Using Non-equilibrium Thermodynamics to Develop a Consistent Model of Non-isothermal, Multi-phase Flow Through Porous Media

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Modelling transport of energy, momentum and matter in porous media is challenging, in particular when several phases are present. We demonstrate that non-equilibrium thermodynamics is an invaluable tool to test the correctness and consistency of both the governing equations and their implementation.

We use non-isothermal, multicomponent gaseous transport of moist air through a porous insulation material as an example. There is significant adsorption of water into and onto the porous matrix, which has a large influence on the behavior. In modeling of gas flow through porous media with adsorption, the thermodynamic properties of the adsorbed phase are usually approximated by those of the bulk liquid. By deriving the expression for the local entropy production for this example and computing it numerically, we show that the bulk-phase approximation leads to a negative entropy production and violation of the second law of thermodynamics.

To resolve this violation, we combine information on the adsorption and thermodynamic properties of bulk fluids to derive consistent thermodynamic properties of the adsorbed phase such as the chemical potential, enthalpy and entropy. The resulting chemical potential of the adsorbed phase can be used as a starting point for rate-based models for adsorption based on non-equilibrium thermodynamics. Incorporating the consistent thermodynamic description into the energy, entropy and momentum balances restores agreement with the second law of thermodynamics.

We show that the temperature evolution in the porous medium from the consistent description differs from the standard formulation only if the adsorption depends on temperature. This highlights the importance of characterizing the temperature dependence of the adsorption with experiments or molecular simulations for accurate non-isothermal modeling of porous media.