THERMOCALC

THERMOCALC is thermodynamic calculation software for tackling mineral equilibria problems. It has two main components: the application itself, and the internally-consistent thermodynamic dataset it uses. The mineral equilibria problems that can be addressed with THERMOCALC include *inverse modelling* ones (geothermometry/barometry using average *PT*), and *forward modelling* ones (calculating phase diagrams for model systems). For the latter there now exists a new program—DRAWPD—that allows manually-assembled THERMOCALC output to be drawn in postscript.

How to run THERMOCALC

- before you fire up THERMOCALC, you must have a datafile for your rock or your model system (depending on whether you are doing inverse or forward modelling)

- THERMOCALC is a standard (old-fashioned) "console" application, without a GUI, so when you fire it up, it operates by Q&A. You proceed by answering questions that it asks you (statements ending in"?": to answer 'yes', you just hit return, or type 1 or y or yes, then return; to answer 'no', you type 0 or n or no, then return) or giving information that it asks you for (statements *not* ending in"?": type the information, then hit return, or, in some cases, just hitting return uses a default).

- As well as the information on the screen, THERMOCALC puts essential output into a file (a TH O file), a complete log of the run into a log file (the TH LOG file), and also specially formatted output, for example, for use by the software DRAWPD, into a file (the TH DR file). the information in these output files will normally be overwritten next time you run THERMOCALC, so copy out the parts you want to keep into another file before continuing.

The steps in phase diagram calculations

- datafile creation (*a-x* relationships, bulk composition etc) for THERMOCALC

- calculation of component parts of phase diagram (often line-by-line) by THERMOCALC

- manual assembly of THERMOCALC output for input to DRAWPD

- generation of a postscript drawing by DRAWPD

- tidying up and labelling the phase diagram with Adobe Illustrator (or other postscript-aware graphics program)

About the software

THERMOCALC, DRAWPD and AX are all written in Pascal using Metrowerks Codewarrior on the Mac platform, and Delphi on the PC platform. The PC development is done on the Mac using the emulation software, RealPC, running Windows 95.

A little history

The first thermodynamic calculation program with the name THERMOCALC was in spaghetti Fortran, written by Roger Powell (RP) in 1971. It went through various incarnations over the years, on everything from mainframes to Hewlett-Packard programmable calculators. In 1982, Tim Holland (TJBH) and RP started talking about the 'best' way of processing the available experimentally-determined mineral equilibria to constrain thermodynamic data, at a meeting we both happened to be attending in London. At that stage, TJBH was interested in the resulting thermodynamic data and what could be done with it, whereas RP was primarily interested in the statistical, mathematical and software problems involved. Although this distinction has blurred substantially in the intervening time, RP is still responsible for the software[1] (and the stats and maths involved), whereas TJBH is responsible for the internally-consistent thermodynamic dataset.

The software is spelt with all capitals—THERMOCALC—to differentiate it from a more recent program, Thermo-calc, coming out of Uppsala, with which it is unrelated.

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[1]But AX is a tjbh program—originally based on a venerable rp mainframe program called RECALC