

## Numerical Analysis on Thermochemical Characteristics of a Hydrogen Iodine Decomposer in Sulfur-Iodine cycle

T. H. Lee<sup>a</sup>, J. S. Choi<sup>b</sup>, K. Y. Lee<sup>a</sup>, Y. J. Shin<sup>a</sup>, J. H. Choi<sup>c\*</sup>

<sup>a</sup> Korea Atomic Energy Research Institute 150 Dukjin-dong, Yuseong-gu, Daejeon, Korea 305-600

<sup>b</sup> Graduate School of Marine Engineering System, Korea Maritime and Ocean University, 727 Taejong-ro, Busan, Korea

<sup>c</sup> Division of Marine Engineering System, Korea Maritime and Ocean University, 727 Taejong-ro, Busan, Korea

\*Corresponding author: choi\_jh@kmou.ac.kr

### 1. Introduction

As the interest and research on nuclear hydrogen technology, which involved decomposing the water directly to produce a large amount of hydrogen using high temperature in nuclear reactor as heat source of the thermochemical cycle, has increased [1]. Especially, on the occasion of the successful continuous operation of a bench-scale closed cycle by the Japanese Atomic Energy Agency (JAEA), the sulfur-iodine (SI) thermochemical hydrogen production technology took center stage as one of the high-practical-potential hydrogen production technologies that could be coupled with the VHTR [2]. However, transferring the high heat output of the gas-coolant for VHTR to the SI (Sulfur-Iodine) thermochemical cycle involves the great challenge of developing a heat exchanger material capable of withstanding high temperatures (1173 K) and pressures (50~70 kg/cm<sup>2</sup>). In the HI decomposition reaction, which was required a lot of heat in SI cycle, if the decomposition efficiency of HI will be able to be maintained at high level pressure, the design and development heat exchanger and reactor can have the flexibility.

In this study, to develop optimum decomposition reactor of HI to apply hydrogen process in thermochemical VHTR-SI cycle, operating characteristics of the HI decomposition reaction were investigated using the CFD code as a commercial program. Several factors, such as hydrogen production, heat of reaction, and temperature distribution, were studied to compare the device performance with that expected for device development.

### 2. Design and CFD Methods

#### 2.1 Model Design

In this study, characteristics of the thermal decomposition device (HI decomposer, Fig. 1(a)) were investigated using the CFD simulator model (Fig. 1(b)). Fig.1(a) shows the HI decomposer model and the heating device consisting of a sealed three-stage electric heaters. A Hastelloy HC276 tube was inserted, the O.D (outer diameter), I.D (inner diameter), and height of

which were 60.5, 52.7, and 1500 mm, respectively. The active carbon catalyst and Al<sub>2</sub>O<sub>3</sub> Raschig ring were filled. Each of the three electric heaters had built-in heating elements (i.e., 3.65 kW Kanthal A-1) and the HC276 tube was surrounded by a low-density ceramic fiber board for insulation. Moreover, a PID controller was used to maintain the temperature of the three electric heaters a set value. The HI-I<sub>2</sub>-H<sub>2</sub>O mixture gas discharged from the condenser of the multistage distillation flowed to the bottom of the inlet of the HI decomposer at an absolute pressure of 5 kgf/cm<sup>2</sup> (506,625 Pa). The temperature gradually increased to reach the set temperature of the electric heater of the HI decomposer and was maintained at this value. Meanwhile, helium (He) gas or N<sub>2</sub> gas was supplied to the HI decomposer to maintain the pressure at 506,625 Pa and thermal equilibrium was reached using an external heating chamber of the HI decomposer.

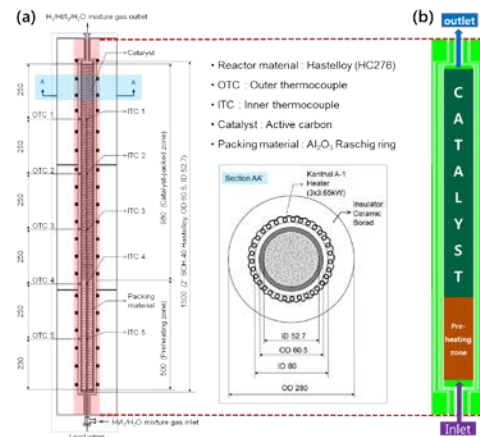


Fig. 1. Designed HI decomposer for SI cycle and CFD Model; (a) Designed HI decomposer (b) CFD domain.

#### 2.2 CFD Analysis Methods

CFD analysis was conducted using the Fluent program. Moreover, to describe the actual operating system, the UDF (i.e., user define function) was applied. At  $t=0$  and 464.85 K (191.7 °C), the HI-I<sub>2</sub>-H<sub>2</sub>O mixture gas with a flow rate of 0.008 mol (HI)·s<sup>-1</sup>, 0.0002 mol (I<sub>2</sub>)·s<sup>-1</sup>, and 0.020 mol (H<sub>2</sub>O)·s<sup>-1</sup> was injected into the HI decomposer at an absolute pressure of 5 kgf/cm<sup>2</sup>.

Maintaining a fixed porosity of 0.4, the temperature of the electric heaters was set at 773.15 K, (500 °C), 873.15 K (600 °C), and 973.15 K (700 °C). The porosity value was approximately predicted by considering several parameters, such as the reactor size, volume, catalyst density, catalyst size, amount of catalyst. The effect of the surface-to-volume (STV) ratio changes on hydrogen production was also considered. When the reactor was developed, the STV ratio was approximately 0.4 in the preliminary simulation.

### 3. Results and Discussion

#### 3.1 Effect of the heater temperature

To investigate the effects of the heater temperature on hydrogen production, the hydrogen production at different set temperatures as 773.15 K, 873.15 K, and 973.15 K of the HI decomposer at STV ratios of 0.3, 0.4, and 0.5 was estimated, as shown in Fig. 2.

Fig. 2(a) shows the hydrogen production measured at 773.15 K (heater temperature). Until 20 min after the operation of the HI decomposer, no hydrogen production occurred regardless of the STV ratio. As presented in Fig. 2(b), at 873.15 K, the amount of hydrogen was very low until 20 min, but after 120 min, it increased according to the STV ratio. After 120 min, hydrogen was produced at 1.11-1.12, 1.98-1.99, and 3.09-3.10 mol/h at STV ratios of 0.3, 0.4, and 0.5, respectively. Fig. 2(c) shows the hydrogen production at 973.15 K. Similar to that at 773.15 K and 873.15 K, the transition process was generated, and then, hydrogen was produced at 1.11-1.12, 1.98-1.99, and 3.09-3.10 mol/h at STV ratios of 0.3, 0.4, and 0.5, respectively.

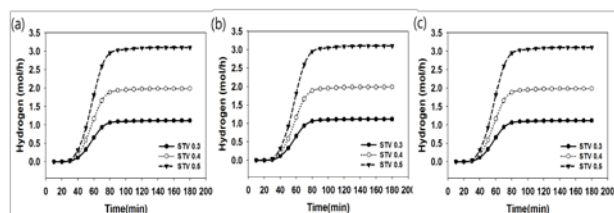


Fig. 2. The prediction of hydrogen production according to heater temperature changes; (a) Heater set value 773.15 K, (b) Heater set value 873.15 K, and (c) Heater set value 973.15 K.

#### 3.2 Inner Temperature distribution of The HI Decomposer on the heater temperature

Fig. 3 shows the inner temperature distribution of the HI decomposer at various STV ratios (0.3, 0.4, and 0.5). The temperature at the center of the catalyst zone was lower than that at the preheating zone for all STV ratios (Fig. 3(a)). Around heat was used to catalyst decomposition reaction. The temperatures of the outlet part which discharged the mixture gas and the temperature of the zone above the catalyst zone were relatively higher than that of the catalyst zone.

At an STV ratio of 0.3, the temperatures of ITC 1, ITC 2, and ITC 3 were higher than the temperature at 773.15 K and 873.15 K for the same STV ratio (Fig. 3(b)). For the decomposition reaction is an endothermic reaction, it seems less reaction heat was supplied so that the inner temperature was higher at 973.15 K than that in the other cases. With different STV ratio, there is no significance different in all of temperature. However, different trends were exhibited at various temperatures even if the difference is small. At the 973.15 K, the inner temperature was found higher than in other cases.

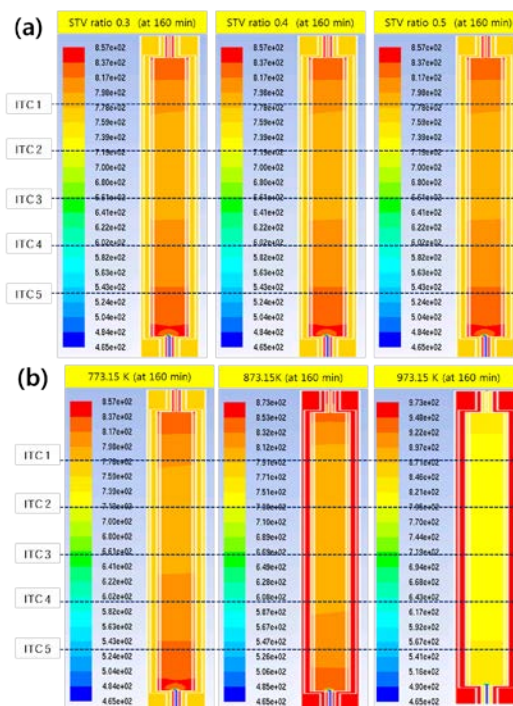


Fig. 3. Inner temperature of HI decomposer according to temperature changes of heater.

### 4. Conclusions

The CFD analysis for HI decomposition simulation was performed by applying the actual operation conditions and HI decomposer design. The hydrogen production depended on the STV ratio. In this study, predicted hydrogen production was 1.12, 1.99, and 3.10 mol/h for STV ratios of 0.3, 0.4, and 0.5, respectively. The hydrogen production at an STV ratio of 0.5 was higher than that at 0.3 by 2 mol/h. The inner temperature of the HI decomposer was studied in the form of contour images at ITC 1-5. A temperature higher than 750 K was required to generate the reaction stably. Also, at ITC 2 and ITC 3 as the center of the catalyst zone, the temperature was 773-801 K and was lower than that at the preheating region.

## **ACKNOWLEDGEMENTS**

This study has been performed under mid-and-long term Nuclear R&D Project by the Ministry of Science, ICT and Future Planning, Republic of Korea.

## **REFERENCES**

- [1] J. E. Funk. Thermochemical hydrogen production: past and present. *International Journal of Hydrogen Energy*, Vol. 26(3), pp.185-190, 2001.
- [2] S. Kubo, H. Nakajima, S. Kasahara, et al. A demonstration study on a closed-cycle hydrogen production by the thermochemical water-splitting iodine-sulfur process. *Nuclear Engineering and Design*, Vol. 233(1-3),347-354, 2004.