

Overview

Chemked-I is a program designed for simulating gas-phase chemically reacting systems. Sets of parameters for calculating thermodynamic functions of species and rate constants of reactions are collected in databases. This data is displayed in tables and easily handled via the user interface. You can edit the data, sort and select species and reactions with particular properties, and move the data from one database to another. The program checks the data and if there are problems will display error messages. Chemked-I provides numerical and graphical information on the thermodynamic functions and the rate constants of reactions. Data and charts can be printed or exported to the clipboard or as a file. As a result you will have verified and consistent databases with easy access to the information.

Chemked-I incorporates a solver to solve problems of gas-phase chemical kinetics at constant pressure and at constant volume. The solver is a FORTRAN program based on the RADAU5 subroutines. The data from the databases is used for generating a desirable reaction mechanism that is entered into the solver. The results of the solution are species concentration and gas temperature vs. time. The program allows you to solve a wide range of problems including simulation of gas-phase chemical reactors and the chemical processes behind shock waves.

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

Citation

To cite Chemked-I, please refer this web page:
M.Jelezniak, I.Jelezniak, "Chemked-I version 5.2. Program for chemical kinetics of gas-phase reactions.", <http://www.chemked.com/>

General Settings

The general settings let you use items that control how some features are displayed. To access these items, you should close all child windows.

Choose **Settings > Colors**. The Colors dialog appears. In the dialog, choose
back color of the main window,
font color for highlighting invalid species and reactions,
color for selecting subsets in charts.
Click OK.

Choose **Settings > Status Bar > Show/Hide**. If **Show** is chosen, the status bar appears at the bottom of the main window. In the status bar, information about current operations in the program is displayed. To remove the status bar, chose the **Hide** item.

Choose **Settings > Physical Constants**; the dialog appears. If necessary, change the values of physical constants; click OK.