Frequently Asked Questions

Chemked – A Program for Chemical Kinetics of Gas-Phase Reactions

Home page: http://www.chemked.com/, email: info@chemked.com

Q. Why do I need Chemked?

A. By means of Chemked tools you can quickly, saving a lot of time, create the reaction mechanism for your chemical kinetics problem and immediately begin examining the problem using the numerical results obtained with the Chemked solver.

Q. What types of problems can I solve?

A. Chemked will be useful for you if you work in the field of chemical kinetics and study combustion, atmospheric chemistry, air pollution or waste gas treatment.

Chemked will also help you if you need to incorporate gas-phase chemistry into problems of fluid dynamics. The program forms a CHEMKIN format text file with reaction mechanism. This file can be used as an input file in the CHEMKIN subroutines or other applications.

Q. What format of thermodynamic data is used in Chemked?

A. The NASA format for specific heats, enthalpies and entropies is used. For each species, seven polynomial coefficients are needed to calculate thermodynamic properties for each of two overlapping temperature ranges.

```
HCO               121286C   1H   1O   1    0G    300.00   5000.00  1000.0      1
 3.55727100E+00 3.34557300E-03-1.33500600E-06 2.47057300E-10-1.71385100E-14    2
 3.91632400E+03 5.55229900E+00 2.89833000E+00 6.19914700E-03-9.62308400E-06    3
 1.08982500E-08-4.57488500E-12 4.15992200E+03 8.98361400E+00 0.00000000E+00    4
```

Each species may be composed of 4 chemical elements. Each Chemked database may be formed on the basis of 10 chemical elements.

Q. What types of reactions are used in Chemked?

A. Elementary reactions commonly used for description of gas-phase reacting systems can be processed in the Chemked. Examples are presented here.

```
! Ordinary reactions
H2O2 + OH <=> H2O + HO2                              5.80E+14          0       9557
OH* + AR <=> OH + AR                                 1.69E+12          0       4135
OH+ + H + e => H2O                                   1.3E+05          0           0

! Reactions with reverse rate parameters
IC3H5OH + HOCHO <=> CH3COCH3 + HOCHO                 2.81E-02     3.286     -4509
    REV / 7.04E+04     1.209       556 /

! Three-body reactions
C + H + M <=> CH* + M                                6.00E+14          0       6940
CO + O + M <=> CO2 + M                               3.00E+14          0       3000
    H2/2.5/ H2O/6./ CO/1.9/ CO2/3.8/ HE/0.5/ CH4/2./ C2H6/3./

! Pressure-dependent reactions; rate constants are described by the Lindemann form with
the Troe or SRI blending functions.
```

More information can be found in User Guide.

Q. Can I use reactions with arbitrary stoichiometric coefficients?
A. No. Chemked does not have such option.
The following reaction will not be accepted.
`2C4H10 + 13O2 = 8CO2 + 10H2O`
The reaction 0.5H2 + 0.5O2 = OH should be rewritten as H2 + O2 = OH + OH.

Q. Where can I find the thermodynamic data and reactions?
A. In Internet there is a lot of information on thermodynamics and reactions; a few links are presented here.

Prof. Burcat's Thermodynamic Data
http://garfield.chem.elte.hu/Burcat/burcat.html
http://garfield.chem.elte.hu/Burcat/THERM.DAT

GRI-Mech 3.0 Reaction mechanism
http://www.me.berkeley.edu/gri_mech/
http://geodynamics.org/svn/cig/vendor/pythia/v0.4/packages/fuego/etc/mechanisms/GRIMech-3.0.ck2

Combustion chemistry
https://www-pls.llnl.gov/?url=science_and_technology-chemistry-combustion-mechanisms

These data have CHEMKIN text format and most of them can be entered in Chemked databases without any additional processing.

Q. What size of reaction mechanism can I process in Chemked?
A. The Chemked solver has limitation on number of differential equations (species) - 1000 and number of reactions - 10000. Actually the size of a reaction mechanism that can be processed for a reasonable time is much less and depends on the capability of your computer. The stiffness of the differential equations, initial concentrations of species and choice of solver control parameters have also a significant impact on the computational time.

You can try the methane-air mixture (GRI-mech 3.0 reaction mechanism, 53 species and 325 reactions) with Chemked-II.
http://www.chemked.com/chemkedII.htm
Depending on initial conditions, the solution takes from several fractions of a second to several seconds.

Q. What should I do if I can't install Chemked?
A. Read the Readme.txt file for more information or send email to info@chemked.com to describe your problem and get help.

Q. Is there technical support?
A. Yes. For technical questions regarding Chemked, please email us info@chemked.com