Simulation of a VHTR/IHX-SI Process Coupling 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 promising technology to produce hydrogen. Hydrogen production by the VHTR-SI process is achieved by following three chemical reactions: a Bunsen reaction (Section 1), sulfuric acid concentration and decomposition (Section 2), and hydriodic acid 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.

To analyze the dynamic behaviors of the SI process, a dynamic simulation program called the Korea Atomic Energy Research Institute-Dynamic Simulation Code (KAERI-DySCo) was developed in 2011[2]. KAERI-DySCo consists of several module programs that can simulate the transient behaviors as well as the steady state of the chemical reactors placed on the helium thermal pathway in the SI process.

As a part of the verification of KAERI-DySCo, the steady state results of VHTR/IHX-SI coupling components, which are predicted through a dynamic simulation of KAERI-DySCo, are compared with the steady state values obtained from Aspen Plus™ Code simulation [3].

2. Method and Results

2.1 Dynamic simulation model

The dynamic simulation model applied to KAERI-DySCo is shown in Fig. 1. As shown in Fig. 1, the model consists of a VHTR, IHX, and SI process for the hydrogen production system.

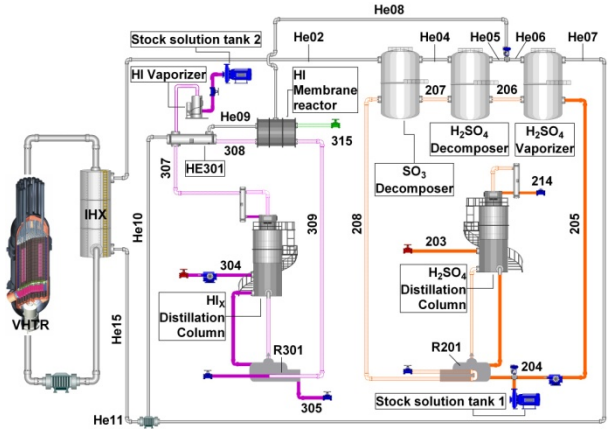

Fig. 1. Dynamic simulation model of KAERI-DySCo.

2.2 Specification of equipment

The purpose of this study is to partially verify the steady state results predicted by KAERI-DySCo. For this purpose, the steady state results of the two chemical reactors in the SI process have been used. One of the two chemical reactors is the SO_3 decomposer in Section 2, and the other is the HI decomposer in Section 3. The equipment specifications applied to KAERI-DySCo are shown in Tables I and II. All specifications are equivalent to a 200 MW_{th} VHTR-SI process with a hydrogen production rate of about 20,000 t·H_2/y.

Table I: Equipment specification and parameters for the SO_3 decomposer

Specification	SO_3 decomposer
Reactor type	Catalyst-packed tube & shell
Applied model	Plug flow
Tube ID/OD(m)	0.013/0.016
Tube L(m)	1.98
# of tube	3712
Shell ID(m)	4.12
Shell L(m)	2.47 (including stationary head)
Heat transfer area(m^2)	292.8
Heat duty(kJ/s)	33768.89

Table II: Equipment specification and parameters for the HI decomposer

Specification	HI decomposer
Reactor type	Catalyst-packed reactors in helium chamber
Applied model	Tank-in-series
System pressure(bar)	40.0
Total number of the reactor	24
Voidage within the reactor	0.2
Hydrogen permeability	0.9
Time lag of pipe(s)	0.001
Apparent volume of the reactor(m^3)	7.89
Volume of the helium chamber(m^3)	8.68
Heat duty(kJ/s)	3817.62

2.3 Boundary conditions

As boundary conditions, outlet stream conditions of the SO_3 decomposer and HI decomposer, such as temperature, pressure, and flow rate are shown in Table III. The conditions listed in Table III are the steady state values calculated using Aspen Plus™ in our previous study [3], and have been used for verifying KAERI-DySCo in this study.

Table III: Boundary conditions of the SO_3 and HI decomposers

Chemical reactor	Stream No.	Boundary conditions	
SO_3 decomposer	208	Temperature	850.0 °C
		Pressure	7.09 bar
		Mole flow rate (mol/s)	H_2O:504.78 H_2SO_4: 0.68 SO_3: 150.62 SO_2: 300.00 O_2 : 150.00
HI decomposer	315	Temperature	450.0 °C
		Pressure	40.0 bar
		Mole flow rate (mol/s)	H_2O: 0.15 HI : 0.15 I_2 : 0.15 H_2 : 300.17

2.4 Comparison of the steady state results

Figs. 2(a) and 2(b) show the steady state of the temperature and compositions of the SO_3 decomposer outlet stream anticipated by KAERI-DySCo and Aspen Plus™. As shown in Figs. 2(a) and 2(b), it is anticipated that the SO_3 decomposer will progress to a steady state within about one second. The mole fractions and temperature in the SO_3 decomposer outlet stream predicted by the KAERI-DySCo agree well within a maximum 10 % error with the steady state results of Aspen Plus™.

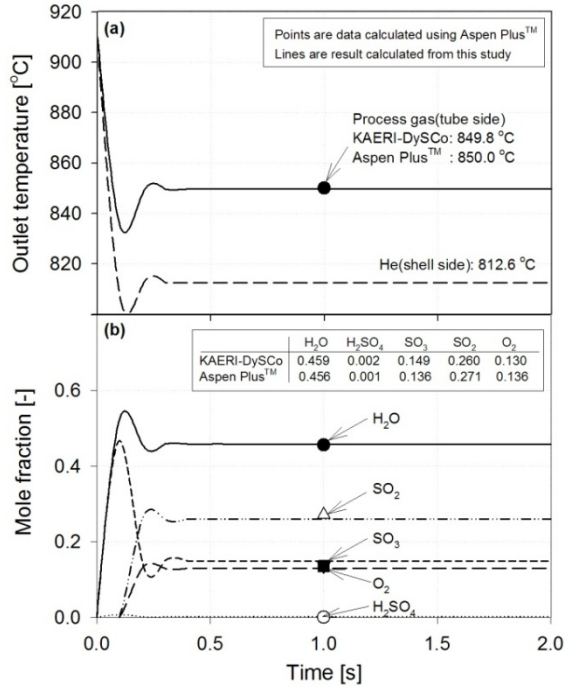

Fig. 2. Steady state results of the SO_3 decomposer predicted by KAERI-DySCo and Aspen Plus™: (a) temperature profile of the outlet process gas and helium and (b) mole fractions of the outlet process gas.

On the other hand, Figs 3(a) and 3(b) show the steady state of the temperature and compositions of the HI decomposer outlet stream predicted by KAERI-DySCo and Aspen Plus™. As shown in Figs 3(a) and 3(b), the temperature and mole flow rate of the HI decomposer outlet stream predicted by KAERI-DySCo approach a steady state within 40 seconds and agree well within a maximum 2 % error with those of Aspen Plus™.

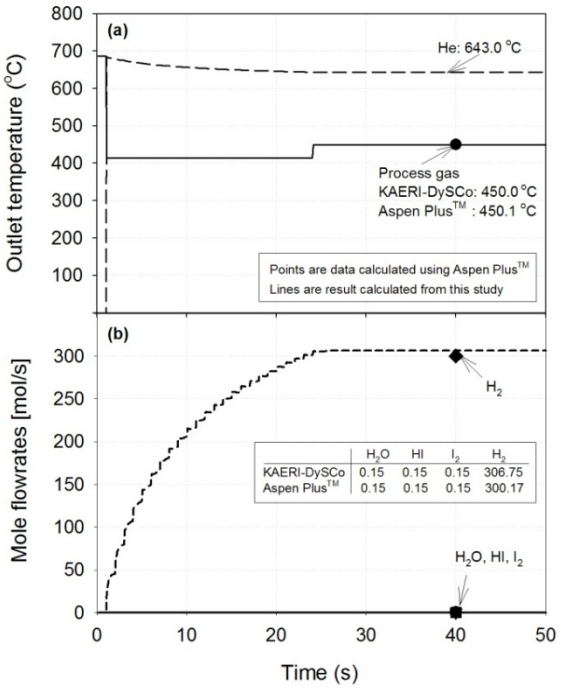

Fig. 3. Steady state results of the HI decomposer predicted by KAERI-DySCo and Aspen Plus™: (a) temperature profile of the outlet process gas and helium and (b) mole fraction of the outlet process gas.

3. Conclusions

The steady state results anticipated through the dynamic simulation of KAERI-DySCo have been partially verified by comparing to the steady state values obtained using Aspen Plus™ code simulation.

Acknowledgments

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