Numerical Study of Real Gas Effects on Shock Tube Problems at Supercritical Conditions

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Investigations of real gas effects of supercritical fluids on shock tube problems were numerically performed. Understandings of fluid behaviors under supercritical conditions are essential for the design of high pressure combustors. We developed a numerical code for simulations of flow fields under the supercritical conditions. Cubic types of equation of state are applied to evaluate properties of nearcritical and supercritical fluids. The present code was tested on shock tube problems, and the present result agreed well with a reference result. Comparisons of results between the real gas equations of state and the ideal gas equation of state showed differences in position of shock waves, contact discontinuities, and expansion fans due to the specific thermodynamic features of the supercritical fluids. In a condition that crosses the critical point, the results showed a large density jump with a small temperature jump at the contact discontinuity because of drastic changes of thermodynamic properties. This indicated that the real gas effects obviously appear when the initial condition is close to the critical point of the working fluids.

Key Words: Supercritical Fluids, Riemann Problem, Liquid Rocket Engine

Nomenclature

c	: sound speed
p	: pressure
R	: gas constant
T	: temperature
t	: time
u	: velocity
V	: volume
ω	: acentric factor
x	: position
ρ	: density
γ	: specific heat ratio

Subscripts

cr	: critical value
left	: initial left state value
right	: initial right state value
ref	: reference value

1. Introduction

Supercritical fluids are widely used in industrial devices such as supercritical nuclear reactors and high pressure combustors. For example, in liquid rocket engines, cryogenic propellants are injected and burnt under high pressure conditions. The pressure reaches over 10 MPa, and the injected propellant is in a supercritical state. Under such conditions, unique behaviors of the fluid jet are observed that do not appear in atmospheric conditions. Past studies¹⁻⁶⁾ have investigated the jet behaviors under the supercritical conditions, however, the its behaviors are still unknown in

detail. Experimental investigations at the supercritical condition are difficult because of extremely high pressure, thus, numerical simulations are effective for the understandings. Present study aims to explore jet mixing in liquid rocket engines, and development of numerical code has been conducted⁷⁾.

The supercritical fluids show unique thermodynamics properties⁸⁾. They have the high density like liquids and high diffusivity like gas. Latent heat and surface tension are decrease with increasing pressure. Near the critical point, the specific heat increases rapidly, and a large expansion appears with a small temperature increase. These features greatly impact the flow fields, thus, treatment of the supercritical fluid as the real gas is essential.

A simulation of the shock tube problem, or Riemann problem, is used to validate the numerical scheme as a common test case. The Riemann problem is a classical initial-value problem for system of hyperbolic equations. The shock tube problem is a particular case of the Riemann problem. The shock tube problem is formed by a long tube separated by a diaphragm into two states that are initially at different pressures. At $t = 0$, the diaphragm bursts and produces three waves: a shock, a contact discontinuity and an expansion fan. The shock and the contact discontinuity propagate down the tube into the low pressure side, and the expansion fan propagates into the high pressure side. An analytical solution in time is known for the initial condition.

The flow field inside the shock tube near the critical point has been investigated in past studies. At this point, compression by shock induces a phase transition, and non-classical waves are observed as a result of the thermodynamic property changes of nearcritical fluid^{9),10)}.

Arina¹¹⁾ developed the numerical method for the supercritical fluid and investigated effects of equations of state. However, there is only little discussion about differences of wave propagation between the real gas case and the ideal gas case.

In the present study, shock tube simulations under the supercritical conditions are carried out to investigate the real gas effects on the wave propagation. The numerical method applies an AUSMDV¹²⁾ scheme which is modified for real gas. Firstly, two types of the equations of state are applied to the numerical code and compared. Secondly, to investigate the real gas effect near a critical point, the shock tube simulations are performed for three cases: the supercritical case, the nearcritical case, and the subcritical case.

(a) Density

(b) Specific heat ratio

Fig. 1. Thermodynamic property of carbon dioxide.

2. Numerical Method

2.1. Governing equations

The governing equations are the three-dimensional compressible Euler equations. Spatial derivative terms in the governing equations are evaluated by the AUSMDV¹²⁾ scheme. To obtain second-order accurate discretization, the MUSCL approach with the van Albada limiter¹³⁾ is applied. The third-order TVD Runge-Kutta scheme¹⁴⁾ is used for time integration.

2.2. Equation of state

For equations of state, the van-der-Waals (vdW) equation of state⁸⁾ and the Soave-Redlich-Kwong (SRK) equation of state¹⁵⁾ are applied to evaluate the thermodynamic properties

under the supercritical conditions. For comparison, the ideal gas equation of state is also used as a calorically perfect gas. The vdW and the SRK equations of state are called the cubic equation of state. The cubic equations of state describe thermodynamic states over a broad range and are computationally efficient compared to more complex equations of state⁸⁾. The SRK equation of state has better accuracy near the critical point. The SRK and vdW equation of states are written as following equations.

$$p = \frac{RT}{V-b} - \frac{a\alpha}{V^2 - ubV} \quad (1)$$

$$\alpha = [1 + (0.48 + 1.574\omega - 0.176\omega^2)(1 - (T/T_{cr})^{1/2})]^2 \text{ :SRK} \quad (2)$$

$$\alpha = 1 \text{ :vdW} \quad (3)$$

The parameters a , b , and u are $a = 0.4275R^2T_{cr}/p_{cr}$, $b = 0.08664RT_{cr}/p_{cr}$ and $u = 1$ in the SRK equation of state, and $a = 0.4219R^2T_{cr}/p_{cr}$, $b = 0.125RT_{cr}/p_{cr}$, and $u = 0$ in the vdW equation of state, respectively. In the present code, thermodynamic relationships are modified for the real gas using cubic equations of state^{8,16)}. Figure 1 shows the changes of the density and the specific heat ratio of carbon dioxide using the SRK equation of state. Critical pressure, density and temperature of the carbon dioxide are $p_{cr} = 7.316$ MPa, $\rho_{cr} = 348.8$ kg/m³, and $T_{cr} = 304.21$ K, respectively. In Fig. 1, large properties change near the critical pressure and the critical temperature is shown.

2.3. Calculation condition

The tube length is 10 m and the initial diaphragm is placed at 5 m from a left wall. Following simulations are performed with a uniformly spaced grid with 0.02 m grid size and 501x5x5 grid points. Both tube ends are opened, and boundary conditions at walls are adiabatic wall. Periodic boundary conditions are used in azimuthal directions. To compare the past study proposed by Arina¹¹⁾, carbon dioxide is used as the working fluid. The carbon dioxide has thermodynamic characteristics similar to oxygen which is used in the liquid rocket engines.

Table 1. Initial condition of validation calculation.

	Left side($0 \leq x$ [m] ≤ 5)	Right side($5 < x$ [m] ≤ 10)
p	$10p_{cr}$	$0.1p_{cr}$
ρ	ρ_{cr}	$0.01\rho_{cr}$
u	0	0

3. Results and Discussions

3.1. Validation

A simulation of the shock tube problem under the supercritical condition is carried out to validate the numerical code. The initial condition is shown in Table 1, which corresponds to a simulation proposed by Arina¹¹⁾.

Figure 2 shows the density profile at $t = 2.745 \times 10^{-3}$ s. In this result, the vdW equation of state is applied. The simulations are performed with the Courant-Friedrichs-Lewy (CFL) number is approximately 0.1. The result by Arina is

also plotted for comparison. Arina used the AUSMDV scheme with the MUSCL as a spatial discretization scheme, and the vdW equation of state. The present result shows good agreement with the Arina's result. The present code captures property jumps across discontinuities, and there are no significant spurious oscillations. This result demonstrates that the present code has accuracy for simulation of shock wave under the supercritical condition. Figure 3 shows a comparison between three equations of state: SRK, vdW, and the ideal gas. The two real gas equations of state predict slower propagation of the shock and the contact discontinuity, and faster propagation of the expansion fan. Behind the contact discontinuity, although the small differences appear in the two real gas equations of state, there are no significant differences in the overall profiles at the present case.

3.2. Real gas effects on the shock tube problem

To investigate real gas effects on wave propagations, the shock tube simulation are carried out at three cases: the supercritical, the nearcritical, and the subcritical pressure. The calculation conditions are shown in Table 2. In each case, the pressure ratio is set to 2 and an initial temperature of 310 K is assumed. Figure 4 shows profiles of density, temperature,

pressure, specific heat ratio, and sound speed, respectively. A result for regarding the working fluid as ideal gas (ideal case) is also plotted. Here, the density, the temperature, and the pressure are nondimensionalized using the initial left side values. Thus, the ideal case shows only one profile regardless of whether the initial pressure is subcritical or supercritical. A reference sound speed is defined using $c_{\text{ref}} = \sqrt{\gamma R T_{\text{cr}}}$.

In Fig. 4, all cases show three waves. The nearcritical case only shows a small density jump at the shock wave and a large density jump at the contact discontinuity in contrast to the other cases. Nevertheless, the nearcritical case shows smaller temperature change at shock and contact discontinuity. In the pressure profiles, the supercritical case and the subcritical case show similar pressure jumps with the ideal case at the shock, while the nearcritical case shows a smaller pressure jump. This is because of strong non-linear changes of thermodynamic properties near the critical point. When the contact surface passes through the critical point, the density increases drastically with a small temperature increase because the specific heat increases toward divergence. Figures 4 (d) and 4 (e) show a peak behind the contact discontinuity,

Fig. 2. Density profile of validation calculation.

Fig. 3. Comparison of the equations of state.

Table 2. Initial conditions.

	$p_{\text{left}},$ MPa	$p_{\text{right}},$ MPa	$p_{\text{left}}/$ p_{right}	T, K	$\rho_{\text{left}},$ kg/m ³	$\rho_{\text{right}},$ kg/m ³
Supercritical	$4p_{\text{cr}}$	$2p_{\text{cr}}$	2	310	845	696
Nearcritical	$1.5p_{\text{cr}}$	$0.75p_{\text{cr}}$	2	310	610	134
Subcritical	$0.5p_{\text{cr}}$	$0.25p_{\text{cr}}$	2	310	76.9	34.4

(c) Pressure

(a) Density

(d) Specific heat ratio

(b) Temperature

(e) Sound speed

Fig. 4. Comparison of results between three cases; supercritical, nearcritical and subcritical.

only at nearcritical case. This indicates that anomalous features obviously appear in the condition near the critical point, and it is important to consider the non-linearity of thermodynamic properties.

3.3. Wave propagation at the nearcritical condition

Figure 5 shows time histories of density and temperature profile in the nearcritical case. The present code captures the density jumps that are kept sharply in time. The shock and the expansion fan propagate with constant velocity in the three cases. In the temperature profile, the small numerical overshoot appears and is kept behind the contact discontinuity. In the nearcritical case, the fluid passes through the critical point at the contact discontinuity, and the rapid increases of thermodynamic properties may cause numerical oscillations. The past studies indicated this problem and proposed some numerical techniques to prevent this oscillation^{17),18)}.

Figure 6 shows time histories of wave positions between the three cases and the ideal case. In all the cases, three waves move proportionally in time. In the supercritical case, both the shock and the expansion fan propagate faster than in the ideal case; whereas, the nearcritical case predicts propagations slower in the shock and faster in the expansion fan. This is explained by the profile of sound speed in Fig 4 (e). In the supercritical case, the sound speeds are high in overall; however, in the nearcritical case, the sound speeds are lower at the right side of the contact discontinuity than ideal case, but higher at the left side. As noted above, only one profile is provided regardless of the initial pressure at the ideal gas conditions. However, even if the initial pressure ratio and the initial temperature are fixed, the results depend on the initial condition when the initial state is close to the critical point.

4. Conclusion

The numerical simulation code for the flow of supercritical fluid is developed with cubic types of real gas equations of state. Using this code, the shock tube problem under the supercritical condition is performed. First, two real gas equations of state and the ideal equation of state are compared. The results show that there are no significant differences in the results between two real gas equations of state at the present condition. Second, the real gas effects on the wave propagation are investigated. There is a large density change with a small temperature increase at the contact discontinuity where the fluid crosses the critical point. This is because of the strong non-linearity of the thermodynamic properties of the supercritical fluids. The obvious real gas effects appear when the initial condition is close to the critical point.

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Fig. 5. Time histories of profile under nearcritical condition.

Fig. 6. Time histories of shock and expansion fan positions.

References

- 1) Oefelein, J. C.: Thermophysical characteristics of shear-coaxial LOX-H₂ flames at supercritical pressure, *Proceedings of the Combustion Institute.*, **30** (2005), pp.2929–2937, doi:10.1016/j.proci.2004.08.212.
- 2) Mayer, W., Schik, A., Woodward, R. and Talley, D.: Atomization and breakup of cryogenic propellants under high-pressure subcritical and supercritical conditions, *Journal of propulsion and power*, **14** (1998), pp. 835–842.
- 3) Zong, N., Meng, H., Hsieh, S.-Y. and Yang, V.: A Numerical study of cryogenic fluid injection and mixing under supercritical conditions, *Physics of Fluids*, **16** (2004), pp. 4248–4261.
- 4) Mayer, W., Telaar, J., Branam, R., Schneider, G. and Husson, J.: Raman Measurements of Cryogenic Injection at Supercritical Pressure, *Heat Mass Transfer*, **39** (2003), pp. 709–719. doi: 10.1007/s00231-002-0315-x.
- 5) Terashima, H. and Koshi, M.: Characterization of cryogenic nitrogen jet mixings under supercritical pressures, *51st AIAA Aerospace Science Meeting including New Horizons Forum Aerospace Exposition*, AIAA 2013–0712, 2013.
- 6) Schmitt, T., Selle, L., Cuenot, B. and Poinot, T.: Large-Eddy Simulation of transcritical flows, *Comptes Rendus Mécanique*, **337** (2009), pp. 528–538, doi:10.1016/j.crme.2009.06.022.
- 7) Muto, D., Tsuboi, N., Terashima, H. and Koshi, M.: Numerical Simulation of Supercritical Jet Structure Using Unsteady Preconditioning Compressible Method, *34th International Symposium on Combustion*, 1–12, 2012.
- 8) Poling, B., Prausnitz, J. and O’Connell, J.: *The Properties of Gases and Liquids*, McGraw-Hill, 5th ed., 2000.
- 9) Argrow, B. M.: Computational analysis of dense gas shock tube flow, *Shock Waves*, **6** (1996), pp. 241–248.
- 10) Guardone, A., Vigevano, L. and Argrow, B.: Assessment of thermodynamic models for dense gas dynamics, *Physics of Fluids*, **16** (2004), No. 11, doi: 10.1063/1.1786791.
- 11) Arina, R.: Numerical simulation of near-critical fluids, *Applied numerical mathematics*, **51** (2004), pp. 409–426. doi:10.1016/j.apnum.2004.06.002.
- 12) Wada, Y. and Liou, M. A.: Flux Splitting Scheme with High-Resolution and Robustness for Discontinuities, *Institute for Computational Mechanics in Propulsion 32nd Aerospace Sciences Meeting & Exhibit*, AIAA 94–0083, 1994.
- 13) Albada, G. Van, Leer, B. Van and Jr, W. R. A.: Comparative study of computational methods in cosmic gas dynamics, *Astronomy and Astrophysics*, **108** (1982), pp. 76–84.
- 14) Gottlieb, S. and Shu, C.-W. Total variation diminishing Runge-Kutta schemes, *Mathematics of Computation*, **67** (1998), pp. 73–86.
- 15) Soave, G.: Equilibrium constants from a modified Redlich-Kwong equation of state, *Chemical Engineering Science*, **27** (1972), pp. 1197–1203.
- 16) Meng, H. and Yang, V.: A unified treatment of general fluid thermodynamics and its application to a preconditioning scheme, *Journal of Computational Physics*, **189** (2003), pp. 277–304. doi:10.1016/S0021-9991(03)00211-0.
- 17) Abgrall, R.: How to prevent pressure oscillations in multicomponent flow calculations: a quasi conservative approach, *Journal of Computational Physics*, **125** (1996), pp. 150–160.
- 18) Kawai, S. and Terashima, H.: A high-resolution scheme for compressible multicomponent flows with shock waves, *International Journal for Numerical Methods in Fluids*, **66** (2011), pp. 1207–1225. doi: 10.1002/fld.2306.