Goldschmidt 2026 Abstract
https://doi.org/10.46427/gold2026.37709

Building novel thermodynamic models for MELTS, vapors, and fluids using ENKI

AARON S WOLF[1], SIMON W MATTHEWS[2], SUZANNE K BIRNER[3], MARK S GHIORSO[4] AND DR. KAYLA IACOVINO[1]

[1]SETI Institute
[2]Nordic Volcanological Center, Institute of Earth Sciences, University of Iceland
[3]Berea College
[4]OFM Research

The evolution of rocky planetary surfaces, atmospheres, and interiors is governed by the properties and energetics of constituent minerals, melts, vapors, and fluids. Computational thermodynamics provides a quantitative framework for understanding the geochemical evolution of worlds by simulating the system's equilibrium state. The challenge lies in the search for the equilibrium energy minimum "needle" hiding in a vast multidimensional "haystack"–representing the space of all possible arrangements of every chemical component within every possible phase that meets bulk composition constraints. Thermodynamic software [e.g. MELTS, THERMOCALC, Perplex, etc.] must combine mathematical phase models from a self-consistent thermodynamic database with algorithms that find the equilibrium state, and then solve this problem iteratively to simulate evolving systems.

We present an overview of the ENKI open-source thermodynamic modeling platform (www.enki-portal.org), which is home to new and forthcoming versions of the MELTS family of models while also providing a generic model-building and inter-comparison toolkit. This includes extended liquid models, robust equilibration algorithms, kinetics modeling for geodynamics simulations, and community-backed modeling applications for vapors, fluids, and more. At the heart of the ENKI project is a generalized code for building phases and finding equilibrium states called ThermoEngine, whose newest release focuses on fast and robust computations, available across all platforms through a python interface supported by pre-compiled C libraries. We will demonstrate extensive updates to the underlying equilibration algorithms, improving speed and extending robust equilibrium determinations to geo-relevant conditions where all prior MELTS codes failed (especially in cases where components go missing due to fractionation). We will also present our new robust Bayesian liquid model MELTS 2.0, which quantifies application-specific simulation uncertainties and accompanies an automated calibration pipeline that reduces development time for future MELTS model extensions. ENKI also supports a variety of community modeling applications that are built upon ThermoEngine, including VapoRock and VESIcal, which model volcanic outgassing and magmatic fluid exsolution, and pyDEW, which provides an integrated python interface for aqueous speciation calculations using the Deep Earth Water model. Finally, we will show results from a new MELTS extension that incorporates S, Cl, & F into coexisting melt/solute-rich fluid systems.