Numerical Analysis on a Thermo-Chemical Decomposer for the Sulfur-Iodine Process

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1. Introduction

Recently, the material problems of thermo-chemical components for the sulfur-iodine process have been issued due to a high temperature (around 850 ^oC) and strongly corrosive environment of the process. Therefore, many researches [1-4] are on-going for the development of high performance materials for the sulfur-iodine process. On the other hand, a design strategy to mitigate the material problem is essential by reducing the temperature of the components.

In this paper, a thermo-chemical decomposer for the sulfur-iodine process has been designed and analyzed by using a computational fluid dynamics (CFD) code in order to relax the material issue of the reactor. A porous media approach has been used to model the region where a chemical decomposition occurs.

2. Decomposer Modeling and CFD Method

A schematic of the thermo-chemical reactor modeled in this study is shown in Fig. 1. RA330 was adopted as the material of the vessel and the guide tube. RA 330 has a good oxidation resistance to a high temperature and an excellent resistance to a thermal shock, etc [5]. The decomposer has the inner dimension of 1.8(W)× 8(H) m, and is filled with Al_2O_3 catalysts with a 32% porosity. The major design values of the decomposer are given in Table 1. The chemical reactions of the mixture gases in the decomposer were not considered. Table 2 and Table 3 show the main thermal hydraulic data of the decomposer. The ratio of the flow rate between the mixture gases and helium is 1:1.445, and it is assumed that the decomposer is able to produce the hydrogen of about 1000 Nm^3/hr for the given flow conditions. A porous media model was applied to the region of the Al_2O_3 catalyst and to the upper and lower side plates .The CFX 5 code [6] was used for the CFD analysis.

Table 1. Design values of thermo-chemical decomposer

	Values
Total decomposer length	16.06m
Decomposer height	8m
Inlet diameter for mixture gases	30cm
He inlet diameter	50cm
Upper & lower Grid plate thicknesses	3cm
Al_2O_3 catalyst diameter	2cm

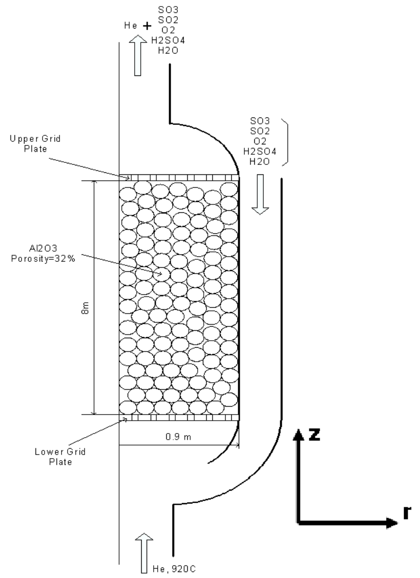

Figure 1. A schematic of thermo-chemical decomposer

Table 2. Mass fraction & mole fraction of mixture gases

	H_2O	O_2	SO_2	SO_3	H_2SO_4
Mass Fraction	22.12%	22.12%	22.15%	33.38%	0.22%
Mole Fraction	1.7777	0.5	1	0.6031	0.0033

Table 3. Operating conditions of thermo-chemical decomposer

	Flow rate	Inlet temperature	Operating pressure
He	2.0628 kg/s	920 ^oC	7.09bar
Mixture gas	1.8046 kg/s	450 ^oC	7.09bar

3. CFD Results

Figure 2 shows the calculated velocity profile along the center line in the z-direction. In Fig. 2, the velocity maintained about 9m/s is decreased drastically at a lower grid plate (z= around 4 m). The flow comes out of the upper grid plate (z=12 m) and the velocity maintained with 3.1m/s in the Al_2O_3 region is increased sharply by about 13 m/s near the outlet of the decomposer. The rapid rise of the velocity at the outlet is due to an augmentation of the flow rate by a mixing the helium gas and the mixture gases.

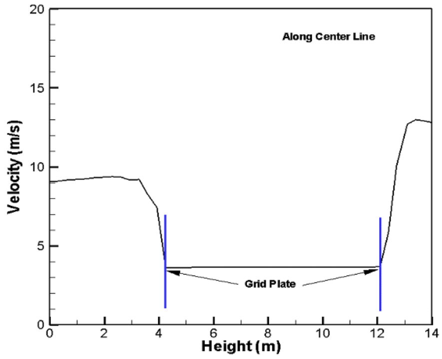

Figure 2. Velocity profile in the z-direction (superficial velocity in the porous region)

Figure 3 and Figure 4 show the calculated temperature contours of the decomposer and the guide tube. It can be seen in Fig. 3 and Fig. 4 that the maximum temperature of RA330 is lower than 800 ℃ which is considered as a limiting temperature in the study. This indicates that RA330 has good conditions as a structure material of a high temperature decomposer.

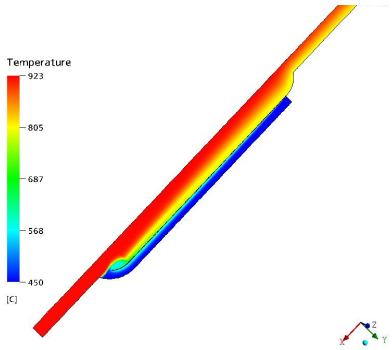

Figure 3. Decomposer temperature contour

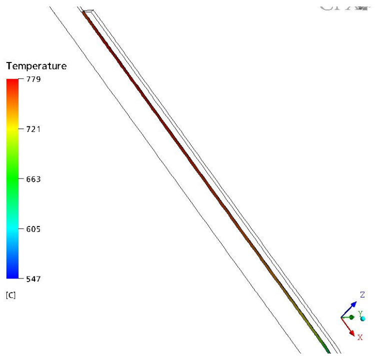

Figure 4. Guide tube temperature contour

Figure 5 shows the temperature profile in the r-direction. In the figure, 'Bottom' represents the upside surface of the lower grid plate, and 'Top' represents the bottom surface of the upper grid plate. 'Middle' indicates the middle position of the Al_2O_3 region. It was also observed that the guide wall maintains a temperature of around 850 ℃ in most of the Al_2O_3 region. This implies that the decomposer modeled in this study satisfies the temperature conditions for a chemical decomposition reaction.

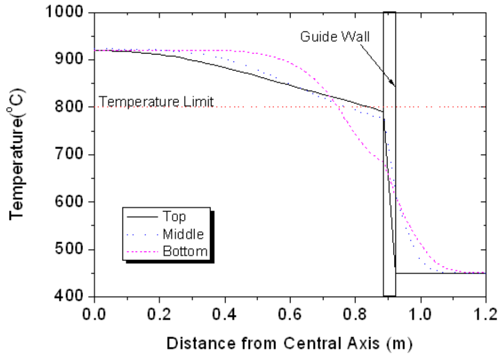

Figure 5. Temperature profile in the r-direction

4. Conclusions

A numerical analysis for a thermo-chemical decomposer has been made. When the conceptual design conditions of the decomposer presented in this research were used, the maximum temperature of the structure material (RA330) could be maintained at 800℃ or less. Also, it can be seen that the mean temperature of the reaction region (Al_2O_3 region) in the thermo-chemical decomposition reactor could be satisfied fully with the temperature condition of around 850 ℃ which is a target in this study. An improved heat transfer model of a catalyst layer including a chemical reaction is required.

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