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Effect of Carbon Dioxide Loading on the Solubility of Nitrous Oxide in Aqueous Solutions of 2-(*tert*-Butylamino)ethanol

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The physical solubility of nitrous oxide was measured in aqueous solutions of 2-(*tert*-butylamino)ethanol. This amine is considered to be sterically hindered and is a candidate chemical absorbent for the selective absorption of hydrogen sulfide in the presence of carbon dioxide. Measurements were made for amine concentrations up to 30 mass % over the temperature range 25 °C to 40 °C. The effect of carbon dioxide loading up to 0.90 mol of CO_2/mole of amine on the nitrous oxide solubility was also investigated. The data obtained in this work may be used to estimate the physical solubility of carbon dioxide in these amine solutions through use of the nitrous oxide analogy method.

Introduction

Aqueous amine solutions are used extensively in the natural gas industry to absorb acid gases such as hydrogen sulfide and carbon dioxide. In general, the H_2S concentration must be reduced to a very low level such as 3 ppm, since this gas is highly toxic and corrosive. On the other hand, the amount of CO_2 to be removed will depend on the end use of the natural gas. For applications where selective absorption of H_2S is desired, tertiary amines are often used, since these amines cannot form carbamates as is the case with primary and secondary amines and the chemical kinetics of the CO_2/tertiary amine reaction is much slower than that for the CO_2 reaction with primary or secondary amines. Sterically hindered primary and secondary amines are alternatives for selective H_2S absorption, since severely hindered amines do not form stable carbamates and have slower kinetics for the CO_2/amine reaction. The stoichiometry for the reaction for severely hindered amines with CO_2 is that 1 mol of CO_2 reacts with 1 mol of amine, as for tertiary amines. For the commonly used primary and secondary amines (that form carbamates), 2 mol of amine are needed per mole of CO_2.

In this work, we have measured the physical solubility of nitrous oxide in aqueous solutions of a severely hindered amine, 2-(*tert*-butylamino)ethanol (TBAE). Measurements of nitrous oxide solubility were made for unloaded and for CO_2-loaded TBAE solutions. TBAE may be an alternative to the use of a tertiary amine such as methyldiethanolamine for selective absorption of H_2S in the presence of CO_2. The physical solubility of CO_2 is a key physicochemical property needed for modeling mass transfer rates. Since CO_2 reacts in the amine solution, the physical solubility of CO_2 cannot be measured directly. Measurements with N_2O can be used to estimate the CO_2 physical solubility through the nitrous oxide analogy method first proposed by Clark.[1]

The experimental results obtained in this work are reported in terms of Henry's law, $p_A = H_A c_A$, which states that the partial pressure of a gas is proportional to the concentration of that gas dissolved in solution at equilibrium. This relation is only valid for sparingly soluble gases at relatively low pressures, as is the case for N_2O solubility in aqueous alkanolamine solutions.

Experimental Apparatus and Procedure

The apparatus and procedure used in this work were similar to those previously described by Rinker and Sandall.[2] The main part of the apparatus consisted of a cylindrical 1-L Zipperclave reactor with an air driven magnetically coupled stirrer on the top, as schematically shown in Figure 1. An internal heating coil as well as external heating jackets were used to adjust and maintain the desired temperature. Additionally, two external gas tanks were used to store a known volume of CO_2 and N_2O, respectively. The volume of the tanks and the reactor was determined by measuring the mass of water needed to fill the volume. The temperature inside the absorption chamber and inside each gas tank was measured by thermocouples with an accuracy of 0.1 K, and the pressure, by pressure transducers with an accuracy of 0.14 kPa.

At the beginning of each experiment, a weighed quantity of approximately 400 g of amine solution was injected into the absorption chamber. The reactor was then sealed and adjusted to the desired temperature, and a vacuum was applied. To degas the solvent, the liquid was stirred under vacuum for several minutes. After the vacuum pump was shut off, the system reached vapor−liquid equilibrium and the pressure was recorded at this point as the vapor pressure, p_v, of the solvent. CO_2 was then allowed to flow into the absorption chamber. The amount of injected CO_2, n_t, was determined by measuring temperature and pressure in the external CO_2 storage tank before (1) and after (2) the gas transfer, taking into consideration the nonideality of CO_2:

$$n_t = \left(\frac{p_1}{Z_1 T_1} - \frac{p_2}{Z_2 T_2}\right)\frac{V_{GT}}{R} \tag{1}$$

V_{GT} is the volume of the CO_2 storage tank, and Z_1 and Z_2 are the compressibility factors. The system reached the simultaneous equilibrium of the CO_2−amine reaction and physical dissolution while stirring for about 60 min. The final pressure, p_f, was measured at this point to determine the CO_2 equilibrium partial pressure and the overall CO_2

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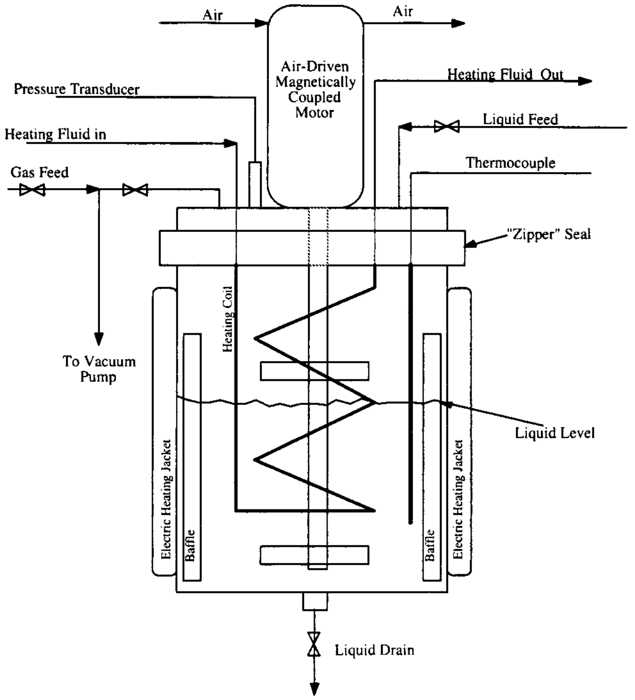

Figure 1. Modified Zipperclave reactor.

loading of the amine solution from the difference in transferred, n_t, and remaining moles of CO_2, n_r:

$$n_r = \left(\frac{p_f}{Z_f} - \frac{p_v}{Z_v}\right)\frac{V_G}{RT} \tag{2}$$

V_G is the gas phase volume in the absorption chamber. Z_v is the compressibility factor of the vapor, and Z_f, that of the final gas mixture in the equilibrium cell, which consisted mainly of water and CO_2. All compressibility factors were determined according to the Redlich−Kwong equation for pure and mixed solvents as given by Model and Reid.[3] The procedure was repeated several times to achieve the desired CO_2 loading, which was calculated by

$$L = \frac{\sum_i (n_t)_i - n_r}{n_{TBAE}} \tag{3}$$

where n_{TBAE} is the moles of TBAE in the liquid.

The N_2O solubility in the CO_2-loaded solution was then measured by adding N_2O into the chamber from the N_2O storage tank and determining the transferred and dissolved moles as well as the N_2O partial pressure in the same way as described for CO_2. Henry's constant is then calculated by the equation

$$H_{N_2O} = \frac{(p_{f,N_2O} - p_{f,CO_2})V_l}{n_{t,N_2O} - n_{r,N_2O}} \tag{4}$$

The density of the aqueous TBAE solution as a function of temperature and concentration, which was needed to determine the liquid volume, V_l, in the equilibrium cell, was measured in a previous work.[4] The quantity of injected N_2O was chosen so as to have a final partial pressure of N_2O close to 1 atm.

A series of preliminary measurements was performed in order to investigate the effect of interactions between physically dissolved N_2O and CO_2. Since the amine−CO_2 reaction is reversible, a small amount of CO_2 remained dissolved in the solution in physical equilibrium with the partial pressure in the gas phase. Through interactions between CO_2 and N_2O molecules after introducing N_2O, some CO_2 could degas, and the measurements of the N_2O partial pressure would be affected. To experimentally confirm that this effect was not significant, different quantities of N_2O were added to amine solutions at the same CO_2 loading. The results for H_{N_2O} thus obtained scattered only within the range of the measuring error. Hence, these interactions could be neglected.

Table 1. Henry's Constants for N_2O in Water (MPa m^3/kmol)

t/°C	this work	Rinker and Sandall[5]	Versteeg and van Swaaij[6]
25	4.314	4.116	4.011
33	4.975	4.982	4.900
40	5.900	5.841	5.791

Table 2. Henry's Constants for N_2O in Unloaded TBAE Solutions

TBAE conc/mass %	t/°C	H_{N_2O}/ MPa $m^3 \cdot kmol^{-1}$	standard deviation/ MPa $m^3 \cdot kmol^{-1}$
10	25	4.357	0.012
	33	5.244	0.045
	40	5.952	0.046
20	25	4.634	0.011
	33	5.421	0.028
	40	5.759	0.114
30	25	4.616	0.032
	33	4.896	0.002
	40	5.390	0.044

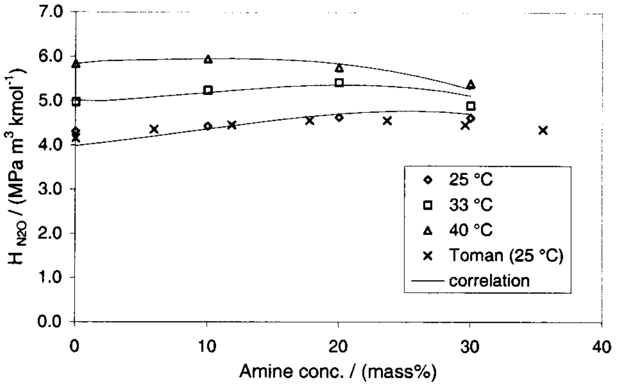

Figure 2. Henry's constants for N_2O in unloaded TBAE solutions.

The TBAE used in this investigation was obtained from Aldrich Chemicals with a stated minimum purity of 99%. The N_2O and CO_2 gases of bone-dry grade were delivered by Puritan Bennett and were of purity greater than 99.8%. Deionized water was used in preparing the amine solutions.

Results and Correlation

A. N_2O Solubility in Unloaded TBAE Solutions. To test the accuracy of the measuring method, the solubility of nitrous oxide in pure water was measured. The results are shown in Table 1 along with data found in the literature. The values are in good agreement with an average deviation of 1.9% from the values reported by Rinker and Sandall[5] and 3.5% from the values reported by Versteeg and van Swaaij.[6]

The Henry's constants for N_2O in unloaded TBAE solutions as measured in this work are listed in Table 2 and plotted in Figure 2 as a function of amine concentration. For comparison, N_2O solubility data at 25 °C as reported by Toman and Rochelle[7] are included in Figure 2 and were found to be in good agreement with the experimental results. Each value reported in Table 2 is the average of at least two measurements with the standard deviation listed in the table. The standard deviation between individual experimental runs indicates that the error is between 1 and 3%, while an estimate of the maximum experimental error is approximately between 7 and 10%.

Recently, Li and Mather[8] proposed a theoretical model to correlate N_2O solubility data in aqueous amine solutions, which is based on the extended scaled-particle theory by Hu et al.[9] Rinker and Sandall[2] applied the Li−Mather model to successfully correlate N_2O solubilities in unloaded aqueous DEA and MDEA solutions and to predict the solubility in aqueous blends of these amines. The model working equations are as follows:

$$\ln(H_1) = \frac{1}{kT}\cdot\frac{\partial A_{\mathrm{h}}}{\partial N_1} + \frac{1}{kT}\cdot\frac{\partial A_{\mathrm{s}}}{\partial N_1} + \ln(kT\sum_j r_j) - \ln\left(\rho\sum_j \frac{w_j}{M_j}\right) \tag{5}$$

and

$$\frac{1}{kT}\cdot\frac{\partial A_{\mathrm{h}}}{\partial N_1} = -\ln(1-y_3) + \left[\frac{y_0}{1-y_3} + \frac{3y_1y_2}{(1-y_3)^2} + \frac{3y_2^3}{(1-y_3)^3} - \frac{y_3y_2^3}{(1-y_3)^3}\right]\sigma_1^3 + \frac{3y_2\sigma_1}{1-y_3} + \frac{3y_1\sigma_1^2}{1-y_3} + \frac{9y_2^2\sigma_1^2}{2(1-y_3)^2} + 3\left(\frac{y_2\sigma_1}{y_3}\right)^2\left[\ln(1-y_3) + \frac{y_3}{1-y_3} - \frac{y_3^2}{2(1-y_3)^2}\right] - \left(\frac{y_2\sigma_1}{y_3}\right)^3\left[2\ln(1-y_3) + \frac{y_3(2-y_3)}{1-y_3}\right] \tag{6}$$

where

$$y_n = \frac{\pi}{6}\sum_j \rho_j\sigma_j^n \tag{7}$$

and

$$\frac{1}{kT}\cdot\frac{\partial A_{\mathrm{s}}}{\partial N_1} = -5.14025\frac{\pi}{kT}\sum_j r_j\epsilon_{1j}\sigma_{1j}^3 \tag{8}$$

where

$$\sigma_{1j} = \frac{1}{2}(\sigma_1 + \sigma_j) \tag{9}$$

The parameters used in these equations are the hard-sphere diameters, σ_i, for the solute and for each of the liquid solvent species, water, and TBAE, and the interaction energy parameters between solute and solvent species, ϵ_{ij}.

The application of the correlation methods includes the estimation of the hard-sphere diameter of TBAE, σ_{TBAE}, and of the energy parameter $\epsilon_{\mathrm{N_2O-TBAE}}$ that characterizes the interactions between the solute N_2O and the amine. Values of the hard-sphere diameters of N_2O and H_2O, $\sigma_{\mathrm{N_2O}}$ and $\sigma_{\mathrm{H_2O}}$, as well as the value of $\epsilon_{\mathrm{N_2O-H_2O}}$ are reported by Li and Mather.[8] Following the method for estimating σ_{TBAE} that was proposed by Li and Mather, solubility measurements in pure amine solvents would have to be conducted. Since TBAE is a solid over the temperature range studied, the hard-sphere diameter could not be determined experimentally in this work. Therefore, the hard-sphere diameter for TBAE was estimated following the Stiel and Thodos method given in Reid and Sherwood.[10] The value of $\epsilon_{\mathrm{N_2O-TBAE}}$ was then determined by a least-squares fit of the N_2O solubility data obtained in this work at each temperature according to the model equations. Both results are given in Table 3, and the best fits are shown in Figure 2. The hard-sphere diameters of all species were held constant with temperature in the fitting procedure, as was proposed by Li and Mather. The average deviation of the fitted curves from the experimental data is 2.0%.

Table 3. Hard-Sphere Diameter and Energy Parameter Estimates from N_2O Solubility Data Fitting

hard-sphere diameter		energy parameter	
molecule	σ/nm	t/°C	$(\epsilon_{\mathrm{N_2O-TBAE}}/k)$/K
TBAE	0.615	25	441.06
		33	448.90
		40	457.87

Table 4. Henry's Constants for N_2O in CO_2-Loaded TBAE Solutions

	10 wt %		20 wt %		30 wt %	
t/°C	$L_{\mathrm{CO_2}}$[a]	$H_{\mathrm{N_2O-TBAE}}$/MPa m^3·kmol^{-1}	$L_{\mathrm{CO_2}}$[a]	$H_{\mathrm{N_2O-TBAE}}$/MPa m^3·kmol^{-1}	$L_{\mathrm{CO_2}}$[a]	$H_{\mathrm{N_2O-TBAE}}$/MPa m^3·kmol^{-1}
25	0	4.428	0	4.629	0	4.612
	0.15	4.667	0.15	5.256	0.14	5.466
	0.29	4.589	0.29	5.533	0.28	6.473
	0.49	5.244	0.41	6.073	0.42	6.893
	0.57	5.114	0.62	5.985	0.56	7.644
	0.67	5.121	0.87	5.656		
	0.9	5.048				
33	0	5.238	0	5.416	0	4.887
	0.16	5.629	0.14	6.165	0.27	6.786
	0.30	5.570	0.41	6.750	0.55	8.298
	0.36	5.718	0.64	7.094		
	0.49	6.165				
	0.53	5.927				
	0.61	6.241				
40	0	5.947	0	5.754	0	5.384
	0.28	6.482	0.29	6.562	0.15	6.051
	0.37	6.414	0.41	6.886	0.28	6.727
	0.61	7.009	0.68	7.523	0.43	7.274
	0.71	7.096			0.57	8.315

[a] mol of CO_2/mol of TBAE.

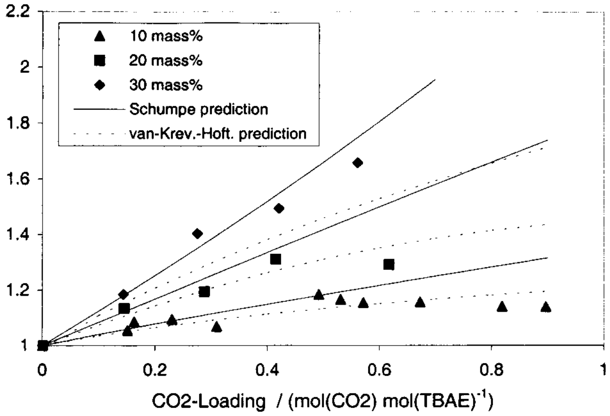

Figure 3. $H_{\mathrm{N_2O}}$ in CO_2-loaded TBAE solutions at 25 °C.

B. N_2O Solubility in CO_2-Loaded TBAE Solutions. The experimental Henry's constants for N_2O in CO_2-loaded solutions as measured in this work are listed in Table 4 and shown in Figures 3−5 as a function of the degree of CO_2 loading related to the corresponding value in unloaded amine solution at the same temperature and initial amine concentration.

The gas solubility depends on the solvent composition and thus on the degree of CO_2 loading. When CO_2 reacts

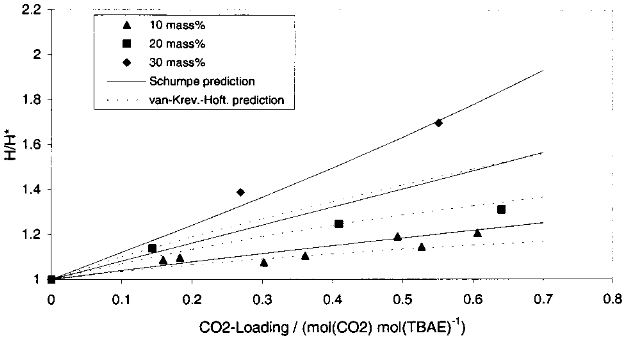

Figure 4. H_{N_2O} in CO_2-loaded TBAE solutions at 33 °C.

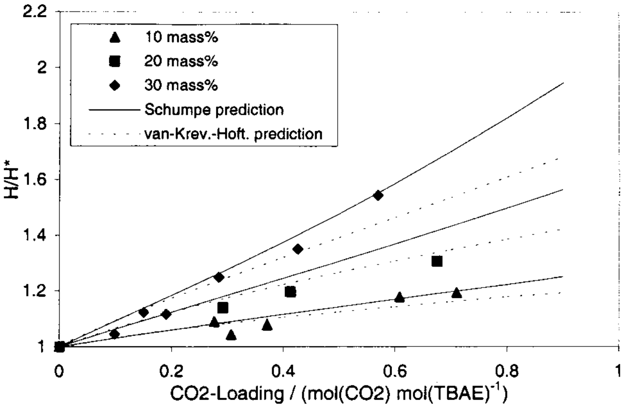

Figure 5. H_{N_2O} in CO_2-loaded TBAE solutions at 40 °C.

with TBAE, the amine concentration decreases and protonated amine and bicarbonate ions are formed. An increased ionic strength of solution is generally assumed to cause a solubility reduction, as is the case with the amine solution studied in this work. Van Krevelen and Hoftijzer suggested the following empirical equation to relate the gas solubility to ionic strength, I, as given by Danckwerts[11]

$$\log\left(\frac{H}{H^*}\right) = \sum_j (k'_+ + k'_- + k'_g)_j I \qquad (10)$$

The parameters k'_+, k'_-, and k'_g (van-Krevelen coefficients) are specific to the cations, the anions, and the gas, respectively, and are assumed to be ion concentration independent. The superscript * refers to solubility in unloaded solution.

A modified correlation was recently proposed by Schumpe:[12]

$$\log\left(\frac{H}{H^*}\right) = \sum_i h_i I_i + \sum_i h_g c_i \qquad (11)$$

The variables h_i and h_g are parameters specific to each solvent species and the gas as introduced by Schumpe,[12] and I_i is the partial ionic strength of each ion, given as

$$I_i = \frac{1}{2} c_i z_i^2 \qquad (12)$$

where c_i is the ion concentration and z_i the ion charge.

For applying the model equations, the ionic strength of the solution as a function of the composition must be calculated. As shown by Kraehnert[4] and Rinker and Sandall,[5] essentially the following reactions are involved in the CO_2 absorption process into an aqueous solution of TBAE, a sterically hindered secondary amine (R_2NH).

Main Reaction

$$R_2NH + CO_2 + H_2O \overset{K_1}{\longleftrightarrow} HCO_3^- + R_2NH_2^+ \qquad (13)$$

Side Reactions

$$CO_2 + OH^- \overset{K_2}{\longleftrightarrow} HCO_3^- \qquad (14)$$

$$HCO_3^- + OH^- \overset{K_3}{\longleftrightarrow} CO_3^{2-} + H_2O \qquad (15)$$

$$R_2NH_2^+ + OH^- \overset{K_4}{\longleftrightarrow} R_2NH + H_2O \qquad (16)$$

$$2H_2O \overset{K_5}{\longleftrightarrow} OH^- + H_3O^+ \qquad (17)$$

The liquid composition can be calculated as a function of the CO_2 loading, the total concentration of TBAE, and the assumption that all reactions are at equilibrium. Table 5 gives the equations for all equilibrium constants needed as taken from refs 5 and 7.

Figure 6 shows the N_2O solubility data in CO_2-loaded solution as measured versus calculated ionic strength. From this plot an overall experimental van-Krevelen constant k' of 0.098 ± 0.0087 L·mol^{-1} is obtained, which was found to be independent of temperature and initial amine concentration, as was expected. The 95% confidence limits of the mean value for k' are included in Figure 6 as dashed lines. The result deviates somewhat from the mean value for k' of 0.075 L·mol^{-1} as reported by Toman and Rochelle,[7] who conducted similar measurements.

The experimentally determined van-Krevelen constant can now be used to predict the solubility according to the transformed van-Krevelen−Hoftijzer equation and the ionic strength as calculated in dependence on CO_2 loading. The results are included as solubility predictions in Figures 3−5.

In addition to the solubility measurements in CO_2-loaded TBAE solutions, a series of measurements was conducted to determine the unknown van-Krevelen coefficient for protonated TBAE. As previously proposed by Browning and Weiland,[13] the production of $R_2NH_2^+$ ions in amine solutions can be simulated by partial protonation of unloaded TBAE solution with hydrochloric acid. The parameter k'_+ can then be obtained by N_2O solubility measurements as a function of the degree of protonation by applying the van-Krevelen−Hoftijzer equation, eq 10, to this simplified system. The solubility data obtained are given in Figure 7 as a function of the total ionic strength. From the slope of the plot and the known van-Krevelen coefficient for the Cl^- ion of 0.021 L·mol^{-1} (Danckwerts[11]), the value for $k'_{R_2NH_2^+}$ was determined. As expected, the parameter is independent of initial amine concentration. The result is listed in Table 6 along with values of other amines as reported by Browning and Weiland[13] and was found to be in reasonable agreement with those values with respect to molecular weight and structure.

However, using this value of $k'_{R_2NH_2^+}$ and the van Krevelen coefficients for all ions present in solution as given by Danckwerts[11] to estimate the N_2O solubility in CO_2-loaded solvents leads to an overall van Krevelen coefficient k of 0.139, as shown in Table 7. This is significantly higher than the value experimentally determined as $k = 0.098$.

In an analogous way as described for the van-Krevelen−Hoftijzer model, the solubility measurements in partially HCl-protonated TBAE solutions were used to estimate the parameter $h_{R_2NH_2^+}$ for protonated amine according to the

Table 5. Equilibrium Constant Correlations (T in K)

K_i	units	correlation	temp range	ref
K_5	$mol^2 \cdot cm^{-6}$	$\log(K_5) = 8909.483 - 142613.6/T - 4229.195 \log(T) + 9.7384T - 0.0129683T^2 + (1.15068 \times 10^{-5})T^3 - (4.602 \times 10^{-9})T^4$	293−573 K	5
K_2K_5	$mol \cdot cm^{-3}$	$\log(K_2K_5) = 179.648 + 0.019244T - 67.341 \log(T) - 7495.441/T$	293−573 K	5
K_3K_5	$mol \cdot cm^{-3}$	$\log(K_3K_5) = -10.35$; $\Delta H_R = 18.3$ MJ·mol^{-1}	at 25 °C	7
K_4K_5	$mol \cdot cm^{-3}$	10−20 wt %: $\log(K_4K_5) = -10.65$ s 30 wt %: $\log(K_4K_5) = -10.35$ $\Delta H_R = 83.2$ MJ·mol^{-1}	at 25 °C	7

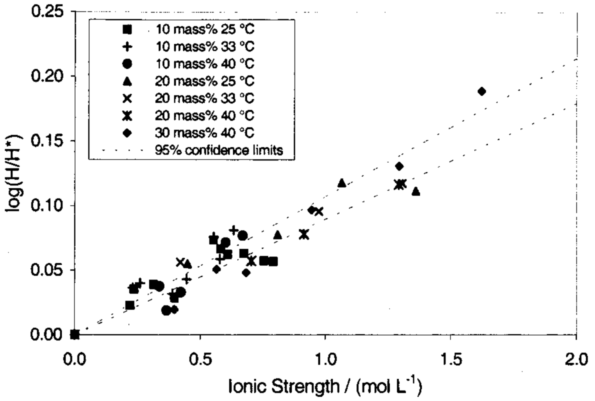

Figure 6. H_{N_2O} in CO_2-loaded TBAE solutions.

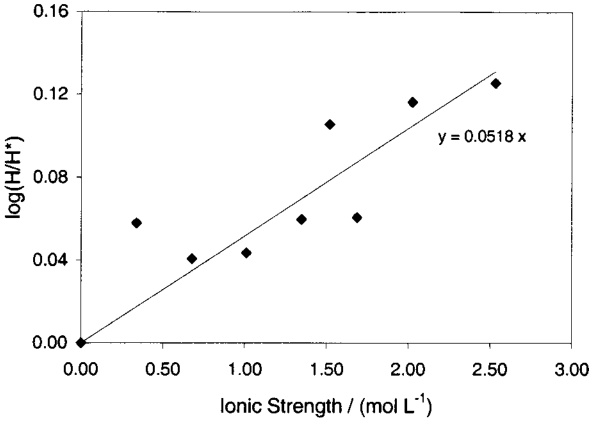

Figure 7. H_{N_2O} in partially protonated TBAE solutions.

Table 6. Van-Krevelen Coefficients for Protonated Amines

ion	k_+/L·mol^{-1}	ion	k_+/L·mol^{-1}
protonated MEA	0.055[a]	protonated MDEA	0.041[a]
protonated DEA	0.047[a]	protonated TBAE	0.031

[a] Taken from ref 13.

correlation proposed by Schumpe. The parameters needed for Cl^- ions of 0.0334 L·mol^{-1} and for N_2O at 25 °C of −0.0110 L·mol^{-1} are reported by Schumpe. A value for $h_{R_2NH_2^+}$ of 0.0404 L·mol^{-1} was thus obtained. The result was then used to correlate the N_2O solubility in CO_2-loaded TBAE solution as shown in Figures 3−5. The parameters h_i used for each ion present in the solvent are listed in Table 8 as taken from Schumpe. The model constant for nitrous oxide h_g depends slightly on temperature. The value at 25 °C is given in the literature.[12] At 33 °C and 40 °C, h_g was adjusted by a best fit of the experimental solubility data in CO_2-loaded solution.

Table 7. Estimation of the Van-Krevelen Coefficient in CO_2-Loaded Solution

ion/gas	k_i/L·mol^{-1}
H^+	0.0[a]
OH^-	0.066[a]
HCO_3^-	0.021[a]
CO_3^{2-}	0.021[a]
$R_2NH_2^+$	0.031
N_2O	0.0[a]
$\sum k_i$	0.139

[a] Taken from ref 11.

Table 8. Schumpe Model Parameters

ion	h_i/L·mol^{-1}	gas	h_g/L·mol^{-1}
H^+	0.0[a]	N_2O at 25 °C	−0.011[a]
OH^-	0.0756[a]	N_2O at 33 °C	−0.016
HCO_3^-	0.1372[a]	N_2O at 40 °C	−0.025
CO_3^{2-}	0.1666[a]		
$R_2NH_2^+$	0.0404		

[a] Taken from ref 12.

Table 9. Deviation between Experimental Data and Correlation

temp	model	10 mass %	20 mass %	30 mass %
25 °C	Van-Krevelen−Hoftijzer	2.2%	2.2%	9.1%
	Schumpe	3.3%	5.0%	3.3%
33 °C	Van-Krevelen−Hoftijzer	2.2%	1.5%	8.2%
	Schumpe	3.3%	8.1%	2.5%
40 °C	Van-Krevelen−Hoftijzer	2.1%	2.0%	2.7%
	Schumpe	1.8%	5.4%	2.7%

Table 9 shows the deviation of the experimental results from both correlations. For an initial TBAE concentration of 10 mass%, both models predict the nitrous oxide solubility fairly well. However, at 20 mass % initial TBAE concentration, the Schumpe model prediction deviates strongly from the measured values, whereas the data calculated using the van-Krevelen−Hoftijzer method are in acceptable agreement. The opposite is found for 30 mass %. One can conclude that the van-Krevelen−Hoftijzer model is applicable in the range of low ionic strengths of solution. For higher ionic strengths, the Schumpe model seems to provide a better estimation of Henry's constant.

Conclusion

The physical solubility of N_2O in unloaded and in CO_2-loaded TBAE solutions was measured as a function of the degree of CO_2 loading. Henry's constant for N_2O in unloaded solutions was correlated according to a method proposed by Li and Mather.[8] The experimental results were found to fit the correlated curves within 2% deviation in the average.

The N_2O solubility in CO_2-loaded TBAE solution decreases with increasing CO_2 loading. It was shown that this behavior can be explained by the increased ionic strength of solution by correlating the data according to the van-Krevelen–Hoftijzer equation as given in Danckwerts[11] and an empirical model proposed by Schumpe.[12] In addition, the van Krevelen coefficient and the Schumpe model parameter for protonated TBAE were determined by conducting solubility measurements on TBAE solutions partially neutralized with hydrochloric acid. The N_2O solubility can be translated into CO_2 solubility by application of the N_2O analogy.

Nomenclature

Latin Letters

A = Helmholtz energy, J
c = concentration, $mol \cdot L^{-1}$
H = Henry's constant, $MPa \cdot m^3 \cdot kmol^{-1}$
H' = Henry's constant, MPa
h = Schumpe model parameter, $L \cdot mol^{-1}$
I = ionic strength, $mol \cdot L^{-1}$
K = equilibrium constants
k = Boltzmann constant, $1.381 \times 10^{-23}\ J \cdot K^{-1}$
k' = van-Krevelen coefficients, $L \cdot mol^{-1}$
L = CO_2 loading, mol of $CO_2 \cdot$(mol of TBAE)$^{-1}$
M = molecular weight, $g \cdot mol^{-1}$
N = average number of molecules
N_0 = Avogadro's number
n = mole number, mol
p = pressure, MPa
R = general gas constant, $8.314 \times 10^{-3}\ MPa \cdot m^3 \cdot kmol^{-1} \cdot K^{-1}$
r = number density of molecules, m^{-3}
T = temperature, °C
V = volume, cm^3
w = mass fraction
Z = compressibility factor
z = ion charge

Greek Letters

ϵ = energy parameter
ρ = solvent density, $g \cdot cm^{-3}$
σ = hard-sphere diameter, m

Subscripts

f = final
g, G = gas phase
GT = gas tank
h = denotes change from ideal gas system to hard-sphere system
j = solvent species (H_2O, TBAE)
l = liquid phase
r = remaining in gas phase
s = denotes change from hard-sphere system to real liquid system
t = transferred
v = denotes equilibrium vapor pressure

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