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# A Study on the Evaluation of Real Gas vs. Ideal Gas for its Application to the $CO_2$ Leak Flow Model

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## 1. Introduction

It has been proposed to couple Sodium-cooled Fast Reactor (SFR) with the supercritical $CO_2$ (S-$CO_2$) Brayton cycle. As an alternative power conversion system to the current steam Rankine cycle, the S-$CO_2$ Brayton cycle can free SFRs from the sodium-water reaction (SWR) issue. However, high pressure $CO_2$ insurgent to the sodium side will still be a safety issue.

If a crack is generated at the pressure boundary of the sodium-$CO_2$ heat exchanger, $CO_2$ will be injected into the sodium side. At this time, the flow will be choked due to a high pressure difference between the sodium side at 0.1 MPa and the $CO_2$ side at 20MPa. The leak can cause various mechanical and thermal problems [1]. Moreover, $CO_2$ also reacts with sodium by producing some solid reaction products (i.e. $Na_2CO_3$, $Na_2O$, etc.), toxic gas (i.e. CO) and heat [2].

Prior to applying the S-$CO_2$ Brayton cycle to the SFRs, the important safety issues that can occur in the Na-$CO_2$ heat exchanger should be evaluated. For this, it is essential to predict a $CO_2$ leak mechanism when the pressure boundary fails. The degree of sodium-$CO_2$ reaction is determined by several factors; a crack or rupture size, the interfacial area between sodium and $CO_2$, the amount of released $CO_2$, and so on. Unfortunately, there are limited research works in this field.

A numerical study has been performed to simulate the system dynamic response and its consequences with consideration of Na-$CO_2$ reaction. An accident has been assumed to occur in the case of a double-ended guillotine break in a shell-and-tube type heat exchanger [3]. In other studies, a numerical model has been developed to investigate the behavior of $CO_2$ leak flow as a jet [1] and to obtain the depletion rate of a single droplet and bubble inside an under-expanded $CO_2$-gas jet into sodium [4].

In order to simulate more reasonable and realistic $CO_2$ leak flow, one needs to evaluate and improve some limitations found from the previous studies. The dynamic response in the $CO_2$ side should be considered for varying mass flux at the nozzle exit over time. Thus, it is necessary to investigate more practical flow model to evaluate the system condition change and its consequences during the $CO_2$ leak.

For the flow modeling, it is obvious that a real gas effect and friction force should be considered. However, due to its complexity and difficulty, it is generally assumed that $CO_2$ behaves as an ideal gas, and an isentropic critical flow without considering the friction force was applied for the analysis so far. The numerical model in the preceded studies was also based on the isentropic flow and ideal gas law. But it was not confirmed whether assuming $CO_2$ as an ideal gas is reasonable under given conditions.

In this paper, before incorporating the real gas effect and friction force to the model, gas properties are evaluated as the first step. The fluid properties of $CO_2$ is studied to observe how strong the real gas effect can be under SFR operating conditions. From this result, it is determined that which gas model is applicable to the $CO_2$ leak flow model for simulating the accident scenario in the given conditions of Na-$CO_2$ heat exchanger.

## 2. Methodology

### *2.1 Condition for Accident Scenario*

A $CO_2$ leak accident in the Na-$CO_2$ heat exchanger is generally assumed to be taken place in the normal operating conditions. The reference initial condition for an accident scenario was selected based on the condition of KALIMER-600 design [5], and it is listed in Table I. Since the fluid properties (i.e. density, specific heat ratio, etc.) are compared to each other, only the information of pressure and temperature is necessary.

Table I: Initial conditions for accident scenario

| | $CO_2$ | | Na | |
|---|---|---|---|---|
| | Inlet | Outlet | Inlet | Outlet |
| $P_0$ (MPa) | 19.94 | 19.74 | 0.1 | |
| $T_0$ (°C) | 370.3 | 508.0 | 381 | 526 |

### *2.2 Description of Fluid Properties*

In order to determine if the fluid properties of $CO_2$ should be calculated with a real gas model or an ideal gas model for given conditions, NIST Standard Reference Database 23 (Version 8.0) was used as the reference value. All properties of $CO_2$ as a real gas is directly obtained from the pressure and temperature conditions. On the other hand, in the case of ideal gas model, just some properties (i.e. density, specific enthalpy, and specific entropy) are provided. Thus, it needs to find other properties (i.e. specific heat at constant pressure, specific entropy, specific heat ratio, and speed of sound) with some values satisfying the condition of ideal gas law. For checking the properties, the following equations were used:

$$Z = \frac{P}{\rho RT} \tag{1}$$

$$P = \rho RT \tag{2}$$

$$dh = c_p dT \tag{3}$$

$$Tds = dh - \frac{dP}{\rho} \tag{4}$$

$$\gamma = \frac{c_p}{c_v} = \frac{c_p}{c_p - R} \tag{5}$$

$$c = \sqrt{\gamma RT} \tag{6}$$

### 3. Results and Discussion

The properties obtained from the NIST Standard Reference Database for different pressure and temperature are shown in the following Figs. 1~7.

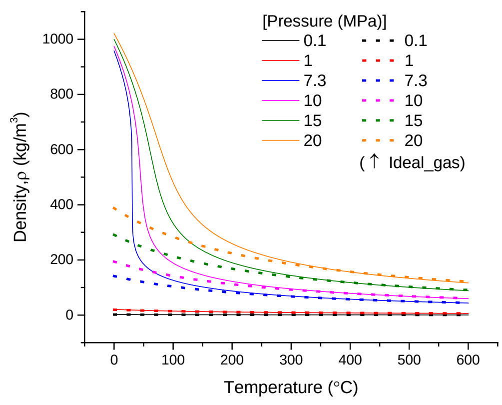


Fig. 2. Density varying with pressure and temperature

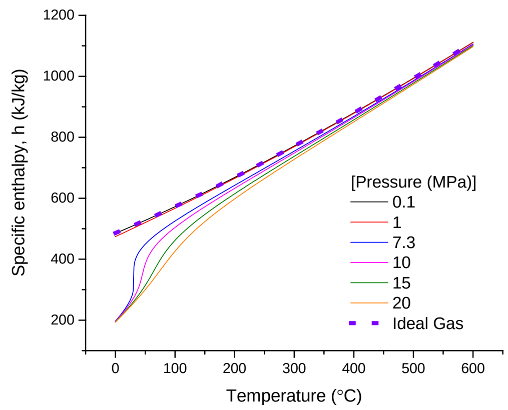


Fig. 3. Specific enthalpy varying with pressure and temperature

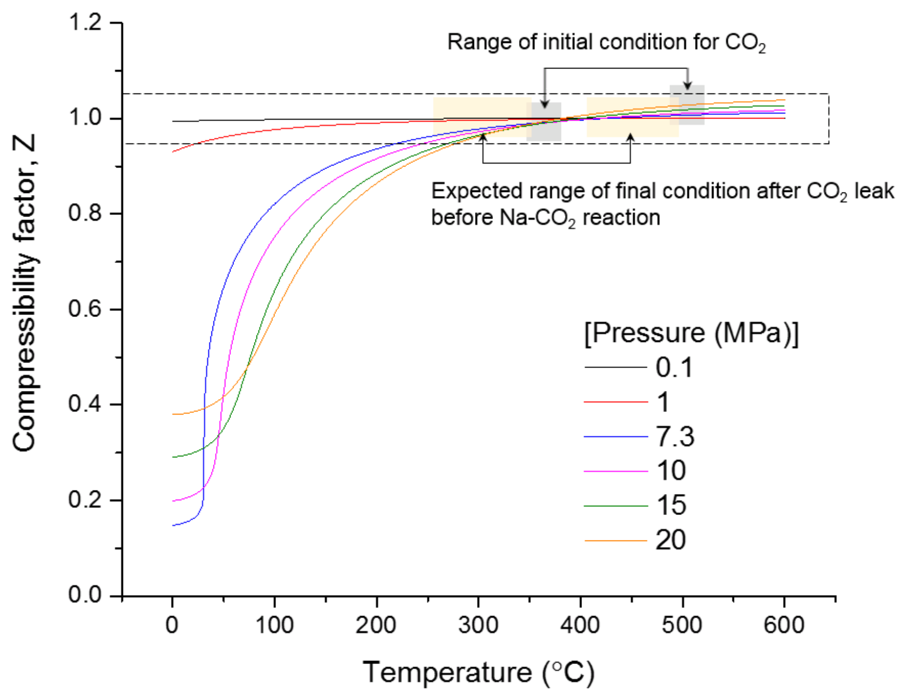


Fig. 1. Compressibility factor varying with pressure and temperature

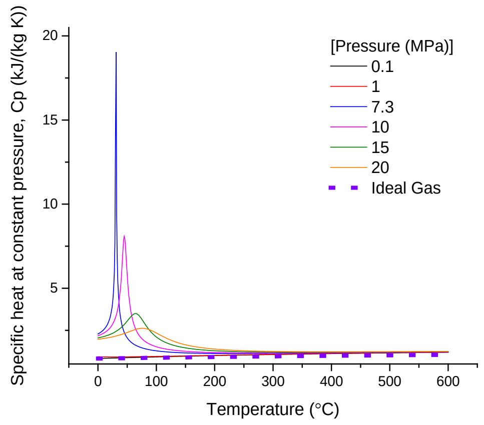


Fig. 4. Specific heat at constant pressure varying with pressure and temperature

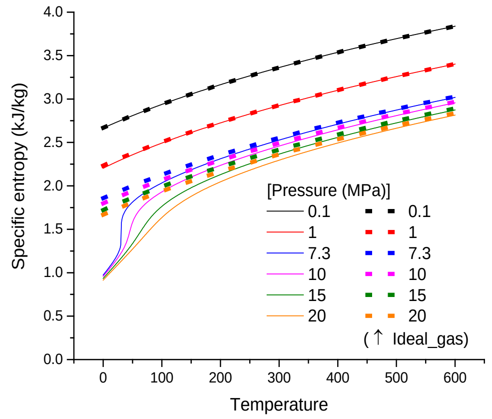


Fig. 5. Specific entropy varying with pressure and temperature

From the results, it is confirmed that the difference between two gas models and the range in which assuming $CO_2$ as an ideal gas is reasonable.

Figure 1 shows the compressibility factor, which is the most representative factor for showing the real gas effect. It indicates that the behavior of $CO_2$ is far from an ideal gas as the temperature is lower and the pressure becomes larger in general. Especially, the compressibility factor drops sharply near the critical point at 7.38MPa and 30.98ºC.

If a deviation from the ideal gas (Z = 1) within 5% is acceptable for applying the ideal gas model, the properties can be calculated with the ideal gas model under the conditions in a dash line box. From this analysis, the ideal gas law is applicable to obtain the properties under the initial/final condition for an accident scenario. However, the real gas effect may become important during a transient. Since the $CO_2$ leak leads to the temperature and pressure changes in sodium side and the depressurization of $CO_2$ side occurs, $CO_2$ state can be predicted with high uncertainty for using the ideal gas law.

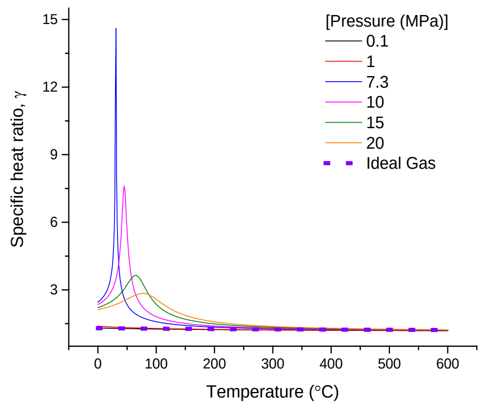


Fig. 6. Specific heat ratio varying with pressure and temperature

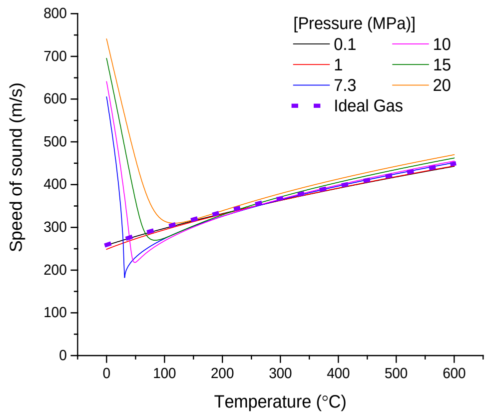


Fig. 7. Speed of sound varying with pressure and temperature

Furthermore, the isentropic critical flow model is generally used for predicting the flow rate of leak $CO_2$, but it is based on the ideal gas law. Thus, it might be necessary to develop a new flow model with an incorporation of the real gas effect.

## 4. Conclusions and Further Works

The ideal gas law and the isentropic critical flow model are generally applied to predict the state and the flow rate of $CO_2$ leak in the Na-$CO_2$ heat exchanger previously. However, to simulate a transient response of the system, the real gas effect may become more important since the properties become deviate from the ideal gas when the pressure is still high but the temperature is low. Since the coherence of the model is important, more studies are required for the application of reasonable gas model in the range of operating conditions of SFR coupled to the S-$CO_2$ power system. This study is expected to provide a baseline of more realistic flow modeling for evaluating the safety of SFR in the future.

## ACKNOWLEDGEMENT

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