COMPUTER SOFTWARE REVIEWS

HSC Chemistry for Windows, 2.0

William R. Smith

School of Engineering and Department of Mathematics and Statistics, University of Guelph, Guelph, Ontario, Canada N1G 2W1

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The "HSC" in the name of the HSC Chemistry for Windows[1] package derives from the symbols for Enthalpy (H), Entropy (S), and Heat capacity (C), and the software is a collection of seven different modules accessed from a single main menu. The modules are entitled (1) Reaction Equations, (2) Heat and Material Balances, (3) Equilibrium Compositions, (4) Electrochemical Cell Equilibria, (5) Formula Weights, (6) Phase Stability Diagrams, and (7) Eh-pH Diagrams. All modules are integrated with a large built-in database. The current version is 2.0, which runs under Windows 3.1[2] (a Windows 3.0 version is apparently available). Hardware requirements are a 386 or faster CPU, 2M of memory, color EGA or better graphics, and 4.3M or more hard disk space.

HSC is one of several related software packages currently available from a number of vendors, all of which are built around a core capability of calculating chemical equilibrium compositions for complex systems[3] (the 1995 CEP Software Directory[4] lists 14 such packages). Similar to most of these packages, HSC primarily treats multiphase ideal-solution problems (although the program also allows the user the option of providing nonideality data). Equilibrium calculations are important in a wide variety of areas, including chemistry, chemical engineering, metallurgy, geochemistry, and physics. Each package has a slightly different "flavor" and different capabilities, so it behooves the prospective purchaser of such software to carefully match its capabilities to their needs.

HSC is produced by Outokumpu Research Oy of Finland, whose primary orientation is metallurgy. Thus, for example, the Eh-pH (Pourbaix diagrams), electrochemical cell equilibria and phase stability (Kellog diagrams) modules are unique to HSC. These types of calculations and diagrams are especially important in metallurgy and much of the underlying research originated in this field. As a consequence, the thermodynamic theory and algorithms underlying these three modules are relatively state-of-the-art. The Reaction Equations, Heat and Material Balances, and Formula Weights modules are of general interest to a broad audience, and the calculations underlying these types of problems are quite straightforward. However, the availability of the integrated database makes these calculations very convenient using HSC. The weakest module of HSC in terms of its use of current technology and capabilities is the Equilibrium Compositions module.

The two principal general aspects of any software package are its user interface and its computational capabilities. The current yardstick of measurement for a user interface is shaped by the high-quality interfaces of horizontal market applications like wordprocessors and spreadsheets. It may be considered unfair to judge HSC from such a viewpoint, but it is a fact that current programming technology embodied in products like Microsoft Visual Basic (VB)[2], Microsoft Visual C++,[2] and Borland Delphi[5] make possible, in the hands of a moderately skilled programmer, the development of software with a similarly high-quality user interface.

HSC appears to be written almost entirely in VB (with at least one exception; the SGM component is a DOS program invoked by a Windows[2] Shell command). The best part of the HSC user interface is its graphical output, which is excellent. Many types of graphs can be prepared for equilibrium calculations, and the Eh-pH and Phase Stability diagram modules produce similarly excellent graphical output. However, elsewhere HSC only manages to scratch the surface of the capabilities of VB. A related aspect of this is the fact that HSC functions as a *collection* of seven different programs, rather as than a seamless whole. The modules generally function by means of data files, which must first be prepared by the user, and which are then reread in another part of the software. For example, to perform an equilibrium calculation and view the results requires the user to first create and save an input file and then to perform the calculation. The latter requires the navigation of four different screen forms before the results can be viewed. Also, within some forms the user interface is rather clumsy. A case in point is the initial formulation of an equilibrium problem, in which the user first selects a list of elements from a periodic table, and then is presented with a form containing a list of the species that HSC has found in its database. The user must select from this list the species that are to be included in the calculation by deleting species from the displayed list. The method for performing this is poorly designed, sometimes requiring the user to begin all over again to recover from a simple keystroke error. This shortcoming is admitted in the User Manual on p 37, where it is stated: "The first time it might be a good idea to make a paper copy of the species by pressing the **Print** button."

Another important aspect of a user interface is its on-line help facilities. In HSC, rather than displaying a familiar Windows[2] hypertext helpfile, the Help button causes the display of a large text file that appears to match portions of the hard-copy manual, which the user must simply scroll through.

Concerning the computational capabilities of HSC, the standard of the Eh-pH, electrochemical cell equilibria, and phase stability modules is high, as mentioned previously. This is unfortunately not the case for the Equilibrium Compositions module (although it is nonetheless capable of performing calculations for a wide variety of problems). Also, the most of the computational modules of HSC are them-

selves also written in VB. Since VB is not a true compiled language this makes the calculations for the Equilibrium Compositions module quite slow for complex problems, especially on a 386 machine. This is not a drawback for the other modules, which are not nearly as computationally intensive.

The underlying algorithms of HSC (and of most of the other available equilibrium calculation software) are variations of the basic NASA algorithm,[6] originally developed over 30 years ago. One reason for the proliferation of equilibrium software may be due to a general view that the equilibrium problem was "solved in principle" many years ago, and all that is required is to combine a seemingly "standard approach" (like the NASA algorithm) with a user interface. In fact, the underlying mathematical structure of the equilibrium problem still presents significant theoretical and numerical challenges. This is still partly true in the case of ideal-solution systems,[3] but even more so for nonideal systems.[7]

In HSC, the user can choose between two different algorithms, one called GIBBS and the other called SGM. GIBBS is based directly on the NASA algorithm,[6] and SGM is a modified version of the public domain program SOLGASMIX, due originally to Erikkson,[8] which is similar in structure. Due to this structure, such algorithms have a number of inherent limitations for important types of equilibrium problems. There are several indications of such limitations in the User's Manual. On page 45, item 7 states the following: "Sometimes when calculating equilibria in completely **condensed** systems it is also necessary to add small amounts of an inert gas as the gas phase, for example, Ar(g) or N2(g). This makes calculations easier for the equilibrium programs." In a similar vein, item 8 on the same page states the following: "It may also be necessary to avoid **stoichiometric raw material ratios** by inserting an additional substance which does not interfere with the existing equilibrium. For example, if you have given 1 mol Na and 1 mol Cl as raw materials and you have NaCl as a pure substance, then all raw materials might fit into NaCl. The routines meet difficulties in calculations, because the amounts of all the other phases and species go to zero. You can avoid this situation by giving an additional 1E-5 mol Cl2(g) to the gas phase, see Figure 34." Again, on p 47, the following is stated: "The most important limitation of GIBBS is that, in some rare cases, only one pure substance is allowed. Otherwise the program may give unpredictable results. If invariant phases do not, however, contain the same elements, several pure phases are usually accepted. You can avoid this limitation by putting a minor amount of dissolving species into such a pure substance and define it as a solution phase".

It is important to note that the types of equilibrium problems with which HSC encounters difficulties are not esoteric and unimportant but arise often in practice. A very simple example is the system consisting of the species CO_2(g), $CaCO_3$(s), and CaO(s). When a calculation was attempted starting from pure $CaCO_3$(s) using the GIBBS module at $p = 1$ bar over the temperature range 400 to 440 K in 2K intervals, the calculation failed to converge for all but three temperatures. The SGM module failed at all temperatures.

A mathematically more subtle but important practical example is a problem consisting of the gaseous species H_2O, CO_2, HCl, CO, O_2, H_2, Cl_2, starting from initial amounts of 1 mol of each of CO and O_2, 0.5 mol Cl_2, 1.5 mol H_2, and zero amounts of the other species. HSC performed somewhat better in this case, although there were still some problems. At $p = 1$ bar over the temperature range (300, 1200 K) in 100 K intervals, when using the default setting on the calculation screen of "Use previous results as initial guess", the Gibbs module produced inaccurate (but not unreasonable) results except at 1200 K. When this option was turned off, correct results were obtained. (This suggests that the default value for this option should be set differently.) The SGM module failed to converge at the first two temperatures but gave accurate results elsewhere.

Final comments concern the built-in database of HSC, which contains over 7600 compounds. This is a very useful feature of the program. The underlying data were obtained from a number of reliable quoted sources, but some remarks by the authors concerning the accuracy of the HSC calculations in reproducing the literature data would be useful. The user may add to the database via an additional useful module accessed from the main menu of HSC. Finally, a problem noted by the reviewer is that no warnings are issued by HSC when data is used in a calculation that is extrapolated outside its stated validity range.

In summary, the best features of HSC are as follows:

1. its generally excellent graphical output, 2. the generally high quality of the Electrochemical Cell Equilibria, Phase Stability Diagrams, and Eh-pH Diagrams modules, and 3. the built-in database of more than 7600 compounds and the ability of adding to this.

Features of HSC which are deficient include the following:

1. a sometimes clumsy user interface, including poor helpfile facilities and 2. a chemical equilibrium computation module that is computationally adequate only for fairly straightforward problems.

If your requirements include the second of the "best features" above, HSC is worth obtaining for these capabilities alone. However, if your needs are primarily to perform equilibrium calculations for a wide variety of systems, HSC is not an "industrial-strength" product in this category.

REFERENCES AND NOTES

(1) HSC 2.0, available in North America from ARSoftware, 8201 Corporate Drive, Suite 110, Landover, MD 20785, USA, $595; elsewhere from Outokumpu Research Oy, P. O. Box 60, FIN-28101 PORI, FINLAND.

(2) Windows, Visual Basic, and Visual C++ are products of Microsoft Corp., 1 Microsoft Way, Redmond, WA 98052-6399.

(3) For a general discussion of such problems, see, for example: Smith, W. R.; Missen, R. W. *Chemical Reaction equilibrium Analysis: Theory and Algorithms*; Krieger Publishing Co.: Malabar, FL, 1991; reprint, with corrections, of the same title by Wiley-Interscience, 1982.

(4) *1995 CEP Software Directory*; supplement to the December 1994 issue of *Chemical Engineering Progress*, American Institute of Chemical Engineering: New York.

(5) Delphi is a product of Borland International Inc., 100 Borland Way, Scotts Valley, California 95066-3249.

(6) Brinkley, S. R. *J. Chem. Phys.* **1947**, 15, 107. Huff, V. N.; Gordon, S.; Morrell, V. E. *Natl. Advis. Comm. Aeronaut.* **1951**, Report 1037, Washington; White, W. B.; Johnson, S. M.; Dantzig, G. B. *J. Chem. Phys.* **1958**, 28, 751.

(7) For example: Castier, M. C.; Rasmussen, P.; Fredenslund, A. *Chem. Eng. Sci.* **1989**, 44, 237.

(8) Erikkson, G. *Chem. Scr.* **1975**, 8, 100.

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