

ODE SOLVERS AND KINETIC SIMULATION SOFTWARE

CHEMKIN software was developed initially at Sandia National Lab and now maintained and distributed by [ReactionDesign, Inc.](#) CHEMKIN by far the most popular Kinetic Simulation software. The modern CHEMKIN modules call widely used, reliable numerical stiff solvers such as VODE and DASPK. We strongly recommend that you learn how to use the new version of CHEMKIN.

Nonetheless, you may run into problems where CHEMKIN won't do exactly what you want, or where there are special numerical problems. Here is a rundown on some alternative ODE solvers and kinetic simulation tools.

Kinetic Simulation Packages

[Cantera](#) has many of the capabilities of CHEMKIN, and some of the modules are open source.

ODE solvers

A complete but still pretty brief explanation can be found in the Numerical Recipes textbooks. Free online versions of the Numerical Recipes books for C, Fortran 77, and Fortran 90 are available; see <http://www.nr.com>.

A very similar stiff solver is available in MATLAB, with the advantage that it is directly connected to some very nice graphics.

DSL48S can be accessed using the ABACUSS interpreter, both available through MIT's Process Systems Engineering Laboratory website (<http://yoric.mit.edu>).