Combination of Molecular Dynamics Simulation and Gravimetric Experiments: The Key to Accurate Dew-Point Densities?

Luca Bernardini [S], Markus Sekulla and Markus Richter [C]
Applied Thermodynamics, Chemnitz University of Technology, Chemnitz, SN, Germany
m.richter@mb.tu-chemnitz.de

Advancing the description of vapor-liquid equilibria of fluid mixtures by thermodynamic property models requires more accurate values for dew-point densities than currently available. Here, gravimetric measurement devices such as tandem-sinker densimeters can produce relief as they belong to the most accurate options to investigate densities in the vicinity of the dew line. Nevertheless, it has to be considered that the investigated fluid may selectively adsorb on the internal quasi-nonporous surfaces of the apparatus, thus, confounding the values of the measured density and composition. In this context, molecular dynamics simulation (MDS) is a powerful instrument to represent the distorting surface effects on an atomistic scale. The evaluation of mixture simulations allows to calculate the local compositions necessary for the correction of the measured density. A first step towards this goal is the validation of simulated adsorption isotherms of pure fluids by means of experimental sorption data. This includes the examination of the impact of "real world effects" such as the non-ideal topography of the apparatus' surfaces as well as deviations between the utilized force fields and actual thermodynamic properties. We will present how the combination of MDS and accurate gravimetric experiments can pave the way to a more accurate determination of dew-point densities. Additionally, the contribution of the four-sinker densimeter, a novel gravimetric apparatus developed in the last few years, will be highlighted, pointing out the importance of a new experimental technique for this investigation.