

Adsorbate Composition in Gravimetric Density Measurements: A Molecular Dynamics Study

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The role of phase equilibria in fluid mixtures is pivotal in numerous industrial applications and, thus, is a central aspect of thermodynamic fluid property research. More accurate measurement data are crucial for developing and improving fluid mixture models. Nowa-days, gravimetric density measurement apparatuses based on magnetic suspension balances are used for carrying out highly accurate density measurements. Although methods using multiple sinkers have been developed to mitigate the adsorption effect for pure substances, Richter and Kleinrahm highlighted in 2014 that measurements of mixtures using these techniques can still be significantly influenced by selective adsorption [1]. Different mixture components adsorb differently on the inner surfaces of the experimental apparatus, altering the composition of the remaining gaseous bulk phase. If this effect is accounted for, the resulting data may reflect correct compositions. In this study, we use molecular dynamics simulations to replicate the adsorption of mixtures of CO₂ and lower alkanes on the internal surfaces of an experimental apparatus. This method enables investigating the variability in the adsorbate's composition along the adsorption isotherm. We present an approach to accurately determine the composition of the adsorbed phase and its consequential impact on the bulk vapor phase composition.

References

1. Richter, M; Kleinrahm, R (2014). Influence of adsorption and desorption on accurate density measurements of gas mixtures. *J. Chem. Thermodyn.* 74, 58-66