Flow Characteristics of High-Pressure Hydrogen Gas in the Critical Nozzle

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Hydrogen gas has been extensively receiving much interest as one of alternative energy sources in future. Of the practical usages of hydrogen gas, a fuel cell car makes use of high-pressure hydrogen gas nearly at atmospheric temperature. In such an application, metering technique of hydrogen gas is of practical importance for mileage and power output of the car. However, the precise measurement of flow rate of hydrogen gas is extremely difficult due to compressibility and real gas effects. For the purpose of practical use of high-pressure hydrogen gas, systematic research is required to clarify the critical nozzle flow of high-pressure hydrogen gas. In the present study, a computational method has been applied to predict the critical nozzle flow of high-pressure hydrogen gas.

Key Words：Critical Nozzle, Compressible Flow, Hydrogen Gas, Real Gas Effects, Internal Flow

1. Introduction

Critical nozzle is one of the flow metering devices which are being extensively used in industrial area dealing with gases. It makes use of the concept of flow choke that occurs at the nozzle throat(1). Under the choked flow conditions, pressure variations in the flow field downstream of the nozzle have negligible influence on the mass flow rate, and the coefficient of discharge is easily obtained only by the flow properties measured upstream of the nozzle.

Recently, Kim et al.(2),(3) have reported the discharge coefficients of a variety of gases for a quite wide range of Reynolds number, using a computational fluid dynamics method. The flow characteristics through the critical nozzle have been well documented at both considerably low and high Reynolds number regimes.

Of many kinds of working gases employed in industrial field, hydrogen gas is one of the most promising gases as alternative energy. For instance, a hydrogen fuel cell, which is being received as the driving power system of vehicles, yields high-pressure hydrogen gas nearly at atmospheric temperature. In such an application, precise measurement of flow rate is of practical importance for mileage and power output of the vehicle.

Only a few researches have been to date made on the mass flow rate of the high-pressure hydrogen gas through critical nozzle. Recently, Nakao(4) has conducted the flow rate measurement of hydrogen gas using a critical nozzle, and has found that the discharge coefficient of hydrogen gas exceeds unity in a specific Reynolds number regime. No detailed explanation has been made for this abnormal discharge coefficient of high-pressure hydrogen gas.

The present study aims at investigating the detailed flow of high-pressure hydrogen gas through a critical nozzle, with the help of a computational fluid dynamics method. The computational results were validated with some experimental data available.

2. Computational analysis

The high-pressure hydrogen gas flow through the critical nozzle is simulated using a Computational Fluid Dynamics method. The

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governing equations are given by the conservation forms of mass, momentum and energy. The axisymmetric, mass averaged, time-dependent Navier-Stokes equations, which use a k-ε turbulent model, are employed in the present computations$^{(1),(2)}$.

Hydrogen gas has little attraction between molecules so that it is inert in character until the molecules are disrupted. From the point of view of kinetic theory or statistical thermodynamics of hydrogen gas, the compressibility factor (Z) is frequently given as a polynomial function of specific volume v,

$$Z = \frac{pv}{RT} = 1 + \frac{B(T)}{v} + \frac{C(T)}{v^2} + \frac{D(T)}{v^3} + \cdots \tag{1}$$

where $B(T)$, $C(T)$ and $D(T)$ are the virial coefficients that are dependent only on temperature.

Similar equation of state of real gas was also reported by Benedict, Webb and Rubin (BWR equation of state)$^{(5)}$, and later on, Lee & Kesler$^{(6)}$ modified BWR equation of state.

Redlich and Kwong have improved the van Der Waals equation to obtain the compressibility factor more accurately, as follows,

$$p = \frac{RT}{v - \tilde{b}} - \frac{a(T)}{v(v + b_0)} \tag{2}$$

where,

$$a(T) = a_0 \left(\frac{T_c}{T} \right)^n, \quad \tilde{b} = b_0 - c_0,$$

$$a_0 = 0.42747 \frac{R^2 T_c^2}{p_c}, \qquad b_0 = 0.08664 \frac{R T_c}{p_c},$$

$$c_0 = RT_c \Big/ \left\{ p_c + \frac{a_0}{v_c (v_c + b_0)} \right\} + b_0 - v_c$$

In case of hydrogen gas, the n value in the function of $a(T)$ is given by $n=0.31$. p_c, T_c and v_c are the pressure, temperature and specific volume, respectively, based on the critical point.

The speed of sound of real gas is determined from the following thermodynamic relation,

$$c = v\sqrt{\{C_p / (R - C_p)\} / (\partial v / \partial p)_T} \tag{3}$$

The dynamic viscosity is given as$^{(7)}$,

$$\mu(T) = 6.3 \times 10^{-7} \frac{M_w^{0.5} p_c^{0.6666}}{T_c^{0.1666}} \left(\frac{T_r^{1.5}}{T_r + 0.8} \right) \tag{4}$$

where T_r is the reduced temperature ($=T/T_c$) and M_w is the molecular weight of real gas. Using this viscosity, the thermal conductivity is obtained from Eucken formula$^{(8)}$.

In the present study, the thermodynamic properties obtained by the above equations are incorporated into the governing equation system and numerically solved to assess the real gas effects of high-pressure hydrogen gas.

In the present study, Redlich-Kwong's equation of state is selected to simulate the high-pressure hydrogen gas through a critical nozzle, since it bears a better agreement with the virial equation of state.

In order to scrutinize the dependence of temperature and pressure on the compressibility factor of hydrogen gas, Figure 1 shows the calculation results using the

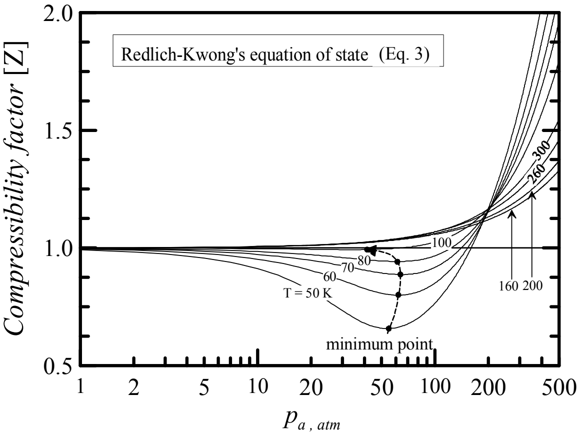

Fig. 1 Dependence of pressure on the compressibility factor of hydrogen gas

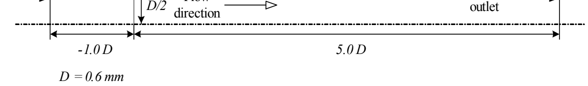

Fig. 2 Schematic diagram of critical nozzle flow field

Redlich-Kwong's equation of state. As the pressure is quite low, the compressibility factor approaches 1.0, being the same to that of ideal gas, regardless of the temperature. However, as the pressure increases, the compressibility factor becomes a strong function of temperature: At low temperature, the compressibility factor decreases and then increases with pressure, after reaching a minimum value. It seems that the minimum value is dependent on the gas temperature. However, at high temperature, such a trend is no longer found, and the compressibility factor is a simply increasing function of the pressure. This is because the molecular weight of hydrogen gas is very low and the intermolecular attraction force is less, compared with the other gases.

The critical nozzle employed in the present study is of a typical conical type(1),(2) and its diameter *D* at the throat is *D*=0.6 mm. A convergent part with a radius of curvature of 2.0*D* is given upstream of the nozzle throat. The straight divergent part has a half angle of 4 degrees and its axial length is 5.0*D*. The computational domain and boundary conditions used in the present study are illustrated in Fig.2. Inlet total pressures and back pressure of nozzle are p_o and p_a, respectively. The symmetric conditions are assumed at the axis of critical nozzle. The adiabatic, no-slip conditions are applied to the solid walls.

In the present study, the nozzle pressure ratio is defined as p_a / p_o and its value maintains constant at 0.5, but the inlet total pressure is varied in the range from 2.0 bar to 350.0 bar at a fixed total temperature, T_0=288 K. A structured grid system with about 35,000 grid points was employed in the present computations.

3. Results and discussion

The present computations were validated with the experimental results(9) using hydrogen gas, where the Reynolds number is based on the diameter of nozzle throat and the total properties at the inlet of nozzle. It is found that the coefficient of discharge is a strong function of Reynolds number, and the predicted coefficients of discharge were in good agreement with the experimental results. It is believed that the present computation method predicts well the gas flow through the critical nozzle.

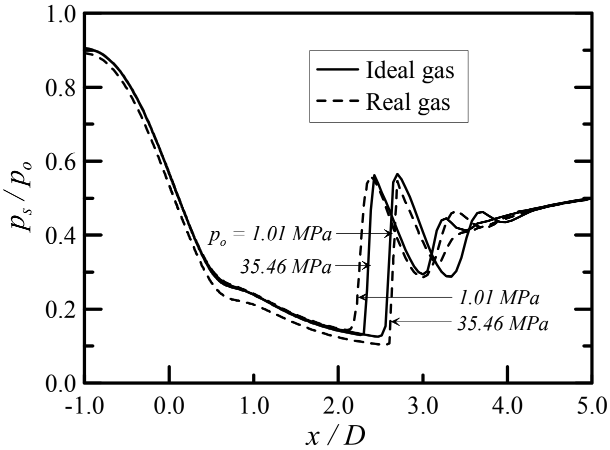

Fig. 3 Predicted static pressure distributions along the nozzle axis

Figure 3 describes the static pressure (p_s) distributions of hydrogen gas flow along the nozzle axis. The pressure ratio (p_a/p_o) is fixed at 0.5. The static pressure decreases with the distance and then suddenly increases when the flow meets the shock wave. The shock wave moves downstream as the inlet total pressure increases. It is noted that for the same p_o, the real gas effect causes the shock wave to be located further downstream, compared with the ideal gas. This is qualitatively the same as what the inlet total pressure influences the shock locations. In this figure, it should be noted that the real gas effect reduces the static pressure at the nozzle throat, compared with the ideal gas. This implies that the mass flow through a critical nozzle can be different due to the real gas effect.

Meanwhile, the coefficient of discharge C_d is usually defined as,

$$C_d = \dot{m} / \dot{m}_{theo} \qquad (5)$$

where $\dot{m}$ is the theoretical mass flow rate through a critical nozzle and $\dot{m}_{theo}$ means the mass flow rate calculated by one-dimensional gasdynamics theory.

Figure 4 shows the comparison of the predicted and experimental$^{(4)}$ discharge coefficients. At present, the only experimental data for high-pressure hydrogen gas are available in Ref.(4). In 1965, Johnson$^{(10)}$ calculated the ratio of specific heats using the Virial equation of state and tabulated the thermodynamic properties of the hydrogen gas flow through a critical nozzle. It is interesting to note that the experimented data show a higher coefficient of discharge than unity, in the range of Reynolds number below 6.0×10^5. At present, this unreasonable trend is not well understood, whether it comes from the real gas effect or from the experimental error. The present computation taking account for the real gas effect is qualitatively similar to Ref. (10) and (4), but still fails in predicting the coefficient of discharge higher than unity. Unfortunately, a clear and persuasive reasoning for this is, at present, not known. More study is needed to elucidate this ambiguous problem.

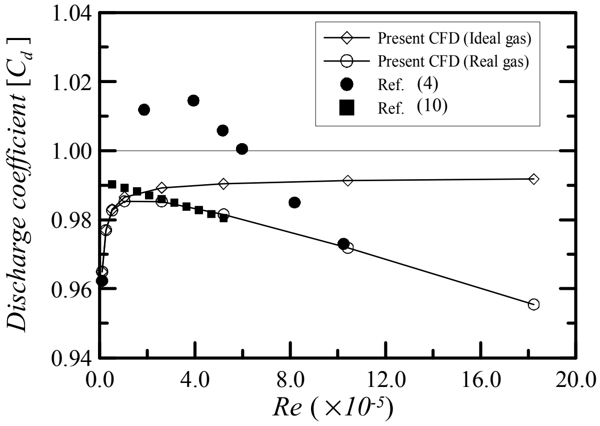

Fig. 4 Variation of the predicted and experimental discharge coefficients with Reynolds number

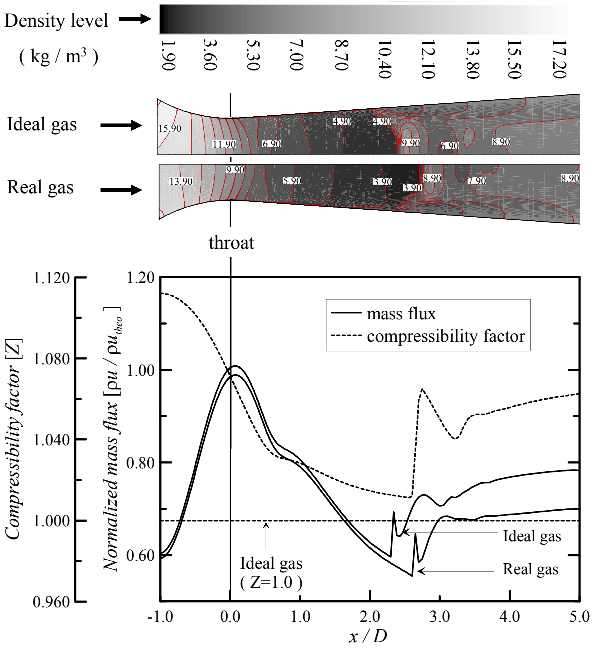

Fig. 5 Distributions of predicted compressibility factors and mass fluxes along the nozzle axis (p_o = 20.27 MPa)

In order to, in more detail, investigate the real gas effect of hydrogen gas flow, the predicted compressibility factor and mass flux along the nozzle axis are presented in Fig.5 (p_0=20.27MPa), together with the computed iso-density contours. Upstream of the shock wave, the compressibility factor greatly decreases with the distance, and at the shock wave location, it sharply increases due to the compression effect of shock wave. There is also some difference in the mass flux distributions upstream of the shock wave. Thus, it is concluded that at high pressure conditions, the compressibility factor of the real gas can be one of the reasons for the coefficients of discharge that were discussed in Fig.4.

Figure 6 shows the axial distributions of the computed values of the ratio of specific heats of hydrogen gas. The ratio of specific heats for ideal gas is constant at 1.41. The specific heat

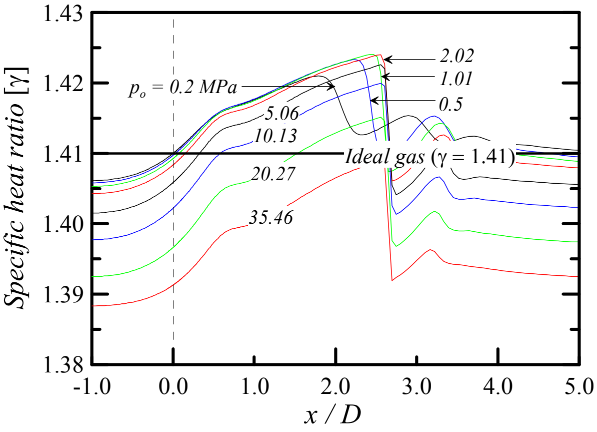

Fig. 6 Influence of inlet total pressure on the specific heat ratio of hydrogen gas

ratio for real gas increases as the flow is accelerated through the nozzle throat, and it sharply decreases at the location of the shock wave. Such a tendency appears similar, regardless of P_0, but the sudden drop in the ratio of specific heats seems to more significant when P_0 increases. It is interesting to note that at the nozzle throat, the ratio of specific heats remains nearly constant at 1.41, when p_0 is less then 1.01MPa, but it significantly decreases as p_0 increases. At the nozzle throat, this variation in the ratio of specific heats with p_0 has an appreciable importance on the mass flow rate of hydrogen gas through a critical nozzle. Therefore, the real gas effect should be included in evaluating the performance and accuracy of critical nozzle as flow metering device.

4. Concluding remarks

Several important and meaningful conclusions obtained from the present study are summarized; Redlich-Kwong's equation of state predicts the real gas effects of high-pressure hydrogen gas comparatively well. However, unlike the coefficient of discharge of ideal gases which have been obtained to date, the coefficient of discharge of real gas through critical nozzle decreases with an increase in Reynolds number, as Reynolds number exceeds a certain value. It is believed that this mainly results from the thermodynamic properties of real gas, such as the compressibility factor and the ratio of specific heats, which appears more remarkable as the pressure of hydrogen gas increases.

Acknowledgement

This study was partially supported by Harada Memorial Foundation.

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