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Coupled heat- and mass transport through a gas-filled nanopore in contact with a liquid

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Transport of water vapor through a membrane with nano- or micropores while being impermeable to liquid water is the basis for many fabrics and materials with widespread use. An application of the concept is membrane distillation (Lawson and Lloyd, 1997), where a temperature difference across the membrane drives transport of heat and mass. The transport is component selective and can purify the fluid. The transport processes through the membrane have recently been analyzed in terms of non-equilibrium thermodynamics (NET) (Kjelstrup and Bedeaux, 2008), resulting in a new understanding of the coupling between them and the roles of the thermodynamic driving forces.

In order to apply the NET formalism to specific cases, it must be supplied with data from experiments, theories, or computer simulations. The purpose of this paper is to examine some of the assumptions behind the NET formalism, such as the assumption of local equilibrium in the system, study the transport process mechanisms on the atomic scale, and provide case data for a model system by using non-equilibrium molecular dynamics (NEMD) simulations (Hoover and Hoover, 2015).

A cylindrical nanopore was filled with vapor in contact with a Lennard-Jones liquid. Equilibrium simulations were made to verify the model's stability and generate equilibrium data against which non-equilibrium data could be compared. A temperature gradient was imposed and similar non-equilibrium data were generated. The data included surface tensions of flat and curved liquid/vapor interfaces as function of temperature, pressure differences across the surface, heat- and mass fluxes through the pore, and estimates of transport coefficients. System variables were temperature, temperature gradient, pore diameter, and vapor/pore wettability.

The main conclusion from this work was that the temperature gradient generated a pressure difference between the two bulk liquid regions shown in Figure 1. The vapor pressure in the pore, as well as the pressure difference, depended on the temperature and the temperature gradient. We found that the non-equilibrium data were consistent with the equilibrium data at the same local thermodynamic states, suggesting that the local equilibrium assumption is valid in this case.

References

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