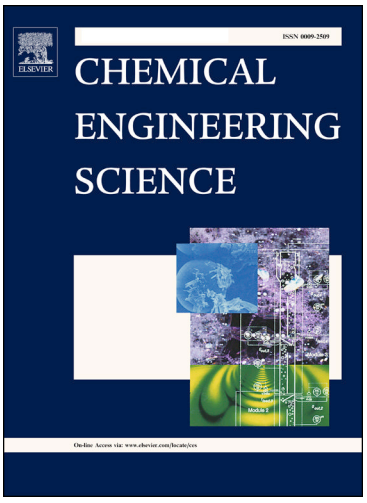

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Application of COSMO-RS and UNIFAC for Ionic Liquids based Gas Separation

Xinyan Liu[a,b], Teng Zhou[c], Xiangping Zhang[b*], Suojiang Zhang[b], Xiaodong Liang[a], Rafiqul Gani[d], Georgios M. Kontogeorgis[a*]

[a] *Department of Chemical & Biochemical Engineering, Technical University of Denmark, DK 2800 Kgs. Lyngby, Denmark*
[b] *Beijing Key Laboratory of Ionic Liquids Clean Process, CAS State Key Laboratory of Green Process and Engineering, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, China*
[c] *Process Systems Engineering, Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstr. 1, D-39106 Magdeburg, Germany*
[d] *PSE for SPEED, Skyttemosen 6, DK-3450 Allerod, Denmark*
*Corresponding authors
Email address: gk@kt.dtu.dk;xpzhang@ipe.ac.cn

Abstract

In recent years, due to their advantages on good stability, non-volatility, tunable viscosity and tailor-made properties, ionic liquids (ILs) have been regarded as novel potential solvents and alternative media for gas separation. However, the various cations and anions representing the ILs, together with limited experimental data, make it challenging to predict gas solubility in ILs and identify the optimal IL for a specific gas separation. In this work, a comprehensive Henry's law constants database is first established for gas-IL which supplements an already established extensive gas solubility database. Because of the insufficient experimental data for both IL-C_2H_4 and IL-C_2H_6 systems, the COSMO-RS model is used after validation to generate additional pseudo-experimental data. Then, together with the sufficient experimental data of CO_2-IL and CH_4-IL systems, UNIFAC-IL is developed for the prediction of four-component shale gas (CH_4, C_2H_4, C_2H_6, CO_2) solubility in ILs. A relatively good agreement between the model predicted and the experimental solubility data is observed. Moreover, the developed UNIFAC-IL model can be used to predict the solubility of gases in new ILs that are not included in parameter fitting due to its group contribution basis. For this reason, the model represents a very useful tool for task-specific design of ionic liquids for gas separations.

Keywords: Ionic Liquids (ILs); COSMO-RS; UNIFAC; Gas solubility; Henry's law constant

1 Introduction

Separation and purification technologies are widely used in modern industry and research area, such as gas separation, material production and environmental protection, and they are indispensable units in many industrial production processes. Currently, the commonly used gas separation technologies are energy intensive distillation, solvent based absorption, flux limited adsorption, and membrane-based operations. Distillation is extensively used for some light hydrocarbon gas separation processes in which the separated gas is recognized as an important raw gas for synthesizing many industrial chemicals. Such distillation processes usually involve columns with large numbers of trays operating at low temperatures and high pressures, which leads to a high energy consumption and negative environmental impact Tula et al., (2017). Thus, solvent based absorption technology is an alternative to overcome these disadvantages. It is widely