Using Equations of State and Non-equilibrium

Thermodynamics to Model Thermal Diffusion

Vegard G. Jervell, Vilde Bråten and Øivind Wilhelmsen

 PoreLab - NTNU, Trondheim, Norway

PoreLab – SINTEF Energy Research, Trondheim, Norway

In mixtures exposed to temperature gradients, transport of heat and mass is coupled. A precise description of transport in these systems therefore relies on knowledge about the coupling coefficient, known as the Soret coefficient, which can be used to describe thermal diffusion. In systems with thermal diffusion, the lighter components are typically driven towards the hottest region, while the heavier components accumulate in the cold part. Thermal diffusion is of importance to many examples, such as transport of reactants and products in heterogeneous catalysis, growth of salt lenses and transport in underground reservoirs, e.g. for CO2 capture.

Several thermodynamic models have been proposed with the intent of predicting the Soret coefficient in a mixture, where many of them require the input from an equation of state. However, these methods have varying degrees of reliability. One of the most frequently discussed methods is the one developed by Kempers [1]. Although the method is an excellent starting point, we show that some of the underlying assumptions of the method are questionable. A consistent modification of the Kempers model will be presented, and compared to alternative models, experimental results and simulations results.

Reference

[1] L. J. T. M. Kempers, " A comprehensive thermodynamic theory of the Soret effect in a multicomponent gas, liquid, or solid", J. Chem. Phys. 115, 6330 (2001).