

Comparing internal and external buffering of oxygen fugacity using phase equilibria modelling

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Pseudosection modelling is the leading tool for the analysis and contextualisation of mineral assemblages within metamorphic rocks. Increasingly, pseudosection modelling is also being applied to igneous rocks, following the development of thermodynamics models for granitic to ultramafic melts. However, a common point of divergence between the two communities relates to how oxygen is considered as a variable. Specifically, metamorphic studies frequently treat oxygen as an extensive variable, typically in terms of a fixed ferric iron content, whereas igneous studies often consider oxygen as an intensive variable, typically in terms of oxygen fugacity (f_{O_2}) relative to an oxygen buffer. These contrasting viewpoints equate to f_{O_2} either being internally buffered by the mineral assemblage, or externally buffered by the environment, with important consequences for phase equilibria calculations.

Herein we document a new tool for maintaining an oxygen buffer relative to quartz-fayalite-magnetite (QFM) in THERMOCALC, enabling pseudosection modelling of both internally and externally buffered systems. We also introduce a new activity-composition model for a Mg-bearing ilmenite. To showcase these new models, we present pseudosections for a range of bulk compositions, including peridotite, basalt, tonalite and pelite, in both 'buffered' and 'unbuffered' scenarios. The results show that for a fixed ferric iron content, f_{O_2} varies by several log units with respect to QFM (typically 2-5) over crustal depths and supra-solidus temperatures. The variation is complex, but closely associated with the modes and compositions of major hosts of Fe^{3+} , principally clinopyroxene, amphibole, biotite and Fe-oxides. Although the variation with respect to QFM is significant, buffered pseudosections show similar topologies to their unbuffered counterparts, with changes typically only manifest in minor phases. Finally, Mg-bearing ilmenite is shown to be more stable than previous ilmenite models, as expected for a model that incorporates more components.

Overall, the new models expand our thermodynamic modelling abilities and provide a simple method for investigating the consequences of internal versus external oxygen buffering. Importantly, this outcome optimises our ability to benchmark thermodynamic model predictions against experimental results, which are typically externally buffered relative to QFM.