A Visualization Program for the Dynamic Simulation of a HIx Distillation Column in the VHTR-SI Process

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1. Introduction

The Sulfur-Iodine (SI) cycle which can be produced hydrogen by using nuclear heat consists of a Bunsen reaction (section 1), a sulfur acid concentration and decomposition (section 2), and a hydrogen iodine concentration and decomposition (section 3). In particular, an H_2O-HI-I_2 ternary mixture solution which is primarily concentrated by electro-electrodialysis in the section 3 is fractionated in a HIx distillation column. HI-enriched vapor is obtained at the top of the HIx distillation column and HI-diluted solution is obtained at the bottom [1].

In order to simulate dynamic behavior of the HIx distillation column, a vapor-liquid equilibrium (VLE) MATLAB program of the H_2O-HI-I_2 ternary system has been already introduced by KAERI research group in 2006 [2]. The dynamic simulation code for the HIx distillation column was also developed in 2009 [3].

In this paper, a visualization program to effectively monitor the output data in the dynamic simulation of the HIx distillation column is introduced by using Chart FX and Spread 7.0[4]. In addition, a sub program which can represent a vapor-liquid equilibrium curve of H_2O-HI-I_2 ternary system synchronizing with specific stage operation conditions such as operation pressure and I_2 mole fraction has been upgraded.

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.

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

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

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

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.

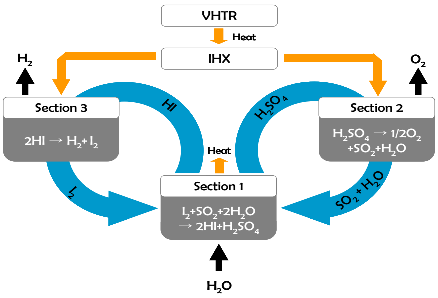

Fig. 1. Schematic chemical reaction flow diagram of the SI process.

2.2 Thermal Pathway

Conceptual diagram of the SI process based on the He-thermal pathway shows in Fig. 2. In the SI process, the 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 Fig. 2.

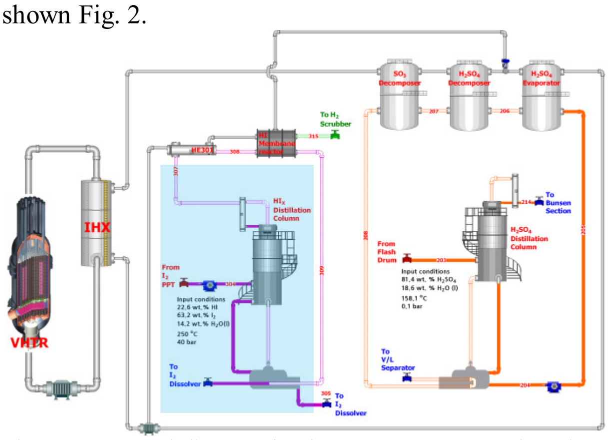

Fig.2. Conceptual diagram for the VHTR-SI process based on the He thermal pathway.

2.3 Dynamic simulation of the HIx distillation column

The current dynamic simulation has focused on the HIx distillation column which is highlighted in blue in Fig. 2. The modified NRTL equation based on the Neumann model and the ideal gas law to calculate vapor-liquid equilibrium values of the H_2O-HI-I_2

ternary system was adopted for liquid and gas phases, respectively.

The design and operation conditions for the dynamic simulation of the HIx distillation column are shown in Fig. 3.

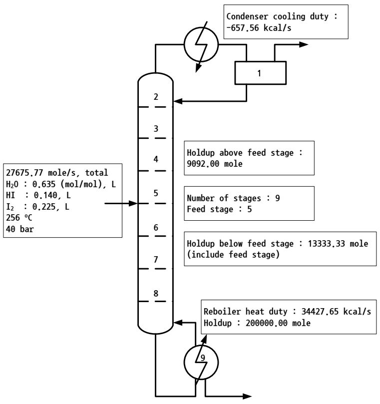

Fig. 3. Design and operation conditions for dynamic simulation of the HIx distillation process.

2.4 Visualization of output data

Lists of output data which can be obtained by running the developed code are shown in Table 1.

Table 1. Lists of output data

Item of output data	Unit
Liquid mole fraction for the H_2O-HI-I_2 ternary system at each stage (xH_2O, xHI, xI_2)	-
Vapor mole fraction for the H_2O-HI-I_2 ternary system at each stage (yH_2O, yHI, yI_2)	-
Total liquid mole flow rate at each stage	mole/s
Total vapor mole flow rate at each stage	mole/s
Temperature at each stage	°C
Boiling temperature at each stage	°C

For visualization of the output data in Table 1, two components such as a chart and a spread sheet were selected. The charts have been embedded in the developed code by using the Windows Forms Control Hosting method [5]. Also, the charts have been classified according to attribution of the listed output data. One is related to the composition of materials, and the other is related to temperature. On the other hand, the spread sheet represents the all of the listed output data in form of numerical value as shown Fig. 4.

For realization of vapor-liquid equilibrium curve, some components such as text box, button and chart have been used. As input values, a pressure and a mole fraction of I_2 in liquid phase can be inputted in two text boxes, the vapor-liquid equilibrium curves can be drawn by clicking the button. In case of a condition that pressure is 40 bar and a mole fraction of I_2 liquid phase is 0.225, an example of VLE curve is shown in Fig. 5. In Fig. 5, the left chart shows the VLE curve corresponding to variation of the H_2O mole fraction, the right chart shows the VLE curve corresponding to variation of the HI mole fraction.

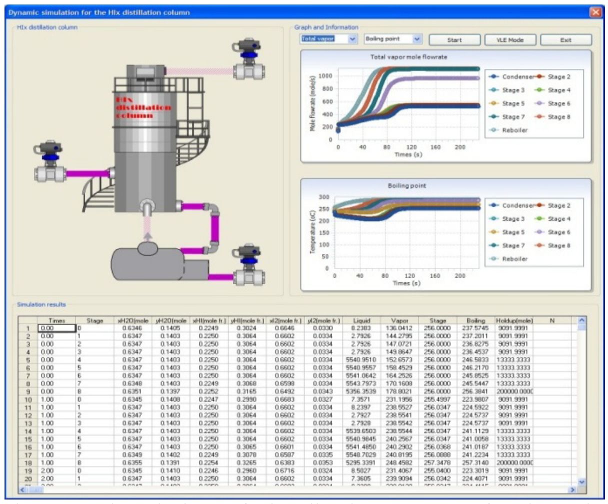

Fig. 4. Main window of visualization program for dynamic simulation of the HIx distillation process.

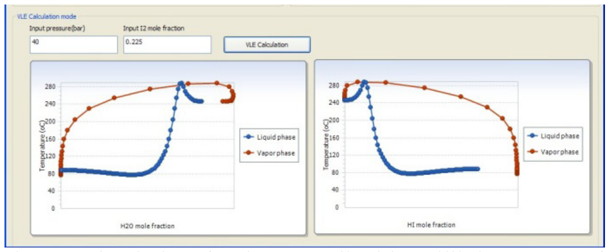

Fig. 5. Sub window for the vapor-liquid equilibrium curve of H_2O-HI-I_2 ternary system.

3. Conclusions

The output data obtained from the dynamic simulation of the HIx distillation column has been visualized as a chart and spread sheet by using Chart FX and Spread 7.0.

This visualization program provides that the user can easily monitor not only the dynamic behavior of the HIx distillation column, but also the approaching status to the steady state.

Acknowledgments

This study has been performed as one of the mid-and-long-term Nuclear R&D projects.

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