

Running Solver

Open a reaction database with the reaction mechanism you are going to examine. All **valid** reactions from the database will be included in the reaction set for the solver. Then carry out the following steps.

1. Activate the reaction database window.
2. Choose **Reaction Kinetics > Run Solver**. The Solver dialog appears.
3. 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.

The screenshot shows the 'Solver File' dialog box with the 'SOLTMP.txt' file selected. The 'Starting Values' tab is active, displaying a table of initial mole fractions for various species. The 'Options and Tips' tab is also visible. The 'Solver Parameters' section includes fields for initial time, final time, initial step size, relative tolerance, and absolute tolerance. The 'Settings' section at the bottom contains buttons for 'Save', 'Enter', 'Default Settings', 'Run Solver', 'Clear Fractions', and 'Cancel'.

No	Species Name	Fraction
90	N2	6.E+00
112	O2	2.2E+00
66	H2	1.86E+00
60	CH4	5.E-01
3	C2	
4	C2C4H6	
9	C2H4	
2	C	
7	C2H3	
8	C2H3O	
5	C2H	
10	C2H4O	
11	C2H5	
12	C2H5O	
13	C2H5O2	
14	C2H5O2H	
15	C2H5O2H	

Reaction mechanism consists of 1027 valid reactions.

Options and Tips

☒ Constant Pressure
☐ Constant Volume

Initial Pressure, atm:

Temperature

☐ Constant ☒ Adiabatic

Initial Value, K:

Solver Parameters

Initial Time, s:
Final Time, s:
Initial Step Size, s:
Relative Tolerance:
Absolute Tolerance:

Settings

Window for setting initial conditions and control parameters

Solver File SOLTMP.txt

Starting Values Options and Tips

Maximum number of computed steps

Output parameters

Write one out of every accepted steps

Maximum number of lines in output

Allowable temperature interval

Minimum Maximum

In the 'Solver Parameters' frame, enter relative (RTOL) and absolute (ATOL) error tolerances. The solver keeps, roughly, the local error of variables below $RTOL * Y(k) + ATOL$, where $Y(k)$ is value of the k-th variable.

☒ Do not close the console window

This option can be useful for debugging problems; some error messages are displayed in the console window. If the console window is opened, the program features are disabled. You should close the window to continue the work.

Settings

Window for setting output parameters and temperature range

Remark -----

All species under consideration should be explicitly presented in reactions as reactants, products or third bodies. The differential equations of mass conservation will be created only for these species. If the system contains a chemically inert species then this species should be introduced explicitly in the reactions as well. There are two ways to do this.

a. Insert a simple reaction with the inert species into the database.

Example. $AR \rightleftharpoons AR$ 1 0 0

b. If the reaction set contains a third-body reaction then the inert species can be included in the list of third bodies.

Example. $N_2H_4 + M \rightleftharpoons NH_2 + NH_2 + M$ $1.60E+17$ 0 223000
 $AR/1./$

Solver Errors

The solver terminates abnormally when an error occurs. In this case you receive one of the following error messages.

1. Temperature is outside of the allowable range.

Restart the problem; change the temperature range in the corresponding text box.

2. Overflow in forward rate constant.

3. Underflow in equilibrium constant.

4. Overflow in equilibrium constant.

5. Overflow in low pressure rate constant.

6. Overflow in Troe or SRI function.

8. In the Troe function, Fc value is negative.

Error messages 2 - 6 and 8 include also information about the reaction where the error has been occurred.

9. Mean specific heat capacity is equal to zero.

10. The user specified maximum number of computed steps is reached.

Restart the problem; change maximum number of computed steps in the corresponding text box (the maximum allowable number is 100000).

11. Step size becomes too small.

12. Matrix is repeatedly singular.

Try to solve the problem with a greater relative tolerance RTOL.

13. The maximum number of species is 300. Reaction mechanism contains #s

14. The maximum number of reactions is 3000. Reaction mechanism contains #r.

15. The user specified maximum number of lines in output is reached.

Restart the problem; change the maximum number of output lines in the corresponding text box (the maximum allowable number is 10000).

Important. When the errors 2 – 6, 8, 9, and 13 - 14 occur your problem cannot be solved with the Chemked solver.

Viewing Results of Calculation

When the solving a chemical kinetics problem finishes successfully the program will display a prompt: 'Show output?'. If Yes is chosen a solver file will open and Solver Output dialog will appear.

Remark -----

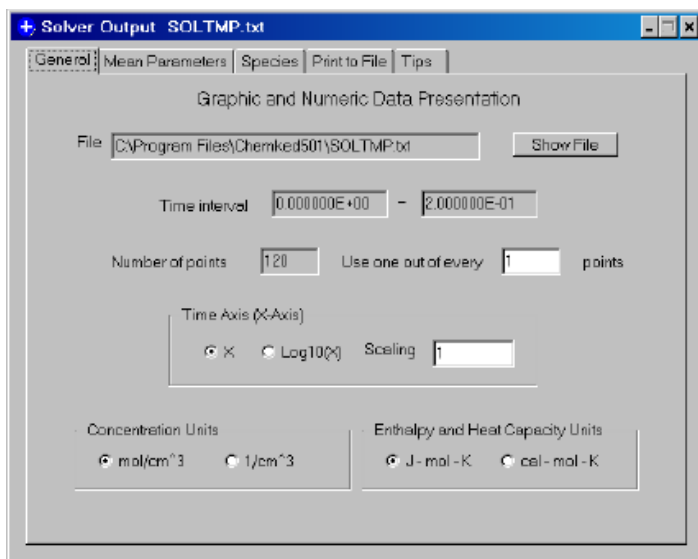
You can save the solver file with output data choosing **File > Save As**. When this file will be opened, you can use all features of the Solver Output dialog for examination of the data. To do this, from the solver file window choose **Reaction Kinetics > Solver Output Dialog**.

The Solver Output dialog contains pages with features for examination of the output information.

General Page

In the frame Time Axis (X-Axis), choose X or Log10(X)) and enter a scale factor.
In the frame Concentration Units, choose mol/cm³ or 1/cm³.
In the frame Enthalpy and Heat Capacity Units, choose J-mol-K or cal-mol-K.
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.

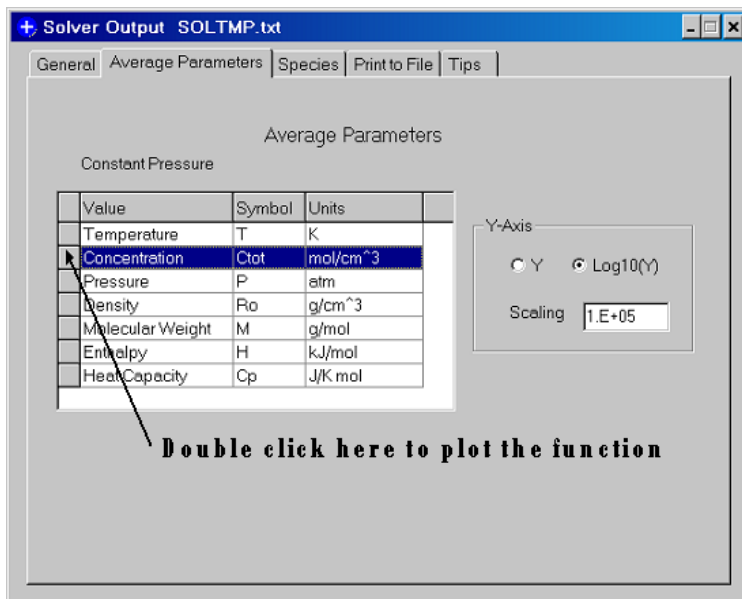
These settings are valid on all pages of this dialog.



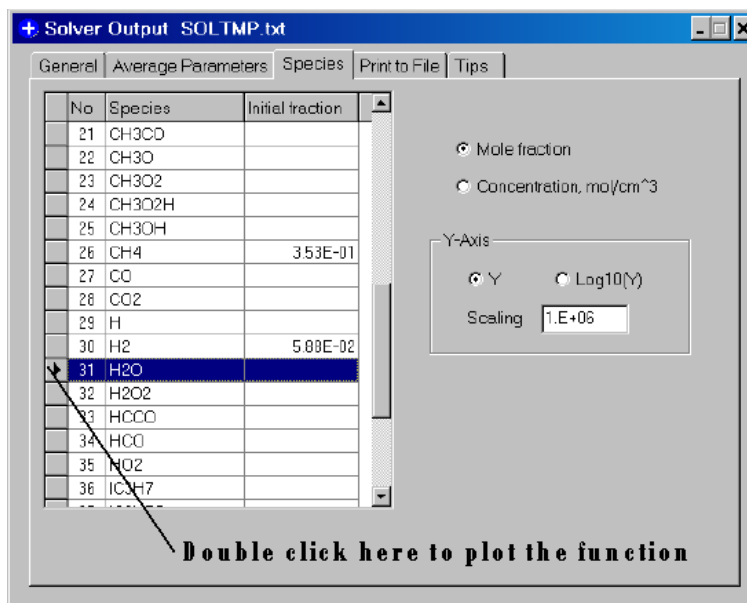
General page

Pages of Mean Parameters and Species

On these pages you can plot the reacting system parameters vs. time.



Average Parameters page



Species page

Follow this procedure to plot the functions.

1. On the Average Parameters page, select a row with the parameter whose function you want to plot.

On the Species page, select a row with the species whose functions you want to plot. Using options, choose the function type: concentration or mole fraction.

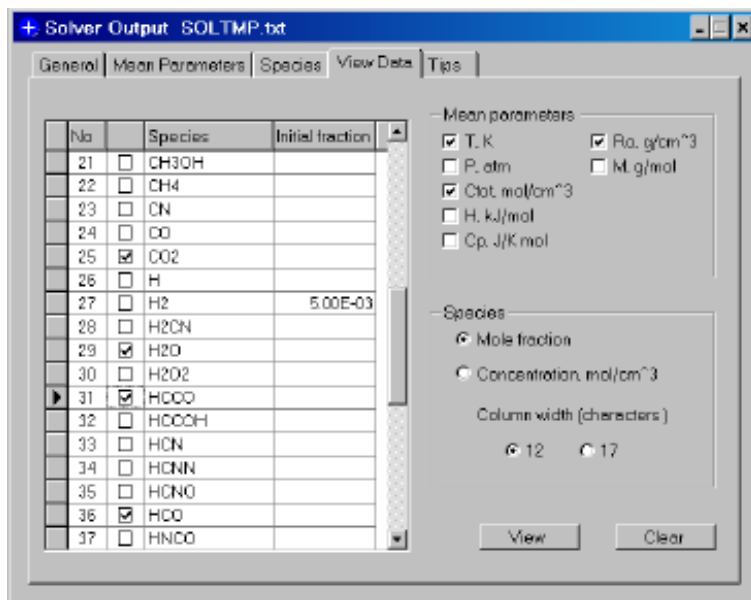
2. Choose the type of Y-values (Y or Log10(Y)) and enter a scale factor; this setting can be chosen for each function separately.

3. Double click the header of the selected row.

The curve appears in Temporary Chart. If this procedure is repeated for different parameters, the existing curve will be replaced with new ones. If you want to add a new curve to existing Temporary Chart, hold down the Ctr key and then double click the corresponding row header.

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.

Viewing Numeric Data



View Data Page

1. Check parameters whose numeric data you want to view.

2. Select type of the function: concentration or mole fraction.

Click the View button; the numeric data of checked parameters will be displayed in a text window.