Modeling Adsorption on Sinker Surfaces in Densimetry:
A Short Story on Surface Wetting and Capillary Condensation

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Phase equilibria of fluid mixtures are pivotal for a great number of industrial applications and are, therefore, a main area of thermophysical property research. More accurate data, particularly in the vicinity and along the dew line, are needed to improve mixture models. However, thermophysical property measurements in the vicinity of the dew line are often significantly distorted by surface phenomena like adsorption and capillary condensation even on the quasi nonporous metal surfaces of an experimental apparatus. To understand these phenomena on an atomistic level, we conducted molecular dynamics simulations (MDS). Besides the representation of the fluid-solid interaction, MDS enables a detailed resolution of selective adsorption out of mixtures and, thus, the consideration of a possible change in the composition of the fluid mixture. However, to convert the experimental setup into a simulation scenario and to subsequently compare the results of both methods is a particular challenge. While sole physisorption can be easily reproduced using an ideal surface in a simple system, effects like capillary condensation and surface wetting require specific knowledge on the real sinker surface of a densimeter as well as adjusted simulation systems. The evaluation of the experimental measurements has shown that such effects must not be neglected: Our isothermal adsorption data show a disproportional increase in adsorbed mass per surface area towards the dew point. The mentioned effects, which may cause this increase to occur on different size scales and differently modeled surface structures and, therefore, require different methods for an accurate analysis. This work provides a critical assessment of these effects that are likely to occur in the experiment - hence, we considered the results from MDS as well as a more detailed analysis of the experimental conditions.