Sulfuric Acid Decomposer Sizing for a Nuclear Hydrogen Production by a SI Process

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1. Introduction

Hydrogen can be an attractive energy if it can be produced cleanly and in a cost effective manner. Nuclear energy can be used as a source of a high temperature process up to 1000℃ for a hydrogen production. The sulfur-iodine (SI) cycle is a baseline candidate thermo-chemical process. It consists of the following three chemical reactions which yield a dissociation of water [1].

$$I_2 + SO_2 + 2H_2O \rightarrow 2HI + H_2SO_4 \qquad (1)$$

$$H_2SO_4 \rightarrow H_2O + SO_2 + 1/2O_2 \qquad (2)$$

$$2HI \rightarrow H_2 + I_2 \qquad (3)$$

The decomposition at a high temperature of the sulfuric acid is the most energy-demanding reaction both from fundamental and applied points of views which represents the key reaction of the whole SI cycle.

In this paper, shell-and-tube type is selected and its fluidic characteristics are applied to an overall heat transfer coefficient calculation. As a result of the study, the sulfuric acid decomposers for 300mole/s (200MW$_{th}$ VHTR 40% thermal efficiency) and 60mole/s (40MW$_{th}$ VHTR 40% thermal efficiency) hydrogen production rates are presented and discussed.

2. Sizing Procedure for Sulfuric Acid Decomposer

2.1. Modeling

The rate equation for the decomposition of sulfuric acid was based on equation (4), whereas the reaction rate constant is equation (5).

$$-r_{SA} = -k_d[C_{SA} - \frac{1}{K_c}C_{SO_3}] \qquad (4)$$

$$k_d = A\exp(-E_a / RT) \qquad (5)$$

The rate equation is a reversible 1st order equation and the reaction rate constant is the Arrhenius equation which is a function of the temperature.

For sulfuric acid decomposition, the activation energy and pre-exponential factor are -10570kcal/(mol K) and 298 h^{-1} [2] respectively. And the equilibrium constant is obtained from HSC5.1 [3]. Fig. 1 shows the non-isothermal plug flow reactor model for the sulfuric acid decomposer.

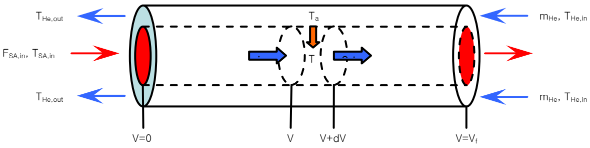

Fig. 1. Non-isothermal plug flow reactor model for sulfuric acid Decomposer

$$\frac{dF_{SA}}{dV} = -r_{SA} \qquad (6)$$

$$\frac{dT_{SA}}{dV} = \frac{Ua(T_{He} - T_{SA}) + r_{SA}\Delta H_{RX}}{\sum F_i c_{p,i}} \qquad (7)$$

$$\frac{dT_{He}}{dV} = \frac{Ua(T_{He} - T_{SA})}{F_{He}c_{p,He}} \qquad (8)$$

Equation (6) is the material balance equation for the plug flow reactor and equations (7) and (8) are the ordinary differential equations of the process gas temperature change and the Helium temperature change respectively. Heat of reaction is obtained from HSC5.1 [3].

2.2. Overall Heat Transfer Coefficient Calculation

Fluidic characteristics of a process stream are applied to calculate the overall heat transfer coefficient, which are as follows [4].

$$\frac{1}{U} = \frac{1}{h_o} + \frac{1}{h_i(D_i / D_o)} + \frac{1}{h_w} + \frac{1}{h_s} \qquad (9)$$

$$h_i = \frac{0.023c_{p,i}G_i}{(c_{p,i}\mu_i / k_i)^{2/3}(D_iG_i / \mu_i)^{0.2}} \qquad (10)$$

$$h_o = \frac{0.273c_{p,o}G_o}{(c_{p,o}\mu_o / k_o)^{2/3}(D_oG_o / \mu_o)^{0.365}} \qquad (11)$$

$$h_w = \frac{2k_t}{(D_o - D_i)} \qquad (12)$$

Equations (10) and (11) are the tube and shell side heat transfer coefficient equations and equation (12) is the coefficient for the tube material. 5670 W/(m^2 K) for the fouling factor(h_s) is applied from the literature [4].

Thermal conductivity and viscosity are calculated by an equation for a highly pressurized gas phase [5] and the heat capacity is obtained from HSC 5.1 [3]. These properties are calculated at an operating temperature and are assumed to be constant throughout the temperature range. The thermal conductivity of a tube is 16.27 J/(s m K). Inside and outside diameter of a tube is fixed at 1/2in and 5/8in.

2.3. Sulfuric Acid Decomposer Sizing

Table 1. Input/output conditions of the sulfuric acid decomposer

		H_2O	H_2SO_4	SO_3	He
Input (Gas)	Mole Flow Rate [mol/s]	332.57	201.11	280.08	17800
	Temperature [℃]	414			815
Output (Gas)	Mole Flow Rate [mol/s]	532.52	1.16	480.03	17800
	Temperature [℃]	750			712

Input/output conditions for a sulfuric acid decomposer are represented in Table 1 based on a 300mole/s hydrogen production rate and the heat duty is 38048kJ/s. For the condition based on 40MW$_{th}$, each of the flow rates and heat duties is multiplied by 1/5 times.

Then, the heat transfer area and tube length should be calculated by the following equations.

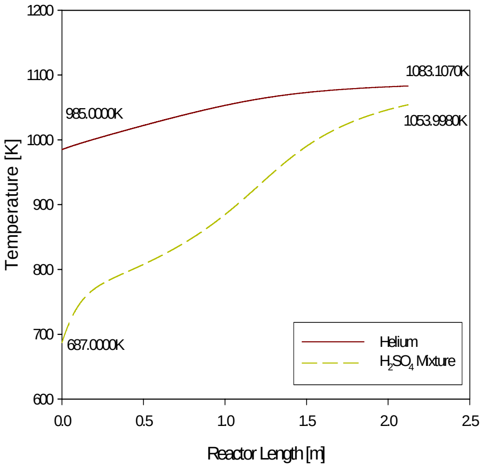

Fig. 2. Temperature profiles for a sulfuric acid decomposer.

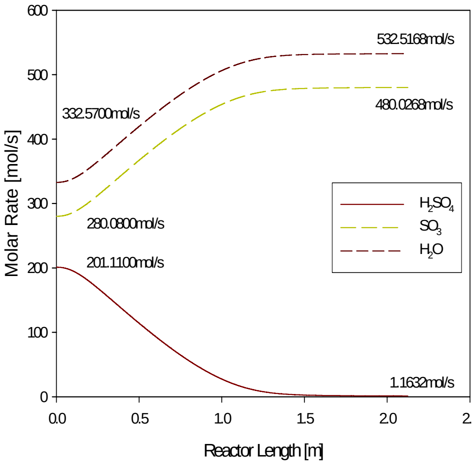

Fig. 3. Mole flow rate changes for a sulfuric acid decomposer.

$$A = \frac{Q}{U \Delta T_{lmtd}} \tag{13}$$

$$L_t = \frac{A}{\pi n_t D_i} \tag{14}$$

Tubes are arranged in a triangular pitch and the tube pitch is 1.25 times that of the tube inside diameter. A gap of the tube bundle to the shell is 10cm.

Fig. 2 and 3 shows the steady state results for the sulfuric acid decomposer.

3. Conclusion

The sulfuric acid decomposer sizing was accomplished and the results are as follows;

Table 2. Sizing results of the sulfuric acid decomposer

Hydrogen production rate		300mole/s	60mole/s
Tube	Inside diameter [in]	1/2	
	Outside diameter [in]	5/8	
	Length [m]	2.12	1.3
	Number [ea]	2470	1100
Shell	Diameter [m]	1.18	0.78
	Height [m]	2.65	1.63
Heat transfer area [m^2]		208.88	57.10
Overall heat transfer coefficient [kJ/(^{o}C m^2 s)]		1.19	0.87

Table 2 shows the calculation results for 200MW$_{th}$ and 40MW$_{th}$. When its scale is 40MW$_{th}$, the superficial mass flow velocity is lowered and the overall heat transfer coefficient is also decreased. Then, the heat transfer area does not decrease linearly.

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