

The 190th birthday of Adolf Fick: Still the same procedure for diffusion in fluids as every year?

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Adolf Fick's work represents in many ways an important starting point for modern scientific research on diffusion. Diffusion itself is a slow process taking long time to progress. In this talk, we aim to discuss the progress of diffusion science. For this purpose, we present a highly subjective review of the study of diffusion since the times of Adolf Fick. Our focus is on mutual diffusion in liquids which is at the heart of many processes in (bio)chemical systems. Here, diffusion is often the rate-limiting step and thus decisive for overall process performance.

We review both experimental methods and theoretical approaches to study diffusion in liquids and highlight the advances made in recent years. Here, our presentation will be strongly biased towards contributions from our own group. We examine three pathways to obtain diffusion coefficients in liquids: 1) experiments, 2) analytical models, and 3) molecular simulations.

For experiments, we discuss the use of spectroscopy and microfluidics to measure multicomponent diffusion coefficients in liquids. Spectroscopy allows to resolve all species in a mixture simultaneously with high spatial and temporal resolution. Combining spectroscopy with microfluidics provides direct access to the diffusion process leading to fast experiments using only small amounts of material and allowing for automation. Experimental diffusion data still provides the most accurate input for process modeling and design. At the same time, diffusion data allows to test advanced theoretical methods to predict diffusion in liquids.

Predictive analytical models have significantly advanced in recent years due to our improved molecular understanding of diffusion. Here, we present Darken-based models to predict the concentration dependence of diffusion coefficients. While the Darken-equation can be derived from statistical thermodynamics for ideal mixtures, non-ideal effects can now be accounted for expanding the application domain for analytical models.

Molecular dynamics simulations support the development of analytical models by providing unique data and insight into diffusion behavior. At the same time, molecular dynamics also allows the direct prediction of diffusion coefficients. In the past, molecular simulations focused mostly on self-diffusion. We discuss recent approaches to enable the efficient calculation of mutual diffusion coefficients by molecular dynamics.

The presented three pathways to diffusion coefficients in liquids are shown to complement each other and allow us to advance our understanding of diffusion demonstrating that diffusion science is not slow.

André Bardow studied mechanical engineering and chemical engineering at RWTH Aachen University, Germany, and Carnegie Mellon University, USA, and received his Ph.D. in process systems engineering from RWTH working on model-based experimental analysis of multicomponent diffusion in liquids. He did postdoctoral research at ETH Zurich and was Associate Professor in the Department of Process & Energy at TU Delft. Since 2010, he has been Full Professor and Head of the Institute of Technical Thermodynamics at RWTH Aachen University and co-appointed at Forschungszentrum Jülich as director at the Institute for Energy and Climate Research (IEK-10) since 2017. His current research ranges from physical property measurements and prediction to adsorption-based energy systems and integrating energy & process systems engineering with life cycle assessment.

