

The computation of equilibrium assemblage diagrams with Theriak/Domino software

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ABSTRACT

In this paper, the term “equilibrium assemblage diagrams” refers to diagrams strictly based on assemblages predicted by Gibbs free energy minimization. The presented Theriak/Domino software uses a unique algorithm of scanning and bookkeeping, which allows to compute completely and automatically a great variety of diagrams: phase diagrams, pseudo-binary, pseudo-ternary, isopleths, modal amounts, molar properties of single phases or bulk-rock properties like total ΔG , volume of solids, etc. The speed and easiness of use makes thermodynamic modeling accessible to any student of Earth sciences and offers a powerful tool to check the consistency of thermodynamic databases, develop new solution models, plan experimental work, and to understand natural systems. The examples described in this paper demonstrate the capacity of the software, but also to show the usefulness and limitations of computed equilibrium assemblage diagrams. For most illustrations, a metapelite (TN205) from the eastern Lepontine Alps is used. The applications include the interpretation of complex diagrams, mineral reactions, the effect of Al content on the equilibrium assemblages, the interpretation of Si per formula unit in white mica, understanding some features of garnet growth, dehydration and isothermal compressibility, a broadening of the concept of AFM diagrams, combining equilibrium assemblage diagram information with thermobarometry, and comparing the results produced with different databases. Equilibrium assemblage diagrams do not always provide straightforward answers, but mostly stimulate further thought.

Keywords: Phase diagram, software, Gibbs free energy minimization, equilibrium assemblage, metapelites