



STELLA diagram modelling an enzyme-catalysed system. The product, after release from the active site (rate constant k), can either be adsorbed onto excess low-affinity sites on the enzyme surface (with rate constants k_1 and k_2 for the on and off reactions respectively) or enters a coupled assay system (non rate-limiting). Both k and k_2 are modulated by the level of calcium ions. The model enables the effect on the coupled assay of addition/removal of calcium at steady state to be explored.

outcome can be immensely valuable and informative.

STELLA uses the familiar windows/icon/mouse/pull-down menus interface. Structures are generated on the Macintosh screen as a (flow) diagram, using just four basic icons which denote stocks, flows between stocks, convertors (factors which influence flows) and connectors (lines denoting a logical connection between a stock or convertor and a flow). In the case of a chemical reaction, for example, these could correspond to reactants/intermediates, reaction pathways, catalysts and linkages of catalyst to the step catalysed, respectively. Input screens then enable the user to enter the parameters to be assumed. It is even possible to do back-of-an-envelope modelling, by sketching out assumed relationships on a graph pad. The program numerically solves the appropriate differential equations, and displays results as graphical or tabulated data as the user requires.

A newcomer to *STELLA* (if not to modelling), I found it easy to learn how to use the package. One could quibble over minor things. The immense user's guide of 392 pages is wordy and uneven — though the vital bits are clear. Mathematicians will find the choice of numerical methods limited, and I was disappointed that the graphics window could not display the main parameters assumed. No matter. This is a package which may well do for modelling what BASIC (also from Dartmouth, New Hampshire) did for programming — make it accessible to the many and lead at least some onto more complex work. *STELLA* will surely be widely used. □

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Information from data

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CLEOPATRA: A Chemometrics Library. Elsevier Scientific Software. Basis version Dfl. 2,220, \$1,080. Extension 1 Dfl. 1,010, \$495.

CHEMOMETRICS can be broadly defined as the application of information technology to the analysis of chemical data. The essential goal is to process and convert data into information as efficiently and effectively as possible. Good experimental design provides the maximum amount of information from the minimum amount of experimentation. Other chemometric methods are aimed at obtaining the maximum amount of information from large and often complex data sets.

CLEOPATRA is a modular chemometrics teaching package which, although it can't be said to be comprehensive, covers several important areas of the subject. A lot of thought has gone into the presentation of the material, which has a modular structure, allowing individual units to be selected by menu. The package is available for both the IBM-PC and HP microcomputers. I have used the IBM version on four PC clones without any problems, provided (even though the program does not use colour) that the microcomputer has a colour graphics adapter card. A particularly useful feature is that the program disks are supplied in two sets, one of interpreted BASIC and one of compiled BASIC. With the interpreter version, the user can incorporate his own BASIC teaching programs as extra modules or modify the existing modules. Some of the modules involve a great deal of calculation for which the faster compiled version is preferable.

Nine modules come in the 'basis' version, including Fourier filtering, curve-fitting and autocorrelation, with six modules covering demonstrations and calculations in sampling, process monitoring and process reconstruction. An extension is available for simplex optimization, Kalman filtering and sequential analysis. The package is unusually well documented — the handbook clearly describes how to use each module and outlines the theory, though newcomers to the subject will need to refer to a textbook or the references given on the header page of each module.

I particularly liked the graphic presentation of the data. In the Fourier-filtering module, for example, as a spectrum is acquired the signal varies slowly (the peaks are broad), while the noise varies rapidly (narrow peaks), and the signal and noise are superimposed in the spectrum.

But on applying the fast Fourier transform algorithm, the data are converted to a frequency or power spectrum where the signal and noise are separated. A filter can cut out the high-frequency noise before carrying out an inverse transform to regenerate the smoothed spectrum. The screen is split into four, showing the original noisy spectrum, the power spectrum, the shape of the filter used and the reconstructed spectrum.

There is a great deal of flexibility in the data used; up to three peaks with varying levels of noise and sinusoidal distortion, and several different types of filter, can be investigated. Similarly, in the curve-fitting module, up to three peaks of different height, position, width and shape (gaussian, lorentzian or mixed) can be studied with various levels of noise superimposed. The Kalman filter, a recursive method which can be applied to multi-component spectroscopic analyses, can be used with the overlapping spectra of four components of variable concentrations and in the presence of baseline drift and variable amounts of noise.

Such flexibility is one of the most important features of any good teaching package. It makes exercises open-ended and more challenging by enabling students to ask such questions as how well can the Kalman filter or curve-fitting routines cope with a high level of noise, or what happens if two peaks are fitted to data which also contain a third underlying peak.

The simplex optimization module provides an excellent visual demonstration of how an optimum response can be obtained for two variables, essentially by climbing to the top of the hill and representing the response by the steepest path. In practice most simplex optimizations will use far more than two variables, but then visualization in more than three dimensions is not possible.

In my experience students enjoy using *CLEOPATRA*, provided care is taken to give them both guidance and the freedom to experiment with open-ended exercises. The main frustration arises from the self-contained nature of the package; with the exception of the calculation modules on grab sampling, process monitoring and process reconstruction, the data are internally generated and the modules cannot be used with the students' own experimental results (with a few modules it is possible to modify the programs, for example the Fourier filtering and curve-fitting units, to allow data files to be read from disk). This drawback does not detract greatly from the usefulness of the package as a teaching aid. In my view, *CLEOPATRA* is an essential component of any chemometrics software library. □

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