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# Chemical Reaction Network Toolbox

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The Chemical Reaction Network Toolbox is made up of two integrated parts: ChemLab and Network Analyst.

ChemLab is a simulation environment. In response to a user-specified mass action system -- that is, a reaction network taken together with a specification of rate constants -- ChemLab will formulate the mass action ordinary differential equations that govern the species concentrations. These equations are sometimes lengthy and complex. So as not to intimidate the mathematically faint of heart, they are kept from view, but users who want to see them can request a display.

An "experiment" with a mass action system is a specification of initial concentrations for the various species taken together with a stopping time. For each experiment specified, ChemLab solves the appropriate differential equations numerically. The evolution of species concentrations with time can then be shown in tabular form or in a variety of two and three dimensional graphical displays.

Experiments with the mass action system under consideration can be saved in a "library". The results of several experiments can be exhibited simultaneously in two and three dimensional phase portraits. (For our purposes, a phase portrait is a collection of curves, called "trajectories", that show how the reactor state travels through "composition space" as time progresses. Each curve corresponds to a particular choice of initial composition.) Phase portraits provide excellent means for understanding the qualitative behavior of mass action systems. Rate constants can be changed while the library of initial conditions is retained, so it is easy to study how phase portraits are affected when parameters in the governing equations are modified.

You can also have the results of an experiment saved to a text file that can, in turn, be imported into a spreadsheet program such as Excel, Quattro Pro or Lotus 123.

Platform: Windows

License restrictions: none

Number of copies: unlimited

Requested by: J. Chalmers

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