

Simulation of a Heat Transfer between Gases in SO₃ Decomposer

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1. Introduction

Korea Atomic Energy Research Institute (KAERI) is developing hydrogen production process called thermo-chemical SI(Sulfur Iodine) cycle utilizing the heat from the High Temperature Gas Cooled Reactor (HTGR) with outlet coolant temperature up to 950 °C, which is considered as an efficient reactor for the hydrogen production[1].

The sulfur trioxide decomposer is one of the key components in SI cycle, because the sulfur trioxide is decomposed into sulfur dioxide and oxygen by a heat transferred from the helium gas.

In this paper, the sulfur-trioxide decomposer was simulated with a chemical process simulator[2]. A standard shell-and-tube heat exchanger model in the simulator was chosen for the simulation.

2. Description of Sulfur-trioxide Decomposer

The sulfur-trioxide decomposer was assumed to be a standard shell-and-tube heat exchanger model.

The helium gas is flowing into the shell side of the heat exchanger while the gaseous mixture of sulfur trioxide, water vapor, and un-reacted sulfuric acid is flowing in the tube side of the sulfur-trioxide decomposer.

While the gaseous mixture in the tube side receives the heat from the helium gas flowing in the shell side, the decomposition reaction of sulfur-trioxide into sulfur-dioxide and oxygen is catalytically taking place in the tube side of sulfur-trioxide decomposer.

The SI cycle that is connected with 200 MWth VHTR can produce hydrogen at 300 moles/sec, if we assume 40% of thermal efficiency.

The flow conditions of the shell and tube side of the sulfur-trioxide decomposer at steady state are as Fig.1 and Table 1[3];

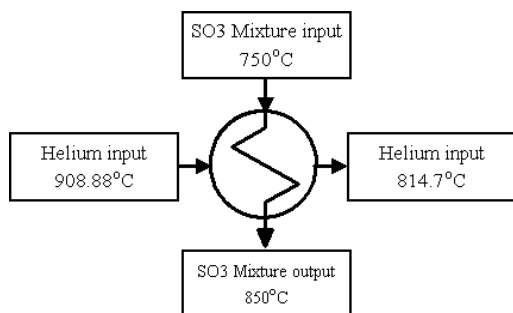


Fig.1. Temperature Distribution at Steady State

3. Simulation of a Sulfur-trioxide Decomposer

The sulfur-trioxide decomposer is modeled as a combination of stoichiometric reactor and a heater in the simulation.

The assumption that was used in the simulation is that the decomposition of sulfur-trioxide begins at 675 °C, and its decomposition ratio increases with temperature with about 0.8 at 825 °C [4].

The temperature of the helium gas at the exit of decomposer is determined by taking heat balance around the sulfur-trioxide decomposer.

From the fact that the heat supplied from helium gas is partly involved in the sulfur trioxide decomposition reaction and remaining heat is used to raise the gas mixture temperature.

$Q_{He} = Q_d + Q_s$
 , where Q_{He} is the heat transferred from helium gas, Q_d is the heat needed for sulfur-trioxide decomposition and Q_s is the heat needed to raise the temperature of product gas mixture.

Simulation model for sulfur-trioxide decomposer is shown in Fig. 2.

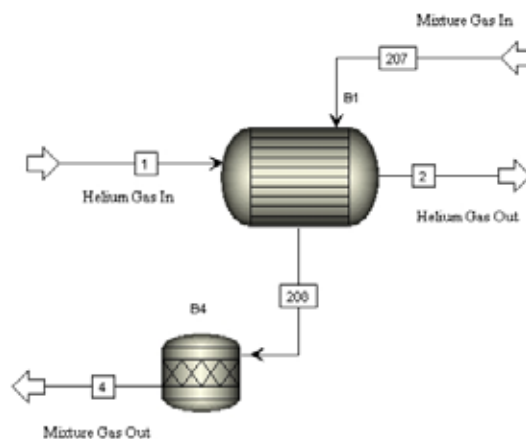


Fig.2. Simulation Model for Sulfur-trioxide Decomposer

The temperature, pressure and molar flow rate for each stream are given in Table 1.

Table 1. Material Balance for the Sulfur-trioxide Decomposer

Streams	1	2	4	207	208
Temperature, C	908.88	892.28	850	750	850
Pressure, atm	69,983	62,984	9,998	9,998	8,9978
Mole Flow, kmol/hr					
H ₂ O	0	0	1910	1914	1913.9
H ₂ SO ₄	0	0	11.33	7.293	7.2926
SO ₃	0	0	1549	1725	1725.1
SO ₂	0	0	172.5	0	0
O ₂	0	0	86.25	0	0
HE	64157	64157	0	0	0
Total Flow, kmol/hr	64157	64157	3729	3646	3646.3
Mole Frac					
H ₂ O	0	0	0.512	0.525	0.5249
H ₂ SO ₄	0	0	0.003	0.002	0.002
SO ₃	0	0	0.415	0.473	0.4731
SO ₂	0	0	0.046	0	0
O ₂	0	0	0.023	0	0
HE	1	1	0	0	0

4. Simulation Result

The temperature profile along the sulfur-trioxide decomposer is obtained as in Fig.3. The simulation result shows no pinch point in the sulfur-trioxide decomposer under the operating condition. The temperature distribution of helium and mixture gas is almost linear along the decomposer.

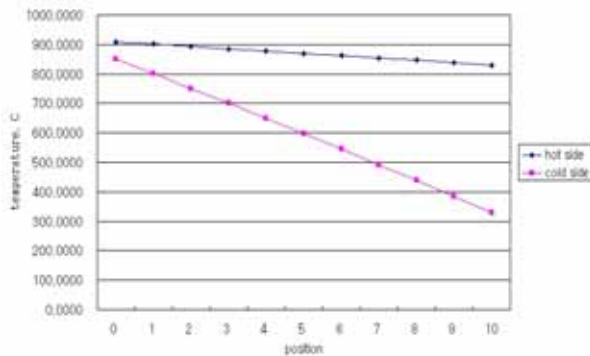


Fig. 3. Temperature Profile along the SO₃ Decomposer

5. Summary

Material and energy balance were established for the sulfur-trioxide decomposer with unit operation models with a chemical process simulator. Temperature profile along the decomposer indicated that there is no pinch point in the decomposer.

ACKNOWLEDGEMENTS

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