# Hydrogen Iodide Decomposer Sizing for a Nuclear Hydrogen Production by a SI Process

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## 1. Introduction

Hydrogen can be an attractive energy if it can be produced cleanly and in a cost effective manner. Nuclear energy can be used as a source of a high temperature process up to 1000℃ for a hydrogen production. The sulfur-iodine (SI) cycle is a baseline candidate thermo-chemical process. It consists of the following three chemical reactions which yield a dissociation of water [1].

$$I_2 + SO_2 + 2H_2O \rightarrow 2HI + H_2SO_4 \quad (1)$$

$$H_2SO_4 \rightarrow H_2O + SO_2 + 1/2O_2 \quad (2)$$

$$2HI \rightarrow H_2 + I_2 \quad (3)$$

The decomposition of the hydrogen iodide is the key reaction of hydrogen production by the SI cycle. But at a temperature of process gas(450℃), equilibrium conversion yield is too low to obtain high decomposition yield. Then, reaction condition is needed to maintain non-equilibrium condition which is accomplished by multiple cascade reactors with selective membranes. In this paper, each cascade consists of catalyst-packed reactors and selective membranes in a helium chamber.

As a result of the study, the hydrogen iodide decomposers for 300mole/s (200MW$_{th}$ VHTR 40% thermal efficiency) and 60mole/s (40MW$_{th}$ VHTR 40% thermal efficiency) hydrogen production rates are presented and discussed.

## 2. Sizing procedure for hydrogen iodide decomposer

### *2.1. Reaction rate equation*

The rate equation for the decomposition of hydrogen iodide was based on equation (4), (5), (6) and (7) by Oosawa [2]. The reaction rate constant (equation (8)) is the Arrhenius equation which is a function of the temperature in the presence of activated carbon. Equilibrium constant (equation (9)) is obtained from HSC5.1 [3]. According to equations, reaction rate is function of input/output concentration, pressure and temperature.

$$r_{HI} = -kPR_{HI} \quad (4)$$

$$R_{HI} = \frac{x_{HI}}{1 + K_{I2}Px_{I2}} - \frac{\sqrt{x_{H2}x_{I2}}\,(1 + K_{I2}P\Phi^e/2)}{K_p(1 + K_{I2}Px_{I2})^2} \quad (5)$$

$$K_{I2} = 5.086 \times 10^{-11} \exp\left(\frac{68667}{RT}\right) \quad (6)$$

$$\Phi^e = 1 - \frac{C^e_{HI}}{C_{HI,0}} \quad (7)$$

$$k = 0.158 \exp\left(\frac{-34375}{RT}\right) \quad (8)$$

$$K_p = \frac{\sqrt{C^e_{H2}}\sqrt{C^e_{I2}}}{C^e_{HI}} \quad (9)$$

### *2.2. Hydrogen iodide decomposer modeling*

Fig. 1 shows the tank-in-series model for the hydrogen iodide decomposer. Each reactor is catalyst-packed reactor and it is connected to selective membrane. These are placed in helium chamber. Reactors and helium chamber assumed perfectly mixed tanks and reaction progresses to equilibrium conversion and hydrogen separates simultaneously in selective membrane.

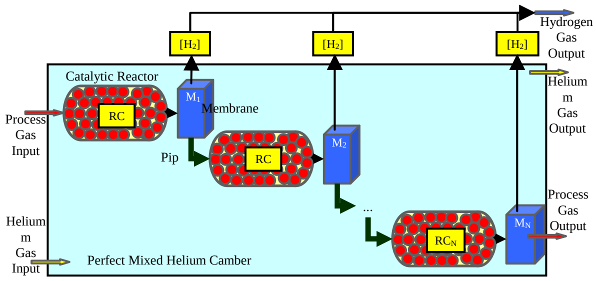


Fig. 1. Tank-in-series model for a hydrogen iodide decomposer

Equation (10) is the material balance equation for the tank-in-series reactor and equations (11), (12) and (13) are material balance equations for selective membrane [4]. Equation (14) presents energy consumption in hydrogen iodide decomposer respectively [5]. It means that only reaction heat exists for the model. Heat of reaction is obtained from HSC5.1 [3].

$$V_i = \frac{(C_{HI,i-1} - C_{HI,i})v_{i-1}}{(-r_{HI,i})} \quad (10)$$

$$F_{HI,i} = k_h\left[v_{i-1}C_{H2,i-1} + v_{i-1}\frac{(C_{HI,i-1} - C_{HI,i})}{2}\right] \quad (11)$$

$$F_{HI,i} = \alpha_{HI}F_{H2,i} \quad (12)$$

$$F_{I2,i} = \alpha_{I2}F_{H2,i} \quad (13)$$

$$Q_r = \sum_{1}^{N} \left[ \left( -r_{HI,i} V_i \right) \left( -\Delta H_{HIr} \right) \right] \quad (14)$$

### *2.3. Hydrogen iodide decomposer sizing*

Table 1. Input/output conditions of the hydrogen iodide decomposer

| | HI | $I_2$ | $H_2O$ | $H_2$ | He |
|---|---|---|---|---|---|
| Input [mole/s] | 989.4 | 275.9 | 2612.1 | 0 | 1268 |
| Total Membrane Output [mole/s] | 0.15 | 0.15 | 0 | 302.8 | 1268 |
| Residual Output [mole/s] | 382.7 | 579.0 | 2612.1 | 0.471 | |
| Input Temp. [K] | 723 | | | | 985 |
| Output Temp. [K] | 723 | | | | 792 |
| Pressure [Pa] | $22*10^5$ | | | | $22*10^5$ |
| Voidage | 0.2 | | | | - |
| Hydrogen permeability | - | - | - | 0.9 | - |
| Relative permeability | 0.0005 | 0.0005 | 0 | 1 | - |

Input/output conditions for a hydrogen iodide decomposer are represented in Table 1 based on a 300mole/s hydrogen production rate and the heat duty is 3790kJ/s. For the condition based on 60mole/s hydrogen production rate, each of the flow rates and heat duty are multiplied by 1/5 times.

Fig. 2 shows the steady state results for the hydrogen iodide decomposer. According to the calculated result, total 24 stages are needed to accomplish 300mole/s hydrogen production rate.

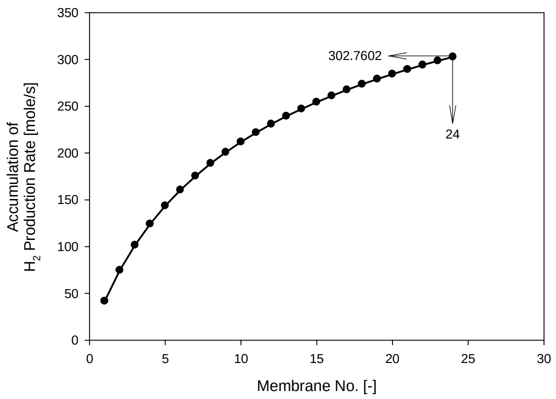


Fig. 2. Accumulation of hydrogen production rate for the membrane in hydrogen iodide.

## 3. Conclusion

A hydrogen iodide decomposer sizing was accomplished and the results are as follows; Table 2 shows the calculation results for $200MW_{th}$ and $40MW_{th}$. Apparent volume is calculated by adopting reactor voidage (0.2) and total chamber volume is 110% of apparent volume; 96.18 and $19.24m^3$.

Table 2. Sizing result of hydrogen iodide decomposer

| Stage No. | Hydrogen Production Rate | | | |
|---|---|---|---|---|
| | $300mole/s(200MW_{th})$ | | $60mole/s(40MW_{th})$ | |
| | Reaction Volume $[m^3]$ | Apparent Volume $[m^3]$ | Reaction Volume $[m^3]$ | Apparent Volume $[m^3]$ |
| 1 | 3.268404 | 16.34202 | 0.653681 | 3.268404 |
| 2 | 1.675015 | 8.375073 | 0.335003 | 1.675015 |
| 3 | 1.306672 | 6.533361 | 0.261334 | 1.306672 |
| 4 | 1.085935 | 5.429676 | 0.217187 | 1.085935 |
| 5 | 0.937447 | 4.687236 | 0.187489 | 0.937447 |
| 6 | 0.829902 | 4.149509 | 0.16598 | 0.829902 |
| 7 | 0.747917 | 3.739585 | 0.149583 | 0.747917 |
| 8 | 0.683029 | 3.415146 | 0.136606 | 0.683029 |
| 9 | 0.630183 | 3.150916 | 0.126037 | 0.630183 |
| 10 | 0.586166 | 2.930829 | 0.117233 | 0.586166 |
| 11 | 0.548832 | 2.744158 | 0.109766 | 0.548832 |
| 12 | 0.516691 | 2.583454 | 0.103338 | 0.516691 |
| 13 | 0.488674 | 2.443371 | 0.097735 | 0.488674 |
| 14 | 0.463994 | 2.319969 | 0.092799 | 0.463994 |
| 15 | 0.442055 | 2.210273 | 0.088411 | 0.442055 |
| 16 | 0.422398 | 2.111992 | 0.08448 | 0.422398 |
| 17 | 0.404666 | 2.023332 | 0.080933 | 0.404666 |
| 18 | 0.388573 | 1.942865 | 0.077715 | 0.388573 |
| 19 | 0.373888 | 1.869441 | 0.074778 | 0.373888 |
| 20 | 0.360424 | 1.80212 | 0.072085 | 0.360424 |
| 21 | 0.348026 | 1.740128 | 0.069605 | 0.348026 |
| 22 | 0.336564 | 1.68282 | 0.067313 | 0.336564 |
| 23 | 0.325931 | 1.629653 | 0.065186 | 0.325931 |
| 24 | 0.316034 | 1.580168 | 0.063207 | 0.316034 |
| Total | 17.48742 | 87.43709 | 3.497484 | 17.48742 |

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