Experimental Investigation and Molecular Simulation of Thermophysical Properties of Ionic Liquids [EMIM][B(CN)$_4$] and [HMIM][B(CN)$_4$]

Thomas Koller[1] and Michael H. Rausch[1,4], Peter S. Schulz[2], Peter Wasserscheid[2], Ioannis G. Economou[3], Alfred Leipertz[1,4], and Andreas P. Fröba [C, S,1,4]

[1]University of Erlangen-Nuremberg, Erlangen Graduate School in Advanced Optical Technologies (SAOT), Erlangen, Germany
[2]University of Erlangen-Nuremberg, Institute of Chemical Reaction Engineering (CRT), Erlangen, Germany
[3]The Petroleum Institute, Department of Chemical Engineering, Abu Dhabi, United Arab Emirates
[4]University of Erlangen-Nuremberg, Institute of Engineering Thermodynamics (LTT), Erlangen, Germany
apf@ltt.uni-erlangen.de

The low-viscous tetracyanoborate-based ionic liquids (ILs) [EMIM][B(CN)$_4$] (1-ethyl-3-methylimidazolium tetracyanoborate) and [HMIM][B(CN)$_4$] (1-hexyl-3-methylimidazolium tetracyanoborate) have high solubilities for CO_2 and are thus attractive working fluids for gas separation processes. A literature survey reveals that only a limited number of thermophysical properties required for process and apparatus design is available for both ILs. Motivated by this situation, a comprehensive experimental investigation of these ILs was performed. Since experiments often imply a fundamental investment in costs and time, especially at temperatures and pressures far from ambient conditions, also molecular dynamics (MD) simulation was used as a prediction tool allowing access to various thermophysical fluid properties at any desired state. In the experimental part of the present study, conventional techniques were applied for the determination of density, refractive index, interfacial tension, and self-diffusion coefficients for both ILs at atmospheric pressure in the temperature range from 283.15 K to 363.15 K. In addition, surface light scattering (SLS) experiments provided accurate viscosity and interfacial tension data. As no complete molecular parameterization was available for the MD simulations for both ILs, a new non-polarizable united-atom force field was developed in which the parameters were optimized with respect to the experimental density. The deviations of the simulated from our experimental density data are less than ±0.5%. The models were validated by comparison of the calculated and measured viscosity and self-diffusion coefficient data where good agreement with deviations of less than ±20% was found over the whole temperature range.