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SOFTWARE NOTICE

GEØ-CALC: Software for calculation and display of *P-T-X* phase diagrams

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General software description

GEØ-CALC is a microcomputer software package consisting of a program for calculation of phase diagrams, a thermodynamic database for minerals, and auxiliary programs for plotting and printing of computed phase diagrams. Minimum hardware requirements are an IBM-compatible personal computer with 512 K memory, math coprocessor, and graphics card (CGA, EGA, or Hercules). The version 1.0 release includes the programs described below.

PTX

The main part of the GEØ-CALC package is PTX, a FORTRAN77 program that calculates complete pressure-temperature (*P-T*), temperature-composition (T-$X_{H_2O\text{-}CO_2}$), and pressure-composition (P-$X_{H_2O\text{-}CO_2}$) diagrams. PTX has been adapted for microcomputer use from mainframe programs that are described in detail by Perkins et al. (1986). The major differences between the mainframe version and this implementation are that three mainframe programs have been combined into one program, user input is simplified greatly, several run-time options have been modified or removed, and the program generates and calculates each reaction separately rather than generating coefficients for all possible reactions before calculating any individual reaction. This last modification was necessary because of the limited memory available on most microcomputers for calculating and storing a large number of reaction coefficients.

Run-time options include setting the *P-T-X* limits of the diagram, selection of ideal or nonideal H_2O-CO_2 mixing, and specification of fixed phase activities. The user can also specify that only curves stable in the presence of a given phase or assemblage be computed so that the stability fields of particular phases or assemblages can be identified readily. The program evaluates all possible reactions in the user-specified compositional and *P-T-X* space. Each point of every reaction is tested for stability with respect to all other phases in the system, and metastable extensions are eliminated. If a curve is completely outside the *P-T-X* limits of the diagram, any remaining reactions containing the metastable assemblage are removed from further consideration. Finally, all curves are written to a plot file and labeled with stable assemblages. The output can also be inspected in tabular form. Figures 1 to 3 show examples of the plot output of the three types of phase diagrams that can be calculated with PTX.

Execution times are only moderately dependent on hardware, with AT-compatibles running approximately 10% faster than XT-compatibles. Computation time is more affected by run-time options, increasing when hydrous and mixed volatile systems are considered, and when solid-solution models are included. Total execution time should be on the order of minutes for systems with less than a hundred possible reactions, hours for systems with several thousand possible reactions, and days for systems with more than several hundred thousand possible reactions. Table 1 gives the execution times for the phase diagrams displayed in Figures 1 to 3.

PTX allows one to calculate any phase diagram using the variables *P*, *T*, or X_{CO_2} and faithfully calculates equilibrium curves defined by the equality of Gibbs free energy of reactants and products of each equilibrium. The user should be ever aware that the accuracy of calculated phase diagrams is a direct function of the quality of thermodynamic input data. The database distributed with this software is that derived by Berman et al. (1985) for some 70 minerals in the system Na_2O-K_2O-CaO-MgO-FeO-Fe_2O_3-Al_2O_3-SiO_2-TiO_2-H_2O-CO_2. These authors have described the database in detail and have documented which experimental data are reproduced well and which are not. Further details of the procedures used to derive this data set are given by Berman et al. (1986). The database includes functions for temperature-dependent disordering, first- and second-order

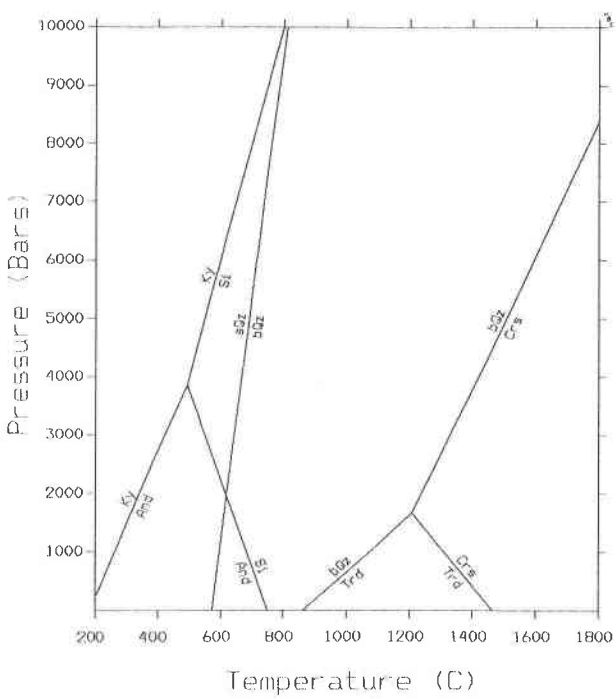

Fig. 1.

[1] The GEØ-CALC software is being distributed by the University of British Columbia at modest cost. If you are interested in obtaining this software, please contact Berman, who can also supply further details regarding this software.

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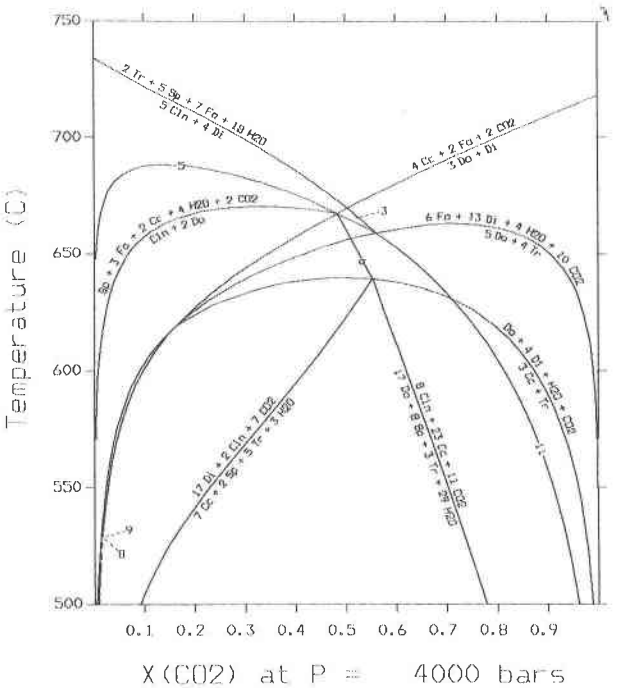

Fig. 2.

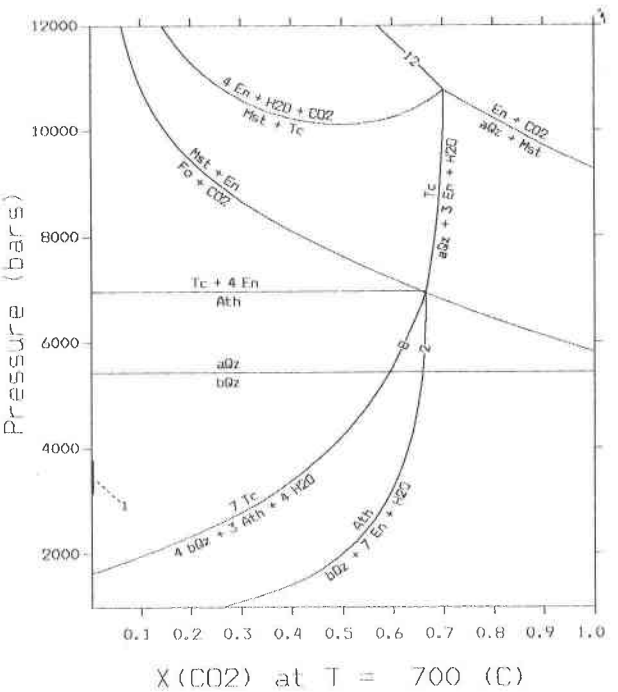

Fig. 3.

TABLE 1. Execution times in minutes for PTX

Fig. no.	No. of reactions	Compaq 286 (AT)	Compaq Plus (XT)
1	35	1.0	1.2
2	36	22.1	25.2
3	126	23.1	21.1

polymorphic transitions, and several specific solid solutions. Options for a variety of other equations of state are provided so that PTX can be used with different sets of thermodynamic data.

PLOT/S/H

These programs are used for viewing the calculated stable phase diagrams on a video monitor. The different versions of PLOT can be used with an IBM color graphics card (CGA), enhanced graphics adapter (EGA), or Hercules graphics card.

PRINTER

This program makes high-resolution hard copies of phase diagrams on dot matrix printers. Figures 1 to 3 show examples of phase diagrams printed on an EPSON dot matrix printer.

CLEAN

This program cleans up the appearance of complicated phase diagrams on which the reaction labels overwrite one another. It replaces all conflicting reaction labels with numbers and writes a list of reactions that correspond to these numbers to a separate file. The CLEANed up plot output (Figs. 2 and 3) can be viewed on screen with PLOT, or on a hard copy with PRINTER.

REFERENCES

Berman, R.G., Brown, T.H., and Greenwood, H.J. (1985) An internally consistent thermodynamic data base for minerals in the system Na_2O-K_2O-CaO-MgO-FeO-Fe_2O_3-Al_2O_3-SiO_2-TiO_2-H_2O-CO_2. Atomic Energy of Canada, Ltd. Technical Report 377, 62 p. (available from SSDO, Atomic Energy of Canada, Ltd., Chalk River, Ontario, K0J 1J0 Canada).

Berman, R.G., Engi, M. Greenwood, H.J., and Brown, T.H. (1986) Derivation of internally consistent thermodynamic data by the technique of mathematical programming: A review with application to the system MgO-SiO_2-H_2O. Journal of Petrology, 27, 1331–1364.

Perkins, E.H., Brown, T.H. and Berman, R.G. (1986) PTX-SYSTEM: Three programs for calculation of pressure-temperature-composition phase diagrams. Computers & Geosciences, 12, 749–755.

NOTICE

NEW TEMPERATURE STANDARD

The U.S. National Bureau of Standards has issued a new standard reference material for temperature based on the freezing point of pure indium. The indium freezing-point standard (SRM 1971) supplies a fixed point for temperature calibrations at 156.635 ± 0.002 °C on the IPTS-68. This temperature lies between the two temperature reference points for the freezing points of gallium (30 °C) and tin (232 °C) and so provides an important new point for precision thermometry and temperature control.