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pyDEW: A python interface for calculations with the Deep Earth Water model

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The Deep Earth Water (DEW) model [1,2] enables modelling of fluid-mineral reactions at the conditions of the upper mantle and lower crust. The DEW model has been applied to a range of problems including devolatilisation of subducting slabs [3] and diamond formation [4]. However, the application of DEW has been limited by the software used to solve for the equilibrium state. Most studies using the DEW model have relied on the Fortran EQ3/6 programs for which generating input files is time consuming, restricting application of the DEW model.

The open-source pyDEW python library is built on top of the ENKI Thermoengine [5] and provides a new toolkit for performing fluid-mineral (and fluid-silicate magma) equilibration calculations. The library provides a convenient interface to calculating the thermodynamic properties of aqueous species, writing the input files for the EQ3/6 programs, or fully automating EQ3/6 aqueous speciation calculations. The pyDEW package liberates the user from data files restricted to specific temperature ranges at fixed pressures. It is not restricted to any particular conditions (beyond that which the model is calibrated over), and returns results rapidly, opening new possibilities for modelling complex systems and performing large numbers of computations over wide ranges of temperature, pressure, and compositional space [6](e.g., Sverjensky et al., this conference).

The integration of pyDEW into the ENKI Thermoengine enables equilibrium between aqueous fluid and magma to be modelled [7], as well as the incorporation of complex mineral solid solution models. It also provides the basis for documenting (using Jupyter Notebooks) all the steps in model calibration and ensuring complete reproducibility. pyDEW calculations may be performed in the cloud, making the software accessible to anyone with a web browser [8].

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