Computer Software Reviews

SolEq: Solution Equilibria Principles and Applications[1]

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The aim of this software package, as stated by the authors, is to cover "the principles of equilibrium in solution chemistry: acid−base, redox, solubility and metal−ligand chemistry", in both homogeneous and heterogeneous systems. The "user-interactive" applications and tutorials are prepared for graduate students and advanced level undergraduates in research, individual study, or class teaching. The package presents as a series of "screens" or "windows", well endowed with navigation buttons that allow the user to find topics of particular interest or to browse progressively though the material. The package has been developed in consultation with IUPAC and contains some sections written by R. W. Ramette.

There are two main sections: speciation modeling and supporting tutorials.

The modeling calculations are based on a subset of selected equilibrium parameters (mostly proton and metal−ligand constants) from the IUPAC "Stability Constants Database", which itself was compiled by SolEq's principal authors. Programs exist to calculate, and display in real time, both species distribution and titration curves. It is also possible to evaluate equilibrium constants as a function of temperature using the van't Hoff equation and as a function of ionic strength using the Davies equation.

The supporting tutorials cover both the principles and the applications of equilibria in solution, including homogeneous and heterogeneous systems. The applications include metal speciation in natural waters (seawater and acid rain among others) and metal speciation in biological fluids (blood plasma). Case studies look at the marine CO_2 system and at chelation therapy.

I found the overall presentation good—well structured and with plenty of icons that usually passed the test of being informative rather than distracting. The navigation system works well, particularly once one realizes the need to avoid a proliferation of windows. The package is easy to use.

A review of this kind would not be complete without a few grumbles. A minor initial problem with installation was cured by the alternative route provided. The symbols used were not always conveniently defined (definition screens are generally available but not always where one wants them). Some of the error messages were a bit opaque: for example, I got "is not a valid floating point value" when I did not know I was trying to enter one. These issues were few and generally quite trivial. My only substantive concern is that users are not adequately taught about hazards of the Davies equation. I would have liked to see not only that this equation has a very limited range of ionic strength but also that much better alternatives are now available (in the form of Pitzer and SIT-type equations). The representation of log K versus I on a log scale is unconventional and, I think, counter-instructive.

Otherwise, the authors write with considerable authority, rather more perhaps than is the case with some of the many computer-assisted learning packages in chemistry that are now available. I found their selection of material particularly impressive, providing a coverage that is satisfactorily comprehensive but not excessively detailed. Some of the concepts and terminology are a little dated (such as the reference to "dative" bonds) but only as befits the author's venerable status!

I can recommend the package wholeheartedly to hard-pressed teachers, especially those who are keen to broaden the education of their students but find it difficult to include everything they wish in their curriculum. The subject of "SolEq" is of considerable relevance to a wide range of modern chemical activities and hence would be useful to many chemistry graduates during their subsequent employment. I suspect that such concepts nowadays often receive less than their due. This package provides a convenient means to redress the balance in favor of practical importance over some current heights of chemical fashion.

Literature Cited

(1) This program was written by K. J. Powell and L. D. Pettit. It was published in 2001 by Academic Software, Otley, U.K. Order form and downloadable text files are available via www.acadsoft.co.uk. Price: single copy, $210.00; with generous discounts for multiple copies and network and site licenses.