TC-Investigator: A Matlab Program to Explore Pseudosections

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Forward modelling of bulk rock compositions to constrain pressures and temperatures of metamorphism based on mineral assemblage is a commonly used technique. The pseudosections produced contain a wealth of information about predicted mineral compositions and abundances that goes far beyond variations in mineral assemblage. A grid of these variations can be contoured using Gibbs free energy minimisation software (such as Theriak-Domino) or precise isopleths calculated for specific quantities in THERMOCALC. We have produced a new piece of software called TC-Investigator that amalgamates these approaches to provide a relatively quick and user friendly way to contour all compositional parameters and mineral modes across a THERMOCALC pseudosection.

TC-Investigator takes the postscript pseudosection diagram and creates a grid of points at a user-specified resolution. THERMOCALC is then used to calculate the equilibrium mineral assemblage at each point using an initial starting guess provided by the user (this can be calculated during initial pseudosection calculation). Once all points have been tried, any that failed to calculate are re-tried using interpolated starting guess values from the surrounding points. This procedure is iterated until no more solutions are found. Any remaining unsolved points are then interpolated numerically from surrounding solutions to produce a fully quantified set of mineral modes and compositions. Following calculation, the dataset can be contoured and output as figures, output as a Matlab readable binary structure or selected compositions written to an ASCII text file.

Compositional maps created by TC-Investigator have the power to inform the user about compositional variables that are not conventionally considered. The automated calculation method makes it easy to investigate all variables in one go. For example, in metapelitic rocks, garnet shows the variations in composition that are usually contoured, however, these couple to variations in composition within many other minerals all of which can be seen using TC-Investigator. Plots of water content reveal zones in P-T space where there is extremely rapid water production as hydrous minerals breakdown. As new P-T conditions and bulk compositions are explored using improved thermodynamic datasets this software will provide a quick and simple way to identify key compositional and modal variations in the newly modelled mineral systems.