Transport of Heat and Mass across Planar and Curved Vapor-Liquid Interfaces: from the Lennard Jones Fluid to Water and Beyond

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Transport of heat and mass across interfaces occurs everywhere and is of major importance to a wide variety of processes, ranging from DNA replication to weather forecasts. Such transport can be described by nonequilibrium thermodynamics for heterogeneous systems [1] in terms of thermodynamic driving forces and fluxes across the interface and a set of interface transport coefficients. Recently, a framework was developed to describe transport across also curved interfaces by expanding the interface transport coefficients in the total and Gaussian curvatures [2]. For most fluids however, the interface transport coefficients and the coefficients in their curvature expansion are unknown. In this work, we explain methodologies by experiments, simulations, and theory to obtain these coefficients. We show that the interfacial curvature can have a strong influence on the interface transport coefficients, which can significantly influence growth of nanosized droplets and bubbles. The magnitude and behavior of these coefficients are discussed for the Lennard Jones fluid and for water. We elaborate where new methods are needed in order to handle more complex fluids and new regions of the phase diagram.

References:

[1] S. Kjelstrup and D. Bedeaux "Non-equilibrium Thermodynamics of Heterogeneous Systems", World Scientific, 2008.

[2] Ø. Wilhelmsen "Equilibrium and Nonequilibrium Thermodynamics of Planar and Curved Interfaces", PhD-thesis, Norwegian University of Science and Technology, 2015.