SOLUBILITY OF HYDROGEN AND CARBON MONOXIDE IN WATER AND SOME ORGANIC SOLVENTS

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Abstract— The solubility of hydrogen and carbon monoxide in water, octene, toluene and nonanal in the range 298-373 K and 0.5-1.5 MPa was studied. The experimental values of the solubility of H₂ and CO at 353 K, 363 K and 373 K were determined by the absorption method as a function of gas pressure in the solvents. The estimation of solubility of gases in water and organic solvents was also accomplished. The proposed method is based on the theory of Regular Solutions by the correlations of Prausnitz-Shair and Yen-McKetta corrected by Lemcoff factor for polar solvents. The critical temperature was predicted by Group Interaction Contribution approach. The experimental results were compared with theoretical prediction of solubility and found to agree with an average relative error of 2.6 %.

Keywords— Gas Solubility, Hydrogen, Carbon Monoxide, Theory of Regular Solutions.

I. INTRODUCTION

The solubility of gases in liquid media is an important parameter required for the interpretation of rate data in gas-liquid, gas-liquid-liquid and gas-liquid-solid reactions. Among them, the hydroformylation of alkenes and fine chemicals by biphasic and supported aqueous phase catalysis have gained considerable interest in recent years (Kuntz, 1975; Arhancet *et al.*, 1989; Jáuregui-Haza *et al.*, 2001). A large volume of solubility values of hydrogen and carbon monoxide in a variety of solvents is available (Pray, 1952; Crozier and Yamamoto, 1974; Sokolov and Polyakov, 1977; Young, 1981; Brunner, 1985; Cargill, 1990; Purwanto *et al.*, 1996; Lekhal, 1998; Nair *et al.*, 1999), but limited data are available at higher temperatures and pressures.

In the present work the solubility of hydrogen and carbon monoxide in water, octene, toluene and nonanal in the range 298-373 K and 0.5-1.5 MPa was studied. Taking into account that a few data of solubility for H_2 and CO at 353 K, 363 K and 373 K are available, they were experimentally determined. The estimation of the solubility of these gases in water and different organic

solvents, using a model based on the theory of Regular Solutions, was also accomplished.

II. EXPERIMENTAL SECTION

The solvents octene, toluene and nonanal with a purity greater than 98 %, procured from Aldrich, were used as received. The solubility of H₂ and CO was determined by the absorption method as a function of the gas pressure in the solvents in a 5.0 x 10^{-4} m³ capacity stirred autoclave (Autoclave Engineers). The experimental setup (Fig. 1) was described elsewhere (Purwanto *et al.*, 1996). The temperature of the liquid in the reactor was controlled within ± 1 K. A pressure transducer having a precision of ± 1 kPa was used to measure the pressure. Hydrogen, carbon monoxide and nitrogen with purity of 99 %, supplied by Prodair, were used. The solvents were degassed by three freeze-pump-thaw cycles using nitrogen.

In a typical experiment, a known volume of solvent was introduced into the autoclave and the contents were heated to a desired temperature. After the thermal equilibrium was attained, the void space in the reactor was carefully flushed with the gas and pressurized to the level required. The contents were then stirred for about 10 min to equilibrate the liquid phase with the gas. The pressure change in the autoclave was recorded on-line as a function of time till it remained constant, indicating saturation of the liquid phase. From the initial and final pressure readings, the solubility was calculated in mole fraction. Each experiment was carried out three times.

III. RESULTS AND DISCUSSION

A. Solubility Data

The solubility of hydrogen and carbon monoxide in water, octene, toluene and nonanal was measured at 353 K, 363 K and 373 K in a pressure range of 0.5-1.5 MPa. The effect of pressure was found to be linear for all the systems, according to the Henry's law. The same behavior of gas solubility with pressure at values lower than 10 MPa has been reported before (Brunner, 1985; Purwanto *et al.*, 1996; Lekhal, 1998; Nair *et al.*, 1999).