Solubility of CO$_2$ in Two Bis(trifluoromethylsulfonyl)imide ([Tf2N]) Based Ionic Liquids

Devjyoti Nath, Amr Henni *

Acid Gas Removal Laboratory, Clean Energy Technologies Research Institute (CETRI), University of Regina, Regina, SK, Canada

Abstract

One of the biggest concerns of the present time is the accelerating of global warming due to anthropogenic emission of carbon dioxide (CO$_2$) mainly produced by the combustion of fossil fuels. One of the most technologically advanced methods to capture CO$_2$ for mitigating emission from large stationary point sources is absorption by the liquid solvent. A major challenge of the research on the investigation of CO$_2$ absorption is to find out cost-effective and environmentally friendly liquid solvent. Ionic liquids (ILs) are known as a green solvent due to their special properties (non-flammable, negligible vapor pressure, high thermal stability, etc.), and they have recently emerged as an alternative of reactive solvent because the low energy required for regeneration. Since, ILs were accepted as an important alternative absorbent of CO$_2$ capture recently, very limited studies have been published on CO$_2$ solubility. According to the previous studies, the anion has the significant influence on the solubility of the CO$_2$ in ILs, and the cation has the minor effect. When three ILs with the same cation and with three different anions ([bmim][BF$_4$], [bmim][PF$_6$] and [bmim][Tf$_2$N]) were investigated, there was very little difference of CO$_2$ solubility in between the ILs with BF$_4$ and PF$_6$; but the IL with Tf$_2$N appears to have a much higher affinity for CO$_2$ than the other two ionic liquids. Previous studies exhibited that fluorination and the presence of S=O groups in anion have a great effect on the solubility of CO$_2$ in ILs. Due to high fluorination and the presence of S=O groups in Tf$_2$N anion, ILs with Tf$_2$N demonstrate high solubility of CO$_2$. Again, the viscosity of the ionic liquid with Tf$_2$N anion is low compared with the ILs containing other anions, however, the density of ILs increase with the presence of Tf$_2$N anion. Due to the higher affinity towards CO$_2$ solubility, two ILs with [Tf$_2$N] anion were selected for this study.

Solubility of carbon dioxide (CO$_2$) in two novel ionic liquids (ILs) with the same anion, 1-(3-Hydroxypropyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)imide [HOPMIm][Tf$_2$N] and N,N-diethyl-N-methyl-N(2-methoxyethyl)ammonium bis(trifluoromethanesulfonyl)imide [DEME][Tf$_2$N], was measured at (303.15, 323.15, and 343.15) K and at pressures up to 1.1 MPa with a gravimetric microbalance. A computer-controlled gravimetric microbalance (HidenIsochema Ltd. IGA003) with a stable resolution of 1 µg was used to perform isotherm study of CO$_2$. This microbalance works on the
electrobalance principle contains two arms. A stainless steel bucket with a known weight which is used as sample container is attached to sample arms with a gold hang down chain, and counter/reference weight is attached to the other arms. This microbalance can work in dynamic mode or static mode. All the isotherm experiments for this current study were performed as static mode. In this present study, solubility of CO2 in these ILs increased significantly with the increase in pressure in a nearly linear manner and reduced drastically with an increase in temperature.

The densities of these ILs were also measured with Anton Paar density meter (DMA 4500). The Henry's law constants, enthalpies and entropies for the absorption of CO2 in these ILs were estimated from the solubility data (P, T, x). Gas solubility in ionic liquids depends primarily on the strength of the interaction between CO2 and the anion as indicated by solubility measurements, spectroscopic studies and molecular simulations. Although anions are known to have a significant influence on the solubility of CO2 in ILs, Henry's law constants in these ILs varied due to the different structure of the cations in these ILs. Solubility in [DEME][Tf2N] was higher than in [HOPMIm][Tf2N]. Experimental solubility data were correlated with Peng-Robinson (PR) equation of state using the van der Waals two (vdW2, based on two binary interaction parameters) mixing rules; and the %AAD of these model correlations were less than 3.

* Corresponding author
E-mail address: amr.henni@uregina.ca (A. Henni)