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MELTS 2.0: A Bayesian calibration for silicate melting with a robust redox model

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Molten rocks are primary drivers of thermochemical evolution in rocky planets, but extreme temperature-pressure conditions and compositional variability make it impossible to rely solely on experimental techniques to study them. Thermochemical models thus play a key role in understanding volcanic and magmatic processes, as they provide a physics-based approach to interpolating between and extrapolating away from experimental data. Classic modeling techniques rely on basic least-squares fitting of experimental petrology databases, and have produced our best thermodynamic modeling tools for simulating melting and crystallization processes in natural silicate systems (e.g. MELTS & ThermoCalc). Despite their success, robustness and accuracy remain critical challenges for these models. Since the key value of thermodynamic models is in their predictions of behavior never directly observed in the lab, the ability to quantify variable prediction accuracy for the full range of scientific applications has been sorely lacking.

We present the MELTS 2.0 model, a Bayesian thermochemical model of silicate melting that provides robust simulation uncertainties and relies on an improved underlying redox model. Unlike classical approaches, Bayesian analysis captures a complete family of models that are consistent with the calibration data and modeling assumptions. This first version of MELTS 2.0 focuses on volatile-free natural silicate melts (relevant to de-volatilized systems on Earth and other planets) and demonstrates the predictive power of the Bayesian approach. We combine the experimental mineral saturation constraints for the original MELTS model with additional redox- and phase-assemblage- constraints. We obtain a final model that accurately recovers the entire calibration dataset of coexisting mineral-liquid pairs (to within ~3 kJ) with improved consistency for measured oxygen fugacities (especially at extreme oxidizing or reducing conditions). We use simple Monte Carlo simulation to predict model accuracy for typical geological applications including basaltic evolution and partial mantle melting, obtaining results that match direct experiments as well or better than the original MELTS and pMELTS models. The model even captures 1 GPa peridotite melting experiments [1], paving the way for a single unified model relevant from the surface to the deep mantle.

[1] Baker & Stolper (1994), Geochimica et Cosmochimica Acta, 58(13), 2811-2827.