

## Preliminary Studies of S-CO<sub>2</sub> Critical Flow for Leak Modeling in Sodium-CO<sub>2</sub> Heat Exchanger

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### 1. Introduction

The supercritical CO<sub>2</sub> (S-CO<sub>2</sub>) Brayton cycle has been receiving attention as an alternative power conversion system to the steam Rankine cycle for the SFR system. Even though a S-CO<sub>2</sub> Brayton cycle can eliminate the sodium-water reaction, there is a potential reactive process between sodium and CO<sub>2</sub> if the pressure boundary fails in the sodium-CO<sub>2</sub> heat exchanger. The pressure boundary is an interface enduring a high pressure difference between sodium at 0.1 MPa and CO<sub>2</sub> at 20MPa. Thus, when it fails, high-pressure CO<sub>2</sub> will be injected into the sodium side to react with sodium.

The amount of chemical reaction between sodium and CO<sub>2</sub> will vary depending on several factors; the crack or rupture size, the interfacial area between sodium and CO<sub>2</sub>, the amount of released CO<sub>2</sub>, and so on. These factors are as influential as the reaction temperature of Na-CO<sub>2</sub> interaction. To specify these factors, it is important to predict the CO<sub>2</sub> leak mechanism during the CO<sub>2</sub> leakage. However, only limited number of studies has been performed for understanding the CO<sub>2</sub> leak mechanism.

The system dynamic response with respect to Na-CO<sub>2</sub> reaction was numerically simulated by assuming a double-ended guillotine break in a shell-and-tube type heat exchanger previously [1]. The modeling of the CO<sub>2</sub>-gas jet into water (before CO<sub>2</sub>-gas jet into sodium) has been investigated from both experiment and numerical analyses to obtain kinetic parameters of Na-CO<sub>2</sub> reaction and understand the behavior of CO<sub>2</sub> leak flow as a jet [2].

However, several limitations can be found from the previous studies. The assumptions such as maintaining steady conditions in the CO<sub>2</sub> side or fixing the mass flux at the nozzle inlet at constant over the course of time are neither practical nor reasonable as the CO<sub>2</sub> side conditions. Since the CO<sub>2</sub> side conditions will change during the depressurization due to the leak, more realistic assumptions should be applied to the CO<sub>2</sub> leak model.

Before simulating the CO<sub>2</sub> flow behavior close to the actual scenario, an isentropic critical flow model was numerically developed with several assumptions in this study. From this model, the variation of conditions of sodium and CO<sub>2</sub> sides and the consequences of Na-CO<sub>2</sub>

interaction can be predicted in the future. The numerically obtained results can be used for evaluation of the consequences of Na-CO<sub>2</sub> interaction.

### 2. Methodology

#### 2.1 Description of Model

A simplified flow model including critical flow for CO<sub>2</sub> leak simulation was devised, and the critical flow model is based on an isentropic flow model. The leak was expected to occur in a PCHE (Printed Circuit Heat Exchanger) type of Na-CO<sub>2</sub> heat exchanger. The PCHE is one of the most widely accepted heat exchangers for the S-CO<sub>2</sub> power cycle application. A simplified flow model was developed as conceptually shown in Fig. 1. It was assumed that the CO<sub>2</sub> flows through a nozzle, which simulates a micro-meter size crack, from the CO<sub>2</sub> tank to the sodium tank. In the sodium tank, there is a cover gas space filled with N<sub>2</sub> where the leaked CO<sub>2</sub> or rest CO<sub>2</sub> and generated CO from Na-CO<sub>2</sub> interaction are gathered, and it is pressurized due to the gas mixture.

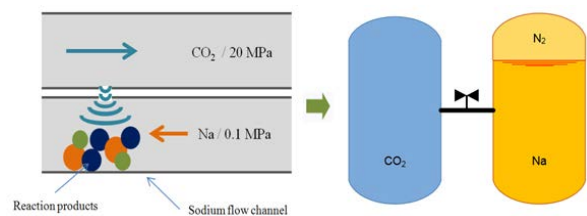


Fig. 1. Expected CO<sub>2</sub> leak in Na-CO<sub>2</sub> heat exchanger (left) and simplified model for numerical analysis (right)

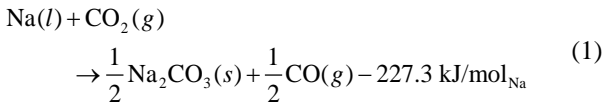
#### 2.2 Assumptions for Model

To simplify the flow simulation model further, the following assumptions were used.

- CO<sub>2</sub> in supercritical state far from the critical point behaves like an ideal gas. (Compressibility factor  $\approx 1$ )
- CO<sub>2</sub> is stagnant in the CO<sub>2</sub> tank.
- The temperature of CO<sub>2</sub> tank is at constant.
- The crack is generated in normal operating conditions.
- Whether the flow is choked or not depends on the nozzle inlet conditions and the back pressure.  
(The flow is choked at the nozzle exit.)

In this flow model, Na-CO<sub>2</sub> reaction model was added to update the boundary conditions in every time step. Thus, the assumptions for the reaction model are as in the following.

- The temperature of CO<sub>2</sub> at the nozzle exit is equalized with that of liquid sodium.
- The pressure of CO<sub>2</sub> leaked into the sodium side is the same as that of sodium regardless of the flow state and the pressure of CO<sub>2</sub> at the nozzle exit.
- 70% of leaked CO<sub>2</sub> reacts with sodium by the dominant chemical reaction equation, Eq. (1) [3].
- The reaction takes place just after the CO<sub>2</sub> gas leaks into the sodium side.
- Un-reacted CO<sub>2</sub> and generated CO are gathered in the cover gas space and affect its pressure.
- The generated CO follows the ideal gas law.
- The generated heat from Na-CO<sub>2</sub> interaction is uniformly dissipated into the entire sodium.



To simplify the model, it was assumed that the temperature and pressure of CO<sub>2</sub> at the nozzle exit are at equilibrium with liquid sodium. It means that the isentropic expansion of CO<sub>2</sub> at the nozzle exit was neglected although the CO<sub>2</sub> pressure at the exit is higher than that of sodium when the flow is choked. For quantifying the amount of chemical reaction, it is assumed that 70% of leaked CO<sub>2</sub> reacts with sodium by the dominant reaction equation. The amount of reacted CO<sub>2</sub> was decided based on the preceded experimental studies [3]. Additionally, the reaction is exothermic reaction, which generates reaction heat.

### 2.3 Modeling for Flow and Chemical Reaction

An isentropic critical flow model neglects the frictional losses and heat transfer thus the flow state can be easily calculated with the following governing equations (i.e. continuity equation, critical-pressure ratio equation, Mach number equation with pressure ratio, and mass flux equation from continuity equation):

$$G = \rho V = \text{constant} \quad (2)$$

$$\frac{P_o}{P_{critical}} = \left(1 + \frac{\gamma - 1}{2}\right)^{\gamma/(\gamma - 1)} \quad (3)$$

$$M = \sqrt{\frac{2}{\gamma - 1} \left[ \left(\frac{P_o}{P}\right)^{(\gamma - 1)/\gamma} - 1 \right]} \quad (4)$$

$$G = \frac{P_o}{\sqrt{RT_o}} \sqrt{\gamma} M \left(1 + \frac{\gamma - 1}{2} M^2\right)^{\frac{\gamma + 1}{2(\gamma - 1)}} \quad (5.1)$$

( $P_{critical} < P_{Na}$ , Unchoked flow case)

$$G_{max} = \frac{P_o}{\sqrt{RT_o}} \sqrt{\gamma} \left(\frac{\gamma + 1}{2}\right)^{\frac{\gamma + 1}{2(\gamma - 1)}} (M_{exit} = 1.0) \quad (5.2)$$

( $P_{critical} \geq P_{Na}$ , Choked flow case)

Based on the above governing equations, the critical pressure obtained from Eq. (3) is compared to the sodium side pressure (back pressure) at every time step then it is determined if the flow is choked or not. If the flow is not choked, Mach number is calculated from Eq. (4) and it is applied to Eq. (5.1). On the other hand, Eq. (5.2) with Mach number of unity is used to calculate the choked mass flux. The configuration of nozzle is shown in Fig. 2.

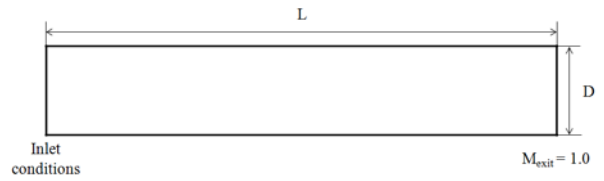


Fig. 2. Configuration of nozzle

Since it is assumed that the generated CO is also regarded as an ideal gas, Eq. (6) is used to calculate the pressure for the next time step and the partial pressure of CO in every time step.

$$\frac{P_1}{n_1} = \frac{P_2}{n_2} \quad (6)$$

Based on the flow model using above equations, the sensitivity study of the transient response during the leak was performed while varying the nozzle diameter and the cover gas space volume. The initial conditions for the model were determined to be the largest values of Na-CO<sub>2</sub> heat exchanger design conditions, which did not considered the pressure drop, shown in Fig. 3, and the assumed conditions are summarized in Table I.

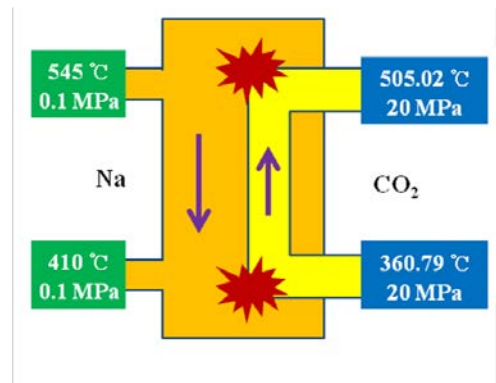


Fig. 3. Preliminary design conditions of Na-CO<sub>2</sub> HX for flow models

Table I: Analytic conditions for the model

Variables		Conditions			
Nozzle diameter (mm) (Volume of cover gas space = 0.1 m <sup>3</sup> )	0.1	P <sub>0</sub> (MPa)	CO <sub>2</sub>	Na	
	0.2		20	0.1	
	0.3	T <sub>0</sub> (°C)	505.02	545	
	0.5		505.02	545	
Volume of cover gas space (m <sup>3</sup> ) (Nozzle diameter = 0.3 mm)	0.03	Mass (kg)	50	58	
	0.07		c <sub>p</sub> of sodium (kJ/kg·K)	1.2619	
	0.1	Nozzle length (mm)		0.3	
	0.25				
	0.5				

### 3. Results and Discussion

The results from the sensitivity study of the transient response during the leak are shown in Figs. 4~11. Calculations are performed while varying the nozzle diameter and the cover gas space volume. From the mass flux results shown in Figs. 4 and 8, the flow was choked in all cases during 600 seconds because the back pressure (the sodium side pressure) was lower than the critical pressure. However, the mass flux shows the same trend in Fig. 8 even though the cover gas space volume is changing. This is because that the mass flux is mainly affected by the pressure of CO<sub>2</sub> side from Eq. (5.2) and the cover gas space volume gives a little influence to the pressure of CO<sub>2</sub> side in this model. This is confirmed from Figs. 5 and 9, which show the pressure change of each CO<sub>2</sub> side and sodium side varying with the nozzle diameter and the cover gas space volume, respectively.

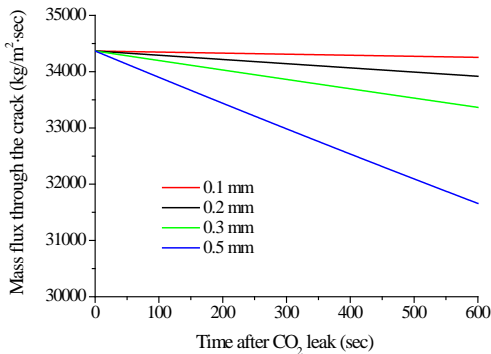


Fig. 4. Mass flux varying with nozzle diameter

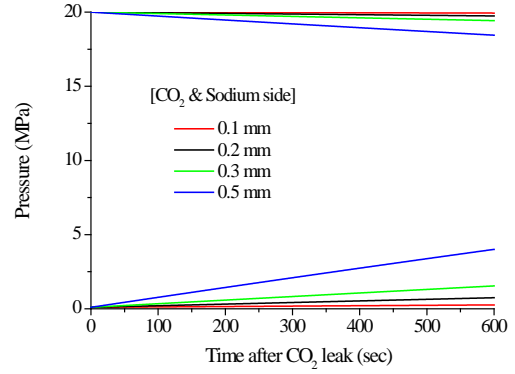


Fig. 5. Pressure change varying with nozzle diameter

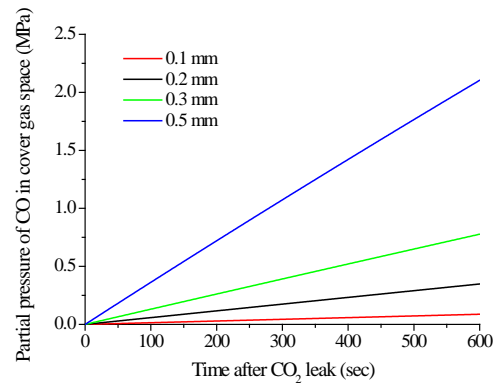


Fig. 6. Partial pressure of CO from Na-CO<sub>2</sub> interaction varying with nozzle diameter

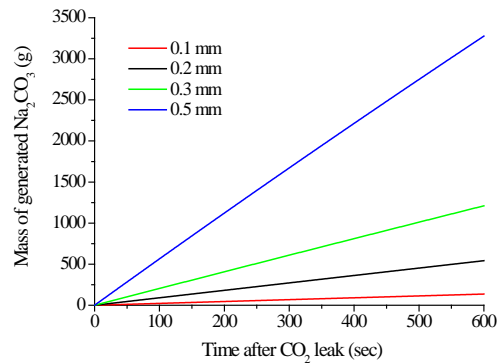


Fig. 7. Mass of Na<sub>2</sub>CO<sub>3</sub> from Na-CO<sub>2</sub> interaction varying with nozzle diameter

Additionally, the partial pressure of CO and the mass of Na<sub>2</sub>CO<sub>3</sub> varying with the nozzle diameter and the cover gas space volume are shown in Figs. 6~7 and 10~11. Thus, the effect of generated heat and CO in terms of pressurization and the amount of main solid reaction product by Na-CO<sub>2</sub> interaction are calculated and quantified.

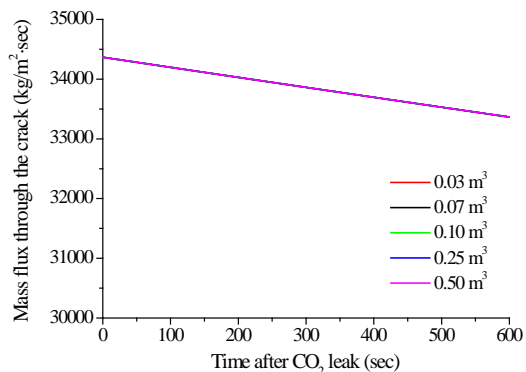


Fig. 8. Mass flux varying with cover gas space volume

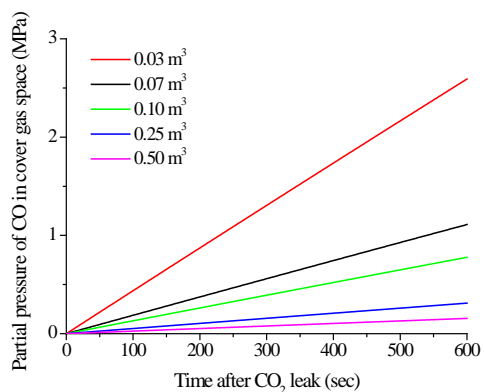


Fig. 10. Partial pressure of CO from Na-CO<sub>2</sub> interaction varying with cover gas space volume

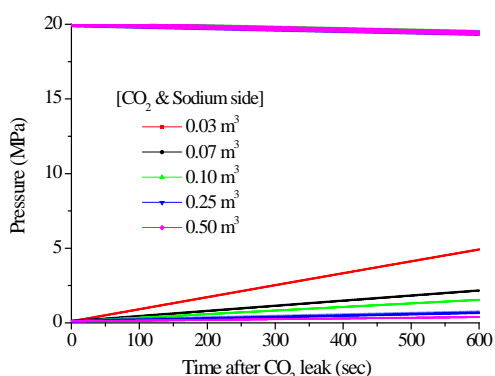


Fig. 9. Pressure change varying with cover gas space volume

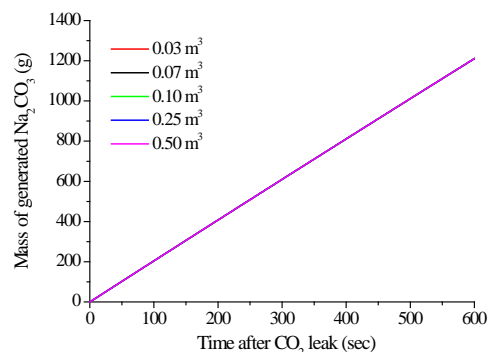


Fig. 11. Mass of Na<sub>2</sub>CO<sub>3</sub> from Na-CO<sub>2</sub> interaction varying with cover gas space volume

#### 4. Conclusions and Further Works

In the process of modeling the CO<sub>2</sub> leak to sodium in a sodium to supercritical CO<sub>2</sub> heat exchanger, an isentropic critical flow model was developed. Based on a simple flow model a preliminary numerical study was carried out by including simplified Na-CO<sub>2</sub> reaction.

However, friction between CO<sub>2</sub> and crack wall should be considered to simulate more realistic CO<sub>2</sub> critical flow, which represents more realistic situation. Thus, the Fanno flow, which considers friction in a compressible flow, will replace the isentropic flow model for better predictability. If this model can reasonably simulate the transient response of the CO<sub>2</sub> leak scenario, several physical models will be added to the current analysis; real gas model, Na-CO<sub>2</sub> interaction, two-phase model for liquid sodium and gaseous CO<sub>2</sub>, heat transport in the sodium tank, and so on.

Under more reasonable assumptions, the model will be gradually updated and more stable numerical scheme will be developed. At this end, it is expected that this study will play an important role in system design and safety evaluation prior to the application of S-CO<sub>2</sub> Brayton cycle to SFRs in the future.

#### ACKNOWLEDGEMENT

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