Goldschmidt 2025 Abstract
https://doi.org/10.7185/gold2025.28811

Predictability of thermodynamic properties of Earth's fluids using molecular level computer simulation and Equations of State: Introducing a new web-based calculation platform

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Presented are reviews on equations of state (EOS) and molecular level computer simulation (MLCS) of thermodynamic properties of Earth's fluid systems. Conclusions are drawn on the predictability of EOS and MLCS. And most importantly, a new online platform is introduced that offers free access to the calculation of various thermodynamic properties of major Earth's fluid systems. The platform can be accessed at: http://efs.idsse.ac.cn/

Experimental data have long been essential in interpreting geochemical mechanisms, yet such data remain persistently scarce for Earth's fluid systems (EFS), as evidenced by those available in three common systems: H_2O, H_2O-CO_2, and H_2O-NaCl. The scarcity underscores the necessity of theoretical approaches as significant alternatives for predicting the thermodynamic properties of EFS in geochemical processes. Among these, EOS and MLCS represent the most significant theoretical tools for this application, and previous studies demonstrated their high predictability for various thermodynamic properties, along with their significance in geochemical applications.

EOS can provide four types of predictability: (1) predicting thermodynamic properties that exceed the pressure-volume-temperature-composition (*PVTx*) range covered by experimental data; (2) deriving unknown thermodynamic properties from known ones, such as transitioning from *PVTx* to fugacity or phase equilibria; (3) serving as an intermediary property (e.g., water density) linking to other geochemically relevant properties (e.g., dielectric constant and conductance); (4) scaling from one type of molecule to other similar ones (e.g., from CH_4 to N_2 or CO_2). MLCS not only complements experimental data by generating a wide *PVTx* range of thermodynamic properties but also simulates dynamic processes associated with EFS, such as carbon capture and sequestration, energy recovery, isotope fractionation, fluid-rock interactions, and fluid flow in shale gas or petroleum reservoirs.

For conveniences of geochemical applications, we have integrated the most important and widely used EOS or thermodynamic models into a new user-friendly online calculation platform (http://efs.idsse.ac.cn). This platform, to be continually updated, is designed to streamline and simplify geochemical computations, enabling researchers to efficiently perform critical calculations.