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A Dynamic Network Model for Thermally-Driven Reactive Transport Near Chemical Equilibrium via Spectral Decomposition

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Predicting the fluid, thermal, and solutal transport in an evolving complex network of pores requires a fundamental description of the transport processes and their coupling to the underlying reaction chemistry. In a single pore, the complex dynamics under various competing timescales and solution-coupled boundary conditions give rise to nonmonotone behaviors in net fluid, thermal, and species fluxes across multiple parameter regimes: reactive (Damköhler), solutal-advective (Peclet) and thermal-conductive (Biot). To tackle a problem posed now in a pore network, we reduce the model order based on a small-amplitude perturbation analysis on the leading-order equations derived from an existing first-principle model [Tilley et al. 2021]. We characterize the dynamics on each edge (treated as a 1D interval) via a spectral decomposition of temperature and species transport near chemical equilibrium. We express the coupled pressure and pore radius evolution in terms of the spectral bases and forcings at adjacent vertices. By imposing flux conservation laws at network vertices via a weakly nonlinear analysis, we close the network model by describing the time evolution of temperature and species at interior vertices. This work introduces a general approach to pore network modeling with PDE dynamics near equilibrium and provides a firm analytical background for adaptation to nonlinear dynamics.

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References

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