

Modeling of a High Temperature Sulfuric Acid Loop using Aspen Plus

DongUn Seo^a, S. D. Hong^b, C. S. Kim^b, J. H. Kim^b, Y. W. Kim^b, J. H. Chang^b, G. C. Park^a

^aSeoul National University, San56-1, Sillim-Dong, Kwanak-Gu, Seoul, 151-742, Korea

^bKorea Atomic Energy Research Institute, Daeduk-Daero 1045, Dukjin-dong, Yuseong-Gu, Daejeon, 305-600, Korea,

¹Corresponding author: duseo@kaeri.re.kr

1. Introduction

Hydrogen energy needs are growing with increased demands for alternatives to fossil fuel. Recently, many researchers have been investigating into hydrogen production technologies from a renewable and a nuclear energy. Very High Temperature gas cooled nuclear Reactor (VHTR) is considered to be suitable for massive hydrogen production systems when it coupled with Sulfur-Iodine (SI) thermo-chemical cycle [1].

Kim et al.[2] are developing a hybrid heat exchanger as a process heat exchanger for the sulfur trioxide decomposition. Hong et al.[3] constructed and are operating a small scale sulfuric acid loop for the integrity and feasibility tests of a process heat exchanger coupled with VHTR and SI cycle. In this study, we performed preliminary analysis of small scale sulfuric acid test loop using Aspen Plus chemical process simulator [4]. In addition, we studied the behavior of main component in the sulfuric acid loop on the basis of experimental results.

2. Methods and Results

2.1 Small Scale Sulfuric Acid Loop

A small scale sulfuric acid (H_2SO_4 98 %wt) loop consists of a H_2SO_4 storage tank, a H_2SO_4 feed pump, a sulfuric acid evaporator and sulfuric acid decomposer, a process heat exchanger (PHE), a high temperature

cooler, a separator, a SO_2 trap, a low temperature cooler, and a H_2SO_4 collector as shown in Figure 1 [3]. Liquid sulfuric acid with room temperature is supplied from a H_2SO_4 storage tank to an evaporator by a sulfuric acid feed pump. Liquid sulfuric acid in the evaporator is heated up to 300 °C. The outlet temperature of H_2SO_4 decomposer is reached up to 500°C. In the decomposer, the evaporated sulfuric acid is dehydrolyzed into water vapor and sulfur trioxide (SO_3). In the PHE, the sulfur trioxide is decomposed into sulfur dioxide (SO_2) and O_2 . The mixed gas, such as SO_3 , SO_2 , H_2O , O_2 , passes through the cooler and the separator. Sulfur dioxide (SO_2) is trapped in the scrubber, and the gas mixture except the sulfur oxides and the sulfuric acid is vented to the outside.

2.2 Modeling of Process Simulator

A modeling of a small scale sulfuric acid loop has been performed using Aspen Plus chemical process simulator. The working fluid is H_2SO_4 with 96 wt%. Mass flow of sulfuric acid is 8cc/min. The inlet temperature of sulfuric acid from feed pump is room temperature and pressure is atmosphere [5]. Figure 2 shows the flow sheet for the small scale sulfuric acid loop in the Aspen Plus simulator. Evaporator and Sulfuric acid decomposer is modeled using the heater and reactor. The stoichiometric model is used for the reactor model of evaporator and Sulfuric acid decomposer.

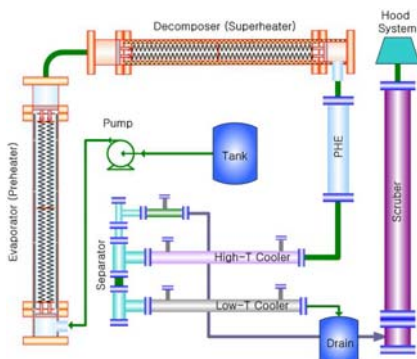


Fig. 1. Schematic Diagram of a Sulfuric Acid Loop

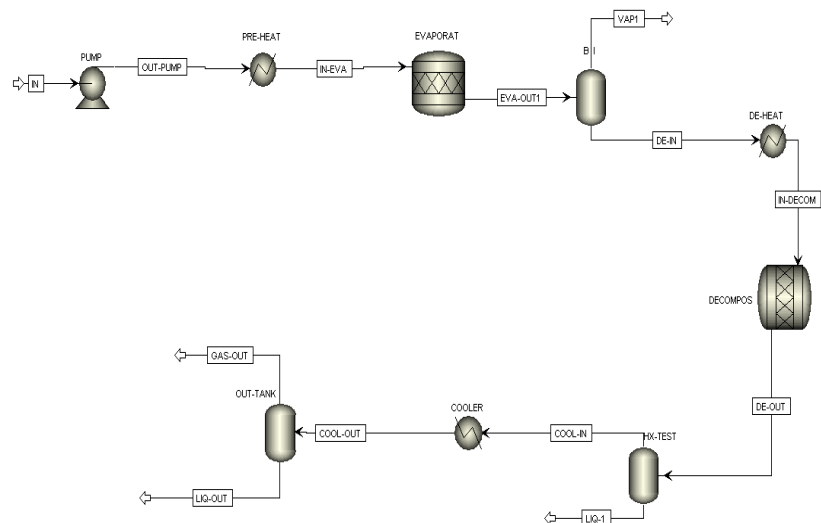


Fig. 2. Flow Sheet of Sulfuric Acid Loop for Aspen Plus

Also, in the reactor model of Sulfuric acid decomposer, it is assumed that the dehydrolyzed fraction conversion (FC) factor of sulfuric is unity at the decomposer outlet. Both high and low temperature coolers modeled with a constant temperature boundary condition as 50°C and 20°C, respectively.

2.3 Results

Figure 3 shows the trend of the operational data at each component including heaters in the experiment. As the power increase of the decomposer heater, decomposer outlet temperature decreases. The reason of this behavior was explained in the previous study [4].

Figure 4 shows the outlet reaction fraction of decomposer in Aspen Plus. As the reaction fraction of sulfuric acid decomposer is increased, the outlet temperature of the sulfuric acid decomposer is decreased as shown in Figure 4.

In the evaporator, some fractional conversion (FC) factor of liquid sulfuric acid was dehydrolyzed into SO₃ and H₂O as shown in Table 1.

If the decomposer outlet temperature is set to 500 °C, the fractional conversion (FC) factor should be 1 with power of 215 W as shown in Table 2. These results suggest that the decomposer outlet temperature with 500 °C requires much higher heated power than the previous study [5].

Table 1. Results of Aspen Plus under Operational Condition

	Evap. Temp.=250 °C Decom. Temp.=180 °C
FC of Evap.	0.01
FC of Decom.	0.08
Evaporator Heat (W)	51 W
Decomposer Heat (W)	10 W

Table 2. Results of Aspen Plus under Design Condition

	Evap. Temp.=250 °C Decom. Temp.=500 °C
FC of Evap.	0.01
FC of Decom.	1
Evaporator Heat (W)	51 W
Decomposer Heat (W)	215 W

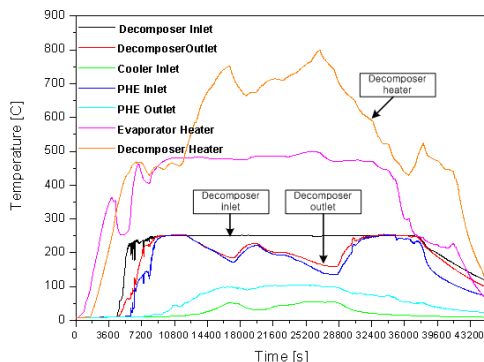


Fig. 3. Trend of Operational Data in Experiment

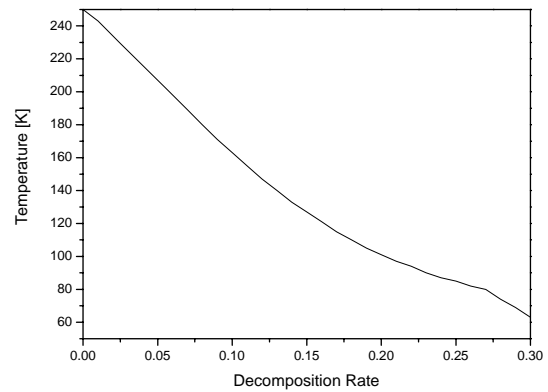


Fig. 4. Reaction Fraction of Decomposer in Aspen Plus

3. Conclusions

A small scale sulfuric acid loop was simulated for the validation of the components for the sulfuric acid decomposition process. We obtained the following results for the modeling of the small scale sulfuric acid loop.

1. As the reaction rate of the sulfuric acid decomposer was increased, the outlet temperature of decomposer was decreased. The reason is due to the endothermic reaction of sulfuric acid at decomposer.

2. Heated power with about 215 W must be added for 500 °C and FC=1 at the decomposer outlet.

ACKNOWLEDGMENTS

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