

Transfer Coefficients for the Liquid-Vapor Interface of a Two-Component Mixture

Isabella Inzoli

Aramco, EXPEC Advanced Research Center, Dhahran, Saudi Arabia

Signe Kjelstrup and Dick Bedeaux

Norwegian University of Science and Technology, Department of Chemistry, Trondheim, Norway

Jean-Marc Simon^{C,S}

University of Burgundy, Laboratoire Interdisciplinaire Carnot de Bourgogne, Dijon, France

jmsimon@u-bourgogne.fr

Evaporation / condensation are important phenomena that are present in many industrial or natural processes. Because they are endothermic / exothermic, they are associated to large transfers of heat through the liquid-vapor interface. As it has already been shown experimentally, and from simulations on single component systems, large thermal diffusion effect, i.e. the coupling between heat and mass transfer, takes place at the surface. It strongly influences the dynamics of the evaporation / condensation that can be well described however within the general framework of non-equilibrium thermodynamics. For the first time, we simulated a liquid-vapor system of a two-component mixture composed of Lennard-Jones atoms, and we applied external heat and mass fluxes through the surface using non-equilibrium molecular dynamics [see Inzoli et al. *Chemical Engineering Science* vol. 66, 4533 (2011)]. From the simulations we could verify that the local equilibrium hypothesis was valid for the whole surface, which is an important hypothesis of non-equilibrium thermodynamics. Based on the transport equations, we computed the transfer coefficients, i.e. the resistivities to heat and mass transfer and their coupling. Like for the one component systems, the results show the large thermal diffusion effect that cannot be neglected in order to model the dynamics of evaporation / condensation, adsorption / desorption processes.