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A new methodology for considering minor elements of geologic importance in phase equilibria modelling

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The development of activity-composition models for melt in phase equilibria modelling has enabled the study of crustal differentiation processes through partial melting. A number of minor and trace elements are not accommodated in the melt models relevant to aluminous sediments, but are of considerable petrological importance (e.g. Zr, P, Ti). In this study, a new methodology is presented for handling minor and trace components that are currently unable to be thermodynamically constrained in supersolidus conditions. A new feature is built into the thermodynamic modelling software Rcrust (Mayne, Moyen, Stevens, et al., 2016), called Component Packet, that can manipulate chemical components that are not accommodated within the activity composition models. Using this functionality, any such element of interest can be modelled for each PT point in Rcrust and partitioned between specified phases. In this study, the usefulness of this new functionality has been demonstrated using the behaviour of Ti. Ti is critical in stabilizing biotite at high temperature. Thus, the lack of Ti in some solution models for melt in aluminous systems, result in a reduced stability of biotite in magma modelled as having fractionated from the residuum. In order to overcome this, a component packet is employed to investigate the proportion of Titanium that would be partitioned to melt during the anatexis of an average amphibolite-facies metapelite. In this scenario, Titanium contents in melt are estimated by linear regression to titanium versus maficity in a global compilation of S-type granites generated for this purpose. The results are compared to that of an internally consistent thermodynamic model, which does include TiO_2. The linear regression method produces trends that agree with the internally consistent model under certain conditions and produces TiO_2 contents for “melt” that are within the lower range of S-type granites and matches the correlation of TiO_2 vs FeO+MgO of S-type granites, indicating that it is built on a strong relation. Melts are extracted once 7 vol% is accumulated, with 1 vol% retained in the residuum. The phase assemblages in extracted melts were investigated through cooling at 3 kbar and 650°C. The presence of Titanium in melt via Component packet results in a biotite mode of up to 2.5 wt% greater than melts formed without TiO_2 at high temperatures, but on average less than 1 wt%. In addition, extracted melts with Ti from Component Packet allow ilmenite to be a liquidus phase. This shows that the component packet can be used to more accurately model titanium in melt, which greatly affects the stability of Ti phases at emplacement. Furthermore, the petrological applicability of the Component Packet is such that the methodology used here could be applied to the approximation of other minor components that thermodynamic models are currently unable to handle for crustal melting, such

as P^2O_5.

REFERENCES

Mayne, M.J., Moyen, J.F., Stevens, G. & Kaislaniemi, L. 2016. Rcrust: a tool for calculating path-dependent open system processes and application to melt loss. Journal of Metamorphic Geology. 34(7):663–682.