Viscosity properties of chemical mixture streams for the VHTR - based SI process

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1. Introduction

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

The SI process consists of a Bunsen reactor and H_2SO_4 , SO_3, and HIx decomposers.

The physicochemical property of the chemical material used in the SI process should be considered when sizing the device. In particular, viscosity is essential for calculating the overall heat transfer coefficient.

In this paper, the viscosity of the previously well known pure material and mixture, calculated based on the equation in Perry's chemical engineers' hand book, is introduced[2].

2. Methods and Results

OriginPro (ver 8.0) was used to develop the correlation equations and graph the results. The best fitted equations were selected from the library of OriginPro (ver 8.0).

2.1 The overall heat transfer coefficient

It is a common method to relate the total rate of heat transfer to the total heat transfer area by using the overall heat transfer coefficient (U), which includes individual terms; the reciprocal of the overall coefficient (U) is given by the following equations [3]:

$$\frac{1}{U} = \frac{1}{h_o} + \frac{1}{h_i(D_i/D_o)} + \frac{1}{h_w} + \frac{1}{h_s} \tag{1}$$

$$h_i = 0.125\frac{\lambda_i}{D_i}\left(\frac{D_pG_i}{\mu_i}\right)^{0.75} \qquad 0.35 < \frac{D_p}{D_i} < 0.60 \tag{2}$$

$$h_i = 0.813\frac{\lambda_i}{D_i}\exp\left(-6D_p/D_i\right)\left(\frac{D_pG_i}{\mu_i}\right)^{0.9} \qquad \frac{D_p}{D_i} < 0.35 \tag{3}$$

$$h_0 = \frac{0.273c_pG_o}{(c_p\mu_o/\lambda_o)^{2/3}(D_oG_o/\mu_o)^{0.365}} \tag{4}$$

$$h_w = \frac{2\lambda_t}{(D_o - D_i)} \tag{5}$$

U : overall heat transfer coefficient [W/(m2 . K)]
h_o : outside heat transfer coefficient [W/(m2 . K)]
h_i : inside heat transfer coefficient [W/(m2 . K)]
D_i : internal diameter of tube [m]
D_o: external diameter of tube [m]
D_p: diameter of packing material [m]
C : conversion factor(British units to MKS units,)
h_w: heat transfer across tube wall [W/(m2 . K)]
h_s : fouling heat transfer coefficient [W/(m2 . K)]
G_o : external superficial mass flow rate per unit area [kg/(s . m2)]
G_i : internal superficial mass flow rate per unit area [kg/(s . m2)]
λ_i : inside thermal conductivity [W/(m . K)]
λ_o : outside thermal conductivity [W/(m . K)]
λ_t : thermal conductivity of tube [W/(m . K)]
μ_i : internal viscosity of fluid [Pa . s]
μ_o : external viscosity of fluid [Pa . s]
c_p : heat capacity of fluid [kJ/(kg . K)]

Where the equations for each heat transfer coefficient of a tube from the inside (hi), from the outside (ho), and across the wall (hw) are given in chemical engineering's handbooks[4], respectively. Two of the equations for the heat transfer coefficient from the inside of a tube can be applied to a ratio of particle diameter (Dp) to inside tube diameter (Di).

2.2 Viscosity of pure material

Based on the equation in the Chemical Engineering Research Information Center (CERIC)[5], the correlation equation for the viscosity of each material is as follows (Table I):

Table I: Equation viscosity of pure material

Material	Phase	μ(cp)	Operating temperature
H2O	Liq	$\mu = -24.71 + 4209/T + 0.04527T - 3.376\times10^{-5}T^2$	273.15~643.15K
	Gas	$\mu = -0.003189 + 4.145\times10^{-5}T - 8.272\times10^{-10}T^2$	273.15~1273.15K
SO3	Liq	$\mu = 28.94 - 2277/T - 0.09392T + 8.064\times10^{-5}T^2$	289.15~483.15K
	Gas	$\mu = 0.0004207 + 4.712\times10^{-5}T - 6.834\times10^{-9}T^2$	173.15~1673.15K
SO2	Liq	$\mu = -6.148 + 936.5/T + 0.01414T - 2.887\times10^{-5}T^2$	203.15~428.15K
	Gas	$\mu = -0.0003793 + 4.645\times10^{-5}T - 7.276\times10^{-9}T^2$	173.15~1673.15K
O2	Liq	$\mu = -4.771 + 214.6/T + 0.01389T - 6.255\times10^{-5}T^2$	55.15~153.15K
	Gas	$\mu = 0.001811 + 6.632\times10^{-5}T - 1.879\times10^{-8}T^2$	113.15~1273.15K
HI	Liq	$\mu = -21.58 + 2337/T + 0.07336T - 9.717\times10^{-5}T^2$	223.15~423.15K
	Gas	$\mu = -0.001765 + 6.976999\times10^{-5}T - 1.365\times10^{-8}T^2$	153.15~1673.15K
I2	Liq	$\mu = -2.083 + 1195/T - 0.0004566T - 1.08\times10^{-7}T^2$	387.15~473.15K
H2	Liq	$\mu = -11.18 + 57.86/T + 0.3244T - 0.006385\times10^{-9}T^2$	15.15~33.15K
	Gas	$\mu = 0.002187 + 0.0000222T - 3.75\times10^{-9}T^2$	113.15~1473.15K

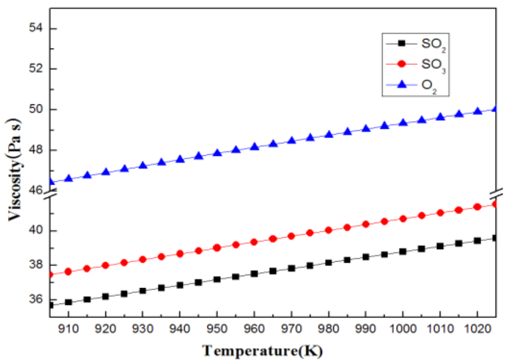

Fig. 1. Viscosity of pure materials at various temperatures

2.3 Viscosity equation of gaseous mixture

Based on the equation in Perry's chemical engineers' handbook[2], viscosities of gaseous mixtures at low pressures can be estimated by using Eqs (6) and (7).

$$\mu_m = \sum_{i=1}^{n}\frac{\mu_i}{1+\sum_{j=1}^{n}(Q_{ij}\frac{y_j}{y_i})} \tag{6}$$

$$Q_{ij} = \frac{1+[(\frac{\mu_i}{\mu_j})^{1/2}(\frac{M_j}{M_i})^{1/4}]^2}{\sqrt{8}[1+\frac{M_i}{M_j}]^{1/2}} \tag{7}$$

The mixing rule is given by Eq (6) with the interaction parameter Q_{ij} for each pair of components defined by (7).

-The viscosity of gaseous mixtures at high pressures.

$$(\mu_{mix} - \mu_{mix}^{0})\zeta_{mix} = (1.08)[\exp(1.439\rho_{\tau,mix}) - \exp(-1.11\rho_{\tau,mix}^{1.858})] \quad (8)$$

$$\rho_\tau = \frac{P_{mix}}{P_{c,mix}} \quad (9) \qquad Z_{c,mix} = \sum_i^n y_u T_{c,i} \quad (10) \qquad P_{c,mix} = \frac{Z_{c,mix} R T_{c,mix}}{V_{c,mix}} \quad (11)$$

$$\zeta_{mix} = T_{c,mix}^{1/6} M \omega_{mix}^{-1/2} P_{mix}^{-1/2} \quad (12) \qquad T_{c,mix} = \sum_i^n y_u T_{c,i} \quad (13)$$

$$V_{c,mix} = \sum_i^n y_u V_{c,i} \quad (14)$$

In the case of aqueous mixture, viscosity can be calculated by using Eq(15).

$$\mu_{mix} = \left(\sum_{i=1}^{n} x_i \mu_i^{1/3}\right)^3 \quad (15)$$

The critical properties of chemical compounds are as follows (Table Ⅱ)[6,7]:

Table Ⅱ: Critical properties of chemical compounds

Material	Tc[K]	Pc[kPa]	Vc [m3/kgmol]	Acentric Factor
H_2O	647.14	22060	0.056	0.343
H_2SO_4	925	6400	0.17	
SO_3	490.85	8200	0.127	0.423
SO_2	430.8	7884	0.122	0.244
O_2	154.59	5043	0.073	0.020
HI	424	8210	0.105	
H2	33.2	1300	0.079	-0.215
I2	112.58	2264.89	0.15498	

The unknown critical properties of H_2SO_4 and I_2 are calculated using Van der Waale's constants, a and b. Van der Waale's constants are as follows (Table Ⅲ)[8]:

Table Ⅲ: Van der Waal's constants

Molecular Formula	a bar L2/mol2	b L/mol
HI	6.309	0.05303
H2	0.2453	0.02651
H2O	5.537	0.03049
He	0.0346	0.02387
O2	1.382	0.03186
SO2	6.865	0.05679
I2	1.632	0.05166

2.4 viscosity of gaseous mixture

- Binary system

The calculated binary system by Eqs (6) and (7) is shown in Fig.2.

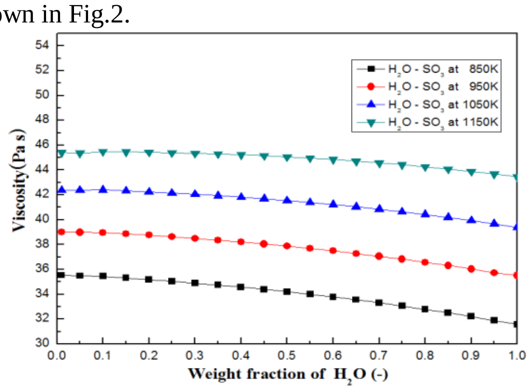

Fig. 2. Viscosity of $H_2O - SO_3$ binary gas mixture as a function of H_2O weight fraction at various temperatures.

- Ternary system

Fig.3 shows the correlation of the mixing ratio and viscosity of H_2-I_2-HI which is a ternary system.

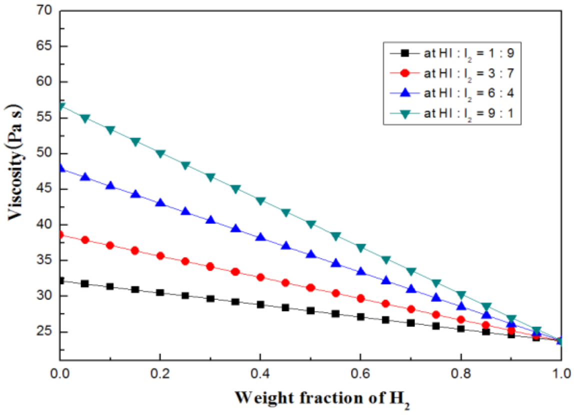

Fig. 3. Viscosity of H_2-I_2-HI Ternary gas mixture as a function of I_2 weight fraction at various ratios of HI and I_2

3. Summary

As a result of this work, the method to estimate viscosities of the binary and ternary chemical systems was introduced. This result is expected to contribute to improving the calculation accuracy of KAERI –DySCO for the dynamic simulation of the SI process.

Acknowledgments

This work was 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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