

Choose your model carefully: comparison of two versions of the MELTS algorithm with sub-liquidus phase relations in mineral – melt equilibration experiments at 1 GPa and 1250°C

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Complex petrologic problems can be approached by experiment or by thermodynamic approximation. The thermodynamic approach has helped in understanding phase relations and geochemistry of igneous and metamorphic rocks over a range of temperatures, pressures, and compositions. One of the most commonly used thermodynamic models is the MELTS algorithm. There are a number of versions of the algorithm, which apply to different compositions. pMELTS is used to model partial melting in peridotite and clinopyroxenite compositions, other versions apply to crystallization and melting in volatile-bearing, silica-undersaturated or silica-oversaturated compositions. We are interested in reactive transport of magma through the mantle, particularly the mineral and melt assemblages that result from prolonged flow of magma through closely-spaced vein systems in peridotite. On the basis of field studies, we expect that the vein – peridotite system should reach equilibrium, since magma was present in the fractures for at least a few thousand years. A number of previous studies of reactive transport in peridotite have used the pMELTS algorithm to replace experiments, though it is not clear if this is the most appropriate model.

Magma – mineral equilibration experiments were performed in which a silica-undersaturated alkaline magma is reacted with orthopyroxene, olivine and clinopyroxene in various proportions under mantle conditions (1250°C and 1 GPa). The experiment charges were finely ground before being sealed into graphite-lined platinum capsules and held at the desired conditions for two weeks. It was expected that the combination of small grains with large surface area and long reaction time should allow chemical equilibrium to be attained. The phase proportions and compositions of glass, olivine, clinopyroxene, and orthopyroxene in the experiments have been determined using imageJ and the electron probe; these data allow the appropriateness of two MELTS versions for modelling peridotite – melt interaction to be assessed.

The experimental results were compared to the outputs from pMELTS (the model appropriate for mantle compositions) and MELTS V 1.2.0 (appropriate for modelling phase relations in quartz-free, volatile-bearing magmatic systems). pMELTS consistently overestimates the silica and alkali content of the equilibrium magma and there are large differences between the observed and calculated phase proportions and mineral compositions. MELTS V 1.2.0 gives much closer agreement of mineral and melt compositions and proportions, though there are still some differences between the experiments and the calculated equilibria. These preliminary results show that great care is needed in choosing the most appropriate thermodynamic model for the system of interest.