Abstract

Experimental and Modeling Study of Carbon Dioxide Absorption in Aqueous Ionic Liquid Blended with Amines

Power plants and chemical process industries face a huge challenge in efficient CO_2 separation from the flue gases over decades. The concern is furthermore important with respect to climate change. Various technologies have been tried for post-combustion CO_2 capture out which chemical absorption using solvents is widely applied and the changes in this technology are well accepted owing to its ease of retrofitting. Development of novel solvents for post-combustion CO_2 capture needs a lot of attention.

The current work examines three potential amine activators, 1-(2-aminotethyl) piperazine (AEP), bis (3-aminopropyl) amine (APA) and 2- methyl piperazine (2-MPZ) for enhancing CO_2 solubility when blended with base solvents. For the current work, selected base solvents are 3-aminopropyl triethoxysilane (TESA), 1-butyl-3-methyl imidazolium acetate ([bmim] [Ac]), *N*-methyldiethanolamine (MDEA), and sulfolane ($TMSO_2$). CO_2 solubility is measured in aqueous systems of [bmim] [Ac], ([bmim] [Ac] + AEP), ([bmim] [Ac] + APA), TESA, (TESA + AEP), (TESA + APA), (MDEA + 2-MPZ), ($TMSO_2$ + 2-MPZ) and ([bmim] [Ac] + 2-MPZ) over a temperature and pressure range of (303.2-323.2) K and (0-400) kPa. ^{13}C NMR and FTIR analysis of unloaded and CO_2 loaded solvents are examined to propose reaction mechanism of the interaction amid CO_2 and solvents. The obtained experimental results are correlated using modified Kent-Eisenberg (KE) model considering the non-ideality in the gas phase. The equilibrium constants of the proposed reactions were estimated using modified KE model through non-linear regressive optimization. The data obtained through modified KE model is further utilized to study the concentration profiles of the associated ionic species at equilibrium conditions and pH of the CO_2 loaded solvents. Further, a new statistical and non-rigorous model is established for correlating the TESA systems. A two layer feed forward artificial neural network (Levenberg-Marquardt back propagation method for training; log sigmoid and linear transfer function for hidden and output layers, respectively) was used to correlated aq. [bmim] [Ac], ([bmim] [Ac] + AEP) and ([bmim] [Ac] + APA) systems. CO_2 cyclic capacity and heat of absorption are also

analysed for aq. (MDEA + 2-MPZ) systems. The obtained CO_2 solubility data is also compared with the literature indicating the efficacy of the proposed solvents.

Important thermophysical properties viz. density, viscosity, surface tension, sound velocity and refractive index of the solvents are measured and reported over the temperature range of (298.15-333.15) K. Along with the nine above mentioned solvents, two more non-aqueous solvents based on 2- hydroxyl ethyl ammonium formate (HEF) i.e. (HEF + AEP) and (HEF + 2-amino-2-methyl-1-propanol (AMP)) are also analysed for physiochemical properties. These properties play significant role in understanding the flow behaviour, inter-molecular interactions, designing of the absorber or regenerator column, pumping costs required for solvents, mass transfer and kinetic rates of CO_2 in the solvents. Density and viscosity were modeled using first principle model i.e. Redlich-Kister and Grunberg-Nissan. New models were proposed for correlating sound velocity, refractive index and surface tension. All the properties were correlated as a function of temperature and composition. The results indicated less deviation amid the experimental and modeled data indicating the accuracy of the models. The experimental results were further used to estimate various important derived properties such as excess molar volume, viscosity deviation, diffusivity of N_2O and CO_2 in the solvents, isentropic compressibility, thermal expansion coefficient, enthalpy and entropy of activation of viscous flow through literature established empirical correlations.