Reduced Reaction Kinetics

Reduction Technique

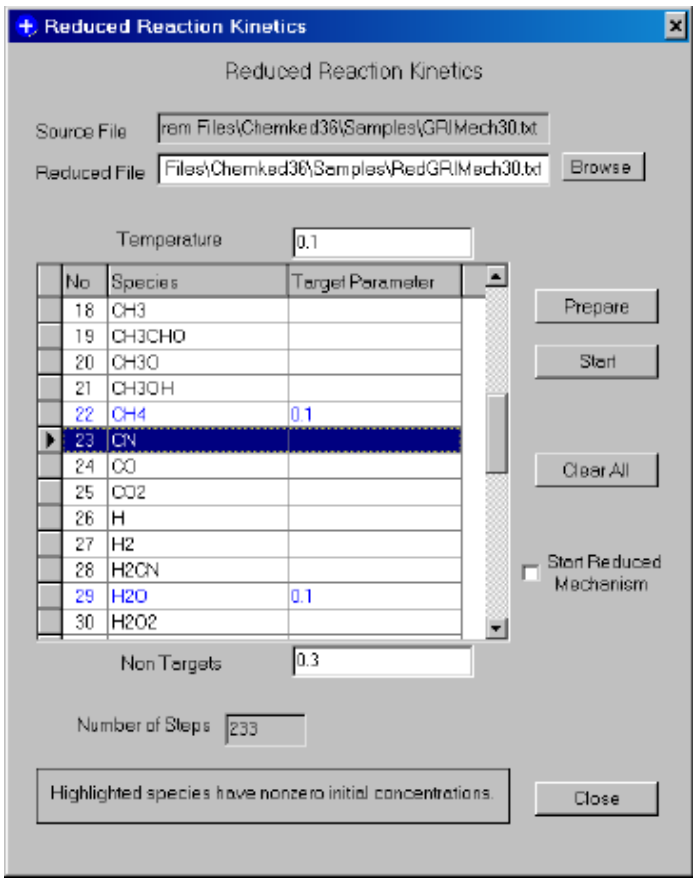
Chemked has a tool for creating reduced reaction mechanism. This procedure includes the following steps.

1. An existing reaction mechanism should be chosen as a detailed reaction mechanism. As a rule, this mechanism consists of a great number of species and reactions.
2. A problem of chemical kinetics is solved with the detailed reaction mechanism for particular initial conditions.
3. The results obtained with the detailed mechanism are used for formation of a particular reduced reaction mechanism. Before starting the formation process, your should define the following control parameters.
   - Specify species, which are believed to be important for the consideration; we will call these species and/or temperature as 'targets'.
   - For the targets and non-targets, enter control parameters that determine accuracy of the selection of important reaction. These values should be set on the interval [0,1].
4. Start the process for creating reduced reaction mechanism.

The reduced mechanism is particular; that is, it is applicable to a certain gas parameters defined by initial condition of the detailed problem. In order to create the reduced mechanism for a domain of parameters, particular reduction mechanisms should be created for separated points within this domain and then the particular mechanisms are united.

Creating Reduced Reaction Mechanism

1. Choose **File** > **Open**. The File dialog appears.
2. In the dialog, select path of the solver file that contains a reaction mechanism you want to reduce (source file). Click the Open button; the window opens. **This file should contain output data of a particular calculation.**
3. Choose **Reaction Kinetics > Postprocessor > Reduced Reaction Kinetics**; the Reduced Kinetics dialog appears.
4. In the **Reduced File** text box of the dialog, enter a file paths where the reduced mechanism will be saved.



The dialog window of reduced reaction kinetics

5. Click the Prepare button. A table with species from the source file appears. In the Target Parameter fields of the table, enter control parameters for species that chosen to be targets.
6. For non-targets, enter a common control parameter in the corresponding text box.
7. Click the Start button. A solver file with a reduce reaction mechanism will be created; this file is ready for execution with the solver.

Converting to CHEMKIN Format

In the created reduced file, reactions have the Chemked specified format. You can convert these reactions to CHEMKIN format. To do this, the following steps should be carried out.

1. Open the solver file you want to convert.
2. Choose **Tools > Reactions in CHEMKIN Format**.

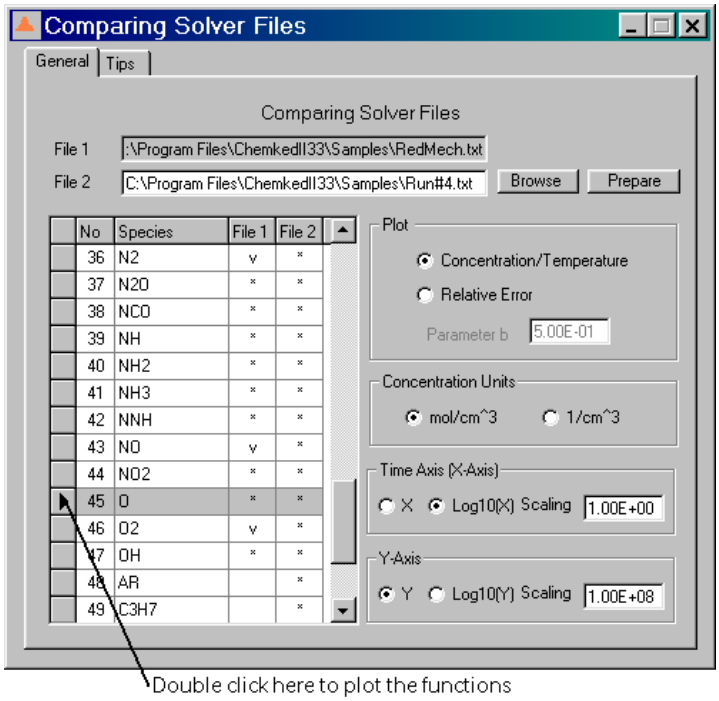
A text document with reaction list will be created.

Comparing Results of Calculations

Chemked-II has tools for comparing time functions of species concentrations and temperature obtained with detailed and reduced reaction mechanisms.

Preparing Information

1. Open a solver file you want to compare. **The file should contain the output data** of a calculation; we call this file as File 1.
2. Choose **Reaction Kinetics > Post-Processor > Compare Results of Calculations**; the Compare dialog appears.



Compare Dialog

3. In the dialog, enter path of File 2 that you want to compare with File 1. **File 2 should contain an output data as well.**
4. Click the Prepare button. A list of species from the files appears. In the table, the asterisks (*) denote species, for which the data is available; the **v** symbols denote targets.

Plotting Concentrations and Temperature

1. In Compare dialog, choose the Concentrations/Temperature option; select the concentration units (mol/cm^3) or (1/cm^3) and enter the scaling factors for axes.
2. Move the table cursor to a species (or Temperature) whose function you want to plot.
3. Double click the row header.

Concentration curves for data from both files appear on Temporary Chart. If you want to add the curves to opened Temporary Chart, hold down the Ctr key and double click the row header.

Error Evaluation

The errors are calculated as follows:

$$\text{Error} = \frac{\text{abs}\,(C_{k,1} - C_{k,2})}{b\,C_{k,1} + (1 - b)\,C_{k,2}},$$

where C_k is the kth species concentration or temperature, the *1* or *2* subscripts correspond to the file number, b is a parameter on the interval [0,1].

In order to create a curve of errors, in Compare dialog, choose the Relative Error option and enter the b parameter in the corresponding text box. Move the table cursor to a row with desirable species and double click the row header. The curve appears on Temporary Chart. If you want to add the curve to existing Temporary Chart, hold down the Ctr key and double click the row header.