Linking Fluid-Mixture Densimetry and Molecular Simulation for the Quantification of Sorption Phenomena on Nonporous Metal Surfaces

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Phase equilibria of fluid mixtures are important in numerous industrial applications and are, thus, a major focus of thermophysical property research. Improved data, particularly along the dew line, are needed to improve mixture models. However, measurements of thermophysical properties in the vicinity of the dew line can be substantially distorted by surface phenomena such as sorption effects and capillary condensation on the nonporous metal surfaces of the experimental apparatus. To investigate these phenomena, our experimental (p, ρ , T, x) studies on binary gas mixtures are typically carried out along isotherms starting at low pressures and increasing pressure towards the dew point. The results reveal three distinct regions: (1) Minor sorption effects in micropores in the low pressure regime; (2) Capillary condensation followed by wetting in macro-scale surface scratches within approximately 98 % of the dew-point pressure; and (3) Bulk condensation. We hypothesize that the true dew point lies within the second region. Further experimental efforts are currently undertaken to gain fundamental understanding of the confounding surface phenomena in the context of fluid-mixture densimetry. This understanding has to be enhanced when the development of a reliable empirical model that would account for, and correct, sorption effects is the goal. Here, we expect molecular simulation to provide us with a qualitative understanding of the sorption processes on an atomistic level. This will help us to identify the location of the true dew point and yield insights into the bulk phase composition. Therefore, a variety of simplified but comparable systems were modelled to study the influence of surface phenomena, which are expected to have an impact on the measurement of mixture properties.