Dynamic Simulation of Temperature Transition on the Secondary Helium Loop of a VHTR-SI Hydrogen Production System

Jiwoon Chang, Youngjoon Shin, Cheong Youn*, Taehoon Lee, Kiyoung Lee, Yongwan Kim
Korea Atomic Energy Research Institute150 Dukjin-dong, Yuseong-gu, Daejeon, Republic of Korea 305-600
**Chungnam National University, 220 Gung-dong, Yuseong-gu, Daejeon, Republic of Korea 305-764*
E-mail;jwjang73@kaeri.re.kr, Tel; +82 42 868 8369, Fax; +82 42 868 8369

1. Introduction

A sulfur–iodine (SI) cycle coupled to a Very High Temperature Gas Cooled Reactor (VHTR) is one of the leading candidates of thermochemical cycles for hydrogen production. The SI cycle can be divided into three sections based on the chemical reactions: a Bunsen reaction (Section 1), sulfuric acid concentration and decomposition (Section 2), and a hydrogen iodine concentration and decomposition (Section 3).

The heat required in the SI cycle 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 IHX and the SI cycle. In the SI cycle, the chemical reactors that receive thermal energy from the helium are a sulfuric acid vaporizer, sulfuric acid decomposer, sulfuric trioxide decomposer, and hydriodic acid decomposer including a pre-heating part.

To simulate the dynamic behavior of the VHTR-SI cycle, the Korea Atomic Energy Research Institute - Dynamic Simulation Code (KAERI-DySCo) based on the Visual C++ has been prepared by the KAERI research group in 2010 [1]. KAERI-DySCo is integration application software, which includes several code modules that can solve the dynamic problem of the seven chemical reactors in the VHTR-SI cycle.

In this paper, the dynamic behavior of the temperature transition on the secondary helium loop of the SI cycle has been simulated using KAERI-DySCo.

2. Methods and Results

2.1 SI cycle

The 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 hydrogen iodine concentration and decomposition section (Section 3).

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

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

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

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 conversion into O_2 and H_2 at high temperature as expressed by Eqs. (2) and (3), respectively.

2.2 Helium Thermal Pathway

Conceptual flow diagram of the SI process based on the He-thermal pathway is shown in Fig. 1. As shown in Fig. 1, the secondary helium from the IHX flows through the sulfuric trioxide decomposer and the sulfuric acid decomposer, and then is split in two ways: connected to the sulfuric acid evaporator and to the hydrogen iodine decomposer [2].

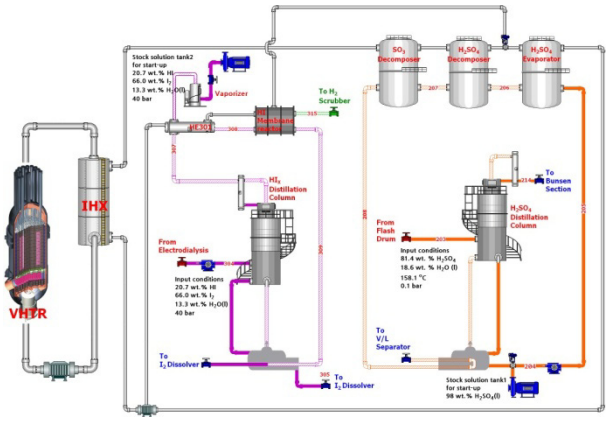

Fig. 1. Conceptual diagram for the VHTR-SI cycle base on the He thermal pathway.

2.3. Assumptions for Start-up

There are some assumptions and operation conditions for a start-up scenario applied to KAERI-DySCo. The principal assumptions and conditions are the following:

1) As an initial internal gas, it is assumed that tubes of the sulfuric acid decomposer and sulfuric trioxide decomposer in Section 2 are filled with helium at a temperature of 910 ℃ and pressure of 7.09 bars, and tubes of the HI decomposer including the pre-heating part in Section 3 are filled with helium at a temperature of 910 ℃ and pressure of 40 bars.
2) Each stage of the H_2SO_4 distillation column is filled with a sulfuric acid solution, which has a concentration of 57 wt. % (H_2SO_4 : H_2O = 563.49 : 451.35 mol/s) and temperature of 158.1 ℃.
3) Each stage of the HI_x solution distillation column is filled with HI_x solution discharged from the electrodialysis equipment. The mole fraction and temperature of the HI_x solution are H_2O:HI:I_2 = 0.635:0.140:0.225 and 256 ℃.

4) In the case of no interaction between process gas and helium discharged from the IHX, it is assumed that there is perfectly thermal equilibrium between the helium discharged from the IHX and the helium filled in the tubes as an initial internal gas.

Fig. 2 shows a data flow diagram for a start-up scenario applied in KAERI-DySCo.

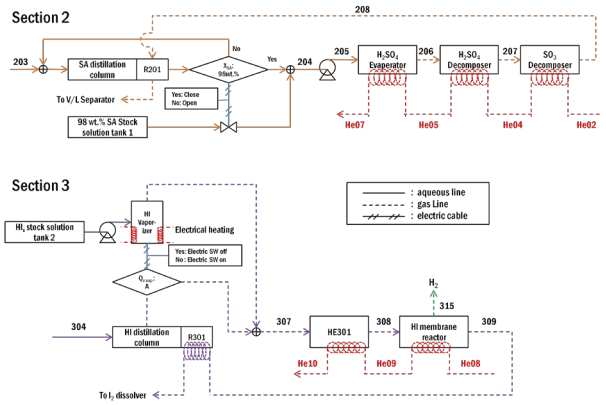

Fig. 2. Schematic data flow diagram for a start-up scenario applied in KAERI-DySCo.

2.4 Operation and Boundary Conditions

The operation and boundary conditions for running KAERI-DySCo are represented in Table I. The conditions listed in Table I are based on a hydrogen production rate of 300 mole/sec [2, 3].

Table I: Conditions for running KAERI-DySCo

Equipment	Item	Operation and boundary conditions
IHX	Outlet mole flowrate Temp., Pressure	He: 16697.74 mol/s 910 ℃, 50 bar
solution tank1	Concentration Temperature	98 wt.% H_2SO_4 158.1 ℃
solution tank2	Concentration Temperature	$H_2O/HI/I_2$ = 13.3/20.7/66.0 wt.% 30 ℃
H_2SO_4 distillation column	Feed mole flowrate Feed temperature	H_2SO_4:H_2O=563.49:451.35 mol/s 158.1 ℃ (Condenser: 38 ℃)
	System pressure	0.1 bar
	Spec. of stages	Num. of stage: 3 (Feeding: 1)
	Holdup (Stage: 0 / 1 / 2)	800 / 280 / 80 kg
	Reboiler heat duty	37300.00 kW_{th}
HI_x Distillation column	Feed mole fraction Feed temperature	H_2O:HI:I_2= 0.635:0.140:0.225 [-] 256.0 ℃
	System pressure	40 bar
	Spec. of stages	Num. of stages: 10 (Feeding: 5)
	Reboiler heat duty	34427.65 kcal/s
	Condenser duty	-657.56 kcal/s
	Holdup	Above feed stage: 9092.0 mole Below feed stage: 13333.3 mole Reboiler: 1000000 mole

2.5 Dynamic Simulation Results

The dynamic simulation results for the temperature transitions in the VHTR-SI cycle using KAERI-DySCo are shown in Figs. 3 and 4. Fig. 3 shows the outlet temperature of process gas as a function of time, while Fig. 4 shows the inlet and outlet temperature of helium as a function of time.

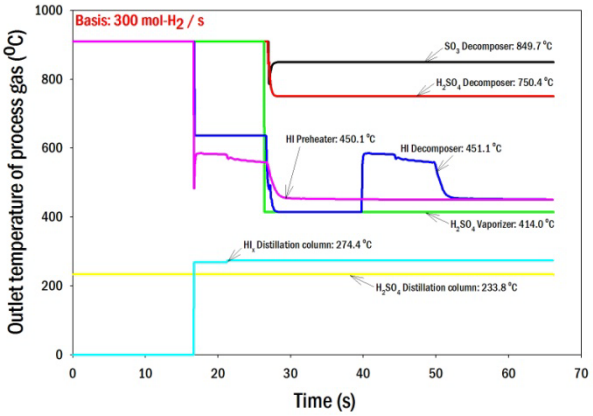

Fig. 3. Outlet temperature of process gas.

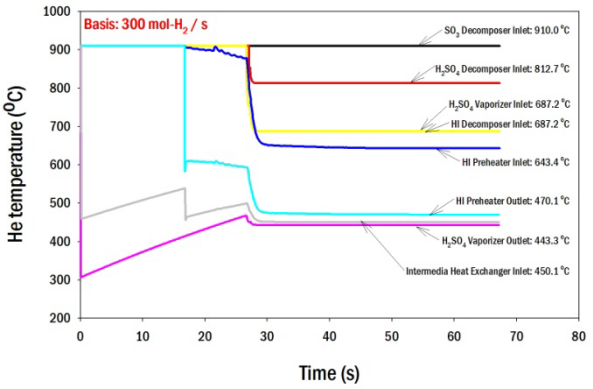

Fig. 4. Inlet and outlet temperature of helium.

3. Conclusions

The dynamic behavior of temperature transitions on the secondary helium loop of a VHTR-SI cycle have been successfully simulated using KAERI-DySCo.

Acknowledgments

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[2] Youngjoon Shin, Kiyoung Lee, Jonghwa Chang, Thermal Efficiency of EED-embedded Sulfur Iodine Cycle, Calculation Note (NHDD-KA07-HP-001-00), 2007.
[3] Jiwoon Chnag, Jihwan Kim, Youngjoon Shin, Cheong Youn, Taehoon Lee, Kiyoung Lee, Yongwan Kim, Jonghwa Chang, Computer Program for Equipment Sizing on the Secondary Helium Loop of a VHTR-SI Hydrogen Production System, Korean Nuclear Society Autumn Meeting, 2010.