Iodine solubility in a HI-H_2O binary solvent system for a VHTR – based SI process

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1. Introduction

The sulfur-iodine (SI) cycle and Westinghouse hybrid sulfur (HyS) cycle, coupled to a very high temperature gas-cooled reactor (VHTR), are well known as feasible technologies for hydrogen mass production [1].

Although solubility information is important to prevent tube clogging due to iodine deposition inside the tube wall and to successfully transport HIx solution in the SI process, the experimental data of the iodine solubility in the HI-H_2O binary solvent system is scarce [2].

In the present study, the solubility correlation of iodine in a hydriodic acid aqueous solution has been obtained using the experimental data reported in reference [3] and [4]. The correlation equation can be applied to estimate I_2 solubility according to the operation condition of the SI cycle.

2. Methods and Results

SigmaPlot (ver 10.0) was used to find the correlation equation. The best fitted equation was selected from the library of SigmaPlot (ver 10.0).

2.1 I_2 Solubility in the system HI-H_2O (0~57 wt%)

Kracek in 1931 summarized previous reliable data for the solubility of iodine in water in the temperature range of 0 to 60 °C and expanded his experimental data up to 200°C. Furthermore the iodine solubility in the HI-H_2O binary system is absolutely required when the precipitation technology to recover excess iodine dissolved into the hydriodic acid solution is adopted in the SI process. Based on this necessity of solubility information, a Korea University research team carried out an experiment to obtain the iodine solubility data in the HI-H_2O binary system [4].

Previous experimental data of the solubility of iodine at various HI concentration and temperatures in the mixed solvent of hydrogen iodide (HI) + water (H_2O) are shown in Table Ⅰ.

Table Ⅰ: Experimental Data of the Solubility of Iodine in Hydriodic Acid Solution

Initial solvent composition		T(K)	I_2 solubility (mole fraction)
HI (mole fraction)	H_2O (mole fraction)		
0	1	298	0.0024
		303	0.0033
		318	0.0046
		333	0.0075
		359	0.0204
0.107	0.893	298	0.117
		303	0.138
		318	0.153
		333	0.147
		359	0.267
0.123	0.877	298	0.161
		303	0.185
		318	0.171
		333	0.193
		359	0.311
0.142	0.858	298	0.205
		303	0.220
		318	0.228
		333	0.260
		359	0.383
0.157	0.843	298	0.237
		303	0.259
		318	0.245
		333	0.299
		359	0.465

2.2 Correlation of experimental data

Iodine solubility (x_{I_2}) has a function of initial concentration (HI^{o}) of HI in the mixed solvent as shown in Eq.(1).

$$x_{I_2} = Ax_{HI^o}^2 + Bx_{HI^o} + C \quad (1)$$

Coefficients A, B and C in Eq.(1) can be represented as follows in the polynomial equations.

$$A = a_1T^2 + b_1T + c_1 \quad (2)$$

$$B = a_2T^2 + b_2T + c_2 \quad (3)$$

$$C = a_3T^2 + b_3T + c_3 \quad (4)$$

where x_{I_2} : I_2 solubility (mole fraction)
x_{HI^o} : HI inital solvent composition (mole fraction)
T : Temperature (K)
a_i, b_i, c_i : Constants in Eq.(2) to (4)

When Eq.(1) is correlated with experimental data of Table Ⅰ, the value of constants a_i, b_i and c_i were found as shown in Table Ⅱ.

Table Ⅱ: Constants in Eq.(2) to (4)

Coefficient	a	b	c
A	1.59E-03	-0.9643	152.7598
B	1.87E-04	-0.116	18.4415
C	5.63E-06	-3.40E-03	0.51664

Eq. (5) has a standard error of $\pm 1.998 \times 10^{-3}$ and agrees well with experimental data as shown in Fig .1.

$$x_{I_2} = (1.59\times10^{-3}\,T^2 - 0.9643T + 152.7598)\,x^2_{HI^0} + (1.87\times10^{-4}\,T^2 - 0.116T + 18.4415)\,x_{HI^0} + 5.63\times10^{-6}T^2 - 3.40\times10^{-3}\,T + 0.51664 \quad (5)$$

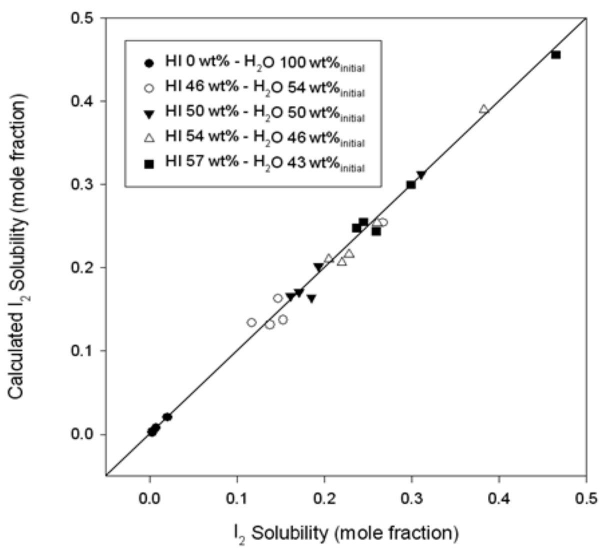

Fig.1. Comparison of calculated values with experimental data

3. Summary

As a result of this work, the engineering equation used to calculate the solubility of iodine at various HI concentrations and temperatures has been obtained. This equation can be applied to anticipate the solubility of iodine within $\pm 1.998 \times 10^{-3}$ standard error and will be used to design the excess I_2 precipitator for a VHTR-based SI process.

Acknowledgments

This work has been performed under mid-and-long-term Nuclear R&D Projects by the Ministry of Education, Science and Technology, Republic of Korea.

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