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Thermodynamic Modeling the Solubility of CO_2 in Aqua System of Methyldiethanolamine and 2-(2-Aminoethylamino)ethanol Using the Nonelectrolyte Wilson Nonrandom Factor

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ABSTRACT

Alkanolamines are used to remove acidic gases such as CO_2 and H_2S from natural gas. In this study, thermodynamic modeling of the binary component CO_2+MDEA, three component MDEA+H_2O+CO_2 and the quaternary MDEA+AEEA+H_2O+CO_2 systems were developed using an additional Gibbs argillic model for the first time in the modeling of CO_2 solubility in different solutions. The appropriate model was considered using the assumption of an entirely molecular system without any occurrence of chemical reactions and saturated gas phase from the CO_2 gas. The nonelectrolyte Wilson nonrandom factor (N-Wilson-NRF) model and the activity coefficient method (γ_φ Aproach) were used to calculate solubility of CO_2. The two-component water- CO_2 model was modeled and the results were obtained by the accuracy of 1.38 of experimental results. In a three-component, water-CO_2-MDEA system with the amount of 6.913, the optimization was developed. The quaternary water-CO_2-MDEA-AEEA system was optimized with an overall approximation of 19.537 for all experiment data.

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1. INTRODUCTION

The removal of CO_2 and H_2S from the flue gas is essential in the process of natural gas purification. In addition, for the design and construction of gas transport equipment, experimental data on the solubility of CO_2 and H_2S in aquatic alkanolamines are required [1]. Due to the weakness or power of various alkanolamines in absorption of various acid gases, the choice of a suitable combination of these materials in the process of natural gas purification has been studied [2-4]. Also, at wide range of temperatures and pressures, various experiments are carried out to obtain a suitable thermodynamic model for desired estimation of experimental data [5-7]. It became clear that, because of the ionization of these mixtures, the models that utilize the activity coefficient have been used extensively in research projects [8-10]. Typically, in these models, various equations have been used to predict wide-range of interactions using the Pitzer-Debye-Huckel method and narrow-range of interactions using other types of methods [11-13].

Separation factor is an important feature in the choice of alkanolamine solution to eliminate acidic gas or to interpret the kinetic mechanism of acidic absorption in alkanolamine solution. Recently, Barzagli et al. [14] have studied CO_2 absorption and desorption experiments with alkanolamine mixtures in non-aqueous solvents (ethylene glycol mixtures and 2,1 propanediol with methanol or ethanol) [13]. They reported relatively low separation temperature (about 80°C) and less

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evaporation. They have shown that amine recovery in non-aqueous solvents can be easily done [6]. The results of their study are given with the average and maximum relative deviation between experimental data and linear matching values. These numbers provide information about the linear extrapolation. Also, the decrease in the strength of the protonated alkanolamines was observed with an increase in fractions of organic composition and temperature. The greatest effect is observed for butanol-water mixtures as solvent. This result was expected since the butanol-water solvents had the lowest dielectric values compared to sulfolane-water and methanol-water solvents.

In the case of acid gases, thermodynamic modeling of the equilibrium solubility is also an important topic for the design of gas purification and CO_2 capture processes. Zoghi and Feizi [15] calculated the solubility of CO_2 in aqueous solutions of 2, 2-aminoethyl amino ethanol (AEEA) and compare the results with the Deshmuch-Mather model. Finally, for the quaternary system water-CO_2-N-methyldiethanolamine (MDEA)-AEEA, the modified Peng-Robinson cube parameters which were modified by the electrolyte are correlated with the emPR-CPA equation of state (EoS) and finally, the solubility of CO_2 is calculated. They studied equilibrium solubility of CO_2 in the mentioned solution in the range of 308.2 to 368.2 K and the 101 to 4448 kPa [9].

2. THERMODYNAMIC MODELING

In this work, we have used gamma-phi (γ-φ) method for modeling the behavior of under investigation systems. Specifically, to calculate the activity coefficients of the components in the gas phase, the N-Wilson-NRF state equation and to calculate the fugacity coefficients in the liquid phase, the Peng Robinson equation has been used [16]. Using the qualitative properties (PVT), we can calculate all thermodynamic properties and thermodynamic potential energies. Here, we will investigate the behavior of PVT of a pure substance in gas and liquid states.

Parameters (a and b) which are called gravity and repulsion parameters, respectively. Here, k_1 and k_2 are numerical constants that obtained by the critical properties for each pure substance.

Peng-Robinson presented his equation as follows Equation (2) where k_1= 2 and k_2=-1 [17]:

$$P=\frac{RT}{v-b}-\frac{a(T,\omega)}{v(v+b)+b(v-b)} \tag{1}$$

In this equation, a, b are:

$$a=0.457235\frac{R^2T_c^{\,2}}{P_c},\ b=0.077796\frac{RT_c}{P_c}$$

The k equation is obtained by fitting steam pressure data from boiling point to critical point in Equation (2):

$$k=0.37464+1.54226\omega-0.26993\omega^2 \tag{2}$$

The cubic equations of state for the blends are written as follows in Equation (3):

$$P=\frac{RT}{v-b}-\frac{a(T,\omega)}{v^2+k_1bv+k_2b^2} \tag{3}$$

Also, v is the molar volume of the mixture. In this case, using the mixing rule, the values of a and b can be set according to the a_i and b_i parameters for the pure substance.

2. 1. Mixture Fugacity Coefficient Using Peng-Robinson Equation

The Peng- Robinson equation of state can be divided as follows in Equation (4) [8-9]:

$$P=\frac{RT}{v-b}-\frac{a\alpha(T,\omega)}{(v+(1+\sqrt{2})b)(v+(1-\sqrt{2})b)} \tag{4}$$

By proper derivation from Equation (2), the fugacity coefficient of component i is obtained as follows in Equation (5):

$$\ln\varphi_i=\frac{b_i}{b}(Z-1)-\ln(Z-B)-\frac{A}{2\sqrt{2}B}\left[\frac{2\sum_{j=1}^{c}y_ia_{ij}}{a\alpha}-\frac{b_i}{b}\right]\ln\frac{Z+B(1+\sqrt{2})}{Z+B(1-\sqrt{2})} \tag{5}$$

2. 2. An Integral Method for the Calculations of Vapor-liquid Equilibrium

In the integral method, the equation of fugacity is used directly for equilibrium calculations. Therefore, for the equilibrium of two phases of vapor and liquid, the equation of fugacity is used based on the following Equation (6) [18, 19]:

$$f_i^{\,v}=f_i^{\,l} \tag{6}$$

In this case, the following two methods are proposed for the calculations of vapor-liquid equilibrium, each method depending on the nature of the components:

I. The equation of state approach (φ_φ Approach)
II. The activity coefficient approach (γ_φ Approach)

In the equation of state approach, the fugacity of each component in the vapor and liquid phases is written as follows:

$f_i^{\,v}=y_i\varphi_i^{\,v}P$ for vapor and $f_i^{\,l}=x_i\varphi_i^{\,l}P$ for liquid and x_i, y_i are the molar fractions of component I in liquid and vapor phases, respectively. Hence Equation (7):

$$K_i=\frac{y_i}{x_i}=\frac{\varphi_i^{\,l}}{\varphi_i^{\,v}} \tag{7}$$

where K_i is the ratio of components (K-value) for component i. Therefore, with the proper equation of state, the coefficients of fugacity can be calculated.

The activity coefficient is the quantity that represents the deviation of the non-ideal behavior of liquid mixtures from the ideal behavior of Lewis-Randal. When we have an ideal solution, the activity coefficient is 1 and the fugacity of component i is ideally written as follows in Equation (8):

$$f_i^{id} = x_i f_{i,pure} \tag{8}$$

In other words, liquid solutions can be divided into (ideal dilution solution) and (non-ideal solution). Therefore, in order to calculate the activity coefficients, it is necessary to calculate the first fugacity from the pure material. Therefore, fugacity can be achieved by using a dense phase fugacity in Equation (9):

$$f_{i,pure} = P_i^{sat}\varphi_i^{sat}\exp[\frac{v_i^0(P-P_i^{sat})}{RT}] \tag{9}$$

The saturation fugacity coefficient (φ_i^{sat}) is obtained at a saturation point at temperature T, which can be calculated using the ratio of the fugacity coefficient for the pure component.

2. 3. Activity Coefficient in Liquid Solutions For liquid solutions, the activity coefficient is used as the standard deviation from the ideal state, so for the component in liquid solution and constant temperature it can be written as Equation (10) [20-22]:

$$\gamma_{i,0} = \frac{f_i(T,P,x_i)}{f_i^{LR}} = \frac{f_i(T,P,x_i)}{x_i f_i^0(T,P)} \tag{10}$$

The Lewis-Randal activity coefficient is used for the solutions in which the components are either dissolved or convergent, in any ratio from dilute to concentrated. On the other hand, some solutions have a positive deviation $(\gamma_i \succ 1)$ from the Lewis-Randal law, and others have negative deviations $(\gamma_i \prec 1)$. For some solutions, you cannot use the Lewis-Randal activity factor. In this kind of systems, components are not resolved in each other with any ratio. In this case, it is not possible to use the Lewis-Randal activity factor for vapor in the solution. In this case, pure vapor may not be available as a standard solution at system temperature and pressure. Another example is the solubility of electrolytes and polymers in solvents. In this case, the activity coefficient for component i is defined as Equation (11):

$$\gamma_i^* = \frac{f_i(T,P,x_i)}{x_i H_{ij}(T,P)} \tag{11}$$

Thus, for equilibrium calculations in liquid and solid phases, using the gamma-phi method, we need to have a proper function for calculating the activity coefficient of the components in the solution. On the other hand, we know that in order to obtain an appropriate model of the activity coefficient, the Gibbs energy function (G^E) is necessary for the solution which is shown in Equation (12).

$$\ln\gamma_i = (\frac{\partial(G^E/RT)}{\partial N_i})_{T,P,N_{j\neq i}} = (\frac{\partial(Ng^E/RT)}{\partial N_i})_{T,P,N_{j\neq i}} \tag{12}$$

2. 4. Local Composition Models The local composition model is a semi-experimental method that derives from the concept of the local composition of molecules in a network. The local composition concept was first introduced by Wilson in 1964 [23].

In 2009, the Haghtalab and Mazloumi present new N-Wilson-NRF model which provided a random mode for each cell based on the literature stated [24]. Local molecular fractions are defined using non-random Γ_{ij} coefficients Equation (13):

$$\begin{aligned} &x_{ij} = x_i\Gamma_{ij},\ \Gamma_{ij} = \frac{\beta_{ij}}{\sum_{k=1}^{N} x_k\beta_{kj}}, \\ &\Gamma_{ii} = \Gamma_{ij}/\beta_{ji}, \\ &\beta_{ij} = \exp(-\frac{h_{ij}-h_{jj}}{ZRT}) = \exp(-\frac{\lambda_{ij}}{Z}) \end{aligned} \tag{13}$$

While $\beta_{ij} \neq \beta_{ji}, \beta_{ii} = \beta_{jj} = 1$ and N is the number of components in the system and Z is the coordination number. Using Equation (13), we can obtain the hypertension enthalpy formula for a two-component mixture. Assuming that the temperature is independent of enthalpy Equation (14):

$$\frac{g^E}{RT} = Z[x_1\ln\Gamma_{11} + x_2\ln\Gamma_{22} + x_1x_2\ln(\beta_{12}\beta_{21})] \tag{14}$$

by deriving the Equation (14), the activity coefficient for a component in a two-component mixture is obtained as Equation (15):

$$\ln\gamma_1 = Z[\ln\Gamma_{11} + x_2(\Gamma_{21}-\Gamma_{12}) + x_2^2\ln(\beta_{12}\beta_{21})] \tag{15}$$

The general format of the equations for a multi-component mixture is obtained as Equations (16) and (17):

$$\frac{g^E}{RT} = Z[\sum_i x_i(\ln\Gamma_{ii} + \sum_j x_j\ln\beta_{ij})] \tag{16}$$

$$\begin{aligned} &\ln\gamma_i = Z[1+\ln\Gamma_{ii} - \sum_j x_j(\Gamma_{ij} - \ln\beta_{ij}\beta_{ji} + \sum_k x_k\ln\beta_{kj})] \\ &\lambda_{ij} = (h_{ij}-h_{jj})/RT,\ \lambda_{ii} = \lambda_{jj} = 0, \beta_{ii} = \beta_{jj} = 1.0 \end{aligned} \tag{17}$$

2. 5. The Process Flowchart of Calculating co_2 Gas Solubility The general method for calculating the

vapor pressure of each of the various system components using the bubble-pressure calculations flowchart is shown in Figure 1. For higher order systems, these equations for the mixtures can be used [17]. As shown in Figure 1 by the help of laboratory pressure, temperature and composition of the components percentage in the liquid phase, by the initial guess for the system pressure, the simulations can be done, and also the composition of the components in the gas phase and the calculated pressure can be gained using this system. It should be noted that for the two-component and multi-component systems the overall process is the same and for the higher order systems, the classic rules of the hybrid can be used.

3. RESULT AND DISCUSSION

3. 1. Quaternary Water-CO_2-MDEA-2, 2-aminoethyl (amino) ethanol System One of the most important factors in the design of absorption unit is the solvent material. The most important features of a solvent for absorption are higher absorption speed, better function in absorption process, high net recycling capacity and better chemical stability. In the previous studies [25], researchers measured the rate of CO_2 absorption among various amines, which showed that 2-2-Aminoethyl(Amino)Ethanol (AEEA) and (2-Aminoethyl) 1,3-Propandiamine solvents can absorb CO_2 more quickly. Ma'mum et al. [26] used a screening test and found that the aqueous solution of AEEA could be used as an absorbent in the process of absorbing CO_2 from combustion gases. AEEA has a high absorption rate and net recycling capacity, which is clearly higher than monoethanolamine indexes. Also, this material has also shown its high absorption capacity at higher CO_2 loads. Recently, Zoghi et al. [27] investigated the effect of various activators in methyl diethanolamine on the CO_2 capture process. They showed that AEEA can greatly increase the rate of CO_2 absorption compared with other activators such as Piperazine. The amount of waste lost in the recovery process is another important factor that should be considered in choosing the appropriate solvent. Wilson [28] measured the vapor pressure of AEEA under the temperature of the recovery process (395 K) and showed that AEEA had much lower vapor pressure (959 Pa) than monoethanolamine (15900 Pa). Also, thermodynamic modeling of the equilibrium solubility of acid gases in the process of sweetening and absorbing CO_2 gas is another vital point. When acid gases are absorbed in an aqueous solution of alkanolamine, different ionic species are produced by chemical reactions. It makes it difficult to calculate the liquid-vapor balance for aqueous solutions of alkanolamine. In this section, we used the gamma-phi(γ-φ) method and the experimental data of Zoghi experiment [15], to develop a thermodynamically model of the quaternary water-CO_2-MDEA-AEEA system. It is important to assume the system physically, in order to reduce the volume of the calculations and to simplify the process of chemical reactions. Based on the results of the above four-component system, the target function was equal to 19.537.

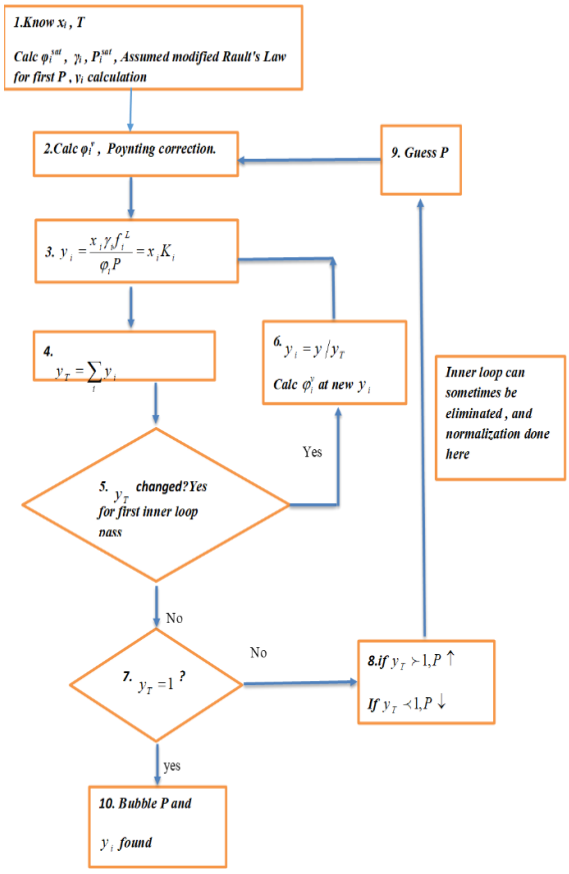

Figure 1. The Process Flowchart of Calculating CO_2 Gas Solubility in Amine Solutions

TABLE 1. Optimized Values of the N-Wilson-NRF Equation for the Quaternary Water-CO_2-MDEA-AEEA System

i-j	λ_{ij} *	a_{ij}	b_{ij}
CO_2-AEEA	λ_{14}	-27/8734	-48669/667
AEEA-CO_2	λ_{41}	-8/3472	-7713/6611
H_2O-AEEA	λ_{24}	278/2278	-941/2250
AEEA-H_2O	λ_{42}	8/4826	1323/4516
MDEA_AEEA	λ_{34}	5/8430	-62/8829
AEEA_MDEA	λ_{43}	2/3283	-221/7266

$\lambda_{ij} = a_{ij} + \frac{b_{ij}}{T}$

3. 2. Interaction Parameter In the previous sections and in the equation of activity coefficients, we used equation 17 to calculate the interaction parameters, where two parameters a and b were obtained and optimized simultaneously. In this section, by developing the interaction parameter equation, we examined the effect of this change on the accuracy of the calculations. The equation of interaction parameter with the three sub-parameters a, b and c is defined in Equation (18):

$$\lambda_{ij} = a_{ij} + \frac{b_{ij}}{T} + c_{ij}\left[\frac{T - T^{0}}{T} + \ln\frac{T}{T^{0}}\right] \quad (18)$$

For the quaternary water-CO_2-MDEA-AEEA system, the target function was equal to 19.084 and the values of interaction parameters are shown in Table 3.

TABLE 2. Experimental and Calculated Pressure in the Quaternary Water-CO_2-MDEA-AEEA System

Loading	Pexp (kPa)	P cal(kPa)	Loading	Pexp(kPa)	P cal(kPa)
	308.2(K)			328.2(K)	
0.735	103.3	130.66	0.516	100.7	90.96
0.753	111.6	140.02	0.544	114.5	114.5
0.807	146.7	171.0261	0.56	128.3	129.3136
0.832	187.4	187.4	0.62	133.5	197.655
0.862	232.9	207.4161	0.652	163.9	242.6039
0.89	350.6	227.9479	0.704	249.7	329.7518
0.906	483.8	240.3064	0.765	373.8	456.6946
0.934	746.8	263.113	0.805	531.8	556.0085
0.944	908.8	271.57	0.846	793.2	672.2862
0.954	1082	280.1942	0.868	963.6	741.1162
0.966	1254.7	290.766	0.885	1165.9	797.5861
0.974	1438.8	298.3437	0.895	1335.3	832.1222
0.988	1652.1	311.3575	0.917	1574.4	911.7242
1.002	1952.7	324.6064	0.934	1798.8	976.6611
	343.2(K)			368.2(K)	
0.489	170.9	158.3485	0.406	281	177.09
0.514	189.4	194.8241	0.429	322	224.31
0.556	230.9	267.88.907	0.47	405.5	327.27
0.626	349.6	426.1947	0.527	585.6	514.45
0.688	468.8	609.5557	0.543	649.5	577
0.73	593.3	759.5985	0.589	821	783.34
0.759	724.3	876.4672	0.626	1010	979.8
0.81	968.3	1110.433	0.67	1241.7	1251.96
0.822	1172.2	1172.2	0.708	1490.3	1523.53
0.835	1316.5	1239.3	0.742	1656.7	1796.68
0.896	2128.4	1596.662	0.852	2758.1	2917.502
0.913	2373.6	1707.78	0.867	3002.9	3101.764
0.916	2898.6	1728.127	0.883	3266.8	3305.867
0.929	3082.6	1817.519	0.899	3502.9	3524.257
0.942	3253.2	1910.189	0.916	3869.6	3766.08

TABLE 3. Optimized Values of the N-Wilson-NRF Equation in the Quaternary Water-CO_2-MDEA-AEEA System

i-j	λ_{ij}	a_{ij}	b_{ij}	c_{ij}
CO_2-AEEA	λ_{14}	-27/8734	-48669/667	-0/01153
AEEA-CO_2	λ_{41}	-8/3472	-7713/6611	-0/01552
H_2O-AEEA	λ_{24}	287/2285	-941/2250	-0/07370
AEEA-H_2O	λ_{42}	8/4826	1323/4516	-0/01154
MDEA_AEEA	λ_{34}	5/8430	-62/8829	0/01758
AEEA_MDEA	λ_{43}	2/3283	-221/7266	0/01680

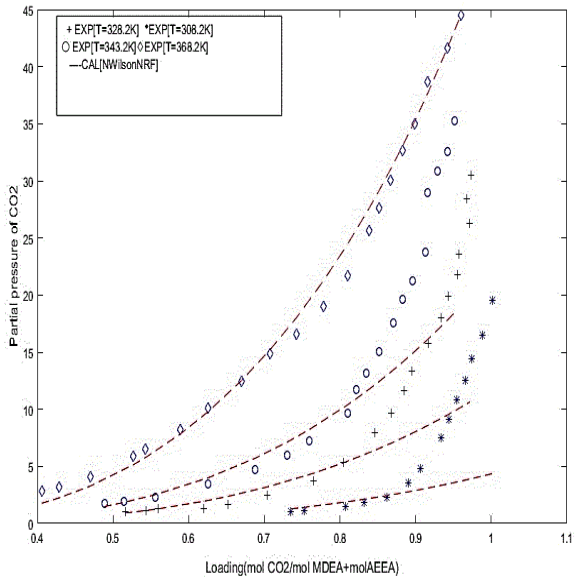

Figure 2. Molecular Concentration of CO_2 in Aqueous Solution of MDEA+AEEA

4. CONCLUSION AND FUTURE PERSPECTIVE

In this project, the solubility of CO_2 gas was investigated in alkanolamine solutions. The N-Wilson-NRF model and the activity coefficient method (γ_φ Approach) were used to calculate solubility of CO_2. The two-component water- CO_2 model was modeled and the results were obtained by the accuracy of 1.38 of experimental results. In a three-component, water-CO_2-MDEA system with the amount of 6.913, the optimization was developed.

The quaternary water-CO_2-MDEA-AEEA system was optimized with an overall approximation of 19.537 for all experiment data. By changing the interaction parameter equation of λ_{ij} to the three-parametric equation in the two-component system, the approximation of 6.581 and in the three-component system, 19.084 were obtained. The systems used in this study have made a completely reasonable approximation considering that the solubility modeling of gas in solutions is based on the physical interaction. To make the calculation and mentioned systems more accurate, some suggestions are presented which are:

1. considering chemical reactions in the liquid phase to improve the accuracy of the model,
2. performing more experiments at higher temperatures and pressures to obtain more operational data,
3. using mixing rules in multi-component system computing procedure,
4. using the equations of electrolyte activation to improve the accuracy of the model.

5. REFERENCES

1. Barzagli, F., Mani, F. and Peruzzini, M., "A comparative study of the CO_2 absorption in some solvent-free alkanolamines and in aqueous monoethanolamine (MEA)", ***Environmental Science & Technology***, Vol. 50, No. 13, (2016), 7239-7246. DOI: 10.1021/acs.est.6b00150
2. Akhmetshina, A.I., Petukhov, A.N., Vorotyntsev, A.V., Nyuchev, A.V. and Vorotyntsev, I.V., "Absorption behavior of acid gases in protic ionic liquid/alkanolamine binary mixtures", ***ACS Sustainable Chemistry & Engineering***, Vol. 5, No. 4, (2017), 3429-3437. DOI: 10.1021/acssuschemeng.7b00092
3. Akbartabar, I., Yazdanshenas, M.E., Tayebi, H.-A. and Nasirizadeh, N., "Physical chemistry studies of acid dye removal from aqueous media by mesoporous nano composite: Adsorption isotherm, kinetic and thermodynamic studies", ***Physical Chemistry Research***, Vol. 5, No. 4, (2017), 659-679. DOI: 10.22036/PCR.2017.83378.1371
4. Patel, H.A., Karadas, F., Canlier, A., Park, J., Deniz, E., Jung, Y., Atilhan, M. and Yavuz, C.T., "High capacity carbon dioxide adsorption by inexpensive covalent organic polymers", ***Journal of Materials Chemistry***, Vol. 22, No. 17, (2012), 8431-8437. https://doi.org/10.1039/C2JM30761H
5. He, X., Fu, C. and Hägg, M.-B., "Membrane system design and process feasibility analysis for CO_2 capture from flue gas with a fixed-site-carrier membrane", ***Chemical Engineering Journal***, Vol. 268, (2015), 1-9. DOI: 10.1016/j.ijggc.2013.03.026
6. Yan, H., Fu, Q., Zhou, Y., Li, D. and Zhang, D., " CO_2 capture from dry flue gas by pressure vacuum swing adsorption: A systematic simulation and optimization", ***International Journal of Greenhouse Gas Control***, Vol. 51, (2016), 1-10. https://doi.org/10.1016/j.ijggc.2016.04.005
7. Shi, W., Siefert, N.S. and Morreale, B.D., "Molecular simulations of CO_2, H_2, H_2O, and H_2S gas absorption into hydrophobic poly (dimethylsiloxane)(PDMS) solvent: Solubility and surface tension", ***The Journal of Physical Chemistry C***, Vol. 119, No. 33, (2015), 19253-19265. DOI: 10.1021/acs.jpcc.5b05806
8. Sadegh, N., Stenby, E.H. and Thomsen, K., "Thermodynamic modeling of hydrogen sulfide absorption by aqueous n-methyldiethanolamine using the extended uniquac model", ***Fluid Phase Equilibria***, Vol. 392, (2015), 24-32. https://doi.org/10.1016/j.fluid.2015.01.024
9. Barati-Harooni, A., Najafi-Marghmaleki, A. and Mohammadi, A.H., "Efficient estimation of acid gases (CO_2 and H_2S) absorption in ionic liquids", ***International Journal of***

Greenhouse Gas Control, Vol. 63, (2017), 338-349. https://doi.org/10.1016/j.ijggc.2017.05.014

10. Koronaki, I., Prentza, L. and Papaefthimiou, V., "Modeling of CO_2 capture via chemical absorption processes−an extensive literature review", ***Renewable and Sustainable Energy Reviews***, Vol. 50, (2015), 547-566. https://doi.org/10.1016/j.rser.2015.04.124
11. Suleman, H., Nasir, Q., Maulud, A.S. and Man, Z., "Comparative study of electrolyte thermodynamic models for carbon dioxide solubility in water at high pressure", ***Chemical Engineering Transactions***, Vol. 45, (2015). DOI: 10.3303/CET1545099
12. Shekaari, H., Zafarani-Moattar, M.T., Mokhtarpour, M. and Faraji, S., "Effect of 1-ethyl-3-methylimidazolium ethyl sulfate ionic liquid on the solubility of indomethacin in aqueous solutions at various temperatures", ***Journal of Molecular Liquids***, Vol. 260, (2018), 166-172. https://doi.org/10.1016/j.molliq.2018.03.061
13. Castañeda, C.A., Wolfson, N.A., Leng, K.R., Kuo, Y.-M., Andrews, A.J. and Fierke, C.A., "Hdac8 substrate selectivity is determined by long-and short-range interactions leading to enhanced reactivity for full-length histone substrates compared with peptides", ***Journal of Biological Chemistry***, Vol. 292, No. 52, (2017), 21568-21577.
14. Barzagli, F., Mani, F. and Peruzzini, M., "Efficient CO_2 absorption and low temperature desorption with non-aqueous solvents based on 2-amino-2-methyl-1-propanol (AMP)", ***International Journal of Greenhouse Gas Control***, Vol. 16, (2013), 217-223. https://doi.org/10.1016/j.ijggc.2013.03.026
15. Zoghi, A.T. and Feyzi, F., "Equilibrium solubility of carbon dioxide in aqueous 2-((2-aminoethyl) amino) ethanol and n-methyldiethanolamine solution and modeling by electrolyte mpr-cpa eos", ***The Journal of Chemical Thermodynamics***, Vol. 67, (2013), 153-162.
16. Haghtalab, A. and Shojaeian, A., "High pressure measurement and thermodynamic modelling of the solubility of carbon dioxide in n-methyldiethanolamine and 1-butyl-3-methylimidazolium acetate mixture", ***The Journal of Chemical Thermodynamics***, Vol. 81, (2015), 237-244. https://doi.org/10.1016/j.jct.2014.10.011
17. Smith, J., Van Ness, H. and Abbott, M., "Chemical engineering thermodynamics", ***Sat***, Vol. 18, (1996), 1-3.
18. He, P. and Chu, J., "Low pressure vapor-liquid equilibrium validation with special pseudo-components", in Control Conference (CCC), 2017 36th Chinese, IEEE. 10381-10386.
19. Løvseth, S.W., Austegard, A., Westman, S.F., Stang, H.G.J., Herrig, S., Neumann, T. and Span, R., "Thermodynamics of the carbon dioxide plus argon (CO_2+ ar) system: An improved reference mixture model and measurements of vapor-liquid, vapor-solid, liquid-solid and vapor-liquid-solid phase equilibrium data at the temperatures 213–299 k and pressures up to 16 mpa", ***Fluid Phase Equilibria***, Vol. 466, (2018), 48-78. https://doi.org/10.1016/j.fluid.2018.02.009
20. Chen, M., Xie, Y., Wu, H., Shi, S. and Yu, J., "Modeling solubility of nitrogen in clean fire extinguishing agent by peng-robinson equation of state and a correlation of henry's law constants", ***Applied Thermal Engineering***, Vol. 110, (2017), 457-468. https://doi.org/10.1016/j.applthermaleng.2016.08.179
21. Ashassi-Sorkhabi, H. and Kazempour, A., "Application of pitzer and six local composition models to correlate the mean ionic activity coefficients of aqueous 1-butyl-3-methylimidazolium bromide ionic liquid solutions obtained by emf measurements", ***The Journal of Chemical Thermodynamics***, Vol. 110, (2017), 71-78. https://doi.org/10.1016/j.jct.2017.02.015
22. Mester, Z. and Panagiotopoulos, A.Z., "Mean ionic activity coefficients in aqueous nacl solutions from molecular dynamics simulations", ***The Journal of Chemical Physics***, Vol. 142, No. 4, (2015), 044507.
23. Renon, H. and Prausnitz, J.M., "Local compositions in thermodynamic excess functions for liquid mixtures", ***AIChE Journal***, Vol. 14, No. 1, (1968), 135-144. https://doi.org/10.1002/aic.690140124
24. Haghtalab, A. and Mazloumi, S.H., "Electrolyte cubic square-well equation of state for computation of the solubility CO_2 and H_2S in aqueous mdea solutions", ***Industrial & Engineering Chemistry Research***, Vol. 49, No. 13, (2010), 6221-6230.
25. Bonenfant, D., Mimeault, M. and Hausler, R., "Determination of the structural features of distinct amines important for the absorption of CO_2 and regeneration in aqueous solution", ***Industrial & Engineering Chemistry Research***, Vol. 42, No. 14, (2003), 3179-3184.
26. Ma'mun, S., Jakobsen, J.P., Svendsen, H.F. and Juliussen, O., "Experimental and modeling study of the solubility of carbon dioxide in aqueous 30 mass% 2-(2-aminoethylamino)ethanol solution", ***Industrial & Engineering Chemistry Research***, Vol. 45, No. 8, (2006), 2505-2512.
27. Zoghi, A.T., Feyzi, F. and Dehghani, M.R., "Modeling CO_2solubility in aqueous n-methyldiethanolamine solution by electrolyte modified peng–robinson plus association equation of state", ***Industrial & Engineering Chemistry Research***, Vol. 51, No. 29, (2012), 9875-9885. doi: 10.1021/ie2026053
28. Dumée, L., Scholes, C., Stevens, G. and Kentish, S., "Purification of aqueous amine solvents used in post combustion CO_2capture: A review", ***International Journal of Greenhouse Gas Control***, Vol. 10, (2012), 443-455. https://doi.org/10.1016/j.ijggc.2012.07.005

Persian Abstract

چکیده

زدودن هیدروژن سولفید و دی اکسید کربن از گاز دودکش در فرایند تصفیه گاز طبیعی و گیرانداختن گازهای اسیدی اهمیت دارد به علاوه، برای طراحی و ساخت تجهیزات اتصال گاز، داده های تجربی انحلال پذیری H_2S و CO_2 در آلکانول آمین های آبی مورد نیاز هستند. به دلیل ضعف یا قدرت آلکانول آمین های مختلف در جذب گازهای اسیدی گوناگون انتخاب یک ترکیب مناسب از این مواد در فرایند تصفیه گاز طبیعی مورد مطالعه قرار گرفته و در دما و فشارهای مختلف آزمایش های گوناگونی برای بدست آوردن مدل ترمودینامیکی مناسب جهت تخمین بهتر دادهای آزمایشگاهی انجام شده است که به خاطر تجزیه یونی این مخلوط ها مدل هایی که از روش ضریب اکتیویته استفاده کرده اند جواب دقیق تری را پیش بینی کرده اند. به طور معمول در این مدل ها برای پیش بینی برهمکنش های برد بلند از روش پیتزر_دبای_هوکل و برای نیروهای برد کوتاه از معادلات مختلفی استفاده شده است. در این مقاله با مطالعه دادهای آزمایشگاهی و محاسباتی مقایسه ای بین حلال های مختلف و مدل های ترمودینامیکی متناظر بر آنها در جهت انتخاب حلال و مدل مناسب انجام شده است.