ENKI: A framework for building, maintaining and using chemical thermodynamic and fluid dynamical models

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ENKI is a software framework designed to facilitate the construction and maintenance of thermodynamic models of naturally occurring materials. It also provides the capability of accessing these models with a standardized user interface and utilizing them for generalized equilibrium calculations (e.g., potential minimization, phase diagram construction) and for supporting kinetic/materials properties models that underlie fluid dynamical simulations. While ENKI provides access to a large number of existing thermodynamic databases (Berman, Helgeson HKF, DEW, Holland and Powell, Stixrude and Lithgow-Bertelloni), a key aspect of ENKI is the ability to formulate thermodynamic models as symbolic expressions, and to automatically generate from these expressions compatible computer code. A consequence of this ability is that models can be more easily documented, more routinely updated, and modifications can be instantly incorporated into application tools (e.g., MELTS). Another key feature of ENKI is the ability to calibrate thermochemical models from experimental data utilizing Bayesian statistical techniques and to document calibration procedures and choices in a manner that encourages reproducibility. We are also making an effort to provide data resources for model calibration, although that effort is incomplete and ongoing.

The user interface to ENKI utilizes Jupyter notebooks and the platform is hosted on a server, which allows user access from a web browser with no additional installation requirements. The API is written in Python, while the underlying computational framework is written in C and derivative languages. The code base is open source and maintained at GitLab (gitlab.com/ENKI-portal). Extensive documentation is provided and may be accessed from the ENKI website (enki-portal.org). Jupyter notebooks illustrating use of the ENKI framework are available at the ENKI compute server (enki.ofm-research.org/hub/login).