

Computational Analysis of a Direct Thermo-Chemical Sulfuric Acid Decomposer Used for Hydrogen Production

YouHo Lee, HeeCheon No

Department of Nuclear and Quantum Engineering, KAIST, Daejunsu Yooseounggu Guseungdong
euo@kaist.ac.kr

1. Introduction

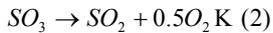
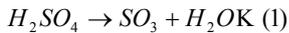
Westinghouse proposed a conceptual design of a new thermo-chemical decomposer called direct decomposer as a mean of mitigating mechanical defects that often arise due to the strongly corrosive environment and structural complexity of the indirect decomposer. However, in-depth feasibility study of the direct decomposer had not been conducted. In this study, profound feasibility analysis of the direct decomposer has been conducted along with proposing a new valve operation to minimize the inherent mass mixing phenomena of the direct decomposer. Basically, the research has been conducted using a CFD code under transient condition.

2. Modeling in CFD

In this section, basic features, boundary conditions and the new valve operation to minimize the mass mixing used to model the direct decomposer are described.

2.1 Basic Features and Boundary Conditions

The packed bed region where the actual reaction takes place is modeled as porous zone filled with 0.06m, in diameter, spherical catalysts. The following two-step chemical reaction is involved in the thermal decomposition of sulfuric acid.



Reaction (1) can be ignored in the simulation due to its negligible effect on the overall kinetics of the reaction.

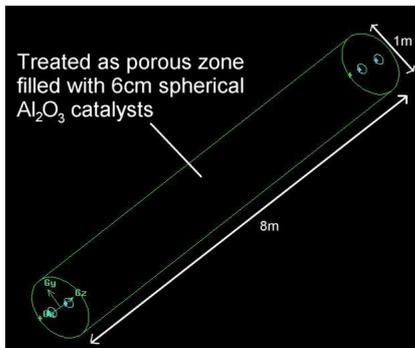


Figure 1. Geometry of the cylindrical direct decomposer

Table 1. *Design values and boundary conditions of the direct decomposer

Input	
Diameter	1m
Height	8m
Diameter of Inlets	0.2m
Diameter of Outlets	0.2m
Diameter of Al_2O_3	0.06m
Decomposer Material	Steel
H_2SO_4 inlet	450 °C SO_3 1.8kg/s
	450 °C H_2O 0.405kg/s
He inlet	900 °C 3kg/s
Initial condition	He 900 °C
Operating pressure	7MPa
Ahhrenius rate	$6.79 \times 10^5 \exp(-20021/T)$

*These values are selected based on the reference papers.

2.2 New valve operation

To reduce the mass mixing of helium and reaction products indicated in the reaction (1), (2), a new valve operation is introduced as follows.

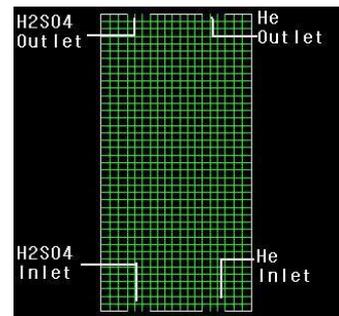


Figure 2. positions of the valves

Given the initial condition He 900 °C and valve positions as indicated in figure2, the new valve operation method as well as the typical valve operation is described below.

Table 2. valve operation

Order	Valves	Typical Operation	New operation
①	H_2SO_4 inlet	Open	open
	He inlet	Closed	closed

	H_2SO_4 outlet	open	closed
	He outlet	closed	Open
②		Temperature dropped sufficiently	Reaction products reached to the top
③	H_2SO_4 inlet	Closed	Open
	He inlet	Open	closed
	H_2SO_4 outlet	Closed	Open
	He outlet	Open	closed
④		Temperature increased to about 900 °C	Temperature dropped sufficiently
⑤	H_2SO_4 inlet	Repeat from ① to ④	closed
	He inlet		Open
	H_2SO_4 outlet		Open
	He outlet		closed
⑥	H_2SO_4 inlet	Repeat from ① to ④	He reached to the top
	He inlet		
	H_2SO_4 outlet		
	He outlet		
⑦	H_2SO_4 inlet	Repeat from ① to ④	closed
	He inlet		open
	H_2SO_4 outlet		closed
	He outlet		Open
⑧		Temperature increased to about 900 °C	
⑨		Repeat from ① to ⑧	

3. Results

Simulation was carried out. Results have been obtained to 70 seconds under the transient condition. It was found that 0.295kg of helium has been lost through H_2SO_4 outlet for 70seconds with the new valve operation. There could have been approximately 18kg helium loss through H_2SO_4 outlet if the new valve operation method was not used.

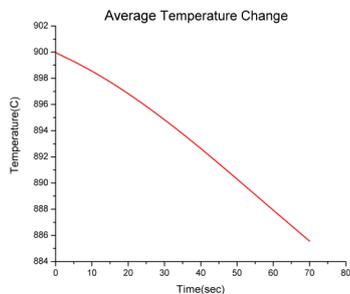


Figure 3. Average temperature change

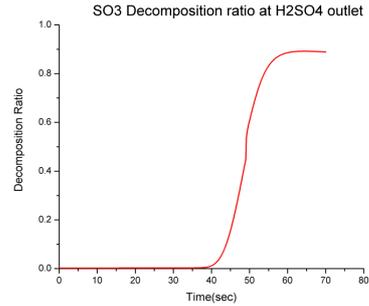


Figure 4. SO_3 decomposition ratio at H_2SO_4 out let

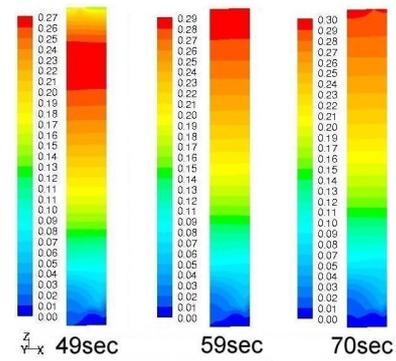


Figure5. SO_2 mole fraction change

4. Conclusion

It was found that the new valve operation could greatly reduce the mass mixing up to a factor of sixty. Thus, in terms of the mass mixing, it seems that the direct decomposer acquires a reasonably strong feasibility through the new valve operation. However, despite the existence of the heat reservoir in the form of packed beds, it was shown that the temperature sharply drops mainly due to a subsequent intake of lower temperature sulfuric acid and endothermic reaction. This leads to such frequent valve manipulations during the operation, which causes a serious impracticality of the direct decomposer.

REFERENCES

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- [2] H. Karasawa, A. Sasahira, K. Hoshino, Thermal Decomposition of SO_3 , Int.J.Nuclear Hydrogen Production and Applications, Vol. 1, No. 1, pp. 134-143, 2006.