

Numerical Studies of CO₂ Leak Modeling in Sodium-CO₂ Heat Exchanger in the SFR coupled with the S-CO₂ Brayton Cycle

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ABSTRACT

For applying the supercritical CO₂ Brayton cycle to the Sodium-cooled Fast Reactor, several technical challenges should be resolved. One of the most significant issues is to comprehend the CO₂ leak mechanism initiated from the pressure boundary failure in a sodium-CO₂ heat exchanger. Since the chemical reaction between sodium and CO₂ is followed, the modeling of CO₂ leak process is essential to predict the system dynamics. So far, a few studies have been performed to understand the CO₂ leak mechanism but some limitations could be found. Thus, to simulate the transient response of the sodium side and CO₂ side during the leak process more realistically, a numerical study was conducted. Prior to fully investigating the CO₂ leak and the reaction mechanism, an isentropic critical flow model as a reference model was developed while reflecting sodium-CO₂ interaction with several assumptions in this study.

A numerical study was performed while varying the nozzle diameter and the cover gas space volume with a conceptually designed simple flow model. Mass flux was calculated by determining the flow state whether the flow is choked or not. Then, the change of system pressure was obtained while calculating the amount of reaction products and generated heat. Even though this model could generally simulate the leak process, it should be modified by adding frictional losses and other assumptions.

KEYWORDS

SFR, S-CO₂ Brayton cycle, CO₂ leak mechanism, flow modeling, Na-CO₂ interaction

1. INTRODUCTION

For developing an innovative future nuclear system, the Generation IV Nuclear Energy Systems were proposed. One of them is the Sodium-cooled Fast Reactor (SFR), which has been actively developed in various countries. In the past, the SFRs have operated with the steam Rankine cycle as a power conversion system. However, the potential sodium-water reaction (SWR) has been one of the major issues of the safety and integrity of the SFRs coupled with the steam Rankine cycle. The risk of SWR, of which chemical reactivity is vigorous and instantaneous, is well known as the formation of corrosive sodium hydroxide (NaOH) and explosive hydrogen gas (H₂) with generating substantial amount of reaction heat.

From this background, the supercritical CO₂ (S-CO₂) Brayton cycle has been receiving attention as an alternative power conversion system to the steam Rankine cycle of SFR systems. Though the S-CO₂ Brayton cycle has several excellent features such as 1) improved thermal efficiency, 2) reduced total plant size by having compact turbo-machineries and heat exchangers, and 3) relatively simplified cycle layout, one of the most pronounced benefits is the elimination of SWR. However, there are still remaining several technical challenges for application of the S-CO₂ Brayton cycle to the SFRs. Furthermore, it has been confirmed in the recent studies that CO₂ reacts with liquid sodium and the reaction shows a different feature depending on the reaction temperature. However, it is still much milder than SWR [1, 2].

This potential reaction between the liquid sodium and CO₂ can occur if the pressure boundary fails in a sodium-CO₂ heat exchanger. Since the pressure boundary is an interface enduring a high pressure difference between sodium at 0.1MPa and CO₂ at 20MPa, high-pressure CO₂ will be injected into the sodium side then react with sodium.

In respect of Na-CO₂ interaction itself, numerous studies have been performed to obtain information of thermodynamic and kinetic features, so far. However, to comprehensively understand and expect the degree of Na-CO₂ interaction, it is necessary to specify the following factors; the crack or rupture size, the interfacial area between sodium and CO₂, the amount of released CO₂, and so on. These factors are as influential as the reaction temperature of Na-CO₂ interaction. To specify these factors, it is important to predict the CO₂ leak mechanism during the CO₂ leak process by simulating the transient response in a Na-CO₂ heat exchanger. However, the studies on the CO₂ leak mechanism initiating the Na-CO₂ interaction are relatively few.

The system dynamic response with respect to Na-CO₂ reaction was numerically simulated by assuming a double-ended guillotine break in a shell-and-tube type heat exchanger previously [3]. The modeling of the CO₂-gas jet into water (before CO₂-gas jet into sodium) has been investigated from both experiment and numerical analyses to obtain kinetic parameters of Na-CO₂ reaction and understand the behavior of CO₂ leak flow as a jet [4].

However, some limitations can be found in the previous studies. The assumptions such as maintaining steady conditions in the CO₂ side or fixing the mass flux at the nozzle inlet at constant over the course of time are neither practical nor reasonable as the CO₂ side conditions. Since the CO₂ side conditions will change during the depressurization while the sodium side is pressurized due to the leak, the flow state also can be changed. This study concentrated more on the flow modeling to apply more realistic assumptions to the CO₂ leak model then to evaluate the effects of system condition change.

Before simulating the transient response of the sodium side and CO₂ side during the leak process close to the actual scenario, an isentropic critical flow model as a reference model was numerically developed with several assumptions as it is shown in this study. From this model, the variation of conditions of sodium and CO₂ sides and the consequences of Na-CO₂ interaction can be predicted. The numerically obtained results can be used for evaluation of the consequences of Na-CO₂ interaction such as the amount of reaction products and generated reaction heat.

2. METHODOLOGY

2.1. Description of Model

It is quite difficult to develop a realistic model to simulate the pressure boundary failure in a Na-CO₂ heat exchanger because both the accident scenario and degree of accident vary with the location and mode of failure. Moreover, in a real accident, the CO₂ flow is compressible flow, which can be choked depending on the pressure difference, and the mass flow rate is affected by the crack size. Also, complex Na-CO₂

interaction varies with the interfacial area. To model the CO₂ leak mechanism realistically, several complex factors should be considered, and making a few assumptions are necessary. Thus, in this study, an isentropic critical flow model as a simple flow model was developed as the first step toward the complete model to predict the CO₂ leak process.

The leak was expected to occur in a PCHE (Printed Circuit Heat Exchanger) type of Na-CO₂ heat exchanger. The PCHE is one of the most widely accepted heat exchangers for the S-CO₂ power cycle application. A simple flow model was developed as conceptually shown in Fig. 1. The expected CO₂ leak is simply depicted to describe when a micro-meter size crack is generated at the pressure boundary. Under this basic concept, it was assumed that CO₂ flows through a nozzle, which simulates a crack, from the CO₂ tank to the sodium tank. In the sodium tank, there is a cover gas space filled with N₂ where the leaked CO₂ and generated CO from Na-CO₂ interaction are gathered, and it is pressurized due to the gas mixture.

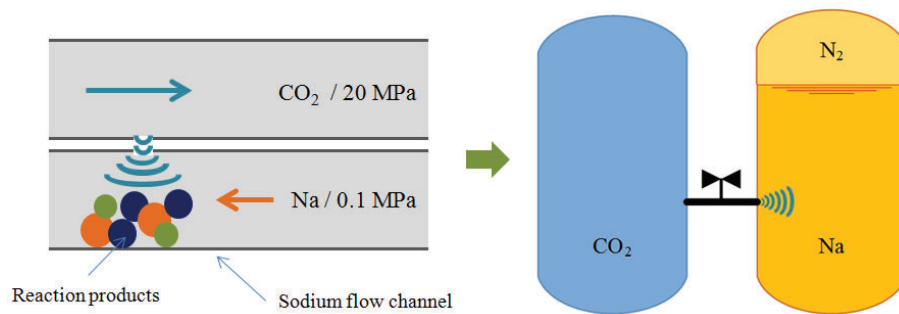


Figure 1. Expected CO₂ leak in Na-CO₂ heat exchanger (left) and simplified model for numerical analysis (right).

2.2. Assumptions for Model Development

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

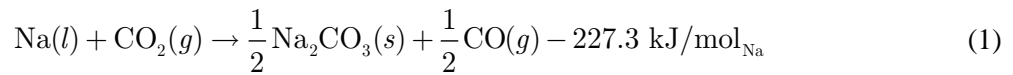
- CO₂ in supercritical state far from the critical point behaves like an ideal gas. (Compressibility factor ≈ 1)
- CO₂ is stagnant in the CO₂ tank.
- The temperature of CO₂ tank is at constant.
- The crack is generated in normal operating conditions.
- Whether the flow is choked or not depends on the critical-pressure ratio.
- In the case of choked conditions, the flow is choked at the nozzle exit.
- The pressure of CO₂ leaked into the sodium side is the same as that of sodium regardless of the flow state and the pressure of CO₂ at the nozzle exit.

CO₂ in the supercritical state is assumed as an ideal gas because the compressibility factor for the supercritical CO₂ is almost close to unity since the condition of CO₂ for this model is far from the critical point (Operating condition: 20MPa 500°C vs. Critical point: 7.38MPa 31.1°C). To simplify the calculation by reducing the variables, the CO₂ flow is assumed to be stagnant and its temperature is at constant in the CO₂ tank. The flow state whether the flow is choked or not is determined by the critical-pressure ratio, which is the ratio of the back pressure (the pressure of sodium side) to the reservoir pressure (the pressure of CO₂ side), because the flow is choked below this ratio. If the flow is choked, it occurs at the nozzle exit. In an actual case, isentropic expansion of CO₂ will occur outside the nozzle because the exit pressure of CO₂ from the nozzle is larger than the back pressure in some cases that the CO₂ flow is choked. But, this

phenomenon is neglected for simplification of calculation in this model by setting the exit pressure of CO₂ to the pressure of sodium.

In this flow model, the Na-CO₂ reaction model was reflected to update the boundary conditions in every time step. Thus, the assumptions for the reaction model are as in the following.

- The temperature of CO₂ at the nozzle exit is equalized with that of liquid sodium.
- 70% of leaked CO₂ reacts with sodium by the dominant chemical reaction equation, Eq. (1) [5].
- The reaction takes place just after the CO₂ gas leaks into the sodium side.
- Un-reacted CO₂ 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-CO₂ interaction is uniformly dissipated into the entire sodium.



It was assumed that the conditions of CO₂ at the nozzle exit are at equilibrium with liquid sodium to simplify the model. In other words, the CO₂ temperature at the nozzle exit and the sodium temperature do not have an effect on the flow modeling. For quantifying the amount of chemical reaction products, it is assumed that 70% of leaked CO₂ reacts with sodium by the dominant reaction equation, Eq. (1). The amount of reacted CO₂ was decided based on the preceded experimental studies [5]. To predict the consequences of reaction, it is assumed that un-reacted CO₂ and generated CO pressurize the sodium system. Additionally, the generated heat is assumed to be uniformly dissipated into the entire sodium in the sodium tank.

2.3. Modeling of Flow and Chemical reaction

For an isentropic critical flow, the frictional losses and heat transfer are neglected 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) [6]:

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

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

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

$$G = \frac{P_o}{\sqrt{RT_o}} \sqrt{\gamma} M \left(1 + \frac{\gamma - 1}{2} M^2\right)^{-\frac{\gamma+1}{2(\gamma-1)}} \quad (P_{critical} < P_b, \text{ Unchoked flow case}) \quad (5)$$

$$G_{max} = \frac{P_o}{\sqrt{RT_o}} \sqrt{\gamma} \left(\frac{\gamma + 1}{2}\right)^{-\frac{\gamma+1}{2(\gamma-1)}} (M_{exit} = 1.0) \quad (P_{critical} \geq P_b, \text{ Choked flow case}) \quad (6)$$

Based on the above governing equations, the critical pressure obtained from Eq. (3) is compared to the sodium side pressure as the back pressure at every time step then it is determined whether 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) to calculate mass flux for the unchoked flow. On the other hand, Eq. (6) with Mach number of unity is used to calculate mass flux for the choked flow.

Since the generated CO is assumed as an ideal gas, Eq. (7) from the ideal gas equation is used to calculate the pressure of sodium side for the next time step. Under the same concept, the partial pressure of CO in the cover gas space is also obtained from Eq. (7).

$$\frac{P_t}{n_t} = \frac{P_{t+1}}{n_{t+1}} \quad (7)$$

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, shown in Fig. 2, were determined to be the Na-CO₂ heat exchanger design conditions without considering the pressure drop. The conditions are based on the input conditions for the analysis of thermal balance in the previous study [7], and the core inlet/outlet temperature was chosen as the sodium temperature to simulate more severe situation. The assumed conditions are summarized in Table I. The analysis time was set as 600 seconds based on the results of the previous study, which analyzed a double-ended guillotine break and showed more conservative results [3].

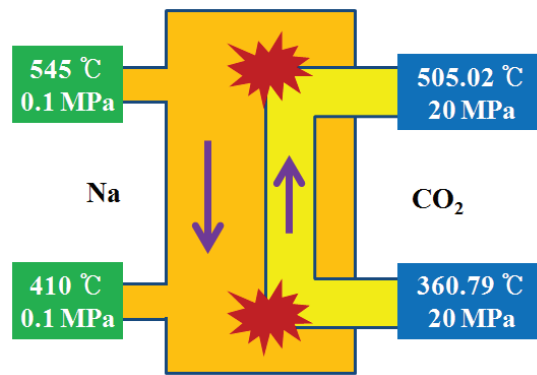


Figure 2. Initial conditions of Na-CO₂ HX for flow models.

Table I. Analytic conditions for the model

Variables		Conditions		
Nozzle diameter (mm) (Volume of cover gas space = 0.1 m ³)	0.1	P ₀ (MPa)	CO ₂	Na
	0.2		20	0.1
	0.3	T ₀ (°C)	505.02	545
	0.5		360.79	20
Volume of cover gas space (m ³) (Nozzle diameter = 0.3 mm)	0.03	Mass (kg)	50	58
	0.07	c _p of sodium (kJ/kg·K)	1.2619	
	0.1			
	0.25	Analysis time (sec)	600	
	0.5			

3. RESULTS AND DISCUSSION

The nondimensionalized results from the sensitivity study of the transient response during the leak are shown in Figs. 3~7. Calculations are performed while varying the nozzle diameter and the cover gas space volume. From the mass flux results shown in Fig. 3, the flow was choked in all cases during 600 seconds because the back pressure was lower than the critical pressure. However, the mass flux shows the same trend in the right figure even though the cover gas space volume is changing. This is because that the mass flux is mainly affected by the pressure of CO₂ side from Eq. (6) and the cover gas space volume has a little influence on the pressure of CO₂ side in this model. This is also confirmed from Figs. 4 and 5, which shows the pressure change of CO₂ side and sodium side, respectively. While the pressure change of CO₂ side in the left figure shows clear distinction varying with the nozzle diameter, the gradient of pressure change is almost the same in the right figure.

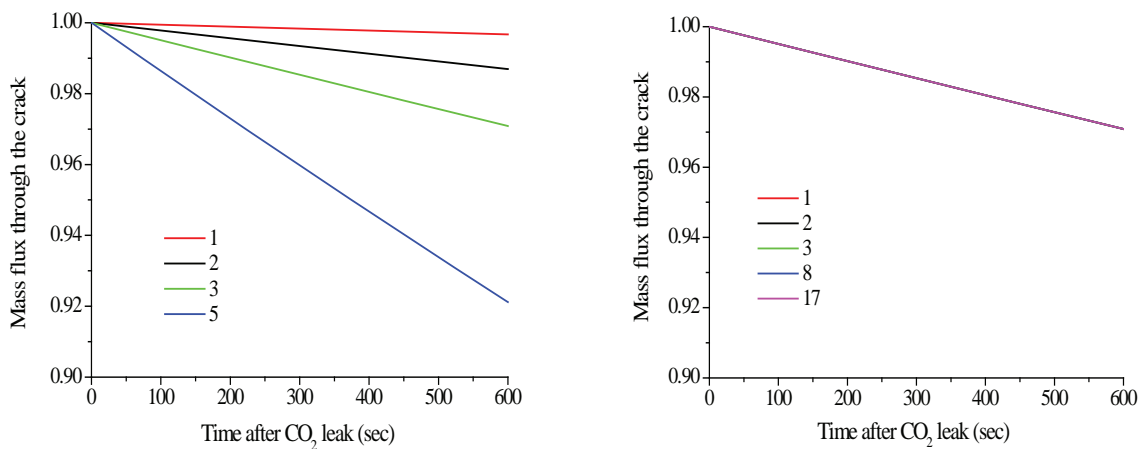


Figure 3. Mass flux varying with nozzle diameter (left) and cover gas space volume (right).

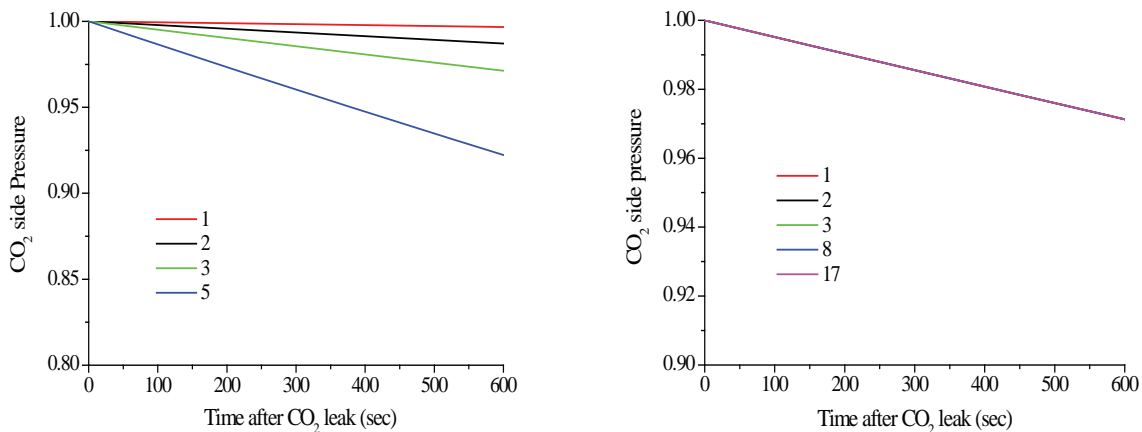


Figure 4. CO₂ side pressure change varying with nozzle diameter (left) and cover gas space volume (right).

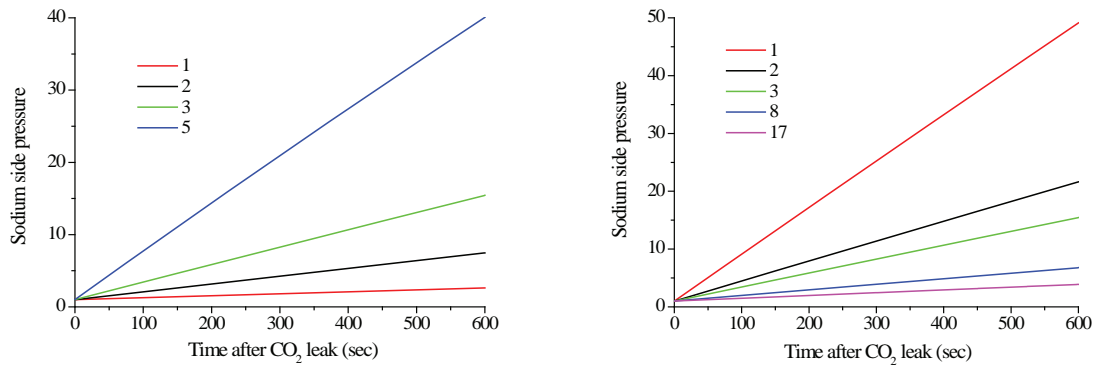


Figure 5. Sodium side pressure change varying with nozzle diameter (left) and cover gas space volume (right).

The partial pressure of CO and the mass of Na_2CO_3 varying with the nozzle diameter and the cover gas space volume are shown in Figs. 6 and 7, respectively. Thus, CO in terms of pressurization and the amount of main solid reaction product by Na- CO_2 interaction are calculated and quantified then the effect of them can be evaluated. Likewise, the nozzle diameter is more influential to most consequences of Na- CO_2 interaction as well as the transient response of the system than the cover gas space volume, except the pressurization of the sodium side.

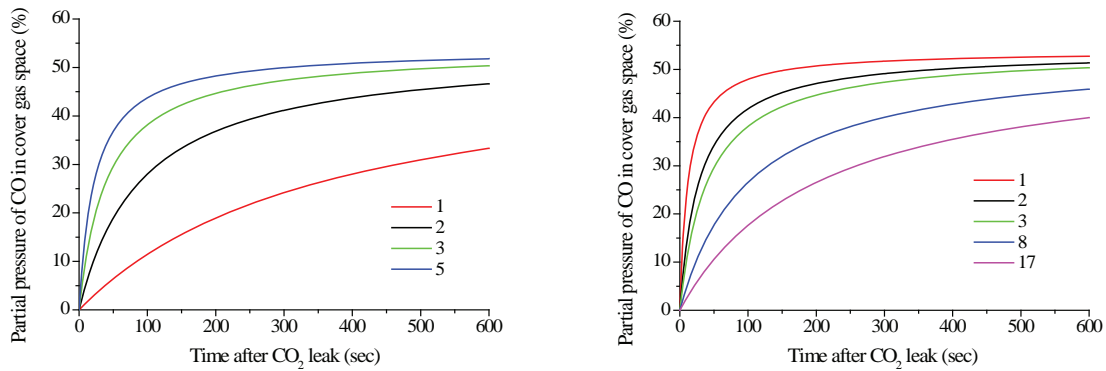


Figure 6. Partial pressure of CO from Na- CO_2 interaction varying with nozzle diameter (left) and cover gas space volume (right).

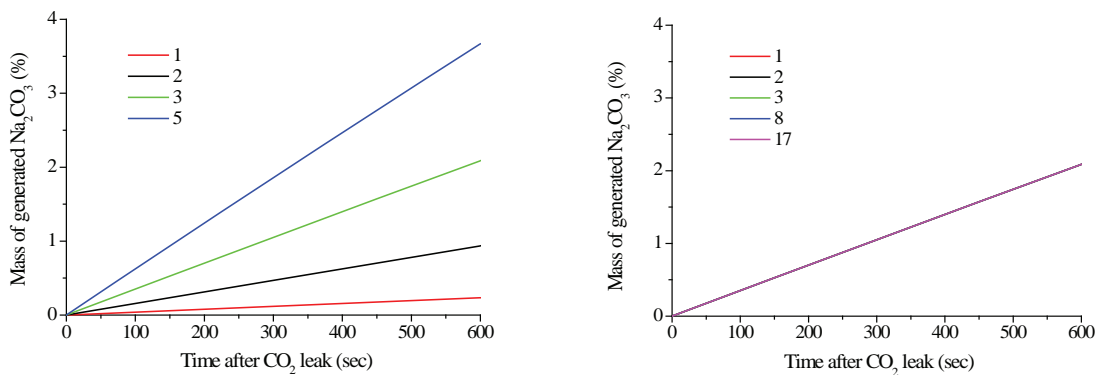


Figure 7. Mass of Na_2CO_3 from Na- CO_2 interaction varying with nozzle diameter (left) and cover gas space volume (right).

4. CONCLUSIONS AND FURTHER WORKS

In the process of modeling the CO₂ leak to sodium in a Na-CO₂ heat exchanger, an isentropic critical flow model was developed. Based on a simple flow model, a preliminary numerical study was carried out with reflecting Na-CO₂ reaction with some assumptions. As a result, the flow was choked in all given conditions and the consequential results were obtained varying the nozzle diameter and the cover gas space volume.

However, friction between CO₂ and crack wall should be considered to simulate more realistic CO₂ critical flow, which represents more realistic situation. Unfortunately, the studies on modeling CO₂ critical flow considering friction have not been performed yet while there are several preceded studies on isentropic flow. Thus, to replace the isentropic flow model for better predictability, the Fanno flow considering friction in compressible flow is under development. However, some limitations of the Fanno flow model were found because more complex boundary conditions and equations are applied to the model. If this model can reasonably simulate the transient response of the CO₂ leak scenario in the near future, several physical models will be added to the current analysis model; real gas model, Na-CO₂ interaction, two-phase model for liquid sodium and gaseous CO₂, 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-CO₂ Brayton cycle to SFRs in the future.

NOMENCLATURE

G	Mass flux	ρ	Density
V	Flow velocity	γ	Ratio of specific heats
M	Mach number	P_o	Stagnation pressure
$P_{critical}$	Critical pressure	P_b	Back pressure
R	Gas constant	T_o	Stagnation temperature
P_t, P_{t+1}	Pressure at the time step t and t+1	n_t, n_{t+1}	Moles at the time step t and t+1

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