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Soret effects in porous media

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Thermal diffusion, the Ludwig –Soret effect, plays an important role in transport of heat and mass in fluid mixtures. The coupling between heat- and mass transport extends Fourier’s law for heat conduction and Fick’s law for mass diffusion and is quantified by the Soret coefficient. The effect has applications in industrial processes, such as utilization of waste heat [1], analyses of composition gradients in oil reservoirs [2], as well as novel use in nanomachines [3]. Many experimental techniques have been used to measure Soret coefficients in bulk fluids [4]. It is known that a porous medium may have an impact on the Soret effect, but experimental data are not conclusive on its origin. For instance, porosity, permeability, wettability, and tortuosity will all change diffusion relative to bulk fluid, but the magnitude and mechanism of the coupling of mass diffusion and thermal diffusion is still unknown.

We will present results from non-equilibrium molecular dynamics simulations [5] of the Soret effect for a Lennard-Jones model with two miscible fluid components in a porous medium. The medium has different porosity and wettability preferences for the two fluid components. We show that the wettability preferences change the Soret coefficient and discuss the mechanisms that lead to such change.

Time Block Preference

Time Block A (09:00-12:00 CET)

References

- [1] L. Keulen, L.V. van der Ham, J. Haanemaier, N.J.M. Kuipers, Thijs Vlugt, S. Kjelstrup, «Membrane distillation against a pressure difference», *J. Membr. Science*, 524 (2017) 151-162.
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- [3] M. Yang and M. Ripoll, «Thermoosmotic microfluidics», *Soft matter*, 12 (2016) 8564 –8573.
- [4] W. Köhler and K. I. Morozov, «The Soret Effect in Liquid Mixtures –A Review», *J. Non-Equilib. Thermodyn.* 41 (2016) 151–197.
- [5] B.Hafskjold, T.Ikeshoji, and S.K.Ratkje, On the molecular mechanism of thermal diffusion in liquids, *Molec. Phys.*, 80 (1993) 1389-1412.

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