Solver File

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The Chemked-II solver is intended for integration of the differential equations of gas phase chemical kinetics at constant pressure without molecular and convective mass and heat transfer. The user can choose the type of the energy equation: constant temperature or adiabatic process.

All information required for starting the solver is stored in one text file; we will call these files as `solver files`. The user can create and keep several solver files. A solver file has the following content:

Control parameters for the solver operation (time interval, initial step size, tolerances and others).
List of species involved in reactions, and thermodynamic data for these species.
List of reactions with parameters for calculating reaction rate constants.
Initial conditions: pressure, temperature and initial mole fractions of species.

The solver uses this information for solving the problem. When the solution finishes the solver writes one more part in the solver file:

Output data: temperature and mass fractions of species as functions of time.

Solver file can be used many times in order to solve the same problem with different initial conditions. However, in this case, old output data will be replaced with new ones. If you want to keep the old output data, you should save the entire file with a new name.

The examination of the output data is performed with post-processor, where the data from the solver file are entered in the subroutine of chemical kinetics to calculate other parameters of the reacting system.

Important. The solver files have a fixed format; we don't recommend you to modify these files.

Remark ----------
In Chemked-II version 3.6 or later, the solver output contains an additional parameter: "Step Size". Use of this parameter improves the accuracy of some program operators. Because of this the post-processing analysis can be performed if the calculation was done with the solver of a version later than 3.6. If the calculation was done with a previous version of Chemked-II or with Chemked-I, you get the message:

“Format of the data output doesn't meet the Chemked-II requirements. Please run the Chemked-II solver with the examined file to create output in the required format.”

After following this recommendation you can analyze the calculation results.

Creating Solver Files (in Chemked-I only)

New solver file can be created **only in Chemked-I** from a reaction database. You should carry out the following steps.

1. Open the Chemked reaction database that contains reaction mechanism you are going to examine.
2. Activate the reaction database window (click the window).
3. Choose **Reaction Kinetics** > **New Solver File (for Chemked-II)**.
4. The File dialo**g** appears. In the dialog, specify the solver file path and click the Open button.

Running Solver

The solver can be started from a solver file only, and first you should open such a file.

1. Choose **File** > **Open**. The File dialog appears.
2. In the dialog, select the solver file path; click the Open button.

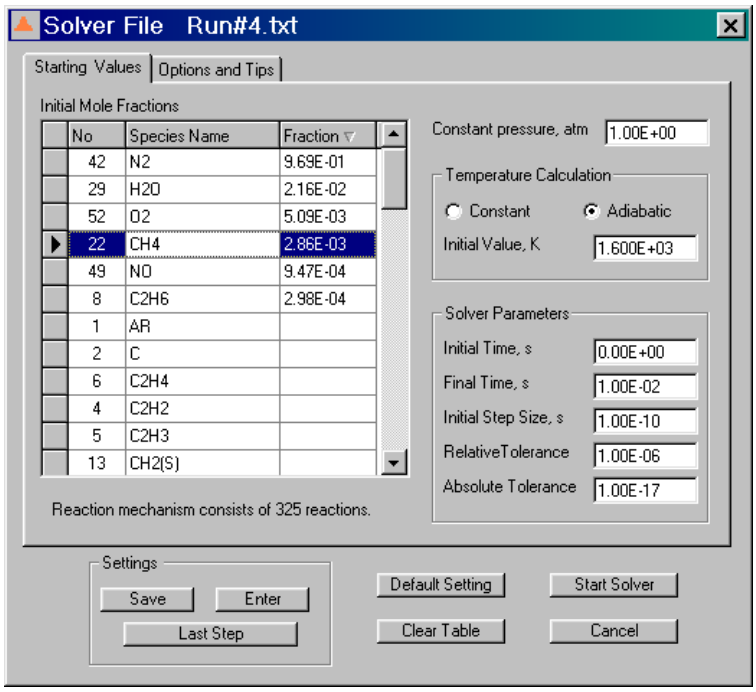
A window with the solver file will open.

To run the solver, carry out the following steps

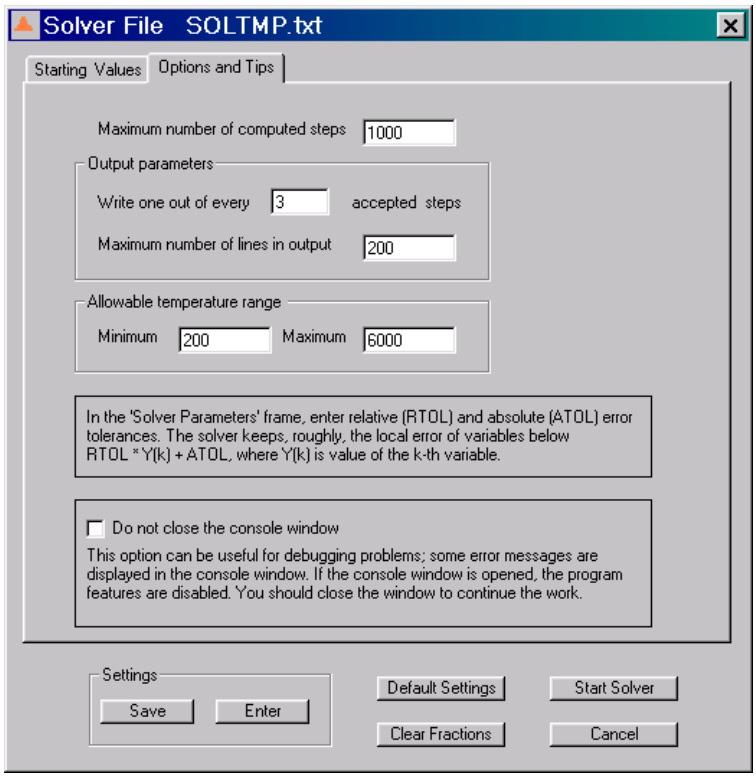
1. Choose **Reaction Kinetics > Run Solver.** The Solver dialog appears.
2. In the dialog, enter initial conditions (pressure, temperature and species mole fractions), specify the solver control parameters; click the Run Solver button.

A console window appears where current information about the problem is displayed. The program will inform you when the solution finishes.

Important. The maximum reaction mechanism size allowed for use in the solver is 300 species and 3000 reactions.



Window for setting initial conditions and control parameters



Window for setting output parameters and temperature range

Analyzing Results of Calculation

When solution of a chemical kinetics problem finishes successfully, the output data (temperature and species mass fractions vs. time) are saved in a solver file. The examination of the output data is performed with the Chemked-II post-processor, where the data are entered in the subroutine of chemical kinetics to calculate other parameters of the reacting system.

In Chemked-II, the two sets of units are used, which are based on the unit volume and on the unit mass. **When analyZing the output data, make sure that you compare data from one set.**

Opening a Solver File

1. Choose **File > Open**, the File dialog appears.
2. In the dialog, specify the solver file path; click the Open button.

A text window opens.

Opening Output Dialog

1. Activate the solver file window.
2. Choose **Reaction Kinetics** > **Post-Processor > Output Dialog**; the dialog appears.

Selecting Rows in Table

In tables of the Output dialog, some operations are performed on selected rows. To select a row, click its header. To use the multiple-selection mode, hold down the Ctrl key and click the row headers. .

Plotting Functions

1. In the Output dialog, click on the tab with item you want to view. The corresponding page appears; the page contains a table with objects of the system under consideration (species or reactions).
2. In the table, select row with the object whose functions you want to plot.
3. Choose a function type , enter an axis scale factor.
4. Double click the row header; the curves of the functions appear in Temporary Chart.

If this procedure is repeated for different rows the existing curves will be replaced with new ones. If you want to add new curves to Temporary Chart, hold down the Ctrl key and then double click the row header.

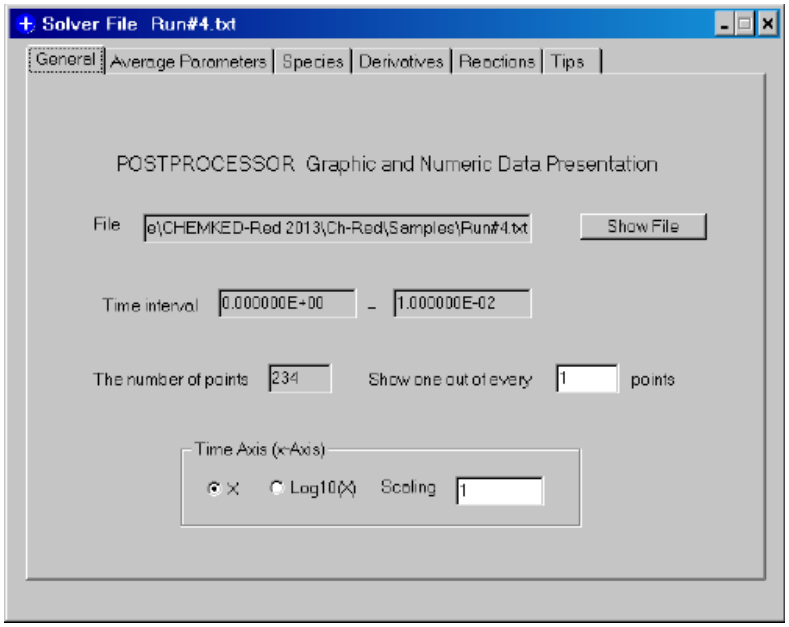
Note. If a functions have negative values, we don't recommend you to create the Log10(*Y*)) axis; the negative values will be omitted.

Note. When a new curve is plotted, the program chooses the types of X,Y axes automatically. In many cases the logarithmic axes are created. To transform them to linear axes, right click mouse on the chart area and choose **X,Y Axes > Linear** from the pop-up menu.

Features of Output Dialog

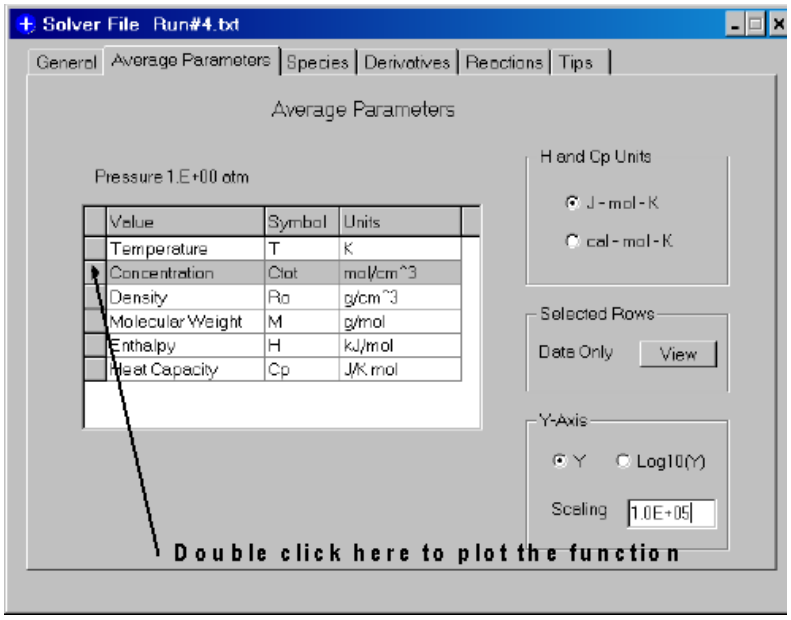
General page

In the frame Time Axis (X-Axis), choose X or Log10(X)) and enter a scale factor. If the number of output steps is too great, you can use every *n*th step; the *n* value should be written in the corresponding text box.
These setting is retained on all pages of this dialog.

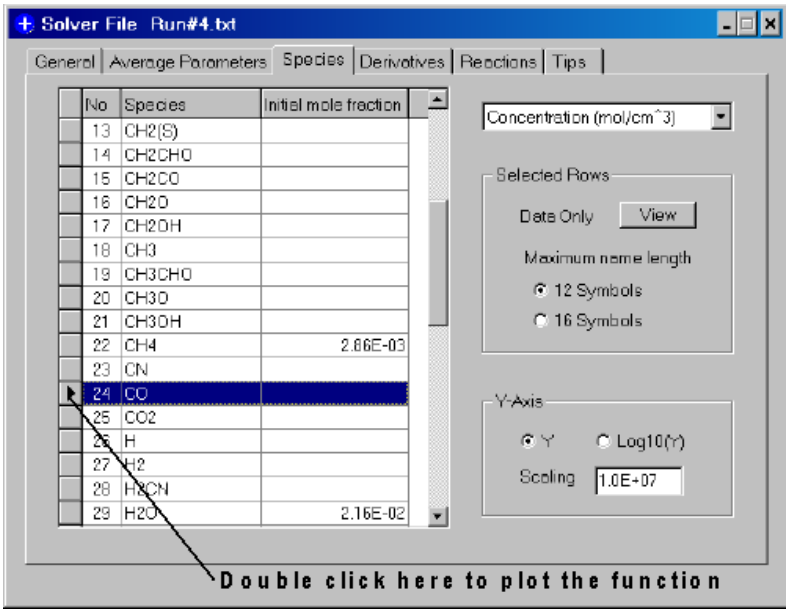


Page of Mean Parameters

Here you can plot functions that are listed in the table. To create a text document with numeric data, select parameters whose data you want to view and click the View button. If needed, you can employ the multiple-selection mode

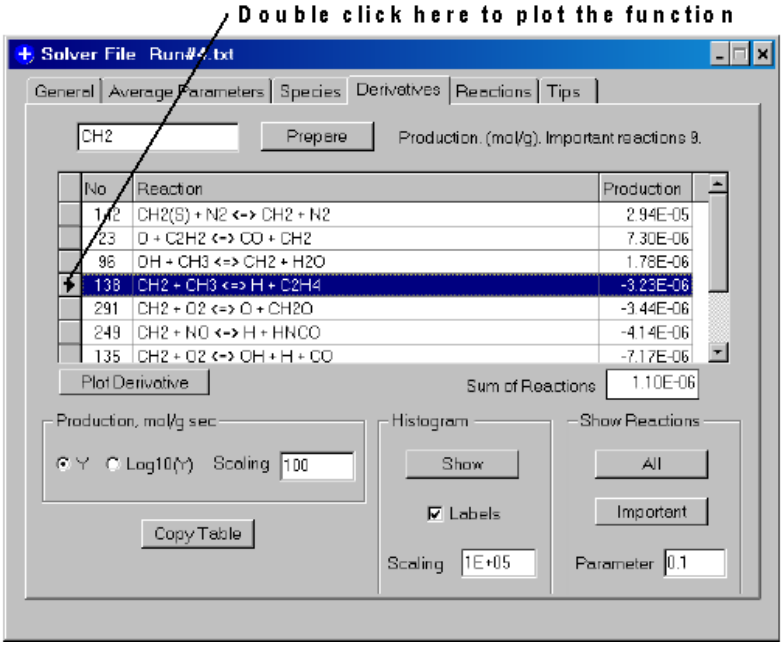


Species Page



For each species you can plot the following functions vs. time:
mole fraction,
mass fraction,
concentration, mol/cm^3
concentration, mol/g.
To create a text document with numeric data, select species whose data you want to view and click the View button. For the selection you can employ the multiple-selection mode

Derivative Page



Here you can analyze contributions of reactions to species derivative (see the help topic **Units of Concentrations and Reaction Rates**)

Primarily you should enter the species name in the text box on the top of the page.This can be done in the following way.

1. Click on the Species tab; the species table appears.
2. Move the table cursor to the species you want to examine.
3. Right click mouse on this species and choose **Copy** from the pop-up menu.
4. Click on the Derivative tab; the Derivative page appears.
5. Right click mouse on the text box and choose **Paste** from the pop-up menu.

You can also simply write the species name in the text box.

Next click the Prepare button. A table with reactions that involve the chosen species appears. The table includes values of the total productions (mol/g) of the chosen species by each reaction. These values can be plotted as a histogram (by clicking the Show button in the Histogram frame) or copy to the clipboard (by clicking the Copy Table button).

For each reaction, the time function of production rate (mol/g sec) of the chosen species can be plotted by double clicking the corresponding row header. To plot the derivative vs. time, click the Plot Derivative button.

Reaction Page

Here you can plot the time functions of forward, reverse and net rates of reactions (mol/cm^3 sec) that involve the species specified in the text box. The way for specifying the species name is discussed in the previous section.

(About reaction rates, see the help topic **Units of Concentrations and Reaction Rates**)