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Redox systematics of COHS fluids in subduction zones: Insights from thermodynamic modeling with ThermoPathX

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The exchange of carbon, sulfur, and other volatiles between Earth's mantle and surface drives long-term geochemical cycling. Modeling the behavior of these volatiles at elevated pressures and tracking their oxidation states remains challenging, as reflected in large uncertainties in global carbon and sulfur budget estimates. Recent advances in thermodynamic modeling have incorporated electrolytic aqueous fluid speciation [1] and open-system frameworks, significantly improving our understanding of slab devolatilization. Managing the resulting large and complex model outputs, however, demands dedicated computational tools.

To address these challenges, we developed ThermoPathX, an automated thermodynamic modelling framework built on PerpleX [2] for Gibbs free energy minimization. It streamlines model preparation and execution across one- and two-dimensional configurations and constructs quasi-3D datasets through iterative workflows. ThermoPathX integrates the subduction zone database of van Keken and Wilson [3] enabling modeling of thermodynamic modelling across wide range of depths and time steps.

We tested ThermoPathX's to explore effects of thermal regimes and initial redox budget on fluid redox capacity by examining the evolution of metapelites during subduction metamorphism. We show that for rock compositions that initially contain significant organic carbon and sulfides, closed-system prograde devolatilization alone can drive a systematic decrease in the $Fe^{3+}/\Sigma Fe$ and redox budget, driven by the loss of oxidized volatile components in aqueous COHS-fluids. If the initial budget of redox-sensitive volatiles is limited, such as in many serpentinites and highly oxidized cherts, Fe^{3+} reduction during prograde metamorphism would require an input of external fluids.

[1] Huang and Sverjensky, 2019 (doi: 10.1016/j.gca.2019.03.027)

[2] Connolly, 2009 (doi: 10.1029/2009GC002540)

[3] van Keken and Wilson, 2023 (doi: 10.1186/s40645-023-00589-5)

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