A Dynamic Simulation Program for a Hydriodic Acid Concentration and Decomposition Process in the VHTR-SI Process

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1. Introduction

The Sulfur-Iodine (SI) cycle which can produce hydrogen by using nuclear heat consists of a Bunsen reaction (Section 1), a sulfur acid concentration and decomposition (Section 2), and a hydriodic acid concentration and decomposition (Section 3). The heat required in the SI process can be supplied through an intermediate heat exchanger (IHX) by a Very High Temperature Gas Cooled Reactor (VHTR).

The Korea Atomic Energy Research Institute-Dynamic Simulation Code (KAERI-DySCo) based on the Visual C++ is an integration application software that simulates the dynamic behavior of the SI process. KAERI-DySCo was prepared to solve dynamic problem of the seven chemical reactors which consist of Sections 2 and 3 [1] [2].

Section 3 is the key part of the SI process, because the strong non-ideality and the partial immiscibility of the binary HI–H_2O and the ternary HI–I_2–H_2O (HI_X solution) mixture make it difficult to model and simulate the dynamic behavior of the system [3]. Therefore, it is necessary to compose separately a dynamic simulation program for Section 3 in KAERI-DySCo optimization.

In this paper, a simulation program to analyze the dynamic behavior of Section 3 is introduced using the prepared KAERI-DySCo, and results of dynamic simulation are represented by running the program.

2. Method and Results

2.1 SI process

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 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.

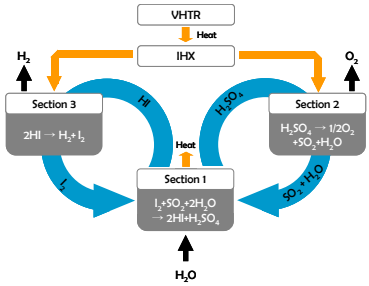

Fig. 1. Schematic chemical reaction flow diagram of the SI process.

2.2 Dynamic model

A conceptual diagram for the dynamic simulation of Section 3 shows in Fig. 2. As shown in Fig. 2, the key chemical reactors that consist of Section 3 are a HI_x distillation column and a membrane reactor, including pre-heating part. In addition, there is a HIx vaporizer including a stock solution tank for start-up.

In the SI process, Section 3 has an electrodialysis equipment to preliminarily concentrate the HIx solution, a HIx solution distillation column for an additional concentration and a vaporization of the HIx solution. A membrane reactor has two functions of a catalysis decomposition of HI and a preferential separation of hydrogen from the decomposed gas mixture of $H_2/I_2/HI/H_2O$. The membrane reactor is heated by the circulated helium and the HIx distillation column is heated by the sensible heat of another process gas as shown in Fig. 2 [4].

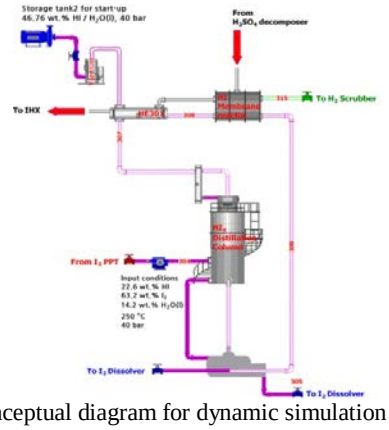

Fig.2. Conceptual diagram for dynamic simulation of Section 3.

2.3 Start-up scenario

A start-up scenario applied the dynamic simulation program for Section 3 is the following:

1) Helium discharged from a H_2SO_4 decomposer in Section 2 flows into the IHX via the membrane reactor including pre-heating part, as shown in Fig. 2. Here, the helium temperature as input value of the membrane reactor is referred to output results of the H_2SO_4 decomposer, as shown in Fig. 3.
2) The HI_x vaporizer including stock solution tank get into operation, until a HI flow rate, at the top of the HI_x distillation column, is reached at steady level.
3) When the HI flow rate is reached at steady level, the operation of the HI_x vaporizer stop and the HI mixture gas generated from the top of the HI_x distillation column flows into the pre-heating part of the membrane instead of the mixture gas generated from the HI_x vaporizer.

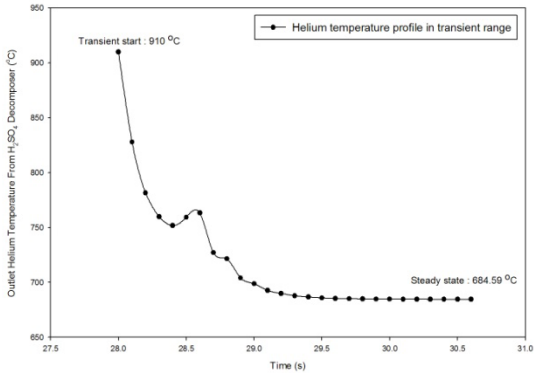

Fig. 3. Helium temperature discharged from the H_2SO_4 decomposer as a function of time.

In Fig. 3, the temperature profile can be divided into two ranges. One is a transient range and another is a steady range. Here the transient range indicates that helium temperature is continuously changed due to heat transfer occurred in the H_2SO_4 decomposer.

2.4 Operating conditions

Based on a production of 300 mol/s of hydrogen, the operating conditions input in the dynamic simulation program are shown in Table 1.

Table 1. Operating conditions

Chemical Reactor	Conditions		
	Feed amount (mole/s)	Temperature (°C)	Pressure (bar)
HI_x vaporizer	H_2O: 1881.92 HI : 351.44	30	40
HI_x distillation column	H_2O: 17569.66 HI : 3878.51 I_2 : 6227.61	250	40
Membrane reactor	He : 5335.82	Fig. 3	50

2.4 Simulation results

The simulation results for Section 3 using the dynamic program are represented in Fig. 4. In Fig. 4, each graph shows the simulated results as a function of time such as temperature (Fig. 4a, 4b) and mole flow rate (Fig. 4c, 4d), respectively.

Fig. 4a shows the temperature profiles of the gas mixture of the H_2O-HI-I_2-H_2 at the each chemical reactor, respectively, and Fig. 2b shows the temperature profiles of the helium at the membrane reactor and its pre-heating part. Fig. 4c and 4d show the mole flow rate of the gas mixture at the HI_x distillation column and the membrane reactor, respectively.

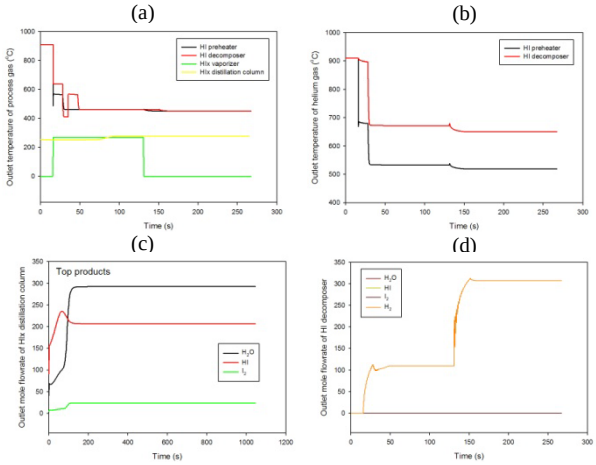

Fig. 4. Simulation results for Section 3.

3. Conclusions

The dynamic simulation program for Section 3 has been discussed. This program provides that the user can easily analyze the dynamic behavior of Section 3.

Acknowledgments

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