

SOFTWARE NOTICE

Computer programs for petrologic *P-T-t* path calculations

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ABSTRACT

Computer programs have been developed for the Apple Macintosh computer that are designed to facilitate metamorphic petrology calculations and to explore the tectonic significance of *P-T-t* paths through thermal modeling. Programs for petrologic calculations include Reaction, which calculates reactions among phase components, Tetplot, which plots three- and four-component tetrahedral phase diagrams in single and stereoscopic views, and Thermobarometry, which calculates and plots lines of constant equilibrium constant for real mineral data and includes a large fraction of all published calibrations of commonly used thermometers and barometers. Program Gibbs is a generalized algorithm to perform *P-T-X-M* (pressure–temperature–composition–mineral abundance) phase equilibria calculations. Two programs model diffusion in garnet: Garnet Diffusion, which performs Fe–Mg diffusion calculations, and DiffGibbs (diffusion + Gibbs), which performs four-component diffusion calculations and supports complex boundary conditions for the garnet.

Thermal modeling programs include Contact, which simulates contact metamorphism, and Thicken, which simulates one-dimensional crustal thickening of an orogen.

A 200-page program manual and tutorial is available to assist the interested user or to use as the basis of class exercises.

INTRODUCTION

On October 26 and 27, 1990, we (F.S.S. and S.M.P.) presented a short course at the Geological Society of America meeting in Dallas, Texas, on the application of computer programs to the calculation and interpretation of metamorphic *P-T-t* (pressure–temperature–time) paths. The bulk of the course consisted of the application of computer programs to solving problems in metamorphic phase equilibria and thermal modeling. The course materials consisted of 11 computer programs and a 200-page program manual (Spear and Peacock, 1990) with detailed computer exercises and tutorials. We have been distributing the programs and manual to interested parties, and the purpose of this notice is to announce their availability to readers of the *American Mineralogist*. The computer programs and program manual are supplementary material to the theoretical coverage of the subject given by Spear and Peacock (1989).

We attempted to write the program manual in a tutorial style that would allow an individual to work through the operation of the programs independently. Our goal was to provide a document that would teach both the use of the computer programs and some important concepts in metamorphic petrology. We believe the programs and manual will be useful to persons doing metamorphic petrology research and to metamorphic petrology

classes. Many program exercises are simple enough for undergraduate students to understand and should be quite useful in undergraduate petrology.

All of the programs are written for a Macintosh in Fortran and will run on any Macintosh microcomputer with at least 1 Mbyte of memory. Versions are available that do and do not require a math coprocessor. Output is in the form of screen graphics and text files. Graphics output that is compatible with the Adobe Illustrator ('88 and v 3.0) graphics programs (Encapsulated Post Script) is also supported. All programs are distributed with source code, executable modules (applications), and auxiliary files necessary to perform the exercises.

DESCRIPTION OF THE PROGRAMS

The programs may be divided into two groups: The first group is designed to aid the petrologist in the analysis of rock phase equilibria and the extraction of meaningful constraints on the pressure–temperature evolution of a sample. The second group of thermal modeling programs is designed to test tectonic interpretations and to examine the consistency of these models with petrologic and geochronologic data.

1. Reaction—A program to calculate a linearly independent set of reactions among phase components of a homogeneous or heterogeneous system. The program will also calculate all possible reactions.

2. Table—A utility program to create/list/tabulate/transform mineral data files used in programs Thermobarometry and Tetplot.

3. Tetplot—A program to plot monoscopic or stereoscopic views of tetrahedral phase diagrams and triangular phase diagrams. The tetrahedral phase diagrams can be rotated and scaled on the screen.

4. Thermobarometry—A program to calculate and plot results of thermobarometry. The program operates on data files created using program Table. The program incorporates most thermobarometric calibrations for metamorphic rocks that have been published in the literature.

5. Gibbs '90—A general Gibbs method algorithm, similar to the program described by Spear and Menard (1989). The current version is enhanced considerably and includes (a) complete compatibility with Berman's (1988) thermodynamic data base, (b) generalized Margules nonideal mixing for single-site solid solutions, (c) calculations involving mixed volatile equilibria (H_2O – CO_2), (d) a "user friendly" Macintosh interface, (e) on-screen graphics plotting, (f) support of encapsulated Post Script graphics output, (g) a completely rewritten computational algorithm involving equilibrium constants rather than Gibbs–Duhem

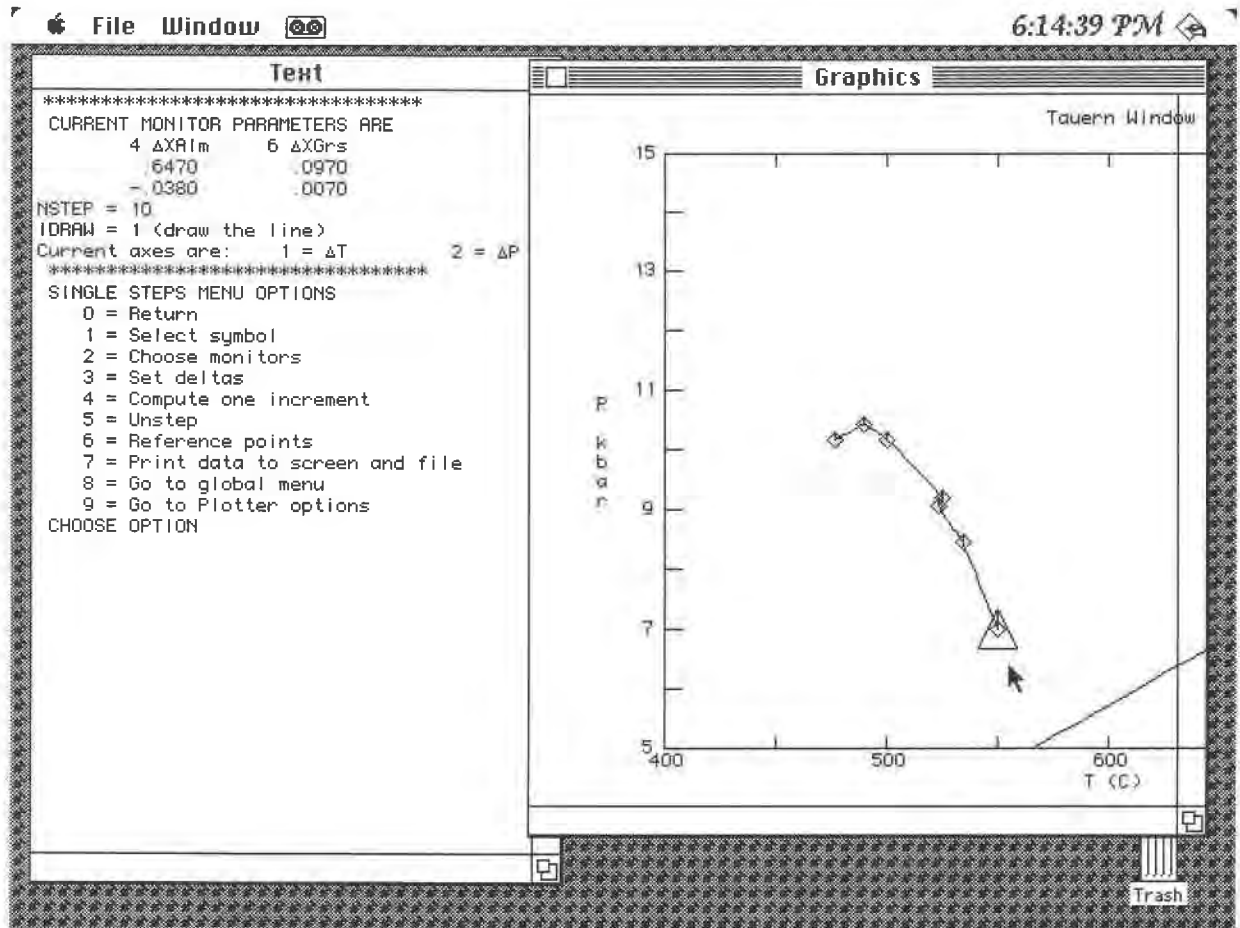


Fig. 1. A Macintosh screen dump showing the appearance of the screen during the operation of program Gibbs '90. The left hand screen (Text) contains menu information for running the program and all nongraphics I/O. The right hand screen (Graphics) contains graphics output. This example depicts a *P-T* path calculated from a zoned garnet from the Tauern Window, Austria, from the data of Selverstone et al. (1984). The arrow points to the rim conditions of the garnet.

equations, which simplifies matrix calculations and enhances speed by a factor of 2–4, and (h) the option of open system calculations. The program is designed to calculate *P-X*, *T-X*, and *P-T* contour diagrams, *P-T* paths from zoned garnets, prograde reaction path models, and other petrologic phase equilibria.

6. Modelplot—A program to plot certain types of results from Gibbs '90 forward modeling experiments.

7. Make Thermo File—A program to read Berman's (1988) thermodynamic data file and convert into a Gibbs '90 compatible file. The program also will allow the user to create data file entries based on estimates of the entropy, volume, heat capacity, compressibility, and expansivity using estimation algorithms in Berman and Brown (1985), Powell and Holland (1985), and Holland (1989).

8. Garnet Diffusion—A binary Fe-Mg finite difference diffusion program to calculate the apparent temperature from garnet-biotite thermometry using user-selected cooling rates and other input parameters.

9. DiffGibbs (diffusion + Gibbs)—A quaternary finite difference diffusion program for garnet integrated into the Gibbs program. The program is designed to examine the consequences of diffusive processes operating simultaneously with net transfer and exchange reactions in either a high-grade rock undergoing

cooling or a low-grade rock undergoing garnet growth and subsequent cooling.

10. Contact—A one-dimensional finite difference program designed to simulate contact metamorphism. The thermal evolution of intrusions and adjacent contact aureoles is demonstrated graphically using temperature-position, T_{max} -position, and temperature-time plots. The user can specify a variety of parameters including intrusion width, intrusion temperature, and country rock temperature.

11. Thicken—A one-dimensional finite difference program designed to simulate regional metamorphism resulting from crustal thickening. Crustal thickening occurs as a result of thrusting or homogeneous (ductile) thickening. The thermal evolution of thickened crust is illustrated by a variety of plots including geotherms as a function of time and *P-T-t* paths for user-selected rocks. A variety of parameters can be specified by the user such as the initial crustal geotherm and the thickness of the thrust sheet.

TWO EXAMPLES

Figure 1 shows an example of the appearance of the Macintosh screen during the calculation of a *P-T* path using program Gibbs

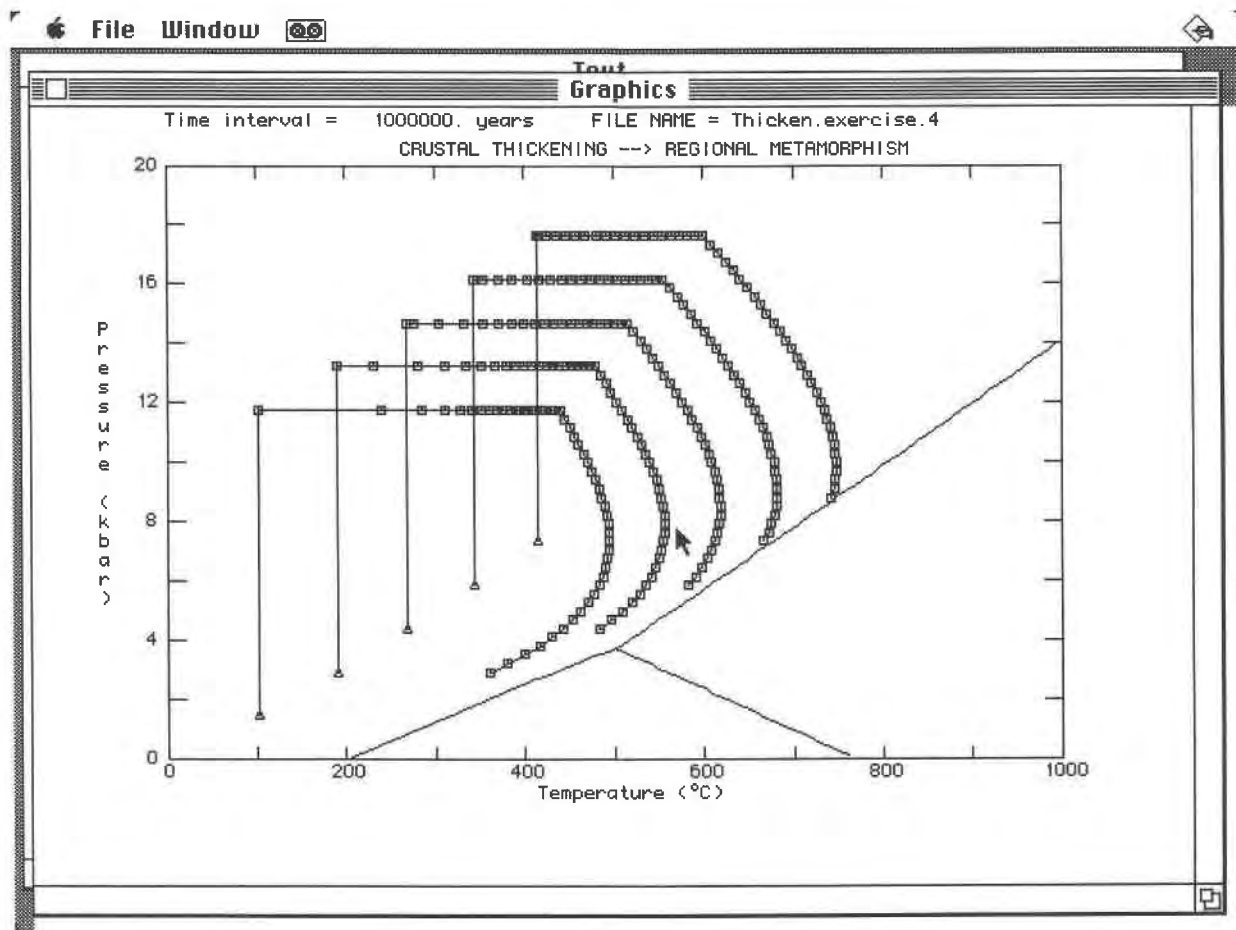


Fig. 2. A Macintosh screen dump illustrating one of the graphics windows produced by the program Thicken. Five metamorphic P - T - t paths are shown for lower plate rocks located 5, 10, 15, 20, and 25 km beneath a thrust sheet 35 km thick. The rocks start at the P - T conditions indicated by the small triangles and undergo isothermal compression as a result of the instantaneous emplacement of the thrust sheet. After thickening, the

rocks heat up isobarically for 20 m.y.; subsequently, rocks undergo decompression as a result of denudation at 1 km/m.y. and reach their maximum temperature during uplift. Each small square represents 1 m.y. of evolution. The P - T - t path indicated by the arrow closely approximates the path determined for the Tauern Window sample shown in Figure 1.

'90. The left screen is the text window, which in this example shows one of the calculation menus in the Gibbs programs. All the programs are menu driven with the menus listed in the text window. The numerical results of calculations are also directed to the text window. Graphics are directed to the graphics window or, if the appropriate switches are set, to a text file in EPS format. The plot shown in Figure 1 is a P - T path calculated from a zoned garnet from the Tauern Window, Austria. The arrow points to the P - T conditions of the rim (see Selverstone et al., 1984, for further details).

Figure 2 shows an example of the Macintosh screen illustrating metamorphic P - T - t paths calculated using the program Thicken. Five different metamorphic P - T - t paths are displayed for rocks located 5, 10, 15, 20, and 25 km below a thrust sheet 35 km thick. In this particular numerical experiment, the thickened continental crust is denuded at 1 km/m.y. starting 20 m.y. after instantaneous crustal thickening. Rocks in the lower plate of a thrust fault follow clockwise metamorphic P - T - t paths. Note that the P - T - t path marked by the arrow closely approximates

the P - T - t path calculated for the rock from the Tauern Window shown in Figure 1.

HOW TO OBTAIN THE PROGRAMS AND PROGRAM MANUAL

The programs are not copy protected, and the source code is provided. Disks are supplied with both nonmath coprocessor versions and math coprocessor versions of every program. Many of the programs are not computationally intensive and run fine without the coprocessor. However, the diffusion and thermal modeling programs run twice as fast using the coprocessor versions. A Mac II or SE/030 (or other coprocessor-enhanced Macintosh) is required for the coprocessor versions.

We are asking a nominal donation to defray the cost of producing the 200-page manual, maintaining and upgrading the programs, and handling distribution of the software. Please remit \$15 per copy of the program manual and \$35 per copy of the software (11 programs total) to the first author (F.S.S.). Please

send a check (made payable to RPI, attention Frank Spear) or money order and include your name and address for shipping. Please do not send blank diskettes.

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