Automated Measurement, Modeling, and Interpretation of Diffusion Coefficients in Multicomponent Liquids

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Accurate modeling of diffusion coefficients is crucial for designing and operating chemical processes. Unfortunately, current diffusion models are not very accurate or precise for liquid mixtures, primarily due to a lack of experimental data for validation and development. Our group, therefore, combined microfluidics and Raman micro-spectroscopy and successfully measured diffusion coefficients in up to quaternary mixtures (Peters *et al.*, 2020). However, the manual procedure prevented routine deployment, limiting the database available for modeling.

This study introduces automation for measuring diffusion coefficients in liquid multicomponent mixtures using microfluidics and Raman micro-spectroscopy. The automation process replaces manual sample preparation, substantially reducing both time and error associated with the experimental setup and allowing for continuous measurements without interruption. Performing a diffusion experiment requires one hour and one milliliter of sample volume.

The automated setup allows for exploring complex diffusion phenomena in detail. In particular, conducting multicomponent diffusion experiments close to a miscibility gap may result in negative main diffusion coefficients, a phenomenon that has been questioned in recent literature (Kozlova *et al.*, 2019). We use different methods, including predictive models for diffusion coefficients, to assess the measurement results. Our findings show that main diffusion coefficients can be negative – but only in rare cases, indicating strong non-ideal behavior.

References

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