On Temperature Profile Estimate

☐ Number of Uniform Grid Points

☐ User-specified

Keyword: NPTS  
Default: 6  
Provides for a uniform computational grid with the specified number of grid points.

# 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.

Continuations (flame\_speed\_parameter\_study:Flame\_Speed (C1))

STEP 1. Select Parameter Group: **Reactor Properties**

STEP 2. Select Type: **No Selection**

STEP 3. Select Parameter: **--- Select a Parameter ---**

Please follow the steps to select a parameter for continuation/new run setting.

**Add Input to Continuation** **Import Input to Continuation**

Continuation #1 Continuation #2 Continuation #3

| Keyword Label                              | Reactor/Stream  | Material/Species | Data Value | Units |
|--|-----------------|------------------|------------|-------|
| Adaptive Grid Control Based On Solution... | C1_ Flame Speed | --               | 0.5        | --    |
| Adaptive Grid Control Based On Solution... | C1_ Flame Speed | --               | 0.5        | --    |
| Ending Axial Position                      | C1_ Flame Speed | --               | 0.5        | cm    |
| Starting Axial Position                    | C1_ Flame Speed | --               | -0.1       | cm    |

**Delete Row** **Clear All** **Insert Cont.** **Delete Cont.**

**Reset # of Continuations** **Clear All Continuations**

Continuation #1 Continuation #2 Continuation #3

| Keyword Label             | Reactor/Stream  | Material/Species | Data Value | Units |
|---------------------------|-----------------|------------------|------------|-------|
| Adaptive Grid Control ... | C1_ Flame Speed | --               | 0.2        | --    |
| Adaptive Grid Control ... | C1_ Flame Speed | --               | 0.2        | --    |
| Ending Axial Position     | C1_ Flame Speed | --               | 2.0        | cm    |
| Starting Axial Position   | C1_ Flame Speed | --               | -1.0       | cm    |

Continuation #1 Continuation #2 Continuation #3

| Keyword Label             | Reactor/Stream  | Material/Species | Data Value | Units |
|---------------------------|-----------------|------------------|------------|-------|
| Adaptive Grid Control ... | C1_ Flame Speed | --               | 0.1        | --    |
| Adaptive Grid Control ... | C1_ Flame Speed | --               | 0.1        | --    |
| Ending Axial Position     | C1_ Flame Speed | --               | 10.0       | cm    |
| Starting Axial Position   | C1_ Flame Speed | --               | -2.0       | cm    |

**Copy Prev. Cont.** **Delete Row** **Clear All** **Insert Cont.** **D**

**Reset # of Continuations** **Clear All C**

## Example 4

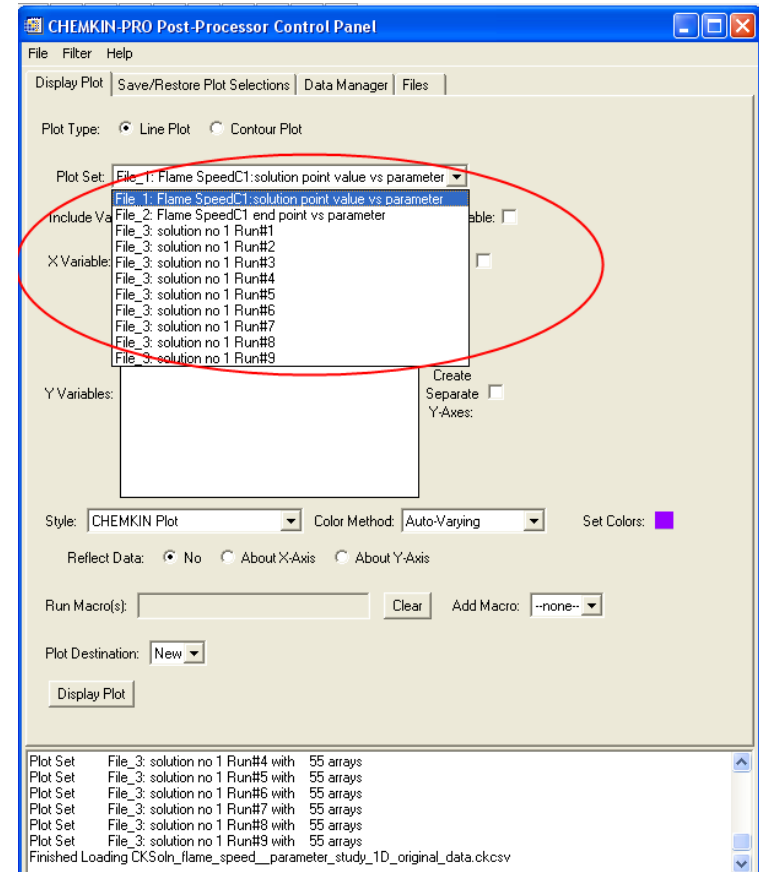
Parameter Study: Propane/Air Flame Speed as a Function of Equivalence Ratio and Unburned Gas Temperature

### 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

File Filter Help

Display Plot Save/Restore Plot Selections Data Manager Files

Plot Type: ☒ Line Plot ☐ Contour Plot

Plot Set: File\_3: Flame SpeedC1 end point vs parameter

Include Variables from Other Plot Sets: ☐ Use Plot Grouping Variable: ☒


Filter X: Y:

X Variable: Equivalence Ratio C1 Inlet1 Flame Speed (C1) Sort X: ☐

Y Variables:

- Mole fraction C3H4 Soln#4 end point
- Mole fraction C3H3 Soln#4 end point
- Mole fraction C3H5 Soln#4 end point
- Mole fraction C3H6 Soln#4 end point
- Mole fraction C3H8 Soln#4 end point
- Mole fraction I-C3H7 Soln#4 end point
- Mole fraction N-C3H7 Soln#4 end point
- Flow rate Soln#4 end point
- Molecular weight Soln#4 end point
- Mole fraction CH3CHOH Soln#4 end point
- Mole fraction CH3CO Soln#4 end point
- Number of grid points end point
- Flame speed end point

Create Separate Y-Axes: ☐

Style: CHEMKIN Plot Color Method: Auto-Varying Set Colors: 

Reflect Data: ☒ No ☐ About X-Axis ☐ About Y-Axis

Run Macro(s): Clear Add Macro: --none--

Plot Destination: New

Display Plot

Plot Set File\_4: solution no 4 Run#17 with 55 arrays  
Plot Set File\_4: solution no 1 Run#18 with 55 arrays  
Plot Set File\_4: solution no 2 Run#18 with 55 arrays  
Plot Set File\_4: solution no 3 Run#18 with 55 arrays  
Plot Set File\_4: solution no 4 Run#18 with 55 arrays  
Finished Loading CKSoln\_flame\_speed\_parameter\_study\_1D\_original\_data.csv

Select Grouping Ranges

Please specify the ranges by specifying the range 2..N starting points (minimum values). The starting point of the 1st range is always the minimum data value and cannot be modified. A separate plot line is created for each range. For instance, if the data ranges from 0(Min) to 100(Max) and you specify 3 range starting points at 25, 50, 75, then there are 4 ranges: Min..24.999, 25-49.999, 50-74.999, 75-Max.

You can specify ranges by multi-selecting starting points in the data values list or by directly entering the start in the start points field.

Grouping Variable: Unburnt Gas Temperature C1 Flame Speed Flame Speed (C1)

Data Values:

- 300.00000
- 700.00000
- 700.00000
- 700.00000
- 700.00000
- 700.00000
- 700.00000
- 700.00000
- 700.00000
- 700.00000

Range 1 Start Point: 300.00000

Range 2..N Start Points:

- 700.00000

OK Cancel



## Example 4

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

### Results and post process

