Beauty and the Beast: phase equilibrium modelling of eclogites

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Phase equilibrium modelling is now a critical tool for quantifying the conditions of high-pressure metamorphism. Two types of forward models based on Gibbs Energy minimization are commonly used (*e.g.*, Lanari & Duesterhoeft, 2019). The first type uses mineral assemblages, modal abundances, and mineral compositions to constrain pressure–temperature (*P*–*T*) conditions on a phase diagram. The goal is to reproduce the observed mineral assemblages and compositions to derive "optimal" *P*–*T* conditions for a given sample. This approach has dominated the high-pressure petrological literature and vastly improved our understanding of the conditions reached during subduction and collision in various metamorphic belts. The second type represents a series of Gibbs Energy minimizations performed along a pre-defined *P*–*T* path for a given bulk rock composition. This approach allows simulation of the successive metamorphic transformations that occur in any rock system where thermodynamic equilibrium is the controlling factor. Recently, these petrological models have been coupled with isotopic calculations resulting in a new generation of so-called petrogeochemical models (Vho *et al.*, 2019, 2020).

Although significant progress has been made in the modeling of high-pressure rocks over the last two decades, the ability of thermodynamic models to accurately reproduce natural observations remains unclear. The modeling of high-pressure rocks is complex for several reasons. Eclogites often carry metastable relicts, such as chemically-zoned minerals, and therefore reached – at best – only local chemical equilibrium. Multiple thermodynamic databases are available for modeling, but there is no systematic quantification of the variability in results caused by differences in thermodynamic properties. This study presents a newly developed algorithm that compares observed and modeled mineral assemblages and compositions for a given reactive bulk composition. The algorithm incorporates the uncertainty on the reference *P*–*T* conditions as well as the mineral and reactive bulk compositions during the model evaluation. We have compiled several, well-characterized, high-pressure rocks which have been used to assess the ability of multiple thermodynamic databases to reproduce nature.

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