

Transport coefficients for liquid-vapor transition.

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In spite of the technical importance of vapor-liquid phase transitions, little is known on the interface resistance to transport. Bedeaux and Kjelstrup [1] showed that it was possible to define transfer coefficients for the interfacial region from the theory of non-equilibrium thermodynamics for surfaces [1]. The coupling between heat and mass transport was large. The coefficient, that describes this coupling, is neglected in most descriptions of evaporation and condensation [2]. It was shown, that the commonly used flux-force relations at the surface do not obey the second law. The main results of these new developments will be presented and illustrating using non-equilibrium molecular dynamics (NEMD).

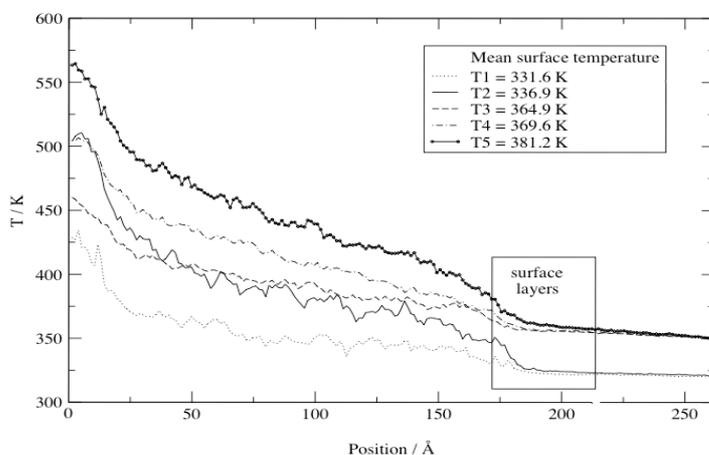


Figure 1- Temperature profile across the simulation box for five n-octane simulated systems with different temperatures and submitted to different heat fluxes. The liquid phase is located on the right side while the gas phase is on the left, the surface extend is located by a rectangle.

Surface transfer coefficients in general, and coupling coefficients in particular are hardly known. They can be calculated using kinetic theory, but practical needs, like modeling of distillation columns, demand realistic coefficients for non-ideal systems. In this study we used non-equilibrium molecular dynamics simulations to obtain them. We simulated n-octane and argon-like liquid-vapour interfaces at different temperatures and applied constant energy fluxes across the liquid-vapor interface following the procedure described in [3, 4]. After a short equilibration period of around 100 picoseconds, the system reached a stationary

state with a non-zero gradient of temperature across the simulation cell, see figure 1 for n-octane. A temperature jump can be seen in this figure inside the surface area in the gas side of the surface that leads to an excess surface heat resistivity.

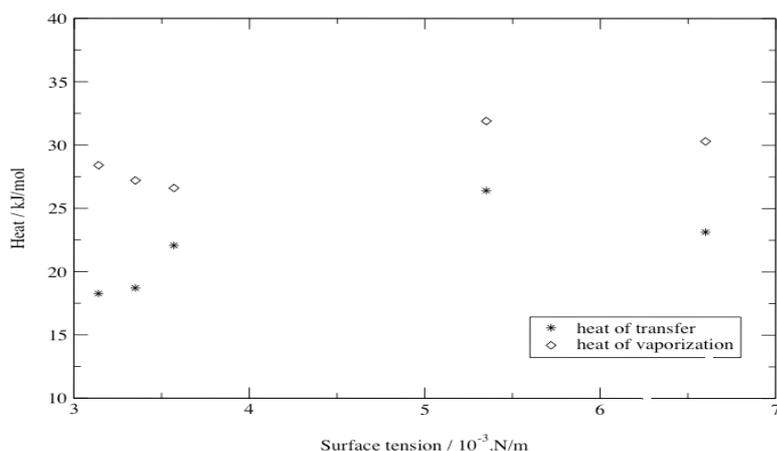


Figure 2- Comparison between the heat of transfer and the heat of vaporization of the liquid-vapor interface as a function of the surface tension.

We calculated the heat flux, the mass transfer resistivities and the heat of transfer [3, 4, 5]. The heat of transfer quantifies the coupling between the transport of heat and mass. The coefficients varied with the surface tension. The heat of transfer was indeed particularly large, it was of the order of the heat of vaporization, as predicted from theory, see figure 2. The contributions to the heat flux from the heats of transfer will then automatically be large as soon as there is a substantial mass flux. When the heat of transfer is neglected in the transport equations, large errors may therefore arise in the heat flux, and consequently in the mass flux.

Acknowledgement

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