Fluorescence Emulation System for Chemistry

Edward Toole, Charles L. R. Barnard
Dept. of Computer Studies & Physical Sciences
Glasgow Caledonian University
Glasgow, G4 OBA

(a) In the Physical Sciences department of the University, students' work in the analytical laboratories includes the use of sophisticated instruments including a Fluorescence spectrometer. It was decided to try to emulate the use of this instrument both in the hardware and software areas. Toolbook has thus been used to provide a user-friendly graphical interpretation of the structure of the instrument.

(b) Toolbook has also been used to provide an emulation of the GEM interface used by the controlling software along with the resulting graphical output of spectral curves and peak tables.

(c) In the chemometric part of their course , the students also study various optimisation techniques for use in the experimental work mentioned above.

The present Toolbook package will also allow the user to study the Nelder & Mead version of the "Simplex method" of optimisation both for a simple 2-variable mathematical minimisation problem (to explain the basic ideas behind the algorithm), and a more realistic 6-variable experimental set-up used to attempt to maximise the output Intensity in the work with the Fluorescence instrument.

This package involves considerable use of the "number-crunching" abilities of Toolbook and the use of lists to represent n-dimensional vectors { since at present Toolbook does not allow arrays }. Toolbook is slow in this area, but can handle the job at a reasonable speed for instructional purposes.

An auto-scaling graph handler was written to allow the plotting of general mathematical functions and the experimental response results (Intensity) from the fluorescence experiments { again this is a fairly slow procedure but adequate for instruction }.