214 *J. Chem. Eng. Data* **1997,** *42,* 214−215

Solubility of Hydrogen in Octane, 1-Octanol, and Squalane

Kwang J. Kim,* Timothy R. Way, and K. Thomas Feldman, Jr.

Thermal *Electric* Devices, Inc., Albuquerque, New Mexico 87131

Arsalan Razani

Mechanical Engineering Department, University of New Mexico, Albuquerque, New Mexico 87131

The solubilities of hydrogen in various liquids were measured over the pressure ranges from 690 to 1380 kPa at a temperature of 22 °C by using the modified Benson and Krause method. The liquids include octane, 1-octanol, and squalane. The solubility increases with increasing pressure and is described by Henry's Law.

Introduction

The solubility of hydrogen in the liquid is an important parameter in the design of hydrogen−liquid−hydride slurry (HLHS) reactors (Chaudhari and Ramachandran, 1980; Bjurström, 1991; Johnson and Reilly, 1986; Reilly and Johnson, 1984; Kim et al., 1996). In the literature, there are a limited number of studies related to the solubility of hydrogen in the liquid for the pressure range above 100 kPa. Hydrogen solubilities in undecane and octane were previously measured by Johnson and Reilly (1986). Measurements were also made for decane by Schofield et al. (1992). In this paper, as a part of a study of HLHS reactors, we present solubility data for hydrogen in various liquids including octane, 1-octanol, and squalane at pressures from 690 to 1380 kPa.

For low concentrations of gas in the liquid, a linear relationship between the mole fraction of gas in the liquid, x_s, and the gas pressure, P, known as "Henry's Law" is

$$x_s = H_L P \tag{1}$$

where H_L is the Henry's law constant.

Experimental Section

In Figure 1, a schematic of the test apparatus is shown. The Benson and Krause method (Fogg, 1990) was modified for a falling pressure experiment. The apparatus consists of a packed bed absorber, a liquid pump, and a hydrogen tank. The absorber is made of clear polycarbonate tube having an outside diameter of 3.81 cm with a 0.64 cm wall thickness. The effective length of the absorber is 46 cm. In order to avoid leaks O-rings were placed between the brass end plates and the polycarbonate tube. The liquid phase mixing and the contact area between the liquid and hydrogen gas are improved by flowing the liquid over a compact packing (Pro-Pak, protruded). A centrifugal pump was chosen for the liquid pump. The hydrogen tank is a leak-tight stainless steel tank with a volume of 609.3 mL. The liquid is pumped from the bottom of the absorber into the top of the absorber. Then, it falls as a thin film over the compact packing. After an appropriate time, the liquid in the absorber becomes saturated with hydrogen and no further pressure change in the hydrogen tank is observed. By knowing the pressure change in the hydrogen tank before and after an experiment, hydrogen solubility in the liquid is calculated. The absorber pressure was varied from approximately 690 to 1380 kPa by using a pressure regulator while the temperature was maintained at 22 ± 0.5 °C. The uncertainty of the pressure transducer is within ±1.4 kPa.

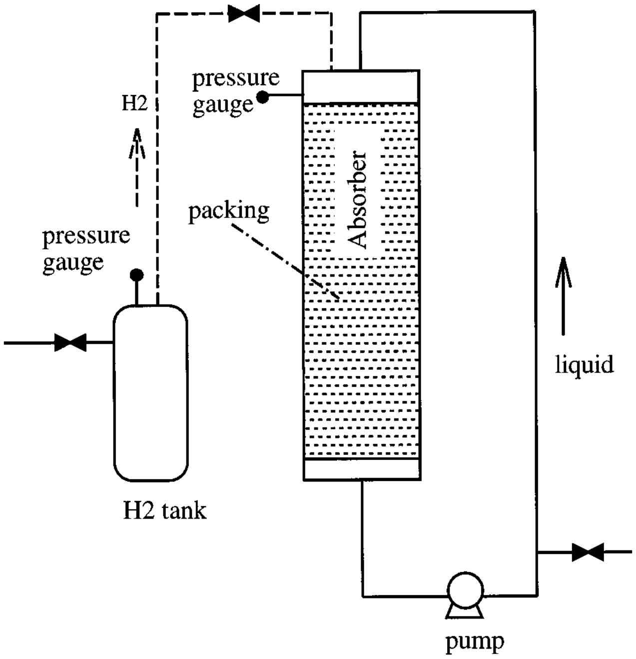

Figure 1. Schematic of the solubility test apparatus.

Octane (99.9+%), 1-octanol (reagent grade), and squalane (99+%) were purchased from SIGMA Chemical Co., Inc., J. T. Baker, Inc., and Aldrich Chemical Co., Inc., respectively. Hydrogen (99.99+%) was obtained from Air Products Corp. No treatment was carried out on any of the chemicals.

Results and Discussion

First, octane was tested for the purpose of comparison between the present work and the published data. In Figure 2, the measured hydrogen solubilities in octane are shown together with the results of Johnson and Reilly (1986). Mole fraction, x_s, was used for the representation of solubility. In general, similar trends are observed.

---

* Author to whom all correspondence should be address. Present address is Heating/Air-conditioning Laboratory, Mechanical Engineering Department, University of New Mexico, Albuquerque, NM 87131. Tel/Fax: 505-277-1335, E-mail: kwangkim@slider.unm.edu.

S0021-9568(96)00268-3 CCC: $14.00

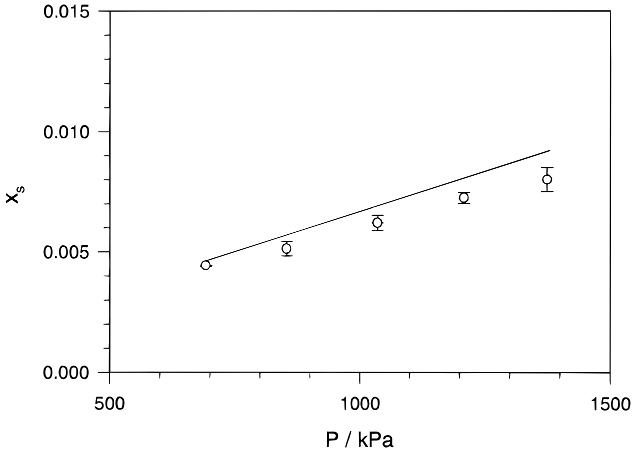

Figure 2. Measured hydrogen solubility in octane: (○) measured; (—) Johnson and Reilly (1986).

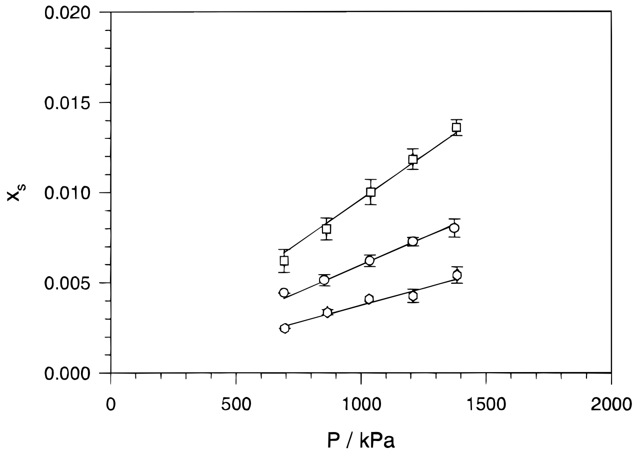

Figure 3. Measured hydrogen solubilities in various liquids: (○) octane; (⬡) 1-octanol; (□) squalane.

Table 1. Mole Fraction Solubilities of Hydrogen, x_s, in Octane, 1-Octanol, and Squalane at 22 °C

liquid	P/kPa	$10^3 x_s$
octane	689.5	4.42 ± 0.01
	861.9	5.13 ± 0.26
	1034.3	6.20 ± 0.28
	1206.6	7.25 ± 0.21
	1379.0	8.01 ± 0.43
1-octanol	689.5	2.46 ± 0.01
	861.9	3.36 ± 0.13
	1034.3	4.10 ± 0.33
	1206.6	4.26 ± 0.33
	1379.0	5.41 ± 0.40
squalane	689.5	6.20 ± 0.57
	861.9	7.97 ± 0.54
	1034.3	10.01 ± 0.64
	1206.6	11.82 ± 0.50
	1379.0	13.58 ± 0.39

Table 2. Measured Henry's Law Constant, H_L, for Various Liquids

liquid	$10^6 H_L$/kPa^{-1}
octane	5.98
1-octanol	3.76
squalane	9.63

The measured solubilities of hydrogen in octane, 1-octanol, and squalane are given in Table 1 along with the standard deviation at the given pressure. They are also plotted in Figure 3 in terms of mole fraction, x_s, against pressure, P. All three liquids adhere to showing a linear relationship between solubility and pressure. This indicates that Henry's law is sufficient to describe the solubilities of hydrogen in these liquids in the pressure ranges from 690 to 1380 kPa. Based upon eq 1, the values of Henry's law constants, H_L, for octane, 1-octanol, and squalane were calculated by regression and are given in Table 2.

The liquids studied range from nonpolar (octane) to polar (1-octanol). For the same number of carbon atoms, the solubility of hydrogen in nonpolar species is much greater than that of polar species as observed by Pollack (1991). Squalane, $[(CH_3)_2CH(CH_2)_3CH(CH_3)(CH_2)_3CH(CH_3)CH_2\text{-}CH_2]_2$, has the largest hydrogen solubility of the liquids studied.

Literature Cited

Bjurström, H. Slurries as Absorbent Fluids. *Proceedings of Absorption Heat Pump Conference '91*, Tokyo, Japan; 1991; pp 171−176.

Chaudhari, R. V.; Ramachandran, P. A. Three Phase Slurry Reactor. *AIChE J.* **1980**, *26*, 177−201.

Fogg, P. G.; Gerrard, W. *Solubility of Gases in Liquids*; John Wiley & Sons: New York, 1990; pp 14−15.

Johnson, J. R.; Reilly, J. J. Kinetics of Hydrogen Absorption by Metal Hydride Suspensions. *Z. Phys. Chem. Neue Folge* **1986**, *147S*, 263−272.

Kim, K. J.; Feldman, K. T., Jr.; Razani, A. Heat-driven Hydride Slurry Heat Pumps. *Int. J. Refrig.* **1996**, submitted for review.

Pollack, G. L. Why Gases Dissolve in Liquids. *Science* **1991**, *251*, 1323−1330.

Reilly, J. J.; Johnson, J. R. The Kinetics of the Absorption of Hydrogen by $LaNi_5H_x$-n-Undecane Suspensions. *J. Less-Common Met.* **1984**, *104*, 175−190.

Schofield, B. A.; Ring, Z. E.; Missen, R. W. Solubility of Hydrogen in a White Oil. *Can. J. Chem. Eng.* **1992**, *70*, 822−824.

Received for review August 5, 1996. Accepted October 31, 1996.[⊗] This work was supported by the Department of Energy (DOE) under contract number DOE/ER-0598. The program manager was Dr. G. C. Carter.

JE960268Z

[⊗] Abstract published in *Advance ACS Abstracts,* December 15, 1996.