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Chemical Engineering Research and Design



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Prediction of carbon dioxide sorption in polymers for capture and storage feasibility analysis



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ARTICLE INFO

Article history: Received 23 December 2016 Received in revised form 15 February 2017 Accepted 21 February 2017 Available online 1 March 2017

Keywords: Carbon dioxide Polymer Capture Solubility

ABSTRACT

The carbon dioxide and its capture and storage has found great importance. Polymeric materials have been used for CO₂ capture where the solubility of CO₂ in polymer is the critical factor that determine the efficiency and performance of selected polymeric materials. For initial assessment and feasibility analysis of considered materials, prior to any experimental measurement, in order to reduce costs, development of a theoretical solubility and sorption model is highly of interest. Thus, here computationally consistent solubility model is developed employing the compressible regular solution theory where inputs parameters include the lattice fluid parameters and Hansen cohesive energy densities that are obtainable using group contribution method of Constantinou and Gani and the group contribution method of van Krevelen respectively. A number of experimental data was collected and used for examination of model accuracy and desirable agreement was found with an R² value of 0.9896.

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1. Introduction

Beside its greenhouse gas effect, carbon dioxide (CO₂) has a wide potential uses in applications such as enhanced oil recovery (EOR), food and beverage manufacturing, pulp and paper manufacturing, and metal fabrication (Olajire, 2010; Leung et al., 2014; Wang et al., 2011). Carbon dioxide capture technologies include absorption with amines, adsorption, membrane gas separation technologies, metalorganic frameworks (MOFs) and etc. (Olajire, 2010; Mondal et al., 2012) where solubility of CO₂ play a critical role in efficiency and feasibility of technologies, especially in membrane based separations and storage in polymeric materials. Therefore, the determination of solubility of CO₂ in polymeric materials is of high importance (Anon, 1999; Paul and Yampol'skii, 1993). A substantial number of research works and publications can be found in literature (Minelli and Sarti, 2013; Minelli and Sarti, 2015; Minelli and Sarti, 2016; Prabhakar et al., 2005).

In literatures (Anon, 1999; Minelli and Sarti, 2013), the solubility measurements have been done for various polymeric materials and large database of solubility data can be found in Anon (1999), Paul and Yampol'skii (1993), Khulbe et al. (2008) and Robeson (2008). However, to reduce the cost of experimental measurement and performance evaluation, cost of material preparation and facility maintenance, the development of theoretical models and methods for prediction, prior to any experimental work has found interest in literatures (Minelli and Sarti, 2013; Minelli and Sarti, 2015; Minelli and Sarti, 2016; Prabhakar et al., 2005; Asgarpour Khansary et al., 2015). Upon establishing such a model, validation of model calculations using any available experimental data is a required need to assess the agreement between model calculated data and those of experimentally measured.

Therefore, here, attempts were made to develop a predictive model employing well-established chemical thermodynamic model of compressible regular solution (CRS) (Gonzalez-Leon and Mayes, 2003; Mayes, 2014; Ruzette and Mayes, 2001) for local pseudo-equilibrium concentration of penetrant gases within the polymeric material as suitability of CRS theory for polymeric solutions has been demonstrated in literature (Ejraei et al., 2016; Keshavarz et al., 2015). The details of model development are given in following sections including the data used for model validation. The details of model development and its evaluation are provided in following sections.

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http://dx.doi.org/10.1016/j.cherd.2017.02.024

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2. Model development

The amount of penetrant i sorped into a polymeric material can be obtained using a local pseudo-thermodynamic equilibrium criterion at the interface of gas bulk stream phase and polymeric material as presented by Eq. (1) (Smith et al., 2005; Prausnitz et al., 1998; Keshavarz et al., 2015).

$$\Delta \mu_i^m = \Delta \mu_i^b \tag{1}$$

Here, $\Delta \mu_i$ is the chemical potential of gas component that can be calculated by using thermodynamic theory of compressible regular solution (CRS) model (Mayes, 2014; Gonzalez-Leon and Mayes, 2003; Ruzette and Mayes, 2001) and superscripts *m* and *b*, refer to polymeric material and bulk stream respectively.

For the case of single gas sorption, here CO₂, the mixture of sorped gas in polymeric material can be considered as a binary mixtures (Ejraei et al., 2016; Farajnezhad et al., 2016). For a binary mixture, the Gibbs free energy model of CRS (Mayes, 2014; Ruzette and Mayes, 2001; Gonzalez-Leon and Mayes, 2003) is given by Eq. (2).

$$\Delta g_{mix} = kT \left[\frac{\varphi_{i}\tilde{\rho}_{i}}{N_{i}\upsilon_{i}} \ln \varphi_{i} + \frac{\varphi_{j}\tilde{\rho}_{j}}{N_{j}\upsilon_{j}} \ln \varphi_{j} \right] + \varphi_{i}\varphi_{j}\tilde{\rho}_{i}\tilde{\rho}_{j} \left(\delta_{i,0} - \delta_{j,0}\right)^{2} + \varphi_{i}\varphi_{j} \left(\tilde{\rho}_{i} - \tilde{\rho}_{j}\right) \left(\delta_{i,0}^{2} - \delta_{j,0}^{2}\right)$$
(2)

Here, k is the Boltzmann constant, $\tilde{\rho}_i$ the reduced density of component i. N_i the number of segments in the hard-core volume (v_i) of component i, $\delta_{i,0}$ the hard-core solubility parameter at 0 K. φ_i is the volume fraction of component i. Subscript i and j refers to gas compound and polymer respectively.

The chemical potential relationship in CRS theory is given by Eq. (3) (Mayes, 2014; Ruzette and Mayes, 2001; Gonzalez-Leon and Mayes, 2003).

$$\Delta \mu_{i} = \frac{N_{i} v_{i}}{\tilde{\rho}_{i}} \left[\Delta g_{mix} + \varphi_{j} \frac{\partial \Delta g_{mix}}{\partial \varphi_{i}} \right]$$
(3)

In the bulk gas phase, for the calculation of gas chemical potential in bulk phase, as the gas bulk phase is pure ($\varphi_i = 1$), one might obtain.

$$\frac{\Delta \mu_i^b}{kT} = -\frac{N_i \upsilon_i \,\tilde{\rho}_j}{N_j \upsilon_j \,\tilde{\rho}_i} \tag{4}$$

Thus, noting to the equality of chemical potentials in two phases according to Eq. (1), one might obtain Eq. (5).

$$\frac{\Delta \mu_i^m}{kT} = \frac{\Delta \mu_i^b}{kT} = -\frac{N_i \upsilon_i}{N_j \upsilon_j} \frac{\tilde{\rho}_j}{\tilde{\rho}_i}$$
(5)

Finally, inserting the chemical potential of gas in membrane from Eq. (3) into Eq. (5), carrying out a number of mathematical manipulations, one would obtain Eq. (6).

$$\ln \varphi_{i} + 1 - \varphi_{i} - \frac{N_{i} v_{i}}{N_{j} v_{j}} \frac{\tilde{\rho}_{j}}{\tilde{\rho}_{i}} \varphi_{i} + \left(\tilde{\rho}_{i} \delta_{i,0} - \tilde{\rho}_{j} \delta_{j,0}\right)^{2}$$
$$\frac{V_{i}}{RT} \left(1 - \varphi_{j}\right) = -\frac{N_{i} v_{i}}{N_{j} v_{j}} \frac{\tilde{\rho}_{j}}{\tilde{\rho}_{i}}$$
(6)

Using Mathematica[®] Software (Wolfram Mathematica, 2014), the solution to Eq. (6) can be given as in Eq. (7).

$$\varphi_{i} = -\frac{W\left(-w_{1}e^{-w_{2}-1}\right)}{w_{1}} \tag{7}$$

$$w_{1} = 1 + \frac{N_{i}v_{i}}{N_{j}v_{j}}\frac{\tilde{\rho}_{j}}{\tilde{\rho}_{i}} + \left(\tilde{\rho}_{i}\delta_{i,0} - \tilde{\rho}_{j}\delta_{j,0}\right)^{2}\frac{V_{i}}{RT}$$
$$= 1 + \frac{N_{i}v_{i}}{N_{j}v_{j}}\frac{\tilde{\rho}_{j}}{\tilde{\rho}_{i}} + \left(\tilde{\rho}_{i}\delta_{i,0} - \tilde{\rho}_{j}\delta_{j,0}\right)^{2}\frac{1}{p}$$
(8)

$$w_{2} = \left(\tilde{\rho}_{i}\delta_{i,0} - \tilde{\rho}_{j}\delta_{j,0}\right)^{2} \frac{V_{i}}{RT} + \frac{N_{i}v_{i}}{N_{j}v_{j}} \frac{\tilde{\rho}_{j}}{\tilde{\rho}_{i}}$$
$$= \frac{N_{i}v_{i}}{N_{j}v_{j}} \frac{\tilde{\rho}_{j}}{\tilde{\rho}_{i}} + \left(\tilde{\rho}_{i}\delta_{i,0} - \tilde{\rho}_{j}\delta_{j,0}\right)^{2} \frac{1}{p}$$
(9)

Here, W (x) is the product log function (Wolfram Mathematica, 2014; Spiegel and Liu, 1999), p is pressure and noting to expressions in Eqs. (8) and (9) one might write $w_1 = 1 + w_2$.

the Taylor series expansion of product log function, W(x), can be used to simplify Eq. (7) using Mathematica[®] Software (Wolfram Mathematica, 2014).

$$W(x) = x - x^2 + \frac{3x^3}{2}$$
(10)

Therefore, Eq. (7) reads Eq. (14).

$$\varphi_{i} = -\frac{W\left(-w_{1}e^{-w_{2}-1}\right)}{w_{1}}$$
$$= -\frac{-w_{1}e^{-w_{2}-1}-\left(-w_{1}e^{-w_{2}-1}\right)^{2}+\frac{3\left(-w_{1}e^{-w_{2}-1}\right)^{3}}{2}}{w_{1}}$$
(11)

$$\varphi_{i} = e^{-w_{2}-1} + w_{1}(e^{-w_{2}-1})^{2} + w_{1}^{2} \frac{3(e^{-w_{2}-1})^{3}}{2}$$
$$= e^{-w_{2}-1} \left[1 + w_{1}e^{-w_{2}-1} + \frac{3}{2}w_{1}^{2}(e^{-w_{2}-1})^{2} \right]$$
(12)

$$\varphi_{i} = e^{-w_{2}-1} \left[1 + w_{1}e^{-w_{2}-1} + \frac{3}{2}w_{1}^{2}(e^{-w_{2}-1})^{2} \right]$$
$$= e^{-w_{2}-1} \left[1 + w_{1}e^{-w_{2}-1} \left[1 + \frac{3}{2}w_{1}e^{-w_{2}-1} \right] \right]$$
(13)

$$\varphi_{i} = e^{-w_{2}-1} \left[1 + w_{1}e^{-w_{2}-1} \left[1 + \frac{3}{2}w_{1}e^{-w_{2}-1} \right] \right]$$
(14)

The volume fraction, then can be converted to the solubility coefficient noting that $S_i = C_i/p$ and $C_i = \rho_i^{\circ} \varphi_i / M w_i$ where p is the pressure.

3. Method of calculations

The $\delta_{i,0}$, hard-core solubility parameter, can be calculated using the Hoftyzer and van Krevelen group contribution method (Krevelen and Nijenhuis, 2017). The reduced density, then can be calculated as $\tilde{\rho}_i = \rho_i / \rho_i^0$ and the hard-core solubility parameter can be calculated as $\delta_i^2 = \delta_{i,0}^2 \left(\rho_i / \rho_i^0 \right)$ (Keshavarz Download English Version:

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