

Non-isothermal diffusion in ternary systems: ground and microgravity experiments

Werner Köhler*, Thomas Triller, Marcel Schraml, Matthias Gebhardt

Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany

*werner.koehler@uni-bayreuth.de

In multicomponent fluid mixtures subjected to a temperature gradient, the number of diffusion coefficients rapidly grows with the number of components. While binaries are sufficiently characterized by two coefficients, ternaries already require four independent diffusion and two thermodiffusion coefficients. Because of this increasing complexity, investigations of thermodiffusion (Soret effect) in truly multicomponent mixtures are scarce, although the latter represent the majority of practically relevant systems, ranging from simple liquids over colloidal dispersions to biological fluids.

Since there are two independent composition variables in a ternary mixture, two independent measurements are necessary to untangle the coupled diffusion and thermodiffusion processes. For this purpose we have developed a two-color optical beam deflection technique for the readout of the composition and temperature gradients in a Soret diffusion cell. The transformation of the signals from the refractive index to the composition space requires a precise knowledge of the optical contrast factors, the partial derivatives of the refractive index with respect to composition and temperature.

Driven by the unsatisfactory experimental situation, a joint international effort has led to the DCMIX microgravity project of the European and Russian space agencies ESA and Roscosmos. In the framework of DCMIX, three experimental campaigns have so far been conducted onboard the International Space Station ISS using different molecular model systems in a guaranteed convection-free setup. The experimental technique employed in the so-called SODI-instrument is two-color digital interferometry, which allows for a spatial reconstruction of the sample composition.

In this contribution both laboratory and microgravity experiments will be discussed. The results of a benchmark campaign have revealed a significant progress but also demonstrated the incompleteness of our present understanding of the underlying physics and, to some extent, experimental difficulties.



Some results for the Soret coefficients of ternary mixtures can qualitatively be interpreted on the basis of the so-called thermophobicity concept developed for binary mixtures, and they are in agreement with trends predicted by nonequilibrium molecular dynamics simulations.

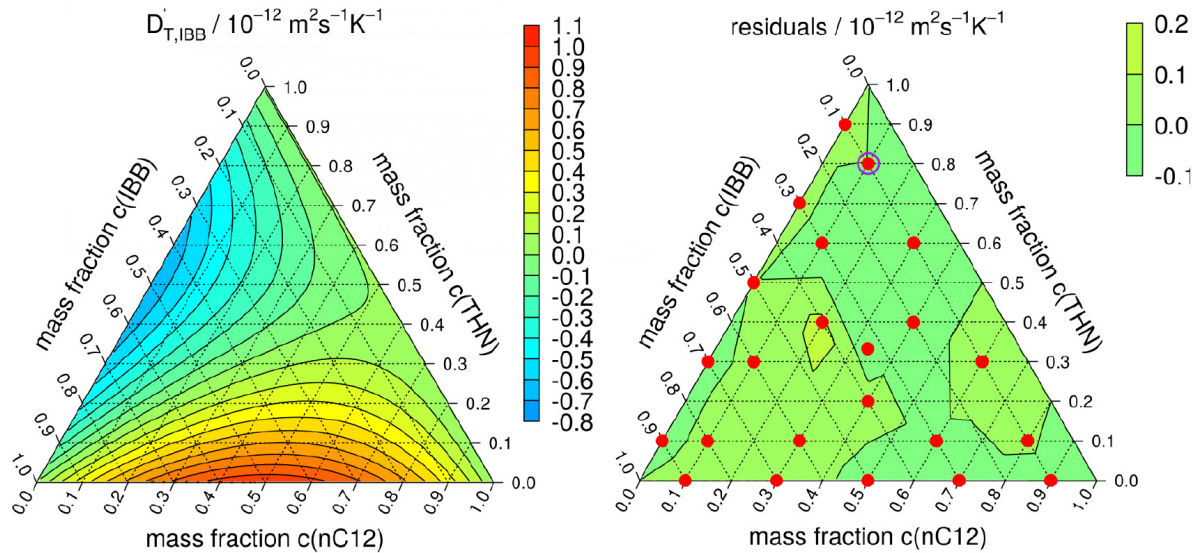


Figure 1: Left: Sign change of thermodiffusion coefficient of IBB in the ternary mixture dodecane/tetralin/isobutylbenzene (nC12/THN/IBB). Right: residues and compositions investigated

References

- [1] M. Gebhardt, W. Köhler: *Soret, thermodiffusion, and mean diffusion coefficients of the ternary mixture n-dodecane+isobutylbenzene+1,2,3,4-tetrahydronaphthalene*. J. Chem. Phys. **143**, 164511 (2015).
- [2] W. Köhler, K. I. Morozov: *The Soret effect in liquid mixtures – a review*. J. Non-Equilib. Thermodyn. **41**, 151 (2016)