



## Thermodynamic modelling of metamorphism: promises, pitfalls and future directions

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Of all the fields of petrology, thermodynamic modelling has had the largest impact in metamorphic petrology. Many of the underlying methods used are predicated on a thermodynamic equilibrium model of metamorphism. While thermodynamic methods have been common in metamorphic studies for decades, for example in thermobarometry, how we use thermodynamic methods have evolved substantially over this time. Of particular importance has been the development of quantitative phase equilibria methods using large internally consistent datasets, sophisticated software and ever evolving and improving activity–composition models. These tools have taken quantitative phase petrology from representing a simple framework in which to consider metamorphic rocks to one that can be directly applied to a wide range metamorphic rocks and processes to understand P–T evolution and the consequences of various key metamorphic processes. However, there remain many outstanding issues with the approach requiring that such methods be applied with caution and the results of modelling not taken too literally. Of all the fields of petrology, thermodynamic modelling has had the largest impact in metamorphic petrology. Many of the underlying methods used are predicated on a thermodynamic equilibrium model of metamorphism. While thermodynamic methods have been common in metamorphic studies for decades, for example in thermobarometry, how we use thermodynamic methods have evolved substantially over this time. Of particular importance has been the development of quantitative phase equilibria methods using large internally consistent datasets, sophisticated software and ever evolving and improving activity–composition models. These tools have taken quantitative phase petrology from representing a simple framework in which to consider metamorphic rocks to one that can be directly applied to a wide range metamorphic rocks and processes to understand P–T evolution and the consequences of various key metamorphic processes. However, there remain many outstanding issues with the approach requiring that such methods be applied with caution and the results of modelling not taken too literally as a “truth”. The ongoing development of thermodynamic datasets and a–x relations for minerals continues to broaden the range of phase petrology studies that can be undertaken. A recent update of the Holland and Powell internally-consistent dataset and the formulation of a–x models more applicable to mantle conditions represent two important recent developments. Even for common crustal rock that can be adequately modelled currently, there is a need to continue to develop original and innovative phase diagrams to illustrate a greater number of processes. This is particularly important for complex rocks that contain reaction textures for example, where only through the simultaneous consideration of both the P–T changes that drove reaction and the diffusional regime that controlled the spatial evolution of the textures can such features be better understood and interpreted. Despite the many caveats in the application of thermodynamic methods to metamorphic rocks it still provides the most robust framework in which to understand the metamorphic evolution of rocks. Further and more explicit integration of phase petrology with a range of geochemical, geochronological and geodynamic methods stand out as important future directions for thermodynamic modelling of metamorphic rocks as a “truth”. The ongoing development of thermodynamic datasets and a–x relations for minerals continues to broaden the range of phase petrology studies that can be undertaken. A recent update of the Holland and Powell internally consistent dataset, and the formulation of a–x models more applicable to mantle conditions represent two important recent developments. Even for common crustal rock that can be adequately modelled currently, there is a need to continue to develop original and innovative phase diagrams to illustrate a greater number of processes. This is particularly important for complex rocks that contain reaction textures for example, where only through the simultaneous consideration of both the P–T changes that drove reaction and the diffusional regime that controlled the spatial evolution of the textures can such features be better understood and interpreted. Despite the many caveats in the application of thermodynamic methods to metamorphic rocks it still provides the most robust framework in which to understand the metamorphic evolution of rocks. Further and more explicit integration of phase petrology with a range of geochemical, geochronological and geodynamic methods stand out as important future directions for thermodynamic modelling of metamorphic rocks.