# Effect of Catalyst on Thermal Design of a Lab-Scale SO<sub>3</sub> Decomposer for Nuclear Hydrogen Production

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# 1. Introduction

The current literature survey [1-4] revealed that a SO<sub>3</sub> decomposer is one of the main issues in nuclear hydrogen production by a very high temperature gas cooled reactor (VHTR) coupled with hydrogen production system. Active decomposition of SO<sub>3</sub> at very high temperature above 850°C makes the VHTR outlet temperature exceed 950°C for an economical massive hydrogen production. Because material corrosion is much more active in very high temperature (850~ 950  $^{\circ}$ C) and SO<sub>3</sub> environment, the decomposer has to have a much stronger resistance than general structures. In addition, the decomposer should endure a structural load from a large pressure difference (2~6 MPa). Hong et al. [5] designed a gas loop for various tests of labscale decomposers and verification of their design performances. In this study, the catalyst effect of a labscale decomposer at the dynamic conditions is evaluated for its thermal design. A hybrid heat exchanger (Kim et al. [6]) is selected as the decomposer model in this study.

### 2. Methods and Results

### 2.1 Governing Equations & Boundary Conditions

A SO3 decomposer is thermally sized through three following conservations: mass conservation, energy conservation and chemical kinetics. At first, the mass conservation is maintained in all the regions. Local flow velocity is calculated from the local density. Especially, the decomposition fraction of SO<sub>3</sub> is the main factor to determine the mixture density. The homogeneous flow of the SO<sub>3</sub> mixture is assumed for a relatively smaller density difference between the compositions than density difference in a two phase flow. In the case of mixture material properties, the specific heat is calculated from the mass flow fraction and the other properties such as the density and thermal conductivity are calculated from the mole flow fraction.

Two differential equations for energy conservation should be solved to calculate fluid temperatures. In the nitrogen channel, the sensible heat for nitrogen is equal to the exchanging heat through the decomposer. In the mixture, the exchanging heat energy consumes the temperature rise of a mixture gas and the thermal decomposition of SO<sub>3</sub> to SO<sub>2</sub> and O<sub>2</sub>.

$$q'_{ex} = \frac{T_N - T_{mix}}{R_{tot}} = \dot{m}_N c_N \frac{dT_N}{dl}$$
$$= \sum_i \dot{m}_i c_i \frac{dT_{mix}}{dl} + \Delta H_R \dot{N}_v \frac{dx}{dl}$$
(1)  
(a)  $l = 0; N_2 \text{ outlet}, Mixture inlet$ 

The decomposition fraction is governed by the kinetics of chemical reaction, so it can be calculated from the transferring time and the rate constant of catalyst as Karasawa et al. [7,8].

$$\frac{dx}{dt} = u_{mix}\frac{dx}{dl} = k(1-x) \tag{2}$$

The gas loop design [5] provided the boundary conditions for thermal design of the decomposer. The maximum power of this heat exchanger will be about 10 kW. The designed mass flow rates of  $N_2$  and 100%  $H_2SO_4$  are respectively 2 kg/min and 0.5 kg/min. In this study, the boundary conditions for the thermal sizing of a lab-scale SO<sub>3</sub> decomposer were determined based on this loop design. Table 1 shows the boundary conditions in this sensitivity analysis.

Table 1 Boundary Conditions for Thermal Design

Parameters	Nitrogen	SO3 Mixture
Mass Flow Rate [kg/min]	1.0	0.4
Inlet Temperature [ $^{\circ}$ C ]	950	500
Pressure [MPa]	6.0	0.1
Inlet Compositions	-	SO3 & H2O
Total Number of Channel Number	1500	600

### 2.2 Catalyst Effect

Rate constants of the catalysts were referenced from Karasawa et al. [7,8]. Karasawa et al. [7]'s catalyst accelerated the thermal composition for the fraction to approached 1.0 within 2 seconds at 900  $^{\circ}$ C. But the decomposition ratio with Karasawa et al. [8]'s catalyst approached 1.0 within 20 seconds at the same temperature.

Figure 1 shows the rate constants by varying catalysts. Since Karasawa et al. [7]'s catalyst has the largest rate constant, it takes the shortest time for reaction into the equilibrium state. Therefore, the exit fraction of Karasawa et al. [8]'s catalyst is larger than any other catalysts as shown in Figure 2. Figure 3 illustrates temperature profiles varying with catalysts. At 850 °C, the active thermal decomposition causes most of the exchanged heat to be consumed for thermal decomposition of SO<sub>3</sub> with Karasawa et al. [7]'s catalyst. The other catalysts don't have enough transferring times for a chemical reaction to limit rising a mixture gas temperature. Reactive energy in Karasawa et al. [7]'s catalyst is about 24.91 % of the total exchanged heat. Most of the reactive energy is consumed at 840 °C.



Figure 1 Rate Constants for Catalysts





#### 3. Conclusion

The result indicates that the rate constant of the used catalysts is very important material property to determine the outlet decomposing fraction.

A lab-scale length is not enough long to simulate a  $SO_3$  decomposition at the real IS cycle, so the decomposer requires a minimum length to detect the catalyst effect to accelerate the thermal decomposition of  $SO_3$ .

In the future, the sensitivity analysis will be performed to evaluate the effect of other factors on thermal design of the decomposer. They will include number of channels, a separation of steam from a mixture gas, and the actual heated length.

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