



Progress in the development of an activity-composition model for silicate melt in THERMOCALC

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We present illustrative calculations on melt-solid equilibria in compositionally simple systems, made using THERMOCALC. The calculations demonstrate the current state of development of an activity-composition model for silicate melt, which is intended ultimately to cover a range of compositions from mafic to granitic, and to be suitable for addressing natural problems involving melting, melt loss and crystallisation.

The envisaged model will combine and expand two melt models already available for use with THERMOCALC. These are a simple mafic melt model in CaO-MgO-Al₂O₃-SiO₂ (CMAS), described by Green et al (2011), and the haplogranitic melt model in Na₂O-CaO-K₂O-FeO-MgO-Al₂O₃-SiO₂-H₂O (NCKFMASH) of White et al (2001). Throughout the development of both mafic and haplogranitic melt models much attention was paid to the careful calibration of model parameters, particularly through a philosophy of calibrating the models in systems with few components. The haplogranitic model was calibrated in its binary subsystems (Holland and Powell, 2001), with the model subsystems being combined to generate the full model. The mafic melt model was calibrated at this early stage in the CMAS system, because this may be regarded as a simple proxy for the natural mantle system, possessing analogues of the crucial thermal divides that govern the evolution of natural melts. By including compositionally simple systems in the calibration, as well as systems that closely approximate natural ones, the amount of information available to constrain model parameters uniquely is increased, making the model calculations more reliable when extrapolated beyond the compositional range of the calibration data.

Green et al (2011). A thermodynamic model for silicate melt in CaO-MgO-Al₂O₃-SiO₂ to 50kbar and 2000 [U+2103]. Submitted to Journal of Metamorphic Geology

Holland and Powell (2001). Calculation of phase relations involving haplogranitic melts using an internally consistent thermodynamic dataset. Journal of Petrology, 2, 673-683

White et al (2001). Calculation of partial melting equilibria in the system NaO-CaO-K₂O-FeO-MgO-Al₂O₃-SiO₂-H₂O (NCKFMASH). Journal of Metamorphic Geology, 19, 139-153