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Computer Program for Equipment Sizing on the Secondary Helium Loop of a VHTR-SI Hydrogen Production System

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1. Introduction

The Sulfur-Iodine (SI) process coupled to a very high temperature gas-cooled reactor (VHTR) is well known as a feasible technology to produce hydrogen. The SI process can be divided into three sections based on the chemical reactions a Bunsen reaction (Section 1), a Sulfur acid concentration and decomposition (Section 2) and a hydrogen iodine concentration and decomposition (Section 3) [1].

The heat required in the SI process can be supplied through an intermediate heat exchanger (IHX) by the VHTR. On the other hand, Helium is used as a high temperature energy carrier gas between the VHTR and the IHX or the IHX and the SI process. In the SI process, chemical reactors that receive thermal energy from the helium are: A sulfuric acid vaporizer, a sulfuric acid decomposer, a sulfuric trioxide decomposer, and a hydriodic acid decomposer including pre-heating part [2].

The sizing of such chemical reactors is essentially required for dynamic simulation of the VHTR-SI process.

In this paper, a sizing program which can calculate the sizing of each chemical reactor to satisfy mass and energy balance at a given operation condition has been introduced. A graphic user interface (GUI) to visualize calculated sizing results of the chemical reactors has been added for the effective program operation.

2. Method and Results

2.1 SI process

SI process coupled to a VHTR requires an intermediate heat exchanger with chemical reaction sections represented by Eqs. (1)-(3); a Bunsen reaction section (section 1), a sulfuric acid concentration and decomposition section (section 2), and a hydrogen iodine concentration and decomposition section (section 3), as described in Fig. 1.

$$I_2 + SO_2 + 2H_2O \rightarrow 2HI + H_2SO_4 \quad (1)$$
$$H_2SO_4 \rightarrow H_2O + SO_2 + 1/2O_2 \quad (2)$$
$$2HI \rightarrow H_2 + I_2 \quad (3)$$

In Section 1, the exothermic Bunsen reaction (Eq. (1)) produces two kinds of acid (H_2SO_4 and HI) from water, SO_2 and I_2. Reaction products of the Bunsen reaction are separated and sent to the decomposition sections for a conversion to O_2 and H_2 at a high temperature as expressed by Eqs. (2) and (3), respectively.

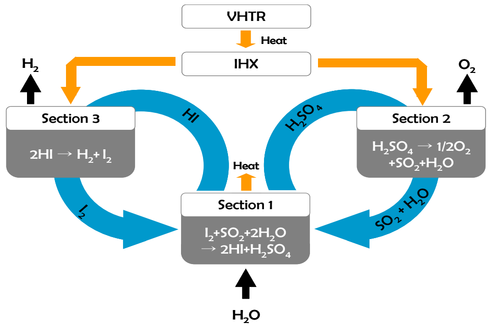

Fig. 1. Schematic chemical reaction flow diagram of the SI process.

2.2 Helium thermal pathway

Conceptual flow diagram of the SI process based on the He-thermal pathway is shown in Fig. 2. As shown in Fig. 2, the secondary helium from the IHX flows through the sulfuric trioxide decomposer and the sulfuric acid decomposer, and then is split in two ways which are connected to the sulfuric acid evaporator and the hydrogen iodine decomposer, respectively.

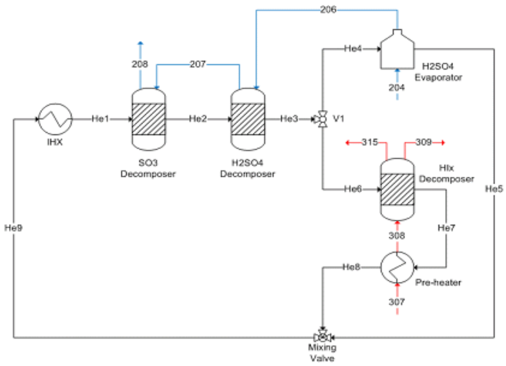

Fig. 2. Conceptual flow diagram for the chemical reactor based on the He thermal pathway.

2.3 Algorithm for sizing and exercise calculation

Boundary conditions and set values to calculate sizing of the chemical reactors in the SI process are shown in Table 1, based on the H_2 productivity of 60 mole/s.

Table 1. Boundary conditions and set values for chemical reactors sizing

Line No. in Fig. 2	Stream Information	Temperature (°C)	Pressure (bar)
He1	Pure helium	910.0	50
He9	Pure helium	450.0	50
204	90 mole % of sulfuric acid and total flow rate of 101.09 mole/s	B.P.	7.09
207	H_2SO_4 decomposer outlet	750.0	7.09
208	SO_3 decomposer outlet, O_2 mole flow rate of 30 mole/s	850.0	7.09
307	H_2O / HI / I_2 mixed vapor, Mole flow rate of each compound: 258.81 / 195.60 / 46.98	274.4	40
308	-	450.0	39.5
309	-	450.0	39.5
315	HI decomposer outlet, H_2 mole flow rate of 60 mole/s	450.0	38

Fig. 3 shows the flow chart for sizing chemical reactors on the secondary helium loop of a VHTR-SI hydrogen production system.

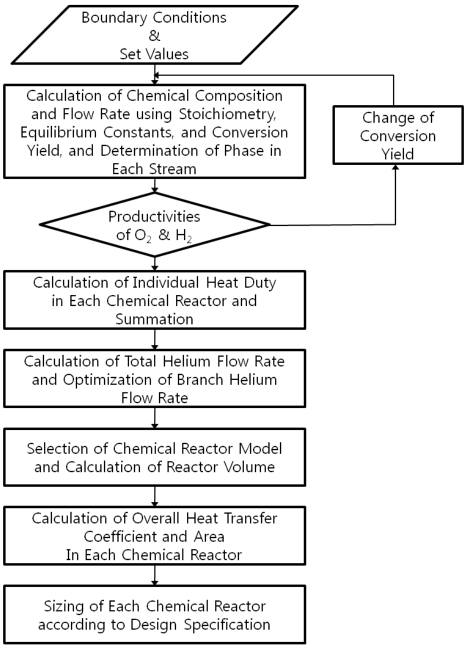

Fig. 3. Flow chart for sizing chemical reactors.

As an exercise calculation, the sizing of a H_2SO_4 vaporizer was performed and the calculation result is shown in Table. 2.

2.4 Graphic user interface of sizing program

In order to visualize the sizing program, a dialog-based window has been configured. Fig. 4 shows a GUI environment of the sizing program. As shown in Fig. 4, the window consists of text boxes, buttons and bit map images. By center of the window, input text box, diagram of the VHTR-SI process and information of the calculated sizing are located on the left side. The specific information of the calculated sizing, selection buttons and operation buttons are located on the right side in the window.

Table 2. Sizing result of H_2SO_4 vaporizer

H_2SO_4 vaporizer sizing result based on the H_2 productivity of 60mole/s					
U[1)] kJ/(m² s °C)	Hi[2)] kJ/(m² s °C)	Ho[3)] kJ/(m² s °C)	Hw[4)] kJ/(m² s °C)	Hs[5)] kJ/(m² s °C)	Q[6)] [kJ/s]
1.80	30.36	4.18	10.25	5.67	12636.27
Lt[m][7)]	Nt[ea][8)]	Ds[m][9)]	DL[m][10)]	LMTD[°C][11)]	
1.79	401	0.8516	3.57	245.22	
Tube inside diameter : 0.0127 m					
Tube outside diameter : 0.0159 m					
Tube (SiC) thermal conductivity : 60.00 J/(m s °C)					
Input mole flow rate [mole/s]					
H_2O	H_2SO_4	SO_3	SO_2	O_2	He
10.8320	90.2620	0.0000	0.0000	0.0000	2596.5003
Output mole flow rate [mole/s]					
H_2O	H_2SO_4	SO_3	SO_2	O_2	He
45.6123	55.4817	34.7803	0.0000	0.0000	2596.5003
Shell side input temperature : 233.80 °C					
Tube side input temperature : 686.75 °C					
Shell side output temperature : 413.09 °C					
Tube side output temperature : 452.62 °C					

1) : Overall heat transfer coefficient 2) : Internal heat transfer coefficient
3) : Outer heat transfer coefficient 4) : Tube heat transfer coefficient
5) : Fouling heat transfer coefficient 6) : Heat duty
7) : Tube length 8) : Number of tube
9) : Shell diameter 10): Shell length
11): Logarithmic mean temperature difference

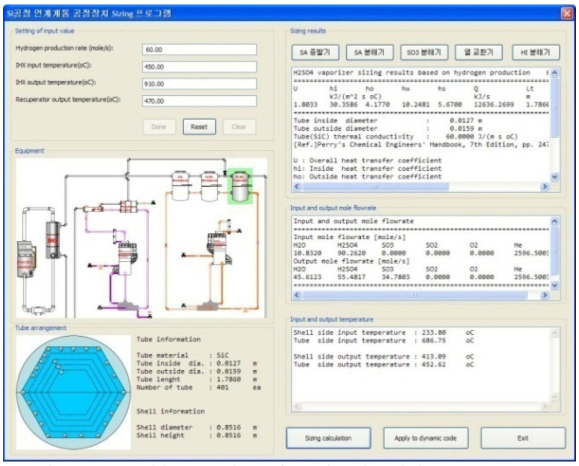

Fig. 4. Graphic user interface for the sizing program.

3. Conclusion

A computer program which can calculate the sizing of each chemical reactor to satisfy mass and energy balance at given operation condition has been introduced. In addition, a graphic user interface (GUI) to visualize calculated sizing results of the chemical reactors has been added for the effective program operation.

Acknowledgments

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REFERENCES

[1]Youngjoon Shin, Kiyoung Lee, Jonghwa Chang, Thermal Efficiency of EED-embedded Sulfur Iodine Cycle, Calculation Note (NHDD-KA07-HP-001-00), 2007.
[2]Wonchul Cho, Dongwon Lee, Kikwang Bae, Youngjoon Shin, Jonghwa Chang, Thermal Efficiency of an Electrodialysis & Membrane Separation-Embedded Sulfur-Iodine Process, Calculation Note(NHDD-HI-CA-10-001), 2010.