American Mineralogist, Volume 74, pages 1390–1393, 1989

SOFTWARE NOTICE

FLINCOR: A microcomputer program for the reduction and investigation of fluid-inclusion data*

PHILIP E. BROWN Department of Geology and Geophysics, University of Wisconsin, 1215 W. Dayton, Madison, Wisconsin 53706, U.S.A.

ABSTRACT

FLINCOR is designed to reduce laboratory data gathered on fluid inclusions and to calculate *P-T* isochores for geologically important fluids composed of H_2O, CO_2, CH_4, NaCl, CO, and N_2. Requirements for input data have been oriented toward the types of values derived from fluid-inclusion observations. Alternatively, fluid mixtures expressed in a variety of units (for instance, mole fraction), can serve as input data. The user can choose from among multiple published equations of state describing the fluid behavior and can readily compare the results obtained by using different equations. Calculated output can be either printed in tabular form or saved as an ASCII text file for exportation to other applications. FLINCOR is a Microsoft® Windows™ application.

INTRODUCTION

Routine heating- and freezing-stage observations of fluid inclusions in the laboratory generate large amounts of data that must be reduced to derived quantities such as mole fractions of observed or inferred species, densities of fluid phases, and concentrations of dissolved solutes. In addition, because observations of fluid inclusions generally provide only constraints on minimum pressures (P) and temperatures (T) of trapping, it is desirable to calculate the extrapolated locus of P and T values (the isochore) consistent with the observational data. Although some of the required equations and calculations are simple, others are long and complicated and are not best solved by individual programming of hand calculators or microcomputers. FLINCOR (Brown, 1989) has been created to fill the needs of geochemists interested in (1) reducing laboratory observations on fluid inclusions, (2) calculating isochores in *P-T* space from fluid-inclusion observations, (3) calculating isochores from hypothetical mixtures of fluids, and (4) comparing the results obtained by using well-known published equations of state to extrapolate fluid behavior and properties.

This program should serve on several levels. As a research tool, FLINCOR allows rapid data reduction of fluid-inclusion observations. As a teaching aid, FLINCOR provides an insight into the kinds of data required to describe a natural fluid system completely. It provides a medium to compare one equation of state to another and to evaluate the ranges of geologic conditions over which differences are significant. In addition it allows rapid determinations of the effects of uncertainties in the input parameters.

At present, FLINCOR includes equations of state and approaches to data reduction from the following: Swanenberg (1980), Bottinga and Richet (1981), Holloway (1981), Jacobs and Kerrick (1981), Kerrick and Jacobs (1981), Heyen et al. (1982), Bowers and Helgeson (1983, 1985), Haar et al. (1984), Saxena and Fei (1987), Zhang and Frantz (1987), and Brown and Lamb (1989). Additional equations such as those by Angus et al. (1976) for the CO_2 liquid-vapor line and Knight and Bodnar (1989) for the critical points of H_2O-NaCl solutions are used where needed to convert observational data to derived quantities.

PROGRAM STRUCTURE

The program has been written in C for the Microsoft Windows environment. Most of the uncompiled code is included on the distribution disk to allow the user to check the equations both for their form and potential typographical errors during programming. However, owing to the complexities of programming the dialog boxes, windows, and icon, the program cannot be modified and recompiled by the user without access to the Microsoft Software Development Kit™ and C compiler.

The distribution disk contains, among others, the following files: README.DOC (documentation), FLINCOR.EXE (the executable program), HELP.HLP (on-line help facility), and FLINCOR.C, CALCS.C, SALTMIX.C (C source code).

The following are required or recommended system attributes. Hardware: IBM-PC or compatible micro with graphics card, 512k of memory, two floppy drives or a hard disk (recommended). A mouse and printer are recommended. Software: MS-DOS (or PC-DOS) 2.0 or later and Microsoft Windows 2.03, Windows 286, or Windows 386. Additional: A color monitor and either EGA or VGA card will enhance the interaction and will be necessary for the graphics output to be implemented in a future version of the program.

Like all Windows applications, FLINCOR is most easily used with a "mouse" or other pointing device. If you do not have a mouse, detailed directions are provided to allow the program to be used. A help section is also on-line during the routine operation of the program. There may be some items that are inaccessible at times to the nonmouse user; in general, however, the entire program can be used without a pointing device. For simplicity, the example discussed below will assume that the user has a mouse.

EXAMPLE

FLINCOR.EXE has been written to conform to the standard Microsoft Windows interface. Most simply, chemical systems and equations of state are chosen from menus in the main window. Appropriate child windows then are opened to prompt for the

* The FLINCOR program and associated files are available from Wisc-Ware, a consortium of colleges and universities that distributes research and instructional software for IBM-compatible microcomputers. Individual copies of FLINCOR cost either $25 or $50 (depending on consortium membership) and can be ordered from Wisc-Ware, 1210 W. Dayton Street, Madison, Wisconsin 53706, U.S.A. Specify disk size and media density. Further information including a current catalog listing over 100 programs and order forms can be obtained by writing to the above address, by calling (800) 543-3201, or by e-mail on Bitnet at wiscware@wiscmacc.

0003–004X/89/1112–1390$02.00

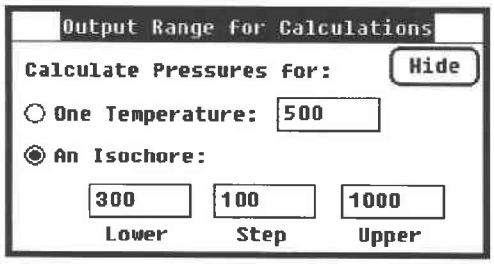

Fig. 1. Output Range window that permits the user to change the range and frequency of calculated P-T points. The numbers shown here are default values and can be readily changed.

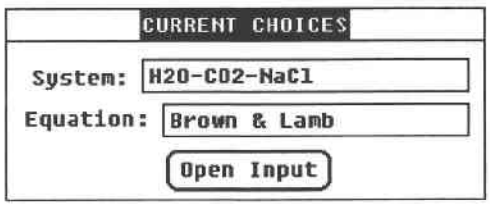

Fig. 2. Current Choices monitor window that displays the current chemical system and equation of state chosen from the menus in the main FLINCOR window. Input windows such as shown in Fig. 3 are called up by pushing the Open Input button in this window.

input data required to completely define the state of the chemical system. Calculated results appear in an output window and can be saved as an ASCII text file or printed out directly.

After starting the program, four windows are open on the screen. The Main window consists of a title bar at the top of the screen, a menu bar containing the File, Windows, Graph, Chemsystems, Equations, and Help menu headings, and the background upon which the other windows are superimposed. The other three windows are "child" windows and include the Output, Current Choices, and Output Range windows. As an example, Figure 1 shows the Output Range window. This figure shows how readily one may change the isochore parameters for subsequent calculations. The four boxes containing numbers are editable text fields that can be changed to reflect the range and frequency of output desired by the user. The Hide button is provided to help unclutter the screen display. This Output Range window can be "unhidden" at anytime by using the Windows menu in the Main window.

The Chemsystems and Equations menus contain the main branching decision points of the program. The Chemsystems menu lists available chemical systems. These systems are mutually exclusive, and only one can be selected at any time. To choose a system (e.g., H_2O-CO_2-NaCl), simply click the mouse button while pointing to the desired menu item. The new choice is immediately shown in the Current Choices monitor window (Fig. 2). If the previous equation of state shown in the Current Choices window is valid for the new chemical system, it will remain. If, however, the previous equation is invalid for the new system, a default change will occur in the equation-of-state choice.

Depending on the chemical system chosen on the Chemsystems menu, the items on the Equations menu are either "grayed out" as inappropriate or are in normal type face with one checked. Clicking on a new valid entry will change the chosen equation, and this change will be reflected in the Current Choices monitor window and in the calculated output.

The Open Input button in the Current Choices monitor window (Fig. 2) will open an input window appropriate to the choices for chemical system and equation of state shown in the window. To open the window in Figure 3, the system H_2O-CO_2-NaCl was selected from the Chemsystems menu. The default equation of state for this system is Brown and Lamb (1989) [Bowers and Helgeson (1983) is also available], and so the user would not have to use the Equations menu to choose this equation. Now the Open Input button in the Current Choices monitor window produces the input window shown in Figure 3.

For this system, one needs to provide salinity information (top portion of the window), information on the CO_2 phase (middle portion of the window), and an estimate of the proportions of water and carbon dioxide in the inclusion (Nicholls and Crawford, 1985). After making these choices, utilizing the Calculate button in the window will result in one of the following responses: (1) A box requesting an identifying name for the data to be reduced (this feature can be turned on and off by the user). (2) An error message telling you that you have entered an incorrect value somewhere in the input. This message is context sensitive and specific; it will generally prompt you with the proper range of values, and, after clearing the message box, the input focus will be returned to the offending entry. (3) The calculation will take place.

The first one third of Figure 4 shows the result of pushing the Calculate button in Figure 3. This and other calculations may be nearly instantaneous or may take several seconds depending on the speed of the computer and the complexity of the calculation. If the delay is substantial (i.e., it took more than a couple of seconds on my 10MHz, 80286 computer), an Hourglass cursor has been programmed to replace the arrow (or I beam) until the calculation is complete. When the calculation is finished, the output box will automatically scroll to the bottom to allow the results to be viewed. However, the input focus will generally

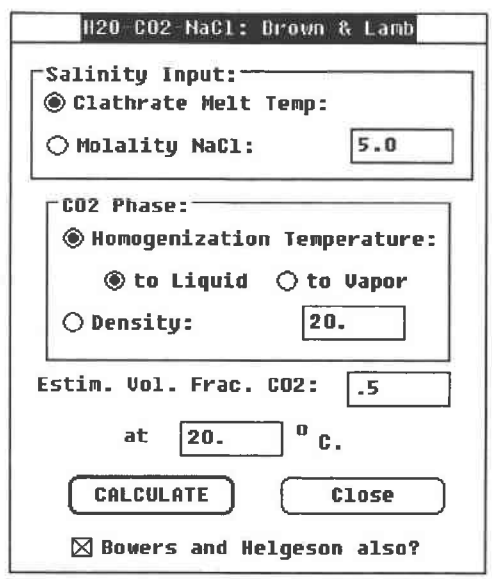

Fig. 3. Input window for reducing fluid-inclusion data in the system H_2O-CO_2-NaCl. The numbers shown are default values that can be easily changed by the user.

```
**************************************
Test Output for Tutorial-1
Chemical System is H2O-CO2-NaCl
Eqn of State: Brown & Lamb
Bulk Inclusion Composition:
  XH2O=0.7368 XCO2=0.2405 XNACL=0.0227
Aqueous Phase Composition:
    Mol.Frac.NaCl= 0.0299
    Molal.NaCl= 1.7092
    Wt.Pct.NaCl= 9.0816
Clathrate Melt Temp.= 5.000
Aqueous Phase Density= 1.06336
CO2 Phase Homog. Temp.=  20.0 (L)
CO2 Phase Molar Volume=  56.82
CO2 Density= 0.7743
Est. Vol. Frac. CO2= 0.50 at 20.0 C.
Bulk Molar Volume=  27.332
Bulk Density=  0.9189
            Brown & Lamb  Bow. & Helg.
 TEMPERATURE    PRESSURE
PRESSURE
    300          2749          1819
    400          3698          3087
    500          4646          4274
    600          5595          5329
    700          6544          6312
    800          7493          7276
    900          8442          8230
   1000          9391          9177
**************************************
Test Output for Tutorial-2
Chemical System is H2O-CO2-NaCl
Eqn of State: Brown & Lamb
Bulk Inclusion Composition:
  XH2O=0.6577 XCO2=0.3220 XNACL=0.0203
Aqueous Phase Composition:
    Mol.Frac.NaCl= 0.0299
    Molal.NaCl= 1.7092
    Wt.Pct.NaCl= 9.0816
Clathrate Melt Temp.= 5.000
Aqueous Phase Density= 1.06336
CO2 Phase Homog. Temp.=  20.0 (L)
CO2 Phase Molar Volume=  56.82
CO2 Density= 0.7743
Est. Vol. Frac. CO2= 0.60 at 20.0 C.
Bulk Molar Volume=  30.498
Bulk Density=  0.8900
            Brown & Lamb  Bow. & Helg.
 TEMPERATURE    PRESSURE
PRESSURE
    300          2402          1684
    400          3224          2754
    500          4045          3750
    600          4867          4624
    700          5688          5431
    800          6510          6222
    900          7332          7007
   1000          8153          7787
**************************************
Test Output for Tutorial-3
Chemical System is H2O-CO2-NaCl
Eqn of State: Brown & Lamb
Bulk Inclusion Composition:
  XH2O=0.8010 XCO2=0.1743 XNACL=0.0247
Aqueous Phase Composition:
    Mol.Frac.NaCl= 0.0299
    Molal.NaCl= 1.7092
    Wt.Pct.NaCl= 9.0816
Clathrate Melt Temp.= 5.000
Aqueous Phase Density= 1.06336
CO2 Phase Homog. Temp.=  20.0 (L)
CO2 Phase Molar Volume=  56.82
CO2 Density= 0.7743
Est. Vol. Frac. CO2= 0.40 at 20.0 C.
Bulk Molar Volume=  24.762
Bulk Density=  0.9478
            Brown & Lamb  Bow. & Helg.
 TEMPERATURE    PRESSURE
PRESSURE
    300          3146          2026
    400          4240          3512
    500          5335          4911
    600          6430          6177
    700          7525          7369
    800          8620          8536
    900          9714          9690
   1000         10809         10834
```

Fig. 4. Example of output from FLINCOR. Note that output was "saved" and imported into a word processor as an ASCII text file.

remain at the last entry in the input window (which will still be active) to allow a new value to be entered. Thus, for example, to explore the effects of varying the estimated volume fraction of CO_2 in Figure 3, simply change the 0.5 entry to 0.6 and recalculate. Repeat this process to calculate the result for 0.4. Now the Output window would contain the complete contents of Figure 4, plus or minus differences in naming of the individual runs. Previous calculations are not lost from the output, they simply scroll out the top of the window and can be later viewed by scrolling the output.

While input windows such as shown in Figure 3 are visible, the user can simply change the equation of state by choosing a new entry from the Equations menu in the Main window. This allows the differences among the various equations to be readily evaluated for the specific chemical system and P-T-X conditions of interest to the individual user. The Close button will remove the input window and ready the program for changing the chemical system or equation of state to be examined.

At any time while using the program, the current contents of the Output window may be printed or saved to a file. The Output window can subsequently be cleared to ready the program to accept data from, for instance, a different locality or compositional range (e.g., CO_2 vs. H_2O). On exiting the program, the user is prompted to save the contents of the Output window to a file. All saved files are in ASCII form and can be readily manipulated by most word-processing or spread-sheet programs. Most spread-sheet programs also will provide a means to graphically plot the calculated isochores, and with more manipulation, will produce histograms of observed data or calculated values.

ACKNOWLEDGMENTS

This research and program development were supported by hardware and software provided by IBM and Microsoft through a software development contract with the University of Wisconsin–Madison. Additional support came from the National Science Foundation through grants EAR 85-08102 and EAR 88-05470, and NASA grant ECG 87-202. W. M. Lamb was intensively involved in the FORTRAN and BASIC programming that served as the precursor to this Windows® application. The program and paper were improved by comments from M. L. Crawford, W. Crawford, D. C. Crowe, A. Musallem, E. Roedder, J. K. Vry, and P. K. Wetherbee.

References cited

Angus, S., Armstrong, B., and de Reuck, K.M (1976) International thermodynamic tables of the fluid state, carbon dioxide, 67 p. Pergamon Press, New York.

Bottinga, Y., and Richet, P. (1981) High pressure and temperature equation of state and calculation of the thermodynamic properties of gaseous carbon dioxide. American Journal of Science, 281, 615–660.

Bowers, T.S., and Helgeson, H.C. (1983) Calculation of the thermodynamic and geochemical consequences of nonideal mixing in the system H_2O-CO_2-NaCl on phase relations in geologic systems: Equation of state for H_2O-CO_2-NaCl fluids at high pressures and temperatures. Geochimica et Cosmochimica Acta, 47, 1247–1275.

——(1985) FORTRAN programs for generating fluid inclusion isochores and fugacity coefficients for the system H_2O-CO_2-NaCl at high pressures and temperatures. Computers & Geosciences, 11, 203–213.

Brown, P.E. (1989) FLINCOR: A fluid inclusion data reduction and exploration program (abs.). Second Biennial Pan-American Conference on Research on Fluid Inclusions, Program with Abstracts, 14.

Brown, P.E., and Lamb, W.M. (1989) *P-V-T* properties of fluids in the system H_2O-CO_2-NaCl: New graphical presentations and implications for fluid inclusion studies. Geochimica et Cosmochimica Acta, 53, 1209–1221.

Haar, L., Gallagher, J.S., and Kell, G.S. (1984) NBS/NRC steam tables. Thermodynamic and transport properties and computer programs for vapor and liquid states of water in SI units. Hemisphere Publishing, McGraw-Hill, New York.

Heyen, G., Ramboz, C., and Dubessy, J. (1982) Simulation des équilibres de phases dans le système CO_2-CH_4 en dessous de 50 °C et de 100 bars. Application aux inclusions fluides. Comptes Rendus, l'Académie des Sciences, Paris, 294, série II, 203–206.

Holloway, J.R. (1981) Compositions and volumes of supercritical fluids in the earth's crust. In L.S. Hollister and M.L. Crawford, Eds., Mineralogical Association of Canada Short Course in Fluid Inclusions, 6, 13–38.

Jacobs, G.K., and Kerrick, D.M. (1981) Methane: An equation of state with application to the ternary system H_2O-CO_2-CH_4. Geochimica et Cosmochimica Acta, 45, 607–614.

Kerrick, D.M., and Jacobs, G.K. (1981) A modified Redlich-Kwong equation for H_2O, CO_2 and H_2O-CO_2 mixtures at elevated pressures and temperatures. American Journal of Science, 281, 735–767.

Knight, C.L., and Bodnar, R.J. (1989) Synthetic fluid inclusions. IX. Critical *PVTX* properties of NaCl-H_2O solutions. Geochimica et Cosmochimica Acta, 53, 3–8.

Nicholls, J., and Crawford, M.L. (1985) FORTRAN programs for calculation of fluid properties from microthermometric data on fluid inclusions. Computers & Geosciences, 11, 619–645.

Saxena, S.K., and Fei, Y. (1987) Fluids at crustal pressures and temperatures I. Pure species. Contributions to Mineralogy and Petrology, 95, 370–375.

Swanenberg, H.E.C. (1980) Fluid inclusions in high-grade metamorphic rocks from southwestern Norway. Geologica Ultraiectina, 25, 147 p.

Zhang, Y., and Frantz, J.D. (1987) Determination of the homogenization temperatures and densities of supercritical fluids in the system NaCl-KCl-$CaCl_2$-H_2O using synthetic fluid inclusions. Chemical Geology, 64, 335–350.

Manuscript received April 26, 1989
Manuscript accepted July 26, 1989