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Solubility of CO_2 in Alcohols, Glycols, Ethers, and Ketones at High Pressures from (288.15 to 318.15) K

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ABSTRACT: The constant-volume method is used to determine the solubility of CO_2 in methanol, ethanol, *n*-propanol, *n*-butanol, *n*-propanol, ethylene glycol, propylene glycol, acetone, 2-butanone, ethylene glycol monomethyl ether, and ethylene glycol monoethyl ether under the pressure of 6 MPa and the temperature variations from (288.15 to 318.15) K in this paper. It is found by contrast that ketones have a greater ability to dissolve CO_2 than alcohols, ethers, and glycols, which also indicate that both the carbonyl group and the ether bond in solvents can promote the CO_2 absorption, but hydroxyl group will inhibit the CO_2 absorption.

1. INTRODUCTION

Global warming and climate change caused by greenhouse gases (GHGs) have become the critical issues of global concern recent years. The CO_2 emissions produced by the fossil fuel powered plants and energy production facilities account for over 80 % of GHGs. With stricter and stricter restrictions on the CO_2 emissions, CO_2 capture from fuel gas using the solid-based process, membrane-based process, and solvent-based process is of primary importance. Compared with other methods, the solvent-based process is a future possibility in developing an economically feasible CO_2 capture process. In general, the solvent-based process can be broadly classified as chemical solvents, physical solvents, and mixed chemical/physical solvents. The most typical and economical solvent-based processes in industry are still based on physical solvents, such as methanol,[1−4] propylene carbonate,[5,6] and poly(ethylene glycol) dimethyl ether.[7,8] As we know, the criteria of a feasible physical-solvent process include: low vapor pressure to prevent solvent loss, high selectivity for CO_2, low viscosity, thermal and chemical stability, and noncorrosive behavior.[9−11]

This study mainly focuses on the research of physical solvents for CO_2 capture. The vapor−liquid equilibrium (VLE) experiments are performed at high pressures up to 6 MPa, over a wide range of temperatures from (288.15 to 318.15) K. New experimental data of CO_2 solubility in alcohols, glycols, ethers, and ketones are presented to illustrate the functional group effect on the solvent ability to dissolve CO_2.

2. EXPERIMENTAL SECTION

2.1. Materials. CO_2 with a volume fraction of 0.9999 was supplied by BeiWen Gas in Beijing. The solvents (methanol, ethanol, *n*-propanol, *n*-butanol, *n*-pentanol, ethylene glycol, propylene glycol, acetone, 2-butanone, ethylene glycol monomethyl ether, and ethylene glycol monoethyl ether) were all obtained from Aladdin-Reagent Company in Shanghai and with the same mass fraction of 0.999. All components were used without further purification.

2.2. Apparatus and Experimental Procedures. The apparatus used in this work was based on the constant-volume method and reported in a previous work.[12] Experiments were carried out respectively at 288.15 K, 298.15 K, 308.15 K, and 318.15 K in the equilibrium cell. When the pressure and temperature were constant in the equilibrium cell, the system was considered to be at equilibrium. Then, according to the data of equilibrium pressure, the mole fraction of CO_2 in liquid phase at this pressure and temperature can be calculated from the material balance. The data calculating process is also described in detail in the literature.[12]

Table 1. Molecular Structure and Functional Group for Methanol, Ethanol, *n*-Propanol, *n*-Butanol, *n*-Pentanol, Ethylene Glycol, Propylene Glycol, Acetone, 2-Butanone, Ethylene Glycol Monomethyl Ether, and Ethylene Glycol Monoethyl Ether

compound	molecular structure	functional group
methanol	CH_3OH	OH
ethanol	CH_3CH_2OH	OH
n-propanol	$CH_3CH_2CH_2OH$	OH
n-butanol	$CH_3CH_2CH_2CH_2OH$	OH
n-pentanol	$CH_3CH_2CH_2CH_2CHOH$	OH
ethylene glycol	$HOCH_2CH_2OH$	OH, OH
propylene glycol	$CH_3CH(OH)CH_2OH$	OH, OH
acetone	CH_3COCH_3	C=O
2-butanone	$CH_3COCH_2CH_3$	C=O
ethylene glycol monomethyl ether	$CH_3OCH_2CH_2OH$	−O−, OH
ethylene glycol monoethyl ether	$CH_3CH_2OCH_2CH_2OH$	−O−, OH

3. RESULTS AND DISCUSSION

3.1. Pure Compound Properties. Experimental results for the phase equilibrium of CO_2 in methanol, ethanol, *n*-propanol,

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Table 2. Mole Fraction (x_i), Partial Pressure (p) of CO_2 at Equilibrium, and Uncertainties (δ_i) of CO_2 in Methanol from 288.15 K to 318.15 K

p/MPa	x_i	δ_i	p/MPa	x_i	δ_i
		T = 288.15 K			
0.1324	0.0114	0.0008	1.7874	0.1543	0.0010
0.3269	0.0282	0.0009	2.1351	0.1843	0.0008
0.5038	0.0435	0.0011	2.5806	0.2228	0.0009
0.8643	0.0746	0.0009	2.9347	0.2534	0.0010
1.1620	0.1003	0.0009	3.0854	0.2664	0.0011
		T = 298.15 K			
0.2213	0.0163	0.0008	1.9685	0.1445	0.0010
0.3998	0.0294	0.0009	2.3634	0.1735	0.0012
0.5446	0.0400	0.0011	2.7921	0.2050	0.0013
0.7742	0.0568	0.0010	3.1538	0.2315	0.0009
0.9623	0.0706	0.0013	3.6043	0.2646	0.0009
1.2869	0.0945	0.0011	3.9219	0.2879	0.0007
1.5535	0.1141	0.0012	4.3365	0.3185	0.0012
		T = 308.15 K			
0.2365	0.0146	0.0007	2.6742	0.1651	0.0004
0.4219	0.0260	0.0006	2.9446	0.1818	0.0007
0.6043	0.0373	0.0011	3.2998	0.2037	0.0006
0.8538	0.0527	0.0004	3.5213	0.2174	0.0009
1.0792	0.0666	0.0007	3.8213	0.2359	0.0007
1.3634	0.0842	0.0008	4.0065	0.2474	0.0006
1.5685	0.0968	0.0010	4.3878	0.2709	0.0008
1.7017	0.1051	0.0009	4.6920	0.2897	0.0010
1.9535	0.1206	0.0008	4.9101	0.3031	0.0011
2.1869	0.1350	0.0010	5.0412	0.3112	0.0013
2.3623	0.1458	0.0006			
		T = 318.15 K			
0.1236	0.0062	0.0011	2.9274	0.1471	0.0011
0.3421	0.0172	0.0009	3.2446	0.1631	0.0013
0.5604	0.0282	0.0012	3.5199	0.1769	0.0012
0.7538	0.0379	0.0009	3.7213	0.1870	0.0013
1.1279	0.0567	0.0011	3.9821	0.2001	0.0011
1.4363	0.0722	0.0009	4.2265	0.2124	0.0009
1.6885	0.0849	0.0011	4.5387	0.2281	0.0008
1.9701	0.0990	0.0013	4.8692	0.2447	0.0007
2.2535	0.1132	0.0008	5.0410	0.2533	0.0006
2.4986	0.1256	0.0010	5.2712	0.2649	0.0008
2.7362	0.1375	0.0008	5.5761	0.2802	0.0011

n-butanol, *n*-pentanol, ethylene glycol, propylene glycol, acetone, 2-butanone, ethylene glycol monomethyl ether and ethylene glycol monoethyl ether at high pressure are given as below. The molecular structure and functional group for the pure alcohols, ethers, and ketones are provided in Table 1.

3.2. Results and Discussion. The temperature T, the CO_2 partial pressure p at the equilibrium state, CO_2 mole fraction x_i in the liquid phase, and the estimated uncertainties δ_i for the binary systems CO_2 + methanol, CO_2 + ethanol, CO_2 + *n*-propanol, CO_2 + *n*-butanol, CO_2 + *n*-pentanol, CO_2 + ethylene glycol, CO_2 + propylene glycol, CO_2 + acetone, CO_2 + 2-butanone, CO_2 + ethylene glycol monomethyl ether, and CO_2 + ethylene

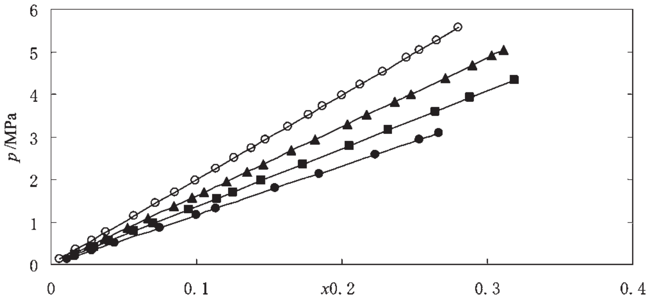

Figure 1. Vapor−liquid equilibrium of the CO_2 + methanol system in this study. x is the mole fraction of CO_2 in the liquid phase, and p is the partial pressure of CO_2 at equilibrium state: ●, 288.15 K; ■, 298.15 K; ▲, 308.15 K; ○, 318.15 K.

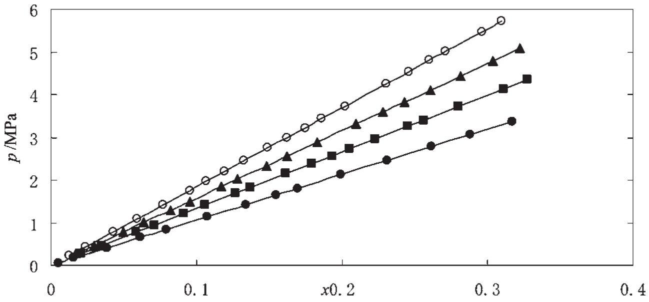

Figure 2. Vapor−liquid equilibrium of the CO_2 + ethanol system in this study. x is the mole fraction of CO_2 in the liquid phase, and p is the partial pressure of CO_2 at equilibrium state: ●, 288.15 K; ■, 298.15 K; ▲, 308.15 K; ○, 318.15 K.

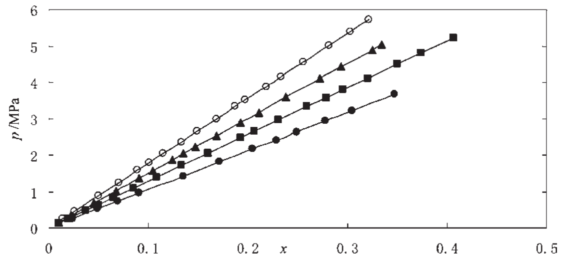

Figure 3. Vapor−liquid equilibrium of the CO_2 + *n*-propanol system in this study. x is the mole fraction of CO_2 in the liquid phase, and p is the partial pressure of CO_2 at equilibrium state: ●, 288.15 K; ■, 298.15 K; ▲, 308.15 K; ○, 318.15 K.

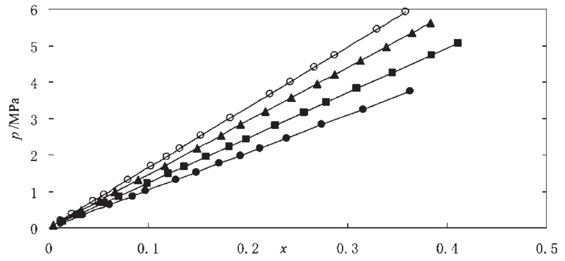

Figure 4. Vapor−liquid equilibrium of the CO_2 + *n*-butanol system in this study. x is the mole fraction of CO_2 in the liquid phase, and p is the partial pressure of CO_2 at equilibrium state: ●, 288.15 K; ■, 298.15 K; ▲, 308.15 K; ○, 318.15 K.

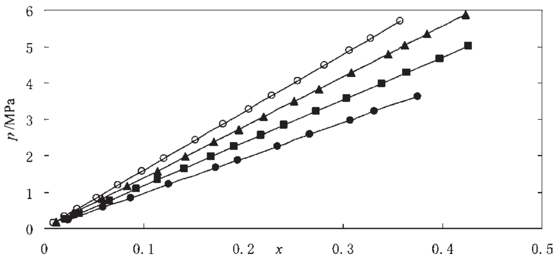

Figure 5. Vapor−liquid equilibrium of the CO_2 + *n*-pentanol system in this study. x is the mole fraction of CO_2 in the liquid phase, and p is the partial pressure of CO_2 at equilibrium state: ●, 288.15 K; ■, 298.15 K; ▲, 308.15 K; ○, 318.15 K.

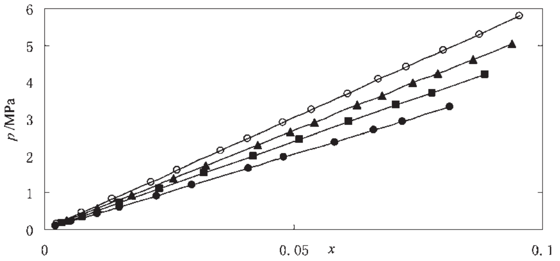

Figure 6. Vapor−liquid equilibrium of the CO_2 + ethylene glycol system in this study. x is the mole fraction of CO_2 in the liquid phase, and p is the partial pressure of CO_2 at equilibrium state: ●, 288.15 K; ■, 298.15 K; ▲, 308.15 K; ○, 318.15 K.

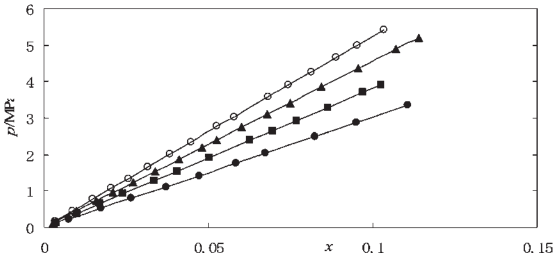

Figure 7. Vapor−liquid equilibrium of the CO_2 + propylene glycol system in this study. x is the mole fraction of CO_2 in the liquid phase, and p is the partial pressure of CO_2 at equilibrium state: ●, 288.15 K; ■, 298.15 K; ▲, 308.15 K; ○, 318.15 K.

glycol monoethyl ether are presented in Tables 2 to 12 and plotted in Figures 1 to 11. The combined standard uncertainty was used in the paper; the uncertainty of the experiment in this paper can be calculated from:

$$\frac{u(x)}{x} = \sqrt{\left(\frac{u(n_g)}{n_g}\right)^2 + \left(\frac{u(n_g + n_l)}{n_g + n_l}\right)^2} \qquad (1)$$

in which $u(n_i)$ can be estimated by:

$$\frac{u(n_i)}{n_i} = \frac{1}{R}\sqrt{\left(\frac{u(P_i)}{P_i}\right)^2 + \left(\frac{u(V_i)}{V_i}\right)^2 + \left(\frac{u(T_i)}{T_i}\right)^2} \qquad (2)$$

and $u(n_l)$ is estimated by:

$$u(n_l) = \frac{\rho}{M}u(V_l) \qquad (3)$$

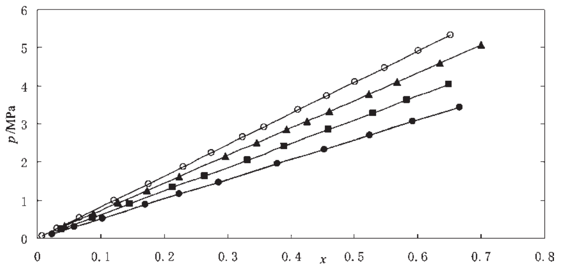

Figure 8. Vapor−liquid equilibrium of the CO_2 + acetone system in this study. x is the mole fraction of CO_2 in the liquid phase, and p is the partial pressure of CO_2 at equilibrium state: ●, 288.15 K; ■, 298.15 K; ▲, 308.15 K; ○, 318.15 K.

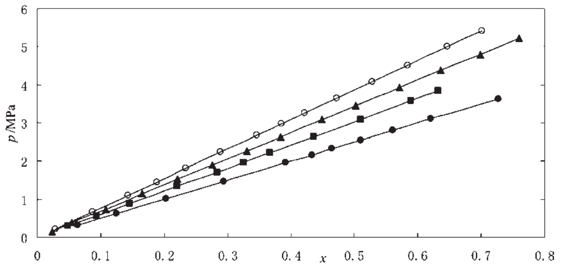

Figure 9. Vapor−liquid equilibrium of the CO_2 + 2-butanone system in this study. x is the mole fraction of CO_2 in the liquid phase, and p is the partial pressure of CO_2 at equilibrium state: ●, 288.15 K; ■, 298.15 K; ▲, 308.15 K; ○, 318.15 K.

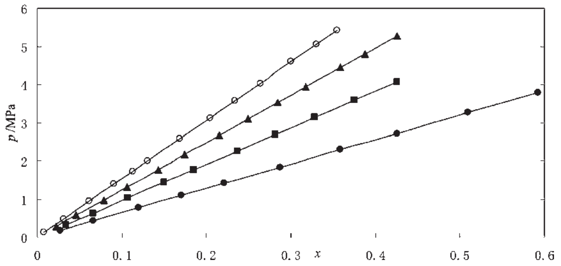

Figure 10. Vapor−liquid equilibrium of the CO_2 + ethylene glycol monomethyl ether system in this study. x is the mole fraction of CO_2 in the liquid phase, and p is the partial pressure of CO_2 at equilibrium state: ●, 288.15 K; ■, 298.15 K; ▲, 308.15 K; ○, 318.15 K.

The measurement errors of temperature, pressure, and volume are $u(T) = 0.1$ K, $u(P_i) = 0.001$ MPa, and $u(V) = 0.05$ mL. n^g is the amount of the CO_2 gas in liquid, n_l is the amount of solvent in the liquid, ρ is the density of the solvent, R is the universal gas constant, and M is the mean molecular weight of the solvent.

When the system attained equilibrium state, the absorbed amount of gas n_g is calculated from:

$$n_g = (n_1 - n_2) - n^E - n^i \qquad (4)$$

where n_1 is the amount of gas in buffer tank before the gas charging step and n_2 is the amount of gas in buffer tank after the gas-charging step. So, the difference value between n_1 and n_2 is the total amount of gas charged into equilibrium cell. n^i can be considered to be the residual amount of inert gas after the equilibrium cell being evacuated. n^E is the amount of CO_2 in the gas phase at the equilibrium state, and the amount of solvent

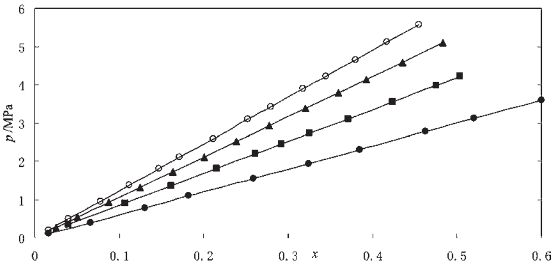

Figure 11. Vapor−liquid equilibrium of the CO_2 + ethylene glycol monoethyl ether system in this study. x is the mole fraction of CO_2 in the liquid phase, and p is the partial pressure of CO_2 at equilibrium state: ●, 288.15 K; ■, 298.15 K; ▲, 308.15 K; ○, 318.15 K.

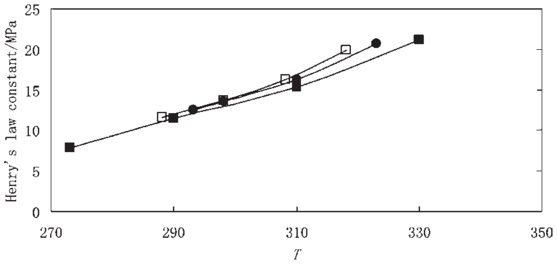

Figure 12. Henry's law constant of CO_2 in methanol from (270 to 350) K. ■, Hong and Kobayashi;[13] □, this study; ●, Secuianu et al.[14]

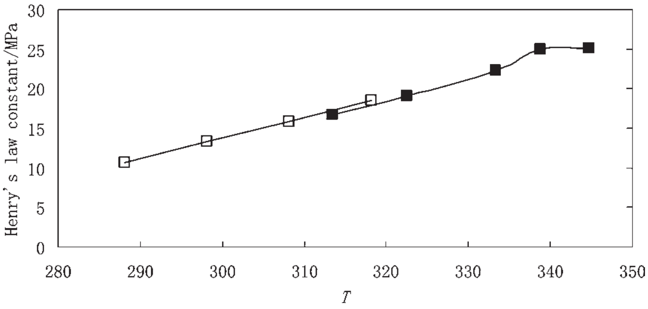

Figure 13. Henry's law constant of CO_2 in ethanol from (280 to 350) K. ■, Joung et al.;[3] □, this study.

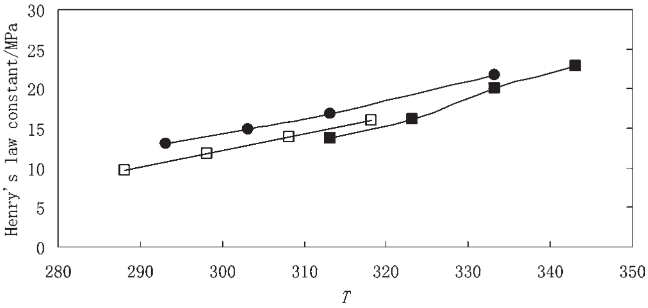

Figure 14. Henry's law constant of CO_2 in n-propanol from (280 to 350) K. ■, Jun et al.;[15] □, this study; ●, Secuianu et al.[16]

n_l added to equilibrium cell is calculated from:

$$n_l = \frac{\rho \Delta V}{M} \tag{5}$$

Table 3. Mole Fraction (x_i), Partial Pressure (p) of CO_2 at Equilibrium, and Uncertainties (δ_i) of CO_2 in Ethanol from 288.15 K to 318.15 K

p/MPa	x_i	δ_i	p/MPa	x_i	δ_i
		T = 288.15 K			
0.0580	0.0055	0.0013	1.6438	0.1545	0.0009
0.1670	0.0157	0.0012	1.8052	0.1697	0.0010
0.4130	0.0388	0.0011	2.1197	0.1992	0.0009
0.6562	0.0617	0.0012	2.4627	0.2315	0.0011
0.8461	0.0795	0.0012	2.7780	0.2611	0.0009
1.1417	0.1073	0.0011	3.0635	0.2879	0.0008
1.4235	0.1338	0.0007	3.3720	0.3169	0.0014
		T = 298.15 K			
0.2732	0.0205	0.0010	2.3846	0.1793	0.0009
0.4635	0.0349	0.0012	2.5662	0.1930	0.0012
0.7787	0.0586	0.0009	2.7320	0.2055	0.0010
0.9462	0.0712	0.0007	2.9678	0.2232	0.0009
1.2119	0.0911	0.0008	3.2584	0.2451	0.0009
1.4052	0.1057	0.0009	3.4043	0.2560	0.0013
1.6846	0.1267	0.0007	3.7219	0.2799	0.0012
1.8235	0.1371	0.0008	4.1336	0.3109	0.0011
2.1479	0.1615	0.0013	4.3579	0.3278	0.0013
		T = 308.15 K			
0.2720	0.0172	0.0006	2.5619	0.1623	0.0012
0.4630	0.0293	0.0005	2.8865	0.1829	0.0013
0.7780	0.0493	0.0009	3.3142	0.2100	0.0009
1.0027	0.0635	0.0009	3.5950	0.2278	0.0008
1.2976	0.0822	0.0013	3.8316	0.2428	0.0013
1.5052	0.0954	0.0010	4.1124	0.2606	0.0012
1.8431	0.1168	0.0012	4.4397	0.2813	0.0009
2.0235	0.1282	0.0007	4.7962	0.3039	0.0009
2.3414	0.1484	0.0011	5.0811	0.3220	0.0012
		T = 318.15 K			
0.2392	0.0130	0.0011	2.9986	0.1625	0.0011
0.4365	0.0237	0.0010	3.2274	0.1749	0.0007
0.7944	0.0430	0.0010	3.4343	0.1861	0.0009
1.0981	0.0595	0.0009	3.7329	0.2023	0.0010
1.4273	0.0773	0.0008	4.2536	0.2305	0.0009
1.757	0.0952	0.0012	4.5378	0.2459	0.0005
1.9656	0.1065	0.0011	4.7992	0.2600	0.0009
2.1961	0.1190	0.0011	5.0011	0.2710	0.0012
2.4453	0.1325	0.0012	5.4649	0.2961	0.0007
2.7528	0.1492	0.0012	5.7168	0.3098	0.0013

where ΔV is the volume of the solvent, ρ is the density of the solvent, and M is the mean molecular weight of the solvent.

The solubility of CO_2 in the solvent expressed in mole fraction is calculated from:

$$x = \frac{n_g}{n_g + n_l} \tag{6}$$

Assume that the solvent follows Raoult's law, and then the equilibrium partial pressure can be calculated from:

$$P_{CO_2} = P - P^S(1 - x) - P^i \tag{7}$$

Table 4. Mole Fraction (x_i), Partial Pressure (p) of CO_2 at Equilibrium, and Uncertainties (δ_i) of CO_2 in *n*-Propanol from 288.15 K to 318.15 K

p/MPa	x_i	δ_i	p/MPa	x_i	δ_i
$T = 288.15$ K					
0.2584	0.0244	0.0011	2.1697	0.2051	0.0011
0.5229	0.0494	0.0010	2.4151	0.2283	0.0007
0.7333	0.0693	0.0010	2.6334	0.2489	0.0007
0.9647	0.0912	0.0009	2.9399	0.2779	0.0007
1.4285	0.1350	0.0008	3.2197	0.3043	0.0013
1.8121	0.1713	0.0012	3.6722	0.3471	0.0011
$T = 298.15$ K					
0.1313	0.0102	0.0012	2.4713	0.1924	0.0009
0.2557	0.0199	0.0011	2.6519	0.2064	0.0012
0.4711	0.0367	0.0011	2.9577	0.2302	0.0010
0.6415	0.0499	0.0012	3.3318	0.2594	0.0009
0.8289	0.0645	0.0012	3.5792	0.2786	0.0009
1.0933	0.0851	0.0011	3.7944	0.2954	0.0013
1.3964	0.1087	0.0007	4.1137	0.3202	0.0012
1.7182	0.1337	0.0009	4.4962	0.3500	0.0011
2.0590	0.1603	0.0010	4.8090	0.3743	0.0013
$T = 308.15$ K					
0.1592	0.0106	0.0011	2.5339	0.1682	0.0009
0.3415	0.0227	0.0010	2.8957	0.1922	0.0009
0.6791	0.0451	0.0010	3.1746	0.2107	0.0013
1.0201	0.0677	0.0009	3.5827	0.2378	0.0010
1.3628	0.0904	0.0008	4.0973	0.2719	0.0012
1.5713	0.1043	0.0012	4.4214	0.2934	0.0006
1.8661	0.1238	0.0011	4.8911	0.3246	0.0013
2.0422	0.1355	0.0006	5.0373	0.3343	0.0014
2.2175	0.1472	0.0005			
$T = 318.15$ K					
0.2544	0.0143	0.0013	2.9976	0.1685	0.0008
0.4539	0.0255	0.0010	3.3333	0.1873	0.0005
0.8851	0.0497	0.0012	3.5084	0.1972	0.0009
1.2448	0.0700	0.0006	3.8851	0.2184	0.0013
1.5831	0.0890	0.0013	4.1477	0.2331	0.0010
1.7878	0.1005	0.0014	4.5469	0.2555	0.0012
2.0433	0.1148	0.0011	5.0073	0.2814	0.0006
2.3651	0.1329	0.0010	5.3873	0.3028	0.0013
2.6457	0.1487	0.0009	5.7216	0.3216	0.0014

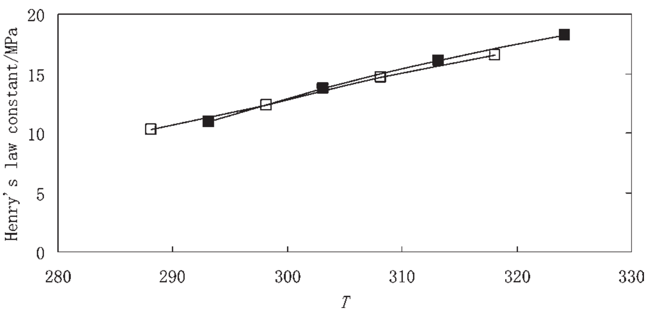

Figure 15. Henry's law constant of CO_2 in *n*-butanol from (280 to 330) K. ■, Lim et al.;[17] □, this study.

where P is the pressure inside the equilibrium cell while phase equilibrium is being established, P^S is the saturated vapor pressure of the solvent at the equilibrium temperature, and P^i is the inert gas pressure. n_1, n_2, and n^E are all calculated by Soave−Redlich−Kwong (SRK) equation of state from PVT data.

Table 5. Mole Fraction (x_i), Partial Pressure (p) of CO_2 at Equilibrium, and Uncertainties (δ_i) of CO_2 in *n*-Butanol from 288.15 K to 318.15 K

p/MPa	x_i	δ_i	p/MPa	x_i	δ_i
$T = 288.15$ K					
0.1273	0.0123	0.0011	1.7637	0.1710	0.0003
0.3534	0.0343	0.0010	1.9866	0.1926	0.0004
0.6283	0.0609	0.0009	2.1898	0.2124	0.0012
0.8715	0.0845	0.0008	2.4667	0.2392	0.0011
1.0026	0.0972	0.0005	2.8258	0.2740	0.0009
1.3175	0.1278	0.0009	3.2522	0.3154	0.0013
1.5307	0.1484	0.0003	3.7473	0.3634	0.0013
$T = 298.15$ K					
0.1747	0.0142	0.0013	2.4426	0.1984	0.0006
0.3522	0.0286	0.0013	2.8015	0.2276	0.0005
0.6825	0.0554	0.0008	3.1628	0.2569	0.0009
0.8667	0.0704	0.0005	3.4354	0.2791	0.0009
1.2198	0.0990	0.0009	3.8127	0.3097	0.0012
1.4866	0.1208	0.00011	4.2529	0.3455	0.0010
1.6763	0.1362	0.0003	4.7348	0.3846	0.0007
1.9530	0.1586	0.0003	5.0667	0.4116	0.0013
2.2375	0.1818	0.0012			
$T = 308.15$ K					
0.0667	0.0045	0.0003	3.1953	0.2178	0.0002
0.4738	0.0323	0.0003	3.5767	0.2438	0.0002
0.7425	0.0506	0.0002	3.9486	0.2691	0.0014
0.9827	0.0670	0.0002	4.2149	0.2873	0.0012
1.3162	0.08971	0.0007	4.5866	0.3126	0.0011
1.7082	0.1164	0.0006	4.9682	0.3386	0.0009
2.1805	0.1486	0.0004	5.3511	0.3647	0.0013
2.5442	0.1734	0.0003	5.6174	0.3829	0.0013
2.8237	0.1925	0.0003			
$T = 318.15$ K					
0.1981	0.0120	0.0002	2.5289	0.1530	0.0008
0.3801	0.0230	0.0002	3.0141	0.1824	0.0007
0.7326	0.0443	0.0002	3.6741	0.2223	0.0006
0.9224	0.0558	0.0001	4.0071	0.2425	0.0005
1.3141	0.0795	0.0004	4.4031	0.2665	0.0008
1.6988	0.1028	0.0004	4.7356	0.2866	0.0006
1.9523	0.1181	0.0003	5.4543	0.3300	0.0013
2.1672	0.1311	0.0003	5.9165	0.3581	0.0010

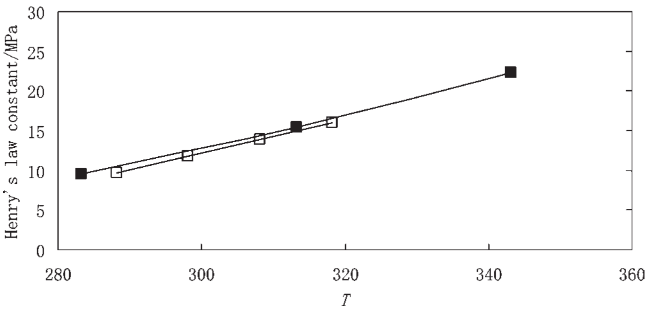

Figure 16. Henry's law constant of CO_2 in *n*-pentanol from (280 to 350) K. ■, Staby and Mollerup;[18] □, this study.

Then eq 1 can be written as eq 8:

$$\frac{u(x)}{x} = \sqrt{\left(\frac{u(n_g)}{n_g}\right)^2 + \left(\frac{u(n_g + n_l)}{n_g + n_l}\right)^2} = \sqrt{\frac{u(n_1)^2 + u(n_2)^2 + u(n^E)^2}{{n_g}^2} + \frac{u(n_1)^2 + u(n_2)^2 + u(n^E)^2 + u(n_l)^2}{(n_g + n_l)^2}} \tag{8}$$

Table 6. Mole Fraction (x_i), Partial Pressure (p) of CO_2 at Equilibrium, and Uncertainties (δ_i) of CO_2 in *n*-Pentanol from 288.15 K to 318.15 K

p/MPa	x_i	δ_i	p/MPa	x_i	δ_i
		$T = 288.15$ K			
0.2331	0.0241	0.0006	2.2629	0.2340	0.0003
0.5725	0.05921	0.0005	2.5782	0.2667	0.0003
0.8443	0.0873	0.0006	2.9686	0.3070	0.0002
1.2129	0.1254	0.0005	3.2072	0.3317	0.0002
1.6656	0.1723	0.0005	3.6243	0.3748	0.0007
1.8790	0.1943	0.0004			
		$T = 298.15$ K			
0.2516	0.0214	0.0002	2.5549	0.2174	0.0008
0.4156	0.0354	0.0002	2.8343	0.2411	0.0007
0.7705	0.0656	0.0002	3.2109	0.2732	0.0006
1.0901	0.0927	0.0001	3.5718	0.3039	0.0005
1.3398	0.1140	0.0004	3.9824	0.3388	0.0008
1.6553	0.1408	0.0004	4.2728	0.3635	0.0006
1.9656	0.1672	0.0003	4.6692	0.3972	0.0011
2.2454	0.1910	0.0003	5.0013	0.4255	0.0010
		$T = 308.15$ K			
0.1669	0.0120	0.0003	3.0598	0.2203	0.0011
0.4046	0.0291	0.0003	3.4824	0.2507	0.0004
0.8092	0.0583	0.0002	3.8268	0.2755	0.0010
1.1570	0.0833	0.0014	4.2764	0.3079	0.0008
1.5821	0.1139	0.0012	4.7953	0.3452	0.0007
1.9722	0.1420	0.0011	5.0286	0.3620	0.0006
2.3728	0.1708	0.0012	5.3358	0.3841	0.0005
2.7126	0.1953	0.0012	5.8762	0.4231	0.0010
		$T = 318.15$ K			
0.1537	0.0097	0.0012	2.8534	0.1792	0.0010
0.3218	0.0202	0.0012	3.2705	0.2054	0.0011
0.5306	0.0333	0.0010	3.6429	0.2288	0.0009
0.8413	0.0528	0.0011	4.0507	0.2544	0.0009
1.1832	0.0743	0.0009	4.4764	0.2811	0.0009
1.5617	0.0981	0.0011	4.8753	0.3062	0.0009
1.9166	0.1204	0.0011	5.2241	0.3281	0.0011
2.4215	0.1521	0.0010	5.6962	0.3578	0.0012

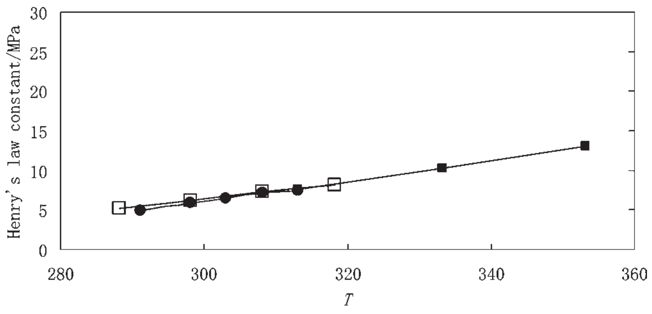

Figure 17. Henry's law constant of CO_2 in acetone from (280 to 350) K. ■, Sato et al.;[19] □, this study; ●, Chang et al.[20]

The solubility of CO_2 at various temperature and the uncertainties of the system are both listed in the following tables.

Table 7. Mole Fraction (x_i), Partial Pressure (p) of CO_2 at Equilibrium, and Uncertainties (δ_i) of CO_2 in Ethylene Glycol from 288.15 K to 318.15 K

p/MPa	x_i	δ_i	p/MPa	x_i	δ_i
		$T = 288.15$ K			
0.0942	0.0023	0.0014	1.6728	0.0410	0.0010
0.2183	0.0054	0.0012	1.9630	0.0481	0.0009
0.4355	0.0107	0.0011	2.3775	0.0583	0.0011
0.6175	0.0151	0.0012	2.6941	0.0660	0.0009
0.9188	0.0225	0.0012	2.9316	0.0719	0.0009
1.2089	0.0296	0.0011	3.3228	0.0814	0.0009
		$T = 298.15$ K			
0.1712	0.0036	0.0011	2.4375	0.0511	0.0008
0.3612	0.0076	0.0009	2.9163	0.0612	0.0011
0.7228	0.0152	0.0012	3.3672	0.0706	0.0009
1.1032	0.0231	0.0009	3.7089	0.0778	0.0010
1.5316	0.0321	0.0011	4.2144	0.0884	0.0009
1.9941	0.0418	0.0010			
		$T = 308.15$ K			
0.2417	0.0045	0.0010	2.9103	0.0542	0.0011
0.5708	0.0106	0.0009	3.3722	0.0628	0.0011
0.9367	0.0174	0.0009	3.6361	0.0677	0.0008
1.3913	0.0259	0.0010	3.9718	0.0740	0.0009
1.7435	0.0325	0.0010	4.2429	0.0790	0.0008
2.2994	0.0428	0.0009	4.6175	0.0860	0.0008
2.6531	0.0494	0.0008	5.0354	0.0938	0.0012
		$T = 318.15$ K			
0.1461	0.0024	0.0011	3.2564	0.0537	0.0012
0.4555	0.0075	0.0011	3.6919	0.0608	0.0009
0.8213	0.0135	0.0010	4.0725	0.0671	0.0011
1.2942	0.0213	0.0009	4.4036	0.0726	0.0006
1.6103	0.0265	0.0011	4.8601	0.0801	0.0005
2.1505	0.0354	0.0010	5.2996	0.0873	0.0005
2.4781	0.0408	0.0011	5.7898	0.0954	0.0009
2.9077	0.0479	0.0009			

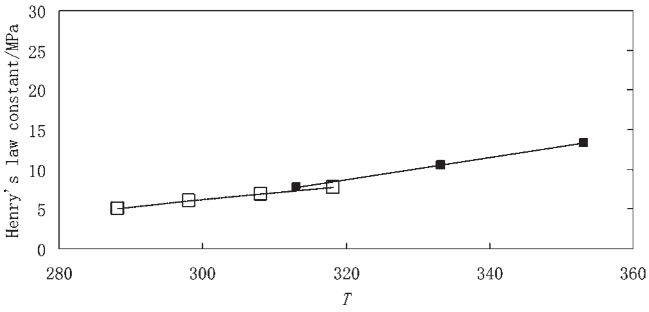

Figure 18. Henry's law constant of CO_2 in butanone from (280 to 350) K. ■, Sato et al.;[19] □, this study.

It can be seen, from Tables 2 to 12 and plotted in Figures 1 to 11, that the solubility of CO_2 in alcohols, glycols, ethers, and ketones decreases with increasing temperature for the same value of partial pressure of CO_2 and decreasing pressure for the same value of temperature, which also illustrates a physical

Table 8. Mole Fraction (x_i), Partial Pressure (p) of CO_2 at Equilibrium, and Uncertainties (δ_i) of CO_2 in Propylene Glycol from 288.15 K to 318.15 K

p/MPa	x_i	δ_i	p/MPa	x_i	δ_i
		$T = 288.15$ K			
0.2322	0.0077	0.0009	1.7652	0.0584	0.0010
0.5217	0.0173	0.0008	2.0320	0.0672	0.0011
0.8029	0.0265	0.0008	2.4953	0.0825	0.0009
1.1195	0.0370	0.0012	2.8729	0.0950	0.0012
1.4236	0.0471	0.0011	3.3473	0.1107	0.0009
		$T = 298.15$ K			
0.1373	0.0036	0.0009	1.9119	0.0501	0.0010
0.3829	0.0100	0.0011	2.3829	0.0625	0.0008
0.6453	0.0169	0.0009	2.6521	0.0696	0.0011
0.9203	0.0241	0.0011	2.9232	0.0767	0.0013
1.2765	0.0335	0.0013	3.2857	0.0861	0.0012
1.5423	0.0405	0.0008	3.6984	0.0970	0.0013
		$T = 308.15$ K			
0.1277	0.0028	0.0008	2.4005	0.0526	0.0009
0.4522	0.0099	0.0009	2.7432	0.0601	0.0009
0.7319	0.0160	0.0007	3.0929	0.0678	0.0013
0.9546	0.0209	0.0008	3.415	0.0748	0.0008
1.2364	0.0271	0.0013	3.8494	0.0843	0.0008
1.5409	0.0338	0.0009	4.3572	0.0955	0.0012
1.8722	0.0410	0.0012	4.8803	0.1069	0.0011
2.1886	0.0480	0.0010	5.2019	0.1140	0.0010
		$T = 318.15$ K			
0.1743	0.0033	0.0009	2.7606	0.0525	0.0012
0.4526	0.0086	0.0012	3.0343	0.0577	0.0011
0.7818	0.0149	0.0010	3.5796	0.0681	0.0002
1.0754	0.0205	0.0009	3.9088	0.0744	0.0002
1.3464	0.0256	0.0009	4.2661	0.0811	0.0007
1.6577	0.0315	0.0013	4.6732	0.0889	0.0006
2.0082	0.0382	0.0008	5.0008	0.0951	0.0004
2.3479	0.0447	0.0008	5.4291	0.1033	0.0003

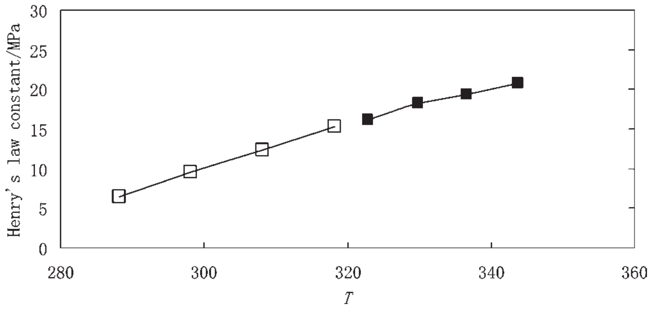

Figure 19. Henry's law constant of CO_2 in ethylene glycol monomethyl ether from (280 to 350) K. ■, Joung et al.;[3] □, this study.

Table 9. Mole Fraction (x_i), Partial Pressure (p) of CO_2 at Equilibrium, and Uncertainties (δ_i) of CO_2 in Acetone from 288.15 K to 318.15 K

p/MPa	x_i	δ_i	p/MPa	x_i	δ_i
		$T = 288.15$ K			
0.1182	0.0229	0.0012	1.4765	0.2857	0.0013
0.3027	0.0586	0.0009	1.9576	0.3788	0.0008
0.5281	0.1022	0.0011	2.3378	0.4524	0.0010
0.8784	0.1700	0.0009	2.7067	0.5237	0.0008
1.1593	0.2243	0.0011	3.0583	0.5918	0.0011
		$T = 298.15$ K			
0.2342	0.0377	0.0012	2.4165	0.3892	0.0009
0.5440	0.0876	0.0012	2.8519	0.4593	0.0011
0.9083	0.1463	0.0011	3.2878	0.5295	0.0009
1.3277	0.2138	0.0007	3.6169	0.5825	0.0008
1.6378	0.2638	0.0009	4.0302	0.6491	0.0012
2.0576	0.3314	0.0010	2.4165	0.3892	0.0009
		$T = 308.15$ K			
0.3154	0.0436	0.0001	2.8453	0.3931	0.0009
0.6377	0.0881	0.0009	3.0749	0.4248	0.0009
0.9205	0.1272	0.0008	3.3326	0.4604	0.0013
1.2481	0.1724	0.0012	3.7813	0.5224	0.0010
1.6176	0.2235	0.0011	4.1057	0.5672	0.0012
2.149	0.2969	0.0006	4.5939	0.6346	0.0006
2.5044	0.3460	0.0005	5.0617	0.6992	0.0013
		$T = 318.15$ K			
0.0617	0.0075	0.0011	2.9194	0.3571	0.0013
0.2593	0.0317	0.0012	3.3617	0.4112	0.0003
0.5410	0.0662	0.0012	3.7288	0.4561	0.0003
0.9871	0.1207	0.0014	4.0920	0.5005	0.0002
1.4332	0.1753	0.0012	4.4776	0.5477	0.0008
1.8794	0.2300	0.0011	4.9135	0.6010	0.0012
2.2453	0.2747	0.0009	5.3291	0.6519	0.0006
2.6501	0.3242	0.0013			

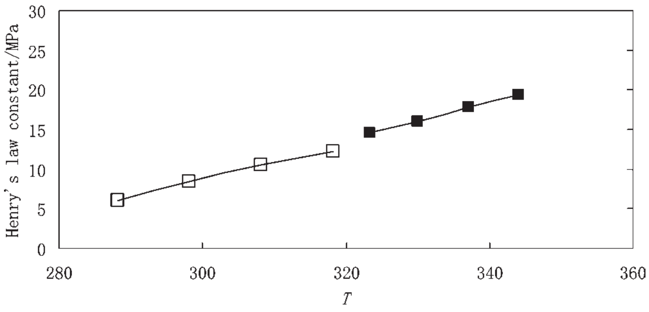

Figure 20. Henry's law constant of CO_2 in ethylene glycol monoethyl ether from (280 to 350) K. ■, Joung et al.;[3] □, this study.

dissolving process of CO_2 in all of these solvents. Henry's law constants of CO_2 in alcohols, glycols, ethers, and ketones are listed in Table 13. It can be seen from Figures 12 to 21 that all of the experimental data present good agreement with the literature data.[13−21] It means that the experimental method in this work is valid for the measurement of gas solubility at high pressures.

As Table 13 shows, under the same conditions, ketones are the best absorption solvents with high performance, and the glycols

Table 10. Mole Fraction (x_i), Partial Pressure (p) of CO_2 at Equilibrium, and Uncertainties (δ_i) of CO_2 in 2-Butanone from 288.15 K to 318.15 K

p/MPa	x_i	δ_i	p/MPa	x_i	δ_i
		$T = 288.15$ K			
0.3161	0.0633	0.0009	2.1632	0.4329	0.0008
0.6257	0.1252	0.0011	2.3236	0.4650	0.0011
1.0116	0.2024	0.0013	2.5491	0.5101	0.0013
1.4689	0.2939	0.0008	2.8018	0.5607	0.0012
1.9547	0.3912	0.0010	3.1014	0.6206	0.0013
		$T = 298.15$ K			
0.2932	0.0484	0.0009	2.2218	0.3668	0.0013
0.5673	0.0937	0.0007	2.6362	0.4352	0.0009
0.8857	0.1462	0.0008	3.0906	0.5102	0.0012
1.3291	0.2194	0.0009	3.5728	0.5898	0.0010
1.7147	0.2831	0.0007	3.8320	0.6326	0.0009
1.9699	0.3252	0.0008			
		$T = 308.15$ K			
0.1583	0.0230	0.0002	2.6391	0.3838	0.0004
0.3778	0.0549	0.0014	3.0874	0.4490	0.0010
0.7396	0.1076	0.0012	3.4569	0.5027	0.0008
1.1362	0.1652	0.0011	3.9237	0.5706	0.0007
1.5218	0.2213	0.0012	4.3722	0.6358	0.0006
1.8957	0.2757	0.0012	4.8010	0.6982	0.0005
2.2714	0.3303	0.0011	5.2193	0.7590	0.0010
		$T = 318.15$ K			
0.2185	0.0282	0.0011	2.9795	0.3851	0.0010
0.6786	0.0877	0.0012	3.2641	0.4218	0.0011
1.1039	0.1427	0.0012	3.6547	0.4723	0.0007
1.4545	0.1880	0.0014	4.0833	0.5277	0.0006
1.8079	0.2336	0.0012	4.5203	0.5842	0.0009
2.2377	0.2892	0.0011	5.0005	0.6462	0.0005
2.6754	0.3456	0.0009	5.4216	0.7007	0.0012

Table 11. Mole Fraction (x_i), Partial Pressure (p) of CO_2 at Equilibrium, and Uncertainties (δ_i) of CO_2 in Ethylene Glycol Monomethyl Ether from 288.15 K to 318.15 K

p/MPa	x_i	δ_i	p/MPa	x_i	δ_i
		$T = 288.15$ K			
0.1738	0.0272	0.0014	1.8379	0.2873	0.0011
0.4257	0.0665	0.0012	2.2927	0.3584	0.0004
0.7643	0.1195	0.0011	2.7202	0.4252	0.0010
1.0908	0.1705	0.0012	3.2588	0.5094	0.0008
1.4158	0.2213	0.0012	3.7908	0.5926	0.0007
		$T = 298.15$ K			
0.3291	0.0344	0.0004	2.2632	0.2366	0.0007
0.6339	0.0663	0.0004	2.6890	0.2811	0.0006
1.0264	0.1073	0.0003	3.1415	0.3284	0.0005
1.4368	0.1502	0.0003	3.5913	0.3754	0.0008
1.7709	0.1851	0.0008	4.0717	0.4256	0.0011
		$T = 308.15$ K			
0.2725	0.0220	0.0006	3.0911	0.2494	0.0009
0.5713	0.0461	0.0009	3.5236	0.2843	0.0011
0.9762	0.0788	0.0011	3.9405	0.3180	0.0003
1.3158	0.1062	0.0010	4.4413	0.3584	0.0002
1.7729	0.1431	0.0011	4.8009	0.3874	0.0006
2.1641	0.1746	0.0009	5.2753	0.4257	0.0005
2.6625	0.2149	0.0012			
		$T = 318.15$ K			
0.1253	0.0082	0.0012	3.1264	0.2044	0.0010
0.4800	0.0314	0.0011	3.5783	0.2339	0.0008
0.9422	0.0616	0.0004	4.0316	0.2635	0.0011
1.3905	0.0909	0.0010	4.5937	0.3003	0.0013
1.7236	0.1127	0.0008	5.0512	0.3302	0.0009
2.0005	0.1308	0.0013	5.4271	0.3548	0.0009
2.5772	0.1685	0.0008			

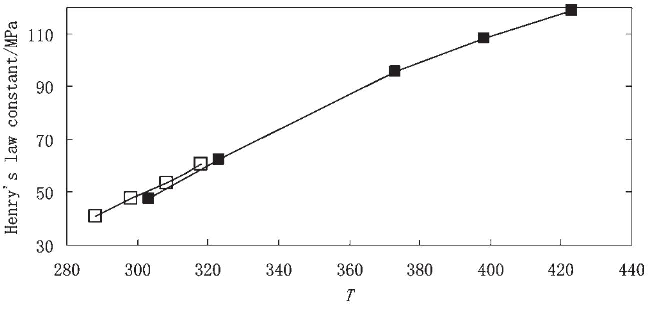

Figure 21. Henry's law constant of CO_2 in ethylene glycol from (280 to 450) K. ■, Francesconi and Galvão;[21] □, this study.

are the worst among the studied solutions. That may be explained by the theory of similarity and intermiscibility. According to similarity theory, it is reasonable that similar structure compounds are easily mutually soluble, so ketones with the similarity of carbonyl group have a greater ability to dissolve CO_2. Then, an analysis on the structure should be made to explain this phenomenon. All of the solvents in this study can be divided as follows: (1) alcohols, with one hydroxyl group; (2) glycols, with two hydroxyl groups; (3) ketones, with one carbonyl group; (4) ethers, with one hydroxyl group and one ether bond. Based on a previous study,[22] it is known that the hydroxyl compound can form the intramolecular hydrogen bond, which will lead to a stronger interaction between the solvent and solvent molecules. Then, the cooperativity effects of the intramolecular hydrogen bond between the solvent molecules are expressed as the formation of multimer hydrogen bonds in alcohols. It is reported that the solubilization of a gas solute in a physical solvent can be divided into two steps:[23] first, the interactions among the solvent molecules must be broken to provide some cavities which can accommodate the solute molecules; second, the cavities formed in the first step are then filled with solute molecules and new interactions between the solute and solvent molecules are also created. Thus, the formation of multimer hydrogen bonds in alcohols leads to a more compact structure of alcohols and cannot provide enough cavities to accommodate the solute molecules in solvent. That is why the glycols are the worst solutions. Moreover, both the ethers and the alcohols have the hydroxyl group, but ethers have a better absorption performance. The experiment data also indicate that the ether bond can

Table 12. Mole Fraction (x_i), Partial Pressure (p) of CO_2 at Equilibrium, and Uncertainties (δ_i) of CO_2 in Ethylene Glycol Monoethyl Ether from 288.15 K to 318.15 K

p/MPa	x_i	δ_i	p/MPa	x_i	δ_i
		T = 288.15 K			
0.1012	0.0169	0.0013	1.9433	0.3247	0.0009
0.3948	0.0660	0.0009	2.3016	0.3846	0.0013
0.7818	0.1306	0.0012	2.7678	0.4625	0.0008
1.0927	0.1826	0.0010	3.1119	0.5200	0.0008
1.5531	0.2595	0.0009	3.5905	0.5999	0.0012
		T = 298.15 K			
0.3375	0.0403	0.0003	2.4451	0.2919	0.0012
0.8987	0.1073	0.0002	2.7269	0.3255	0.0012
1.3522	0.1614	0.0014	3.1065	0.3708	0.0011
1.8018	0.2151	0.0012	3.5484	0.4236	0.0004
2.1903	0.2615	0.0011	3.9798	0.4751	0.0010
		T = 308.15 K			
0.2671	0.0253	0.0007	2.9203	0.2772	0.0007
0.5349	0.0508	0.0006	3.3734	0.3202	0.0006
0.9280	0.0881	0.0005	3.7898	0.3597	0.0005
1.3165	0.1249	0.0010	4.1335	0.3923	0.0008
1.7226	0.1635	0.0003	4.5842	0.4351	0.0006
2.1147	0.2007	0.0003	5.0933	0.4834	0.0012
2.5190	0.2391	0.0008			
		T = 318.15 K			
0.1985	0.0162	0.0003	3.0922	0.2525	0.0011
0.4873	0.0398	0.0002	3.4198	0.2793	0.0004
0.9539	0.0779	0.0014	3.8874	0.3175	0.0011
1.3764	0.1124	0.0012	4.2196	0.3446	0.0009
1.7962	0.1467	0.0011	4.6508	0.3798	0.0011
2.1007	0.1716	0.0012	5.1077	0.4171	0.0011
2.5870	0.2113	0.0012	5.5651	0.4545	0.0010

Table 13. Henry's Law Constant of CO_2 in Alcohols, Glycols, Ethers, and Ketones from 288.15 K to 318.15 K

compound	Henry's law constant/MPa			
	288.15 K	298.15 K	308.15 K	318.15 K
methanol	11.5830	13.6210	16.1970	19.8990
ethanol	10.6391	13.2959	15.7822	18.4554
n-propanol	10.5793	12.8466	15.0687	17.7927
n-butanol	10.3121	12.3107	14.6715	16.5242
n-pentanol	9.6687	11.7542	13.8898	15.9219
ethylene glycol	40.7968	47.6813	53.6857	60.6819
propylene glycol	30.2431	38.123	45.6389	52.5711
acetone	5.1681	6.2091	7.2389	8.1751
butanone	4.9973	6.0576	6.8762	7.7379
ethylene glycol monomethyl ether	6.3968	9.5669	12.3924	15.2983
ethylene glycol monoethyl ether	5.9846	8.3775	10.5367	12.2451

counteract the negative effect generated by the hydroxyl group to some extent.

4. CONCLUSIONS

The main conclusions of the study can be summarized as follows:

1. The constant-volume method is used to determine the solubility of CO_2 in alcohols, glycols, ethers, and ketones under the pressure of 6 MPa and the temperature variations from 288.15 K to 318.15 K.
2. The solubility of CO_2 in all of the alcohol, ether, and ketone solvents decreases as temperature increases and pressure decreases.
3. It is found by contrast that ketones have a greater ability to dissolve CO_2 than alcohols, ethers, and glycols. This also indicates that carbonyl group and ether bond in solvents can promote the CO_2 absorption, but the hydroxyl group will inhibit the CO_2 absorption.

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