Comparison of COSMO-SAC and the Multi-Fluid Mixture Model with Binary and Ternary Mixtures

Erik Mickoleit [C, S], Constantino Grau Turuelo, Andreas Jäger and Cornelia Breitkopf
Chair of Technical Thermodynamics, Technische Universität Dresden, Dresden, Saxony, Germany
erik.mickoleit@tu-dresden.de

Predictive and likewise preferably accurate equation of states for mixtures have been very important in science and industry in order to screen and identify solvents, find suitable working fluids, optimize processes, etc. In the context of the EU regulation 517/2014 on fluorinated greenhouse gases, new alternative environmentally friendly refrigerants are required in order to replace existing refrigerants which exhibit a high global warming potential (GWP). Refrigerant mixtures are a promising alternative, however, suitable candidates need to be identified by a broad screening and subsequent experimental validation. It has been demonstrated, that the combination of the "Conductor-like Screening– Segment Activity Coefficient"-model (COSMO-SAC) with the multi-fluid mixture model yields good predictive results for binary mixtures. However, the model has not been evaluated for ternary or higher mixtures. In this study, experimental phase equilibrium data for binary and ternary mixtures have been compared to results from COSMO-SAC (with original parameters and a reparametrization) used in the multi-fluid mixture model and to results from COSMO-SAC when assuming ideal gas behaviour for the vapor phase. All results have been calculated with the thermophysical property software TREND 4.0.