Thermal Marangoni Effects, Thermodiffusion, and Thermo-osmosis in Membranes

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We will report results on fluid flow through a membrane by molecular dynamics simulations. The membrane is a porous material surrounded by a one-component fluid. The porous membrane is a slit pore between two solid walls. The fluid is subject to temperature and pressure gradients. The questions we will discuss in this presentation are (1) where are the resistances to heat- and mass flow located, and (2) what have we learned about the transport mechanisms? The results were analyzed in terms of nonequilibrium thermodynamics and mechanical forces acting on the fluid particles in the pore.

Both fluid and solid are Lennard-Jones/spline particles. A heat flux was created by thermostating chunks in the hot ends and cold center of the periodic system. At fully developed stationary state with a temperature gradient, a Poiseuille-type velocity profile was established in the pore. Simulations were also done under isothermal conditions and with a volume flux generated with the Reflecting Particle Method [1].

Transport of heat and mass in the x-direction was analyzed with nonequilibrium thermodynamics. The system was divided into five regions; (1) hot bulk, (2) hot pore end, (3) pore, (4) cold pore end, and (5) cold bulk.

It is convenient to choose the difference in pressure, P, and in inverse temperature, $1/T$, as function of the fluxes, because the total resistance to heat and mass transport can then be considered as a sum of local resistances. The difference in pressure and in inverse temperature across the membrane can be described by the equations

$$\Delta\left(\frac{1}{T}\right) = R_{qq} J'_q + R_{qP} J_V \text{ and } \Delta P = R_{Pq} J'_q + R_{PP} J_V$$

where the R's are resistances and J'_q and J_V are the measurable heat flux and volume flux, respectively. Each product of a resistance and a flux has contributions from each of the five regions in the system, of which regions (2) – (4) are of special interest here. These contributions were determined from the simulations. In this analysis, the pore ends (the surfaces of the membrane) were considered as surfaces with excess properties.

In the second part of this work, we studied the thermal Marangoni effect, also called thermo-capillary convection, which is fluid creep flow along a surface caused by a temperature gradient. The creep flow from the cold to the hot end of the pore was determined, suggesting that its driving force was the temperature gradient along the pore wall. This was examined in more detail by computing the temperature profile and the corresponding force profile in the pore. We found that the thermo-capillary convection was driven by local forces on the fluid near the pore walls. The effects of the boundaries, *i.e.* the periodic boundary conditions, and the surfaces between the bulk fluid and the membrane will be discussed.

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References

1. J. Li, D. Liao, and S. Yip, Phys. Rev. E 57, 7259 (1998)