Gas−Liquid Solubility of Hydrogen in *n*-Alcohols (1 ≤ *n* ≤ 4) at Pressures from 3.6 MPa to 10 MPa and Temperatures from 298.15 K to 525.15 K

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The gas−liquid solubility of hydrogen in methanol, ethanol, 1-propanol, and 1-butanol at pressures in the range 3.6 to 10 MPa and at temperatures in the range 298.15 to 525.15 K has been measured in an autoclave type phase equilibrium apparatus using the total pressure method. Pseudo-Henry's law constants, $H_{2,1}^{PS}$, were calculated. The solubility of hydrogen increases with increasing temperature and pressure for all solvents used, and it also increases as the carbon chain length of the alcohol molecule increases.

Introduction

In the fine chemicals industry, α,β-unsaturated alcohols are very important products, related to the production of flavors, pharmaceuticals, perfumes, cosmetics, and many others. Catalytic hydrogenation reactions for converting aldehydes into these alcohols usually take place in a "slurry" reactor, where three phases are present: reactants, solvents and the products of the reaction (liquid phase), catalyst (solid) and hydrogen (gas). Alcohols that are used as solvents for the reaction products influence the selectivity and velocity of the reaction and the catalyst activity. This influence is associated with the solubility of hydrogen in the solvents. The aim of this work was to study the solubility of hydrogen in four selected solvents (methanol, ethanol, 1-propanol, and 1-butanol) commonly used in catalytic hydrogenation reactions of aldehydes. Relatively few data for the solubility of hydrogen in alcohols at high temperatures and high pressures are available in the literature. Therefore, by extending the range of experimental pressure and temperature beyond that used in the reactions mentioned above, this work intends to make more of this information available. These results are also useful for testing/developing models that predict thermodynamic properties.

Experimental Section

Apparatus. The experimental apparatus used for measuring the solubility of hydrogen in alcohols is a commercial equipment produced by LECO Co., called a Barnes Volumetric Hydrothermal System, model RA-1A-1. A schematic of this apparatus is shown in Figure 1. The equilibrium cell is a stainless steel mechanically agitated autoclave (volume 1128 cm³), which was placed inside an electrical heated furnace, with a maximum operating temperature of 673 K. To improve agitation, steel spheres (volume 6.2 cm³) were used in the cell. The temperature at the external wall of the autoclave was measured with a K-type thermocouple connected to a digital controller (Eurotherm, model 847, resolution 0.1 K). The temperature inside the
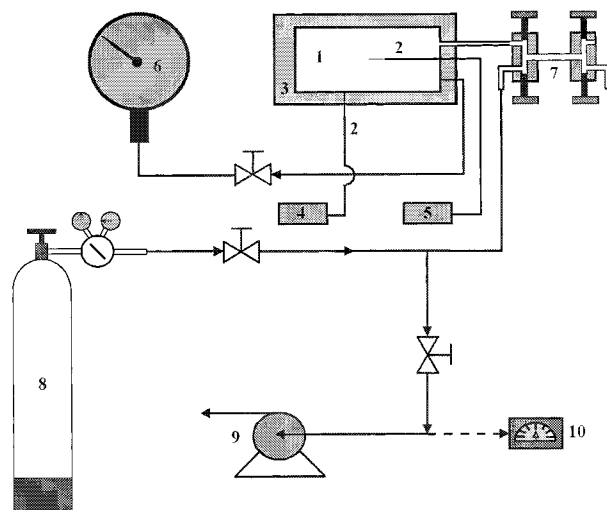
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Figure 1. Scheme of the experimental equilibrium apparatus: (1) equilibrium cell; (2) thermocouples; (3) heating mantel; (4) temperature controllers; (5) temperature indicator; (6) pressure gauge; (7) three-way valves; (8) hydrogen cylinder; (9) vacuum pump; (10) vacuum meter.

autoclave was measured with a J-type thermocouple connected to a digital temperature indicator (Shimaden, model SD20, resolution 0.1 K). Both thermocouples were calibrated by measuring the boiling point of seven different chemicals and comparing the values indicated by them with those presented by a Pt-100 resistance thermometer (Guildline, model 9540, resolution of 10^{-3} K), used as reference. The estimated uncertainty of the temperature measurement was ±0.3 K. The autoclave was connected to a Bourdon gauge covering the range 0 to 40 MPa. This manometer was calibrated by measuring the pressure of saturated steam at several temperatures. The estimated uncertainty of the pressure measurement was ±0.035 MPa.

Materials. Hydrogen (analytical grade, supplied by White Martins) was used without further purification. The purities of the alcohols were checked by three methods: gas chromatography, measurement of refractive index, and measurement of density. For all alcohols used (analytical grade, supplied by Merck) no impurity peaks were found

Table 1. Comparison of Experimental Refractive Indices (η) and Densities (ρ) of Pure Alcohols with Literature Values at 293.15 K

	η		ρ (kg·m^{-3})	
chemical	this work	ref 14	this work	ref 14
methanol	1.3290	1.3288	792.1	791.4
ethanol	1.3619	1.3611	790.7	789.3
1-propanol	1.3854	1.3850	804.2	803.5
1-butanol	1.3995	1.3993	810.1	809.8

in the chromatographic analysis. Table 1 shows the results for refractive index and density measured in this work, compared with values taken from the literature for the alcohols used. All solvents were used without further purification except degassing, which was done by boiling them during a period of approximately 5 min in a beaker. After this time, the beaker was sealed and then put into an ice bath for cooling, before feeding the solvent into the equilibrium cell.

Experimental Method. The experimental method used is similar to that of Cukor and Prausnitz,[1] Olson,[2] Graaf et al.,[3] and Breman et al.[4] Known quantities of the two components (hydrogen and alcohol) are introduced in a vessel (equilibrium cell) of known volume. By measuring accurately these quantities and also the pressure, temperature, and volume of the system at equilibrium, and using thermodynamic relations of phase equilibria and a material balance, the composition of the phases can be determined as well as the gas−liquid solubility, which is given by the mole fraction of the solute in the liquid phase, x_2. This method is known as the total pressure method, and its description and data reduction are given in detail by Breman et al.[4]

Basically the experimental procedure begins by evacuating the equilibrium cell and then filling it with an amount of degassed solvent. Then a small pressurized cylinder containing the solute is attached to the cell to feed this component. Both quantities of solvent and solute are accurately measured from the differential mass of a beaker (for the solvent), and of the cylinder (for the solute), before and after feeding, using a semianalytical balance (accuracy of ±0.005 g).

After both components were fed into and enclosed in the autoclave, the set point of the temperature controller was adjusted to a desired temperature and the rocking mechanism to agitate the system was turned on. When equilibrium was attained in the system at the desired point, the temperature and pressure of the system were written down. The set point was changed again, increasing temperature stepwise, until the highest temperature desired was reached. The system was assumed to be in equilibrium if during an interval of at least 40 min the values of temperature and pressure were constant within 0.3 K and 0.035 MPa, respectively.

Data Reduction

In this work, following the procedure used by Breman et al.,[4] the gas−liquid solubility of solute (2) in solvent (1) is also expressed by a so-called "pseudo-Henry's law constant", given by $H_{2,1}^{PS}$, at a reference pressure that is the solvent saturation pressure (P_1^{sat}) at the temperature of the system.

When equilibrium is attained in the system, the following relation holds[5] for both components:

$$\hat{\phi}_i^V y_i P = x_i \gamma_i f_i^\circ \qquad (1)$$

Table 2. Molar Mass (*MM*), Normal Boiling Point (T_{bp}), Critical Properties (T_C, P_C, Z_C), and Acentric Factor (ω) of the Pure Components (Values Obtained from ref 7)

chemical	MM/(g/mol)	T_{bp}/K	T_C/K	P_C/MPa	Z_C	ω
CH$_3$OH	32.042	337.7	512.6	8.09	0.224	0.556
C$_2$H$_5$OH	46.069	351.4	513.9	6.14	0.240	0.644
1-C$_3$H$_7$OH	60.096	370.3	536.8	5.17	0.253	0.623
1-C$_4$H$_9$OH	74.123	390.9	563.1	4.42	0.259	0.593
H$_2$	2.016	20.3	33.0	1.29	0.303	−0.216

where P is the pressure of the system, y_i is the vapor-phase mole fraction of component i, $\hat{\phi}_i^V$ is the vapor-phase fugacity coefficient of component i, x_i is the liquid-phase mole fraction of component i, f_i° is the fugacity of component i at a reference state, and γ_i is the liquid-phase activity coefficient of component i. Taking as a reference pressure for the solute the saturation pressure of the solvent at the system temperature and taking into account the normalization of the activity coefficient of the solute by the unsymmetric convention (denoted by $\gamma_2^* \to 1$ as $x_2 \to 0$), eq 1 can be written for the solute

$$\hat{\phi}_2^V y_2 P = x_2 \gamma_2^* (P_1^{sat}) H_{2,1}(P_1^{sat}) \exp\left(\int_{P_1^{sat}}^{P} \frac{\bar{V}_2}{RT} dP\right) \qquad (2)$$

where $H_{2,1}$ is the Henry's law constant of solute 2 in solvent 1 at pressure P_1^{sat}, R is the universal gas constant, and $\bar{V}_2$ is the partial molar volume of solute. The exponential term of eq 2 is called the Poynting correction factor and is used to correct the effect of pressure on the fugacity of solute 2 in the liquid phase.

Substituting the product $\gamma_2^* H_{2,1}$ by the so-called pseudo-Henry's law constant, eq 2 can be rewritten as

$$\hat{\phi}_2^V y_2 P = x_2 H_{2,1}^{PS}(P_1^{sat}) \exp\left(\int_{P_1^{sat}}^{P} \frac{\bar{V}_2}{RT} dP\right) \qquad (3)$$

Using the Peng−Robinson[6] equation of state to calculate $\hat{\phi}_2^V$ and $\bar{v}_2$, the equation of Wagner from Reid et al.[7] to calculate the saturation pressure of the solvent, the modified equation of Rackett presented by Spencer and Danner[8] to calculate the molar volume of saturated liquid, and the equation presented by Breman et al.[4] to calculate the liquid density of solvent at increased pressure and also making a material balance for each component in both phases, the composition of the phases at equilibrium can be obtained from the primary experimental data at equilibrium (P, T, V, n_1^T and n_2^T) via an iterative method (Breman et al.[4]), where T = temperature, V = volume of the system (equilibrium cell), and n_i^T = total number of moles of component i fed in the system.

The pseudo-Henry's law constant can then be calculated using eq 3. This constant is inversely proportional to the liquid-phase mole fraction of hydrogen. When its behavior is analyzed as a function of temperature, some conclusions arise about the solubility of hydrogen in alcohols.

Results and Discussion

Table 2 presents the relevant physical quantities of the pure components used in this study. Tables 3−6 show the experimental values of temperature (T), pressure (P), and the charge of solute and solvent for each experiment (n_1^T and n_2^T, respectively) for all the experiments and also the calculated values of mole fraction of solute in the liquid and vapor phases (x_2 and y_2, respectively), pseudo-Henry's law constant ($H_{2,1}^{PS}$), and Poynting correction factor (PCF). Figure 2 shows the behavior of the pseudo-Henry's law constant as a function of the absolute temperature. This

Table 3. Solubility Data for the System Methanol–Hydrogen

T/K	P/MPa	x_2	y_2	$H_{2,1}^{PS}$/MPa	PCF
Run No. 1: $n_1^T = 19.0266$ mol, $n_2^T = 0.7574$ mol
323.8	4.78	0.0116	0.9850	388.7	1.060
347.6	5.00	0.0158	0.9635	289.6	1.066
372.5	5.43	0.0200	0.9214	237.3	1.076
373.9	5.50	0.0201	0.9186	238.3	1.077
385.4	5.83	0.0219	0.8908	223.7	1.085
400.7	6.44	0.0245	0.8457	208.6	1.099
415.2	6.86	0.0281	0.7876	180.8	1.113
424.6	7.45	0.0302	0.7501	173.5	1.129
437.5	8.03	0.0341	0.6848	151.6	1.151
450.8	8.89	0.0388	0.6140	132.7	1.188
460.7	9.68	0.0431	0.5594	118.6	1.228
476.6	10.98	0.0525	0.4643	91.7	1.329
Run No. 2: $n_1^T = 18.6215$ mol, $n_2^T = 0.7612$ mol
314.4	4.49	0.0102	0.9895	418.0	1.056
324.7	4.56	0.0120	0.9838	357.8	1.058
348.2	4.78	0.0161	0.9613	273.1	1.063
358.5	5.00	0.0174	0.9466	259.0	1.067
374.2	5.39	0.0195	0.9167	239.9	1.076
395.8	6.00	0.0233	0.8571	208.6	1.090
414.5	6.73	0.0271	0.7878	184.1	1.109
425.3	7.20	0.0298	0.7393	168.2	1.124
438.9	7.81	0.0339	0.6683	146.0	1.147
448.6	8.38	0.0371	0.6150	132.2	1.171
458.9	9.11	0.0412	0.5554	117.3	1.208
475.3	10.44	0.0498	0.4590	92.1	1.303

Table 4. Solubility Data for the System Ethanol–Hydrogen

T/K	P/MPa	x_2	y_2	$H_{2,1}^{PS}$/MPa	PCF
Run No. 1: $n_1^T = 7.9435$ mol, $n_2^T = 0.9863$ mol
324.2	3.70	0.0177	0.9897	199.1	1.050
347.7	3.91	0.0237	0.9729	154.3	1.055
375.3	4.28	0.0302	0.9313	125.5	1.066
395.8	4.71	0.0342	0.8792	114.8	1.079
411.2	5.10	0.0380	0.8253	104.8	1.092
426.5	5.57	0.0426	0.7587	93.9	1.111
438.2	6.10	0.0452	0.7023	89.8	1.132
449.9	6.69	0.0485	0.6400	83.9	1.161
463.4	7.40	0.0550	0.5603	72.0	1.211
476.5	8.24	0.0629	0.4808	60.1	1.295
Run No. 2: $n_1^T = 12.7704$ mol, $n_2^T = 0.8024$ mol
299.9	4.38	0.0132	0.9973	318.4	1.057
326.8	4.49	0.0204	0.9900	208.7	1.061
352.6	4.64	0.0269	0.9714	158.9	1.067
373.8	4.78	0.0326	0.9404	130.8	1.074
400.2	5.32	0.0386	0.8758	113.4	1.092
449.4	7.45	0.0540	0.6710	85.8	1.185
463.6	8.26	0.0616	0.5911	73.4	1.246
475.8	9.03	0.0704	0.5176	60.9	1.331

Table 5. Solubility Data for the System 1-Propanol–Hydrogen

T/K	P/MPa	x_2	y_2	$H_{2,1}^{PS}$/MPa	PCF
Run No. 1: $n_1^T = 7.0000$ mol, $n_2^T = 0.9186$ mol
301.0	3.64	0.0111	0.9988	314.7	1.048
353.7	4.25	0.0213	0.9844	187.1	1.062
439.5	5.94	0.0438	0.8146	102.4	1.127
462.3	6.77	0.0524	0.7165	85.6	1.173
474.6	7.34	0.0578	0.6546	76.8	1.212
488.7	7.93	0.0679	0.5744	62.2	1.278
500.2	8.60	0.0767	0.5078	52.5	1.365
Run No. 2: $n_1^T = 9.1991$ mol, $n_2^T = 0.8068$ mol
299.9	4.13	0.0119	0.9989	334.0	1.055
326.1	4.35	0.0187	0.9956	220.8	1.060
338.4	4.49	0.0214	0.9923	198.6	1.063
348.4	4.71	0.0223	0.9884	198.4	1.068
363.7	4.92	0.0257	0.9792	177.0	1.074
374.4	5.14	0.0277	0.9699	169.4	1.081
387.9	5.43	0.0305	0.9541	158.7	1.089
402.7	5.75	0.0344	0.9299	144.5	1.101
412.5	5.97	0.0374	0.9092	134.0	1.110
423.5	6.29	0.0407	0.8817	125.3	1.123
433.2	6.58	0.0441	0.8527	116.3	1.136
452.5	7.30	0.0519	0.7814	99.5	1.174
463.5	7.66	0.0577	0.7329	88.1	1.201
475.6	8.13	0.0646	0.6747	76.6	1.242
486.6	8.67	0.0727	0.6119	65.6	1.299
494.8	9.03	0.0800	0.5638	57.0	1.356
504.2	9.61	0.0901	0.5109	48.1	1.451
513.6	10.19	0.1052	0.4650	37.9	1.602

Table 6. Solubility Data for the System 1-Butanol–Hydrogen

T/K	P/MPa	x_2	y_2	$H_{2,1}^{PS}$/MPa	PCF
Run No. 1: $n_1^T = 7.1207$ mol, $n_2^T = 0.8339$ mol
295.3	3.91	0.0137	0.9997	274.4	1.053
322.6	4.06	0.0236	0.9985	164.6	1.057
349.4	4.20	0.0327	0.9943	121.9	1.062
368.8	4.49	0.0360	0.9875	116.8	1.070
373.2	4.56	0.0367	0.9853	115.8	1.072
421.6	5.43	0.0481	0.9347	97.5	1.105
452.2	6.15	0.0584	0.8669	82.8	1.142
472.6	6.65	0.0680	0.8006	70.2	1.179
497.9	7.63	0.0820	0.6979	57.1	1.265
512.6	8.17	0.0938	0.6275	47.2	1.349
524.9	8.82	0.1064	0.5686	39.5	1.464

behavior was fitted by a polynomial regression for each one of the alcohols studied, and the coefficients of this fitting are presented in Table 7.

For all binary systems the solubility of hydrogen increases with increasing temperature and pressure in the experimental range studied. This behavior was also observed by Breman et al.,[4] Brunner,[9] and Radhakrishnan et al.[10] in systems containing hydrogen as a solute.

The solubility also increases with increasing carbon chain length of the alcohols, as can be seen in Figure 2, but ethanol was an exception for this behavior. Although in Figure 2 the curve for the system ethanol–hydrogen is located between the ones of 1-propanol-H_2 and 1-butanol-H_2, the solubility of hydrogen in ethanol is just slightly higher than that in 1-propanol.

The binary interaction parameter (k_{ij}) used in mixing rules in the Peng–Robinson equation of state was taken as zero for all systems studied. It was observed that different values of k_{ij} did not affected sensibly the calculated values of solubility, especially at temperatures below 450 K.

Table 8 shows the uncertainties estimated for each variable measured experimentally. Considering them, a calculation from a worst case approach, assuming all error sources contribute maximally in the same direction to the overall error, has allowed us to estimate the uncertainty in the values of the liquid-phase mole fraction of hydrogen as about ±0.002. This value corresponds to a maximum relative deviation of ±19.6% and a minimum relative deviation of 1.9%, among experimental data for all systems. Such uncertainties are comparable with those obtained for systems containing hydrogen as solute.[4]

Previous solubility data of hydrogen in alcohols at high temperatures and pressures are reported by Brunner,[9] Radhakrishnan et al.,[10] Choudary et al.,[11] Wainwright et al.,[12] and Koneripalli et al.[13] A comparison with some data published by Brunner[9] is possible. Table 9 shows such a comparison for the solubility of hydrogen in 1-propanol. Since the pressure and temperature values presented in Brunner[9] are not the same as those measured in this work, interpolated solubility values from his work were compared with solubility data obtained in this work using curve fitting for experimental P–T data and the thermodynamic equations used in the experimental method to calculate the composition of the phases at equilibrium. A maximum relative deviation of 40% was found. Such deviations may arise because different methods (Brunner has used an experimental method with sampling and decompression of the liquid phase) and equations were used to determine the solubility of hydrogen in alcohols, which may give different results, especially in cases where the solubility is very low.
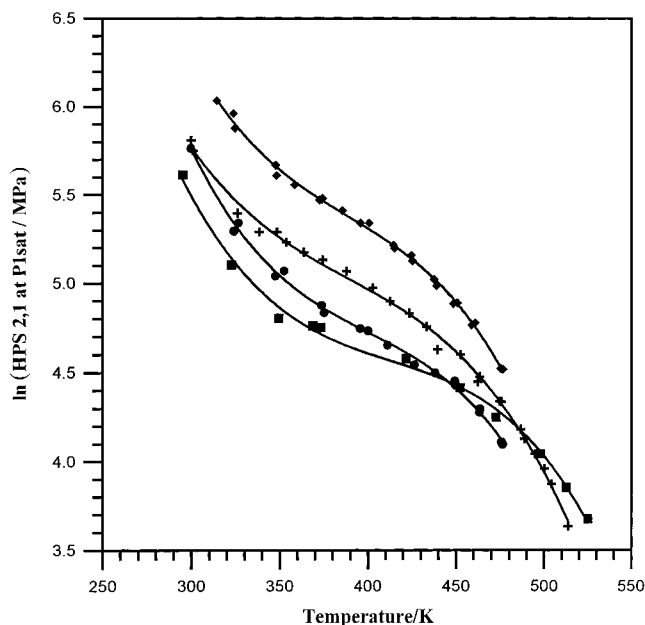
Figure 2. Natural logarithm of the pseudo-Henry's law constant at saturation pressure of the solvent as a function of the absolute temperature: ◆, methanol−hydrogen; ●, ethanol−hydrogen; +, 1-propanol−hydrogen; ■, 1-butanol−hydrogen; −, curve fitting by polynomial regression.

Table 7. Coefficients of the Polynomial $\ln(H_{2,1}^{PS}) = aT^3 + bT^2 + cT + d$ Obtained by Curve Fitting for the Natural Logarithm of the Pseudo-Henry's Law Constant As a Function of the Absolute Temperature

system	polynomial coefficients			
	$10^8 a$	$10^5 b$	$10^2 c$	d
methanol-H_2	−51.2395	59.8201	−23.8834	37.9228
ethanol-H_2	−52.6234	63.2644	−25.8519	40.5862
propanol-H_2	−36.3045	42.4620	−17.0950	28.6388
butanol-H_2	−40.1448	49.7264	−20.8418	34.1033

Table 8. Uncertainties of Variables Measured in the Experiments

variable	uncertainty
pressure	±0.035 MPa
temperature	±0.3 K
volume	±2 mL
mass	±0.005 g

A comparison between the pseudo-Henry's law constant $H_{2,1}^{PS}$, given in this work, and the true Henry's law constant $H_{2,1}$ was made by calculating activity coefficients of hydrogen using the equation of Wilson. The results show that the values of these activity coefficients of the solute vary in the range 0.98 to 1.05 for all alcohols studied. Comparable results were also obtained by Breman et al.[4] for hydrogen dissolved in some hydrocarbons and alcohols. As a result, one can assume that $H_{2,1}^{PS}$ deviates less than 5% from $H_{2,1}$.

Conclusions

Experimental results on the solubility of hydrogen in methanol, ethanol, 1-propanol, and 1-butanol at high

Table 9. Comparison of Solubility Data of Hydrogen in 1-Propanol

		mole fraction of H_2	
T/K	*P*/MPa	this work[a]	Brunner[9][b]
323.15	3.89	0.0154	0.0102
323.15	4.34	0.0175	0.0114
373.15	4.51	0.0255	0.0153
373.15	5.11	0.0276	0.0173

[a] Calculated using *PT* data obtained by curve fitting of experimental data. [b] Estimated through linear interpolation.

temperatures and pressures have been reported. The solubility of hydrogen in all alcohols increases with increasing temperature and pressure. It also increases with increasing carbon chain length of the alcohol molecule, except for ethanol, which presented a solubility for hydrogen slightly higher than that in 1-propanol.

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