### Computational Analysis of a Packed Column for SO<sub>3</sub> Decomposition in Sulfur-Iodine Process



### **Research Background and Purpose**

- The thermochemical and hybrid hydrogen production processes accompanied with the high temperature and strongly corrosive operating conditions basically have material problems.
- The development of a structural material and equipment design technologies is being carried out.

# How to be free and easy from the material issue ?

In order to resolve these problems, the concept of a directly heated SO<sub>3</sub> decomposer for the SI and HyS processes has been introduced and analyzed by using a computational fluid dynamics code(CFD).

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### Nuclear Hydrogen Production System



### Sulfur-Iodine Cycle



### **Preliminary Thermal Pathway for SI Cycle**



### Concept of a Directly Heated SO<sub>3</sub> Decomposer

- •In order to mitigate material problems and complex heatexchanger configurations, the following conceptions are adopted.
- -A direct mixing of process and He gases to maintain an operation temperature.
  -Insertion of molten salt layer to monitor the integrity of IHX.
- -A gas separator to recycle He From VHTR and process gases.



### **Design values for Chemical Decomposer**(1/2)



Schematic of sulfur-iodine decomposer

Design values of thermo-chemical decomposer

	Values
Total decomposer length	16.06m
Decomposer height	<b>8m</b>
Inlet diameter for mixture gases	<b>30cm</b>
He inlet diameter	50cm
Upper & lower Grid plate thicknesses	3cm
Al <sub>2</sub> O <sub>3</sub> catalyst diameter	2cm

□ RA330<sup>[6]</sup> as the material of the vessel and guide tube

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### **Design values for Chemical Decomposer**(2/2)

	H <sub>2</sub> O	<b>O</b> <sub>2</sub>	SO <sub>2</sub>	SO <sub>3</sub>	H <sub>2</sub> SO <sub>4</sub>
Mass Fraction	22.12%	22.12%	22.15%	33.38%	0.22%
Mole Fraction	1.7777	0.5	1	0.6031	0.0033

#### Mass fraction & mole fraction of mixture gases

#### **Operating conditions of thermo-chemical decomposer**

	Flow rate	Inlet temperature	Operating pressure
He	<b>2.0628 kg/s</b>	920 °C	7.09bar
Mixture gas	<b>1.8046 kg/s</b>	450 °C	7.09bar



### **Pressure drop as function of catalyst diameter and gas velocity**



Ergun Model  

$$\frac{dp}{L} = -\frac{150\mu(1-\varepsilon)^2}{\varepsilon^3 D_p^2} - \frac{1.75\rho(1-\varepsilon)u^2}{\varepsilon^3 D_p}$$

$$\mu = vis \cos ity[kg / ms]$$

$$\rho = density[kg / m^3]$$

 $\mu = vis \cos ity[kg / ms]$   $\rho = density[kg / m^{3}]$   $D_{p} = Al_{2}O_{3}diameter[m]$   $\varepsilon = porosity[-]$   $u = su \ erficial velocity[m / s]$ 

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### Velocity profile



### Temperature contour



### Temperature profile in the r-direction



### Guide tube Temperature contour with different He Flow Rate



- The maximum temperature of RA 330 is 690 °C at He=1 kg/s. It is much lower than 800 °C which is considered as a limiting temperature. The mean temperature in the Al2O3 region is 783 °C which is a little low temperature to decompose a sulfur-iodine.
- The maximum temperature of guide tube is 780°C at He=3 kg/s, and The mean temperature in the Al2O3 region is 890°C which is good temperature to decompose a sulfur-iodine.

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## **Conclusions**

- A numerical analysis for a directly heated SO3 decomposer has been made.
- When the conceptual design conditions of the decomposer presented in this research were used, the maximum temperature of the structural material (RA330) could be maintained at 800 °C or less.
- It can be seen that the mean temperature of the reaction region packed with catalysts in the SO3 decomposition reactor could satisfy the temperature condition of around 850 °C which is the target temperature in this study.
- An improved heat transfer model for a catalyst layer including a chemical reaction is required.

# Thank you.

