Overview

Chemked-II is a multi-purpose post-processor for analyzing simulation results of gas-phase chemically reacting systems. The information required for description of a reacting systems is stored in a solver file that is prepared with the Chemked-I tools. The solver file contains the reaction mechanism and the relevant thermodynamic data. For each reaction mechanism you should create an individual solver file.

These files are used in the Chemked solver to solve problems at different initial conditions. The output data is analyzed with the Chemked-II post-processor, which allows you to get numeric and graphic information about average gas parameters, concentrations, mole and mass fractions of species. In addition, the post-processor gives the full information about reaction rates.

Chemked-II contains a program module for creating reduced reaction mechanism on the basis of numerical results previously obtained for full reaction system. Description of the reduction technique and sample problems can be found at http://www.chemked.com/aux_files/samplesred.pdf

The Chemked solver is a Fortran program based on the RADAU5 subroutines.

Supported Operating Systems: Windows XP, Windows Vista, Windows 7, Windows 8, Windows 10.

Citation

To cite Chemked-II, please refer this web page:
M.Jelezniak, I.Jelezniak,"Chemked-II version 3.7. Program for chemical kinetics of gas-phase reactions", http://www.chemked.com/

General Settings

Parameters for general settings are doted in the file
<app_dir> \Chemked361\AssistFiles\OPTIONS.txt
where <app_dir> is a directory chosen for the Chemked-II installation. These parameters are

8.314472	Gas constant J/mol·K
1.987216	Gas constant cal/mol·K
6.022142E+23	Avogadro constan 1/mol
1.38065E-23	Boltzmann constant J/K
101.325	1 atm = 101.325 kPa
9408399	Background color of the main window.

Reading ignores other lines of the file.

If you need to change the data, you must do it manually. You can also replace this file with identical file from Chemked-I.

Software Limitations

This section covers the software limitations of this release.

In Chemked-II, the main sources of information are solver files that you should create using the Chemked-I tools. Chemked-I has a greater scope for simulation of chemical kinetics problems than Chemked-II. Therefore creating the solver files you should consider the following circumstances

1. Chemked-I simulates chemical kinetics at constant pressure and at constant volume. Respectively, solver file can be created for these two types of problems. **Chemked-II simulates and examines chemical kinetics at constant pressure only.** If you try to use a file whit constant volume parameters, you get an error message.

2. Chemked-I versions 5.x can process reactions with reverse rate parameters, such as

```
HO2 + H <=> H2 + O2          1.66E+13 0 823
REV / 3.16E+12 0.35 55510 /
```

Chemked-II does not supports this reaction type; it should not be included in the reaction mechanism for the Chemked-II solver file.

Remark

Time evolution of a chemically reacting system is described by a set of ordinary differential equations with respect to variables $Y(t)$. Solution of this set of equations is searched in a time interval $[t_1, t_2]$, initial values of the variables are defined at the time point t_1. Sometimes it is convenient to specify a non-zero number as initial time t_1. Nevertheless, if $(t_2-t_1)/t_1<<1$ then you can have difficulties with creating charts and diagrams of a good quality. We recommend the following to avoid these problems.

Right hand sides of the differential equations of chemical kinetics are not explicit functions of time. Because of this the time histories of variables don't depend on the initial time t_1 and are functions of the difference $t-t_1$, $Y(t-t_1)$. The final result depends only on the time interval t_2-t_1.

So, if you have a problem where

Initial time t_1 is a non-zero nimbler

Final time is t_2,

we recommend you to solve the same problem where

Initial time is 0

Final time is t_2-t_1.

Results of both calculations are identical but the first data is shifted by t_1. Use of data from the second calculation allows you to avoid some problems with creating charts and diagrams.