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An integrated modeling framework and a software solution for tracing equilibrium relationships in metamorphic rocks

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Equilibrium thermodynamics is a fundamental tool to model how a rock with a specific bulk composition responds to changes in pressure (P) and temperature (T). The success of equilibrium thermodynamics has been largely facilitated by the successive developments of databases as well as by the availability of software solutions for petrological modeling. However, the underlying assumption that metamorphic minerals form and evolve at or close to equilibrium conditions restricts the petrological models to relatively simple scenarios. Examples include [1] isochemical models allowing phase relationships at equilibrium to be mapped out in the P-T space (e.g. pseudosection), or [2] non-isochemical models involving dynamic reactive bulk compositions (e.g. mineral or melt fractionation) along fixed P-T trajectories. By contrast, most of the metamorphic minerals in nature exhibit compositional zoning suggesting sluggish diffusion and partial re-equilibration. Where metastable relics are present, thermodynamic equilibrium was as best achieved locally during the evolution of the rock. This simple observation raises several questions about the limits of the equilibrium models. Is the bulk rock composition of a hand-specimen sized sample representative of a reactive volume at any stage of the P-T path? What are the size and the geometry of the equilibrium volumes that have to be considered for accurate modeling?

To answer these questions, a new modeling framework based on iterative thermodynamic models integrated with quantitative compositional mapping was developed and stitched into the software package Bingo-Antidote. The subroutine Bingo contains a scoring technique to quantitatively compare modeled and observed mineral assemblages modes and compositions. One of the key features is the correspondence between the local bulk composition taken as the reactive bulk composition and the direct observations (modes and compositions) in the same volume. This mutual correspondence permits to build a fully quantitative comparison between model and observations as well as providing a statistical framework for evaluating the quality of the model. In addition, the subroutine Antidote includes mapping functions and a heuristic search method that can determine optimal P-T-X conditions. Bingo-Antidote is a powerful alternative to traditional modeling tools as the textural and compositional complexity of any sample can be taken into consideration when applying equilibrium models.