Solubilities of CO_2 in, densities and kinematic viscosities of poly (propylene glycol) diglycidyl ether and poly(ethylene glycol) monooleate

Yun Li [a,*], Yanhong You [a], Weijia Huang [b], Jie Yang [b]

[a] School of Environment and Architecture, University of Shanghai for Science and Technology, Shanghai 200093, China
[b] School of Energy and Powering Engineering, University of Shanghai for Science and Technology, Shanghai 200093, China

A B S T R A C T

Densities and kinematic viscosities of polymer absorbents such as poly(propylene glycol) diglycidyl ether (PPDE) with molecular weights of 380 and 640, and poly(ethylene glycol) monooleate(PEGM) with molecular weight of 460 were respectively measured at atmosphere and temperatures ranging from 273.15 K to 333.15 K, and correlated with linear equation and Vogel-Fulcher-Tamman equation respectively. The density declines slightly while the kinematic viscosity decreases greatly with the increase of temperature. The result also showed that increasing the molecular weight is beneficial for the decrease of density and the increase of kinematic viscosity. In addition, CO_2 solubilities in the selected polymer absorbents were determined by using an isothermal synthetic method, under pressures up to 1.2 MPa and at temperatures ranging from 273.15 K to 303.15 K. The four-parameter nonrandom two-liquid (NRTL) model was used to fit the experimental data, and model parameters were obtained. According to the absorbents as PPDE380, PEGM460, and PPDE640, the mean relative deviations of the pressure between the experimental and fitted data were 1.03%, 1.15%, and 1.31%, and the maximum deviations of that were 2.73%, 2.57%, and 2.55%. The result showed that decreasing the absorption temperature has a large effect on improving absorption capacity. Henry's constants were calculated from NRTL model and compared with those of experimental data. Relatively good correspondence was obtained with the experimental and calculated data. To assess the selected absorbents for CO_2 capture preliminarily, densities and kinematic viscosities of, CO_2 solubilities in selected absorbents were compared with common solvents used in industrial plants, other polymer absorbents, and some ionic liquids. The result showed the selected absorbent as PPDE640 has moderate density and kinematic viscosity, the highest CO_2 absorption capacities of all the compared absorbents, which showed that PPDE640 has potential research value for CO_2 capture.

© 2018 Elsevier Ltd.

1. Introduction

Carbon capture and storage (CCS) seems to be the most economical and feasible technology that currently used to decrease the release of excessive greenhouse gas into the atmosphere and slow down global warming [1]. There are several methods as physical/chemical/hybrid absorption method [2], adsorption method [3,4], cryogenic method [5], membrane method [6], microorganism method [7] that are used to capture CO_2. Physical absorption method is popular and suitable for large amount of feed gas and extremely high CO_2 concentration, as the equilibrium concentration of the absorbate(CO_2) in the liquid phase is strongly depen-

dent on the partial pressure in the gas phase. In addition, a large amount of energy is saved for solvent regeneration because flash tanks are used instead of rectifying columns. Common solvents typically used in industrial absorption plants include methanol, propylene carbonate(PC), N-methyl-2-pyrrolidone(NMP), and so on. It is indicated that the development of new physical absorbent is one of the core parts for carbon capture technology [8].

Polymer absorbents are receiving attention because of their excellent absorption and separation properties for CO_2. There have been some studies [9–13]––either experimental or predictive––carried out on new polymer absorbents. Li [9] measured the solubilities of CO_2 in poly(ethylene glycol)(PEG) with molecular weights of 150, 200, 300, and 400 over the range of pressure from (100 to 1200) kPa and temperature from (303.15 to 333.15) K. The result showed that PEG with higher molecular weights can enhance solubility with CO_2. Rayer [10] determined solubility of

carbon dioxide in polyethylene glycol dimethyl ethers with molecular weight of 339.9(Genosorb 1753) at the temperatures of 298.15–333.15 K and pressures up to 7940 kPa. High pressure solubilities of CO_2 in Genosorb 1753 were compared with those in six other physical solvents. It indicated clearly that Genosorb 1753 is a better solvent for CO_2 than all others. Moreover, the results were correlated with PR equation of state and three other activity coefficient models, which showed that NRTL model was found to fit data with less standard error deviation. Tang [11] synthesized poly(ionic liquid)s and studied their CO_2 absorption behavior. It seemed that the poly(ionic liquid)s had enhanced CO_2 absorption capacities and fast absorption/desorption rates compared with room temperature ionic liquids. Miller [12] reported the solubility of carbon dioxide in four polymer absorbents as polyethylene glycol dimethyl ether (PEGDME), perfluoro polyether (PFPE), polydimethyl siloxane (PDMS), and polypropylene glycol di-methyl ether (PPGDME), and compared the experimental data to predict phase behavior using the conductor-like screening model for real solvents(COSMO-RS) formalism. In particular, PPGDME exhibited larger CO_2 absorption capacity than the other selected polymers. Moreover, it has been shown that COSMOtherm was able to qualitatively describe all systems and their corresponding Henry's constants. Shah [13] measured the solubility of methane, carbon dioxide, and propane in five silicone rubbery polymers at 283.15 K, 308.15 K and 328.15 K and at pressures up to 26 atm. It turned out that the solubility of carbon dioxide in poly(trifluoropropy1 methyl siloxane) appears to be anomalously high, possibly because of specific penetrant/polymer interactions. In addition, some researchers [14–17] have been devoted to the study of basic thermophysical properties of polymer absorbents. Elbro [14] proposed a new group contribution method for the prediction of liquid densities as a function of the temperature. It seemed that many solvents even strongly polar solvents can be predicted with an average error of 1%. Conesa [15] measured liquid densities and heat capacities at 1 MPa, and kinematic viscosities at atmospheric pressure of PEGDME with molecular weight of 250. All experimental data for the three thermophysical properties have been separately fitted to different empirical equations. Ottani [16] determined densities, kinematic viscosities of PEG with molecular weight of 200 and 400 at 297.15–307.15 K and atmosphere. Awwad [17] measured relative permittivities, densities and refractive indices of PEG with molecular weights of 200 and 600 at 303.15 K.

In this paper, polymer absorbents either with ether group or ester group, as poly(propylene glycol) diglycidyl ether(PPDE) with molecular weights of 380 and 640, and poly(ethylene glycol) monooleate(PEGM) with molecular weight of 460 were selected as a comprehensive study, as ester and ether groups were found to be beneficial for improving CO_2 absorption capacity in our previous work [18]. Thermophysical properties as densities and kinematic viscosities of polymer absorbents are determined at temperatures from 273.15 K to 333.15 K and atmosphere. Effects of temperature, molecular weight on density, kinematic viscosity are discussed. In addition, CO_2 absorption capacities are measured under temperatures from 273.15 K to 303.15 K and pressures up to 1.2 MPa.

2. Experiment

2.1. Materials

A Metrohm 831 Karl Fischer coulometer was used for the determination of the water content in the studied solvents. The purity that stated by the supplier, CAS registry number, water mass fraction content, and source of the used chemicals are listed in Table 1.

The other substances were directly used without any further purification.

2.2. Density and kinematic viscosity measurement

Densities of the selected polymer absorbents were determined with the help of Anton Paar DMA 4500 M with the accuracy of 0.00005 g/cm³, at temperatures ranged from 273.15 K to 333.15 K and atmosphere. The temperature of the sample was controlled with the accuracy of 0.03 K. The U-cell of apparatus was calibrated with dry air and ultrapure water at atmospheric pressure. The total relative standard uncertainty ($u_r(\rho)$) can be calculated with the following equation:

$$u_r(\rho) = \sqrt{u_{1r}^2(\rho) + u_{2r}^2(\rho)} \qquad (1)$$

The relative standard uncertainty of the measurements repeatability ($u_{1r}(\rho)$) for the selected absorbents may be 0.00009 based on our determinations repeated for three times. Additionally, the relative standard uncertainty of the effect of other unknown factors ($u_{2r}(\rho)$) was estimated as 0.0028. Since the digit number of $u_r(\rho)$ should be consistent with those of $u_{1r}(\rho)$ based on the compute rule, the $u_r(\rho)$ was calculated as 0.00280.

Kinematic viscosities of the selected polymer absorbents at temperatures from 273.15 K to 333.15 K were determined by the glass capillary viscometers as discussed in our previous work [19] and the literature [20], which were always used for the determinations for ionic liquids and common solvents. It is based on the principle that the kinematic viscosity(v) at a certain temperature is proportional to the flow time of the solvent(t) in the capillary viscometer. The proportional factor is a viscometer constant(C) which is calibrated with oil by the manufacture. In the experimental process, the capillary viscometers were put into the water bath, which were provided by the refrigerator that used for temperature control of the sample with the assistance of a Julabo LC6 within the accuracy of 0.03 K. Time of sample flowing was recorded by a digital stopwatch with an accuracy of 0.01 s. The kinematic viscosity of the selected absorbents can be calculated as follows:

$$v = Ct \qquad (2)$$

The relative uncertainty of the kinematic viscosity($u_r(v)$) for the absorbents was assumed as 0.015 roughly.

To check the reliability of density and kinematic viscosity determinations, the density and kinematic viscosity of ethylene glycol were measured under the temperatures ranged from 273.15 K to 333.15 K and at atmosphere pressure, as shown in Table 2. The experimental data were compared with the data of density [21–36] and kinematic viscosity [24,25,29,30,33–38] in some literatures, as there are so many literatures. The average absolute relative deviations between the experimental and literature data for the density and kinematic viscosity were shown in Table 3. In addition, the deviations between the data in this work and available in the literatures [21–38] under different temperatures were shown in Figs. 1 and 2. The results showed that the device for the density and kinematic viscosity was accurate and reliable.

2.3. CO_2 solubility measurement

The device schematic with the isothermal synthetic method is shown in Fig. 3. In our previous works, CO_2 solubilities in various absorbents including physical [18,39,40] and hybrid [19] absorbents, were determined with the help of this device. The thermostatic bath was provided as previously discussed. The device mainly consists of a gas chamber, an equilibrium vessel, the temperature control system, and a vacuum-pumping system. Two PTX5072 sensors (General Electric), which are ranged up to