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Investigation of various process parameters on the solubility of carbon dioxide in phosphonium-based deep eutectic solvents and their aqueous mixtures: Experimental and modeling

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ABSTRACT

This research presents the application of predictive regression model such as quadratic regression for estimation of CO_2 solubility in deep eutectic solvents namely allyltriphenylphosphonium bromide-triethylene glycol (ATPPB-TEG) into different molar ratios and their aqueous solutions. In doing so, a design of experiment (DOE) was applied based on Taguchi L_{18} orthogonal array method. Four factors, namely pressure, temperature, molar ratio and water/DES concentration in mixture were selected as input parameters of model. The output parameter of model was the CO_2 solubility in terms of mole fraction of CO_2 (X_{CO2}). A quadratic regression model was developed after validation and confirmation through several strong approaches. The results disclose that the prediction of developed quadratic regression model is in acceptable agreement with experimental solubility data. The overall R-squared (R^2) and absolute relative error (*ARE*) values of proposed quadratic regression model were 0.9966 and 0.0725, respectively. Moreover, analysis of variance (ANOVA) indicates that pressure is the most significant factor influencing the X_{CO2}. Finally, the signal to noise (S/N) ratio shows that the highest levels for pressure, concentration of DES in mixture, and molar ratio, and lowest level for temperature are the optimal levels of input parameters to obtain the highest CO_2 solubility in this system. The developed quadratic regression model and correlation are effective and provide quick, reliable and accurate predictions of CO_2 solubility in DESs without carrying out any time consuming, difficult and expensive experimental measurements. To the best of our knowledge, this is the first time a regression model was developed for prediction of CO_2 solubility in DESs and their aqueous solutions.

1. Introduction

Global energy consumption is currently rising due to increasing population and technology advancement. Fossil fuel supplies about 88% of that world energy demand. However, due to combustion of carbon based fossil fuels, many pollutants are being emitted to the environment and this is causing major environmental issues to rise. It causes a major global problem as most of the pollutants released from burning of fossil fuels consist of greenhouse gases (GHG) which are gases that trap heat in the atmosphere. The CO_2 that is known as one of the main greenhouse gases, is the chief reason brought about climate changing as well as global warming in a gradual way, hence the influence of steadily growing concentration of CO_2 released to the atmosphere has worried worldwide, as shown in Fig. 1.

It can be clearly seen from Fig. 1 that over this span of 50 years, the concentration of CO_2 has been increased moderately at the atmosphere and reached values around 404.34 ppm in September 2017, as reported by Scripps Institution of Oceanography (2017). At the end of this century, it is estimated that the global temperature might increase 2–5 °C, if the emissions of CO_2 do not be reduced instantly (Pachauri and Reisinger, 2007). The increased CO_2 emissions are attributed to an increasing dependence on the combustion of fossil fuels (coal, petroleum and natural gas) which contribute 86% of anthropogenic greenhouse gas emissions, the remainder arising from land use change (mainly deforestation) and chemical processing (Ahmady et al., 2011; Bredesen et al., 2004). Besides, CO_2 content of natural gas reservoirs in Malaysia is the range of 28 up to 87% (Darman and Harun, 2006). CO_2 makes problems in industries such as corrosion pipelines (Moraes and Dias,

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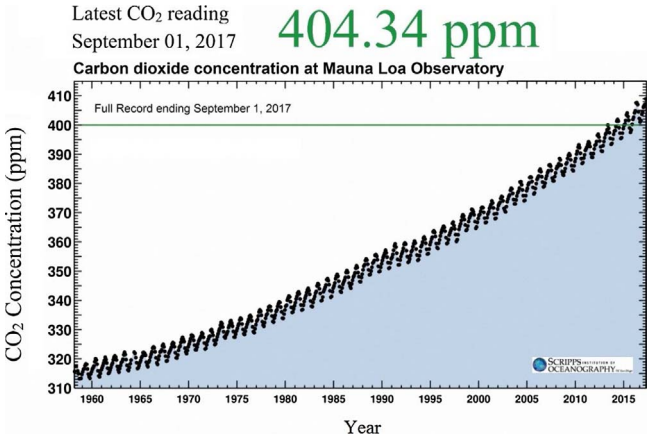

Fig. 1. CO_2 concentration at the atmosphere between 1950 and 2017 reported by Scripps Institution of Oceanography (2017).

1999) and also lower the fuel value of natural gas (Bates et al., 2002). It is also known that presence of CO_2 in gas stream will lead to CO2 crystallization during liquefaction process (Ghiasi et al., 2016). Therefore, there is a demanding need to decline CO_2 in industrial scales and control emissions of CO_2 in the atmosphere.

Three main pathways for capturing CO_2 from fossil fuel energy conversion systems in order to reduce CO_2 emissions are post-combustion capture (CO_2 can be captured from fuel combustion flue gas) (Figueroa et al., 2008; Plasynski et al., 2009), pre-combustion capture (fuel gasification syngas) (Bachu, 2008; Figueroa et al., 2008), oxyfuel combustion (Figueroa et al., 2008; Plasynski et al., 2009). There are well-known processes and techniques for CO_2 removal such as absorption (Cheung et al., 2012; Gupta et al., 2003), adsorption (Cheung et al., 2012; Gupta et al., 2003), cryogenic capture processes (Olajire, 2010; Xu et al., 2012), and membrane separation units (Ambashta and Sillanpää, 2012; Bredesen et al., 2004) that are currently used to manage CO_2 emissions. The choice of the suitable technology depends on the characteristics of the gas stream from which CO_2 will be captured. Such characteristics are heavily dependent on the type of dynamics of the process through which the fuel is processed and used (García et al., 2015).

Amine solvent based technology has been used for CO_2 capture more than 70 years. In 1991s, amine solutions have received more attentions in practical application and industrial processes for CO_2 capture (Baghban et al., 2017). In the amine-based CO_2 capture process, CO_2 recovery rates of up to 98% and product purities in excess of approximately 99% can be achieved. However, this process has some drawbacks including the loss of amine reagents and transfer of water into the gas stream during the desorption stage, chemical degradation to form corrosive byproducts, and high energy consumption during regeneration, as well as insufficient carbon dioxide capture capacity (García et al., 2015). In order to mitigate these problems related to amine process, both industry and academia are trying to synthesis alternative solvents that are chemically more robust, having high CO_2 affinity with viable physicochemical properties.

Over the past decade, ILs have been considered as substitute solvents because of several unique properties such as low melting point, high solvency power for both polar and non-polar solvents, high ionic conductivity, high thermal and chemical stability, tunable physicochemical character, low flammability and volatility (Baranyai et al., 2004; Bates et al., 2002; Carvalho et al., 2014; Figueroa et al., 2008; Hasib-Ur-Rahman et al., 2012; Jain et al., 2005; Kenarsari et al., 2013; Ramdin et al., 2012; Smiglak et al., 2006; Xue et al., 2006). In recent years, the use of ILs for gas capture and in particular CO_2 capture has received interest because of their unique characteristics and high solubilities (García et al., 2015). However, despite these unique properties of ILs, there have been drawbacks, such as costly large scale industrial applications, complex reaction steps and purification procedures for synthesizing, high viscosity, potentially toxicity, limited biodegradability and low CO_2 loading capacity (in comparison with traditional alkanolamines) (Bara et al., 2009; Gardas and Coutinho, 2008).

Researchers are trying to find new solvents as an alternative to ILs. Similar to ILs. Recently, deep eutectic solvent (DESs) have gained popularity among researchers for different purposes, especially in CO_2 capture (Ghaedi et al., 2017c; Ali et al., 2014; Chen et al., 2014, 2016; Deng et al., 2016; Gutierrez et al., 2011; Hsu et al., 2014; Leron et al., 2013; Leron and Li, 2013a,b; Li et al., 2014, 2008; Lin et al., 2014; Lu et al., 2015; Mirza et al., 2015; Sarmad et al., 2017; Sze et al., 2014; Xie et al., 2014). DESs have many unique properties which have been reported by Ghaedi et al. (2018), Ghaedi et al. (2017a,b,d), Alomar et al. (2016), Hayyan et al. (2015), Chen et al. (2016), Kareem et al. (2010), Yadav and Pandey (2014), Liu and Liu (2014) and Siongco et al. (2013). DESs are non-volatile, thermally stable, highly conductive, and are relatively low-cost, non-toxic, and natural. They have easy preparation and synthesizing procedure, lower melting point than the constituents of the mixture, a wide liquid range, high solvation capacity, and made up of biodegradable constituents which are important for the environment and from an economical perspective. Therefore, DESs can be regarded as the potential alternative to ILs in many applications particularly in CO_2 capture.

Generally, CO_2 solubility in pure DESs depends on pressure, temperature, alkyl chain length, molar ratio while in aqueous solutions, on the concentration of water and DESs of the mixture. The CO_2 solubility in DESs increases with pressure and decreases with increasing temperature. There are abundant CO_2 solubility data, particularly that of choline chloride −(ChCl)-based DESs available in literature.

Li et al. (2008) measured CO_2 solubility in choline chloride-based DES and studied the effect of pressure, temperature and molar ratio on CO_2 solubility. Their results showed that CO_2 solubility increased as the pressure is increased. Meanwhile, a downtrend in CO_2 solubility is seen with increasing temperature. Essentially, molar ratio has had a great effect on CO_2 solubility. Therefore, the ChCl to urea (1:2) molar ratio exhibited a higher CO_2 solubility value than DES from a ChCl to urea molar ratio of 1:1.5 and 1:2.5.

The CO_2 solubility in ChCl −based DESs from mixture with dihydric alcohols (1,4-butanediol, 2,3-butanediol, and 1,2-propanediol) with 1:3 and 1:4 molar ratio of ChCl to HBDs was studied by Chen et al. (2014). Their results showed that DESs containing 2,3-butanediol with a ratio of 1:4 have the highest CO_2 absorption capacity. Li et al. (2014) investigated the solubility of CO_2 in DESs of ChCl/phenol (1:2, 1:3, 1:4), ChCl/diethylene glycol (1:3 and 1:4), and ChCl/triethylene glycol (TEG) (1:3 and 1:4). It was found that the CO_2 solubility in ChCl/(TEG) (1:4) is the highest as compared with other DESs. CO_2 solubility in the ChCl −based DES solutions and levulinic acid or furfuryl alcohol as HBDs with the molar ratios of 1:3, 1:4, and 1:5 salt to HBD, was investigated by Lu et al. (2015). ChCl/levulinic (1:5) exhibited the highest CO_2 absorption capacity, which was higher than that of furfuryl alcohol.

Water content also has an effect on CO_2 solubility. Most researchers reported that water acts as an anti-solvent to drive out dissolved CO_2 in the DES. Su et al. (2009) studied CO_2 solubility in aqueous ChCl −based DES at various temperatures and atmospheric pressure. Their results disclosed that CO_2 solubility in DES decreases as water content increases. Xie et al. (2014) reported that CO_2 solubility in aqueous ChCl/urea (1:2) decreases with increasing water content in the mixture. However, Lin et al. (2014) observed an unusual behavior of CO_2 solubility in aqueous ChCl/glycerol (1:2) at temperature of 303.15 K. At this temperature, it was found that CO_2 solubility increases (Henry's law constant decreases) as water content increases in the mixture. This behavior was not observed at 308.15 K and 313.15 K. They mentioned that this indicates a very weak dependence of Henry's law constant on concentration at low temperatures.

Hsu et al. (2014) added Monoethanolamine (MEA) to aqueous