Modeling of the Sulfuric Acid and Sulfur Trioxide Decomposer using Aspen Plus

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1. Introduction

A hydrogen production system using VHTR, which was combined with a Sulfur-Iodine (SI) thermo-chemical cycle, is a good candidate for massive hydrogen production. It is being investigated for Nuclear Hydrogen Development and Demonstration (NHDD) project in Korea Atomic Energy Research Institute [1].

The SI thermo-chemical cycle is a good promise for the economical and eco-friendly hydrogen production. In SI cycle, the decomposition of a sulfuric acid is main concern for the material corrosion and mechanical stress on high temperature and pressure operation condition.

KAERI has designed and constructed a small-scale gas loop that included sulfuric acid experimental facilities as a secondary loop [2]. The main objectives of the loop are to monitor and validate the performances of NHDD component such as the Process Heat Exchanger (PHE) and sulfuric acid decomposer [3].

In this paper, we discussed the results of the modeling of the sulfuric acid and sulfur trioxide decomposer using Aspen plus process simulator [4].

2. Methods and Results

2.1 Small Scale Sulfuric Acid Loop

A small scale sulfuric acid (H_2SO_4 96 %wt) loop is an open loop and consists of a H_2SO_4 storage tank, a H_2SO_4 feed pump, a sulfuric acid evaporator (H_2SO_4 pre-heater) and decomposer (H_2SO_4 super-heater), 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. Liquid H_2SO_4 96 %wt of room temperature is supplied from a H_2SO_4 storage tank to the evaporator through the H_2SO_4 feed pump. Liquid H_2SO_4 in the evaporator is raised from room temperature to 300°C. The outlet temperature of superheater is reached up to 500°C. In the superheater, 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, and O_2, passes through the cooler and the separator. Sulfur dioxide (SO_2) is trapped in the scrubber, and the oxygen is released to the atmosphere via filter system.

Fig. 1. Small Scale Sulfuric Acid Loop

2.2 Modeling of the Process Simulator

A sulfuric acid loop was simulated using an Aspen plus chemical process simulator. Figure 2 shows the flow sheet of the sulfuric acid loop for Aspen plus modeling. The evaporator (evap), sulfuric acid decomposer (decomp 1) and sulfur trioxide decomposer (decomp 2) were modeled using the reactor model. The Gibbs reactor model was used to model the evaporator and sulfuric acid and sulfur trioxide decomposer. In Tables 3 and 4, the test matrixes are divided into two parts: sulfuric acid decomposer and sulfur trioxide decomposer. High and low temperature coolers were modeled using constant boundary conditions of 50°C and 20°C, respectively.

2.3 Results

Table 3 shows the mole fractions of the H_2SO_4 decomposer with constant temperature of 500°C at SO_3 decomposer. As the outlet temperature of the H_2SO_4 decomposer is increased, the mole fraction of H_2SO_4 is gradually decreased and the mole fractions of H_2O and SO_3 are increased. At the SO_3 decomposer outlet temperature of 500°C, remaining H_2SO_4 vapor is dehydrolyzed into SO_3 and H_2O. A small amount of SO_3 also decomposes into SO_2 and O_2.

Table 4 shows the mole fractions of the SO_3 decomposer with constant temperature of 500°C at H_2SO_4 decomposer. As the outlet temperature of the SO_3 decomposer is increased to 900°C, the mole fraction of the H_2SO_4, H_2O and SO_3 are decreased and the mole fractions of SO_2 and O_2 are increased.

Figure 3 shows the mole fractions of the chemical composition of H_2SO_4 and SO_3 decomposer and its dependence on variations in the decomposer outlet temperature based on Aspen plus simulations.

Table 3: Mole fraction results for the cases of H_2SO_4 decomposer

Comp.	H_2SO_4 decomposer			SO_3 decomposer
	CASE 1 (350°C)	CASE 2 (400°C)	CASE 3 (450°C)	(500°C)
H_2SO_4	0.3636	0.1620	0.0611	0.0224
H_2O	0.3869	0.4756	0.5173	0.5284
SO_3	0.2453	0.3484	0.3879	0.3816
SO_2	0.0027	0.0092	0.0224	0.0450
O_2	0.0014	0.0046	0.0112	0.0225

Table 4: Mole fraction results for the cases of SO_3 decomposer

Comp.	H_2SO_4 decomposer (500°C)	SO_3 decomposer			
		CASE 4 (600°C)	CASE 5 (700°C)	CASE 6 (800°C)	CASE 7 (900°C)
H_2SO_4	0.0224	0.0033	0.0005	8.89e-5	1.79e-5
H_2O	0.5284	0.5157	0.4901	0.4701	0.4595
SO_3	0.3816	0.2973	0.1792	0.0897	0.0427
SO_2	0.0450	0.1225	0.2201	0.2934	0.3319
O_2	0.0225	0.0612	0.1101	0.1467	0.1659

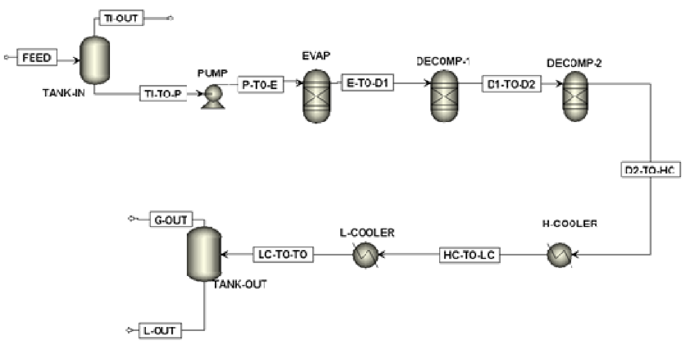

Fig. 2. Flow sheet of the sulfuric acid loop for Aspen+ modeling

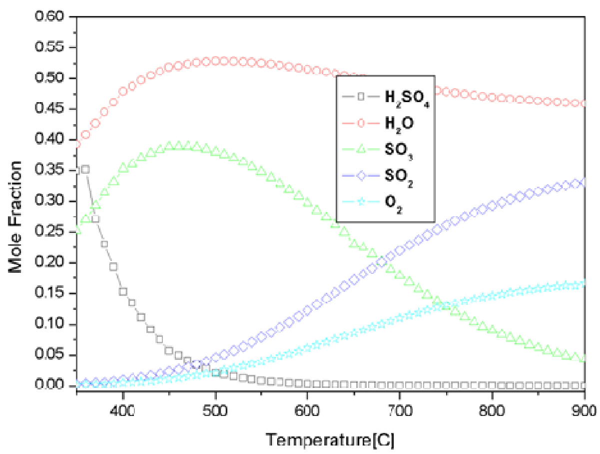

Fig. 3. Mole fraction of H_2SO_4 and SO_3 decomposer in Aspen+

3. Conclusions

A small scale sulfuric acid loop was simulated for the decomposition of the sulfuric acid and sulfur trioxide decomposer using Aspen plus process simulator. We obtained the following results for the modeling of the small scale sulfuric acid loop.

1. As the outlet temperature of the H_2SO_4 decomposer is increased, the mole fraction of H_2SO_4 is decreased and the mole fractions of H_2O and SO_3 are increased.
2. As the outlet temperature of the SO_3 decomposer is increased above 600°C, the mole fraction of the H_2SO_4 becomes very small. The mole fractions of SO_2 and O_2 are increased due to the decomposition of SO_3.
3. At the SO_3 decomposer outlet temperature of 900°C, very small quantities of SO_3 decompose into SO_2 and O_2.

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