Validation of classical mixing rule coupled with a van der Waals–type equation of state for supercritical mixture system of oxygen and hydrogen using molecular simulation

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Abstract
We have validated the classical mixing rule (CMR) applied to the Soave–Redlich–Kwong (SRK) equation of state (EOS) as one of the van der Waals–type EOSs for the thermodynamic properties (pressure–volume–temperature relationship, specific heat at constant pressure) of oxygen–hydrogen mixture in supercritical state using molecular dynamics (MD) simulations. As for oxygen and hydrogen, effect of the intramolecular orientation on the intermolecular interaction is very small; therefore, we employed the Lennard–Jones (L–J) potential between each molecule. The intermolecular interaction between the different molecular species was given by modified Lorentz–Berthelot (L–B) rules, which improved the accuracy of the well–applied original L–B rules in accordance with the more accurate combining rules proposed for the L–J potential. We have validated the CMR applicability through the comparison of thermodynamic variables obtained by MD simulations with those obtained by CMR coupled with the SRK EOS. As a result, the thermodynamic variables by MD simulations corresponded with those from the SRK EOS employing CMR. Further, the relative difference in thermodynamic variables between the MD simulations and SRK EOS hardly increased against single–component fluids. Therefore, we conclude that the CMR can be applied to the oxygen–hydrogen mixture system in supercritical condition.

Keywords: Thermodynamic properties, Molecular dynamics, Equation of state, Mixing rule, Oxygen–hydrogen mixture

1. Introduction

In a typical combustion chamber of a first–stage liquid rocket engine using oxygen and hydrogen as a propellant, since the propellant flow exceeds both the critical pressures of oxygen and hydrogen, the propellant changes the thermodynamic state in a wide range of supercritical states. In the supercritical condition, considering the non–ideality of fluids is necessary because the thermodynamic properties are different from that of normal–pressure gases. Further, since it is known that the flow field near the injector at the inlet region of the combustion chamber has particular influence on the combustion efficiency or combustion stability (Gill, 1976, Hannum and Rocker, 1976, Tamura, 2005), the investigation of detailed flow fields has been required. However, because of high pressures, optical or direct measurements of quantitative data on the flow field by experiments are difficult. On the other hand, numerical simulations such as computational fluid dynamics (CFD) can obtain the quantitative data even for high pressures; it is an effective method for the understanding of mixing, turbulence, and the thermodynamic aspect of jet flow in supercritical pressures.
Since combustion instability can be caused by unsteady motion of the vortices or flow instability, CFD analyses investigating the detailed flow fields without combustion have been also conducted (Liu et al., 2006, Hosangadi, 2008, Schmitt et al., 2012, Terashima, 2014).

In many CFD analyses for the combustion chamber, the van der Waals (vdW)–type equation of state (EOS) reflecting non–ideality has been used, and a classical mixing rule (CMR) (Sengers et al., 2000) has been applied to the EOS to predict the thermodynamic variables of multicomponent systems such as the oxygen–hydrogen mixture system. While the EOS accuracy in a single–component system has been validated, the accuracy of the CMR applied to the EOS has hardly been validated because of the lack of experimental data pertaining to the thermophysical properties of the oxygen–hydrogen mixture, particularly in the conditions corresponding to the combustion chamber. Note that the quantitative error levels in CFD by other factors, e.g., turbulence model, chemical reaction model, have been often investigated and discussed while that by the CMR coupled with the vdW–type EOS has been totally unknown nor investigated. Some comparison of EOSs (Park, 2012, Petit et al., 2013) indicates that EOS can also affect CFD results leading a non–negligible level of error, and the validation of the CMR is one of the important subjects for ensuring reliability of the CFD analyses.

This study aims to validate the accuracy of the CMR applied to the EOS in supercritical conditions using molecular dynamics (MD) simulations. In this study, we discussed the applicability of the CMR coupled with the Soave–Redlich–Kwong (SRK) EOS (Soave, 1972) as one of the vdW–type EOSs for the oxygen–hydrogen mixture system in supercritical state. For the thermodynamic properties of oxygen and hydrogen in a wide temperature range, SRK EOS is the most appropriate among the vdW–type EOSs, and it has been mostly used for typical CFD analyses for the combustion chamber of a liquid rocket engine.

2. Calculation Methods
2.1 Molecular Dynamics Simulation

In this study, we conducted MD simulations for an imaginary model corresponding to the oxygen–hydrogen mixture system. The intermolecular interaction was given by the Lennard–Jones (L–J) potential, which is an empirical model for the vdW force of monatomic fluid. The L–J potential $\phi_{LJ}(r)$ is given as follows:

$$\phi_{LJ}(r) = 4\varepsilon \left( \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right),$$

where $\varepsilon$ and $\sigma$ are the potential parameters for the intermolecular interaction energy and molecular diameter, respectively, and $r$ is the intermolecular distance. The potential parameters which are determined to correspond to the actual critical temperature and density of oxygen and those of hydrogen (National Institute of Standards and Technology) are listed in Table 1.

| Table 1 | L–J potential parameters, $\varepsilon$ and $\sigma$ |
|---------|------------------|
|         | Oxygen       | Hydrogen  |
| $\varepsilon$ | $[\times 10^{-22}\text{J}]$ | 15.79 | 3.37 |
| $\sigma$      | $[\times 10^{-10}\text{m}]$  | 3.399 | 3.290 |

Since the cut–off distance $r_c$ in the L–J potential for bulk liquid or gas is typically chosen as $r_c = 3\sigma \sim 4\sigma$, we employed $r_c = 3.5\sigma$. To reduce the artificial effect by the finite cut–off distance, we have added a correction term for the internal energy and the pressure on the basis of the assumption that the radial distribution function equals to one in intermolecular distances exceeding the cut–off radius (Frenkel and Smit, 2002). Note that both internuclear distances are very small (Huber and Herzberg, 1979), and even if the effect of each intramolecular orientation on the intermolecular potential is ignored, the $P–V–T$ relationship and excess specific heat described below can be properly evaluated. Also, while the supercritical condition in this paper is $T = 200\text{K}$ and $P = 10\text{MPa}$ (the details are shown in Section 3), the intramolecular vibration is perfectly frozen at 200K because the vibrational characteristic temperatures of oxygen and hydrogen are 2274 K and 6331 K, respectively (Helrich, 2009). Further, the intramolecular deformation hardly occurs at 10MPa. Therefore, the intramolecular interaction can be also neglected. In fact, the prediction of the thermal property of
oxygen except for around the critical point is possible by using the L–J potential with a cut–off distance of \( r_c = 3.5\sigma \) (Tsuda et al., 2009). For reference, the comparison results of the \( P–V–T \) relationship and the specific heat at constant pressure between Johnson’s EOS (Johnson et al., 1993), which has a high accuracy among the conventional EOSs for L–J fluid, the NIST data (National Institute of Standards and Technology) and SRK EOS are shown in Fig. 1. Herein, the results of the present MD simulations in the above supercritical condition are also plotted in each figure. Here, the ideal gas term of specific heat was treated as a diatomic molecule and was given by reference to NIST data of oxygen and para–hydrogen. In this paper, we employed the value of para–hydrogen because it is actually used as a propellant of liquid rocket. As shown in each figure, we confirmed that the present MD simulation corresponded well with Johnson’s EOS, which can qualitatively well reproduce the pressure dependence of the thermodynamic properties of the NIST data of oxygen and hydrogen at \( T = 200 \) K. This result shows that the excess thermodynamic variables of oxygen and hydrogen as diatomic fluids are well reproduced by the L–J fluid as a monatomic fluid. Under the supercritical condition of \( T = 200 \) K and \( P = 10 \) MPa, the relative error of density of Johnson’s EOS against the NIST data is approximately 5% in both oxygen and hydrogen, and the relative error of specific heat at constant pressure is approximately 10% in oxygen, and within 1% in hydrogen, we further confirmed that Johnson’s EOS quantitatively roughly reproduces the NIST data.

![Fig. 1. Comparison of thermodynamic properties between EOS for L–J fluid (Johnson et al., 1993), SRK EOS (Soave, 1972) and NIST data at 200K: (a) \( P–V–T \) relationship, (b) Specific heat at constant pressure.](image)

In general, the L–J potential parameters between the different kinds of molecules are given by the well–known Lorentz–Berthelot (L–B) rules as follows:

\[
\varepsilon_{ij} = \alpha \sqrt{\varepsilon_i \varepsilon_j},
\]

\[
\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2},
\]

in which the subscript \( i \) or \( j \) shows a different kind of molecule. These rules are widely used to calculate the thermodynamic properties of mixtures. However, since the L–B rules cannot exactly reproduce the intermolecular interaction between different kinds of molecules, we introduced a set of modified parameters that can arrange the intermolecular interaction between oxygen and hydrogen. The modified L–B rules are given as follows:

\[
\varepsilon_{ij} = \alpha \sqrt{\varepsilon_i \varepsilon_j},
\]

\[
\sigma_{ij} = \frac{\beta (\sigma_i + \sigma_j)}{2},
\]
where $\alpha$ and $\beta$ are modified parameters. Instead of using the L–B rules, the parameter ranges of $\alpha$ and $\beta$ were set according to the Fender–Halsey (F–H) rule (Fender and Halsey, 1962), Waldman–Hagler (W–H) rules (Waldman and Hagler, 1993), and Kong (KG) rules (Kong, 1973), which can reproduce the experimental values of intermolecular interactions for unlike molecules or the virial coefficient of a two–component mixture system consisting of monoatomic molecules, e.g., neon, argon, krypton, and xenon. Concretely, we set the parameter ranges $0.75 \leq \alpha \leq 1.00$, $1.00 \leq \beta \leq 1.02$ to include the ratios of L–J potential parameter between F–H, W–H, KG rules and L–B rules. For reference, the comparison results of coexisting curve of Ne–Kr mixture between experimental data and each combining rule applied to L–J potential are shown in Fig. 2. As shown in Fig. 2, the L–J potential coupled with each combining rules shows good agreement with experimental data except the case of the L–B rules in liquid phase. Further, applying W–H rules or KG rules, the prediction accuracy is improved more than the L–B rules. Therefore, likewise in the present oxygen–hydrogen mixture system whose L–J potential parameter ratio is approximately the same as that of the Kr–Ne mixture system (those potential parameter ratios are $\epsilon_{\text{Kr}}/\epsilon_{\text{Ne}} \approx 4.72$, $\sigma_{\text{Kr}}/\sigma_{\text{Ne}} \approx 1.30$, respectively), good prediction of thermodynamic properties is expected.

![Fig. 2. Coexisting Ne molar fraction in an Ne–Kr binary mixture at $T = 150K$ (Delhommelle and Millié, 2001).](image)

We calculated the thermodynamic variables ($P$–$V$–$T$ relationship, specific heat) of the imaginary oxygen–hydrogen mixture model constructed by the L–J potential with the modified L–B rules using MD simulations. To correspond with the pressure–based CFD analysis, we employed the $NPT$ ensemble, which keeps the following parameters constant: (i) number of molecules $N$, (ii) pressure $P$, which is calculated via the virial theorem, and (iii) temperature $T$. In this calculation, the equations of motions proposed by Martyna et al. (Martyna et al., 1994), which includes the Andersen’s barostat and the Nosé–Hoover chain thermostats, were solved using the reference system propagator algorithm (RESPA) method (Tuckerman et al., 1992). Since the computational domain volume is changed with time at constant pressure and temperature, the corresponding density was evaluated from the time–averaged volume in $P$–$V$–$T$ relationship calculation. In calculating the specific heat, we estimated the excess specific heat $c_{p,ex}$ at constant pressure, which is defined as $c_{p,ex} = c_p - c_{p,id}$, where $c_p$ and $c_{p,id}$ are the isobaric specific heat and its ideal gas term, respectively. The excess specific heat $c_{p,ex}$ is given by Eq. (6) (Piñeiro et al., 2008).

$$c_{p,ex} = \frac{1}{Nk_BT^2} \left( \langle \delta\phi^2 \rangle + 2P \langle \delta\phi \delta\nu \rangle + P^2 \langle \delta\nu^2 \rangle \right) - k_B,$$

where $\delta\phi$ and $\delta\nu$ are the deviation from the time–averaged potential energy between all molecules and that from the averaged volume of the computational domain, respectively. Actually, the specific heat is given by the total of excess specific heat and the ideal gas specific heat. In this paper, the ideal gas specific heats at constant pressure of oxygen and para–hydrogen were estimated theoretically, and they were $c_{p,id} \text{O}_2 \approx 29.1J/mol/K$ and $c_{p,id} H_2 \approx 32.4J/mol/K$. Here, the rotational specific heat of para–hydrogen was evaluated by quantum statistical mechanics (Schwabl, 2002), and the
other terms were given by classical approximation. In this calculation, we employed the periodic boundary condition as the standard condition for the evaluation of bulk properties. The number of molecules was 864. The total number of steps was 3000000, in which the initial 500000 was the relaxation period and the subsequent 2500000 was used as sampling. In this sampling period, we sampled at every 1000 steps, and the time–averaged values of density and excess specific heat during the sampling were used as the calculation results.

2.2 SRK EOS and Classical Mixing Rule

Soave proposed an EOS that can closely reproduce the vapor pressures of a single–component by modifying the parameter of the Redlich–Kwong (RK) EOS (Soave, 1972). The SRK EOS is given as follows:

\[ P = \frac{RT}{V - b} - \frac{a(T)}{V(V + b)}, \quad (7) \]

\[ a(T) = a_0 \left[ 1 + \left( 0.480 + 1.574 \omega - 0.176 \omega^2 \right) \left( 1 - \left( T / T_c \right)^{0.5} \right)^2 \right], \quad (8) \]

where \( R \) is the universal gas constant; \( a(T) \) is a function of the intermolecular attraction dependent on temperature \( T \) as shown in Eq. (8); \( T_c \) is the critical temperature; \( \omega \) is the acetonic factor that reflects the degree of deviation from the spherical configuration of the molecule. However, \( \omega \) was set at zero in this calculation because the spherical configurations were assumed for oxygen and hydrogen in the above MD simulations. Further, \( a_0 \) and \( b \) are the constants determined by the critical temperature \( T_c \) and critical pressure \( P_c \) of each substance, and they are given by \( a_0 = 0.42748R \left( T_c / P_c \right) \) and \( b = 0.08664R T_c / P_c \), respectively (Soave, 1972). To extend to an oxygen–hydrogen mixture system, the CMR has been mostly applied to the SRK EOS. In the CMR, \( a \) and \( b \) in Eq. (7) are given by

\[ a = \sum_i \sum_j x_i x_j \left( 1 - k_{ij} \right) \sqrt{a_i a_j}, \quad (9) \]

\[ b = \sum_i \sum_j x_i x_j \left( 1 - \beta_{ij} \right) \left( b_i + b_j \right) / 2, \quad (10) \]

where \( x_i \) and \( x_j \) are the molar fractions of each component; \( k_{ij} \) and \( \beta_{ij} \) as the fitting parameters are dealt as zero in this study because they have been set at zero in many CFDs for the combustion chamber of a liquid rocket engine.

3. Results and Discussion

In the typical operating condition of the combustion chamber of a first–stage liquid rocket engine, oxygen and hydrogen are injected at approximately 100 K and 300 K, respectively (Yang, 2004), and those propellants are combusted under high pressures of over 10 MPa. We have set the calculation conditions at temperature \( T = 200 \) K and pressure \( P = 10 \) MPa to correspond to the inlet region of the combustion chamber. The critical pressures of oxygen and hydrogen are 5.0 MPa and 1.3 MPa, respectively, and the critical temperatures are 155 K and 33 K, respectively (National Institute of Standards and Technology). Therefore, in the calculation conditions above, oxygen and hydrogen are supercritical or around the critical state, and non–ideality cannot be neglected. Also, for the evaluation of the statistical uncertainty of the MD simulation, we conducted 20 MD runs, each of which includes a sampling period of 2500000 steps and confirmed that the MD simulation has a statistical uncertainty of ±0.15% for \( P–V–T \) relationship and of ±2.5% for specific heat at constant pressure in the mixture system.

The molar density against the molar fraction of hydrogen as a \( P–V–T \) relationship is shown in Fig. 3. Here, for reference, MD result of molar density in oxygen (molar fraction of hydrogen is zero) and that in hydrogen (molar fraction of hydrogen is one) corresponds to \( \rho_{O_2} = 259 \) kg/m\(^3\) and \( \rho_{H_2} = 10.7 \) kg/m\(^3\), respectively, in the unit of mass. As shown in Fig. 3, the results of the MD simulations and SRK EOS employing the CMR corresponded well. The relative density variation by parameter \( \alpha \) was within 3%, and that by \( \beta \) was within 0.5%; the influence of the parameters of the modified L–B rules is very small. Further, the relative difference in density between the MD simulation and the SRK
EOS coupled with CMR in the mixture system is within 3% as shown in Fig. 4. The difference is higher than the single-component system in some cases; however, since the increment from the single-component system was quantitatively very small, we confirmed that the CMR hardly increases the difference in the $P$–$V$–$T$ relationship of a single-component fluid. If the difference between the MD simulation and the SRK EOS coupled with CMR is within this magnitude, the sufficient correction for the $P$–$V$–$T$ relationship is possible using the fitting parameters in Eq. (9) and Eq. (10).

The specific heat at constant pressure against the molar fraction of hydrogen is shown in Fig. 5. Here, for reference, MD result of $c_p$ [J/mol/K] in oxygen (molar fraction of hydrogen is zero) and that in hydrogen (molar fraction of hydrogen is one) corresponds to $c_{p,o_2} = 1.68$ kJ/kg/K and $c_{p,H_2} = 16.2$ kJ/kg/K, respectively, in the unit of mass. Since the variation in specific heat caused by the parameters of the modified L–B rules in the mixture system is approximately 1.7 J/mol/K at a maximum when the molar fraction of hydrogen is 0.25, the influence of the parameters of the modified L–B rules is small. The relative difference in the specific heat between the MD simulation and the SRK EOS coupled with CMR in the mixture system is within 3%, as shown in Fig. 6. Further, even if considering uncertainty of ±2.5% of the MD simulations, the difference is within several percent. Also, the difference is higher than the single-component system in some cases. Considering the uncertainty of the MD simulations, we could not quantitatively assess whether the difference between the relative difference of the mixture system and that of a single-component is significant. However, as is shown in Fig. 5, we confirmed that the SRK EOS with CMR reproduces the dependency of specific heat on the molar concentration within a comparative accuracy to the statistical error of the MD simulations.

As above, that the CMR coupled with SRK EOS can reproduce the thermodynamic properties within the accuracy of several percent was confirmed is meaningful for ensuring reliability of the CFD analysis for combustion chamber. For...
A reliable analysis of turbulence, unsteady calculation by large eddy simulation (LES) or direct numerical simulation (DNS) using sufficiently fine computational grid is necessary. However, since these are not practical in design and development of liquid rocket engine because of those enormous calculation cost, steady calculation using Reynolds averaged Navier–Stokes (RANS) has been mainly conducted (Shima, 2016). Currently, the turbulence models in RANS especially have a great effect on flow field both in the combustion (Ivancic et al., 2013, Chemnitz et al., 2016) and non–combustion state (Park, 2012), and the relative difference in results can be several tens of percent in some cases. Particularly for the CFD of non–combustion state, validation of the CMR for oxygen–hydrogen is more meaningful because the non–ideality of oxygen and hydrogen cannot be neglected in this state, and both the CMR and turbulence model affects mixing of the propellant. As mentioned above, the error of CMR is within several percent even considering the statistical uncertainty of the present MD simulation, we confirmed that the CMR is reliable compared with the current turbulence models. Hence, in the typical CFDs based on RANS, we conclude that the CMR would be valid for the $P–V–T$ relationship and the specific heat at constant pressure for the oxygen–hydrogen mixture in the supercritical state, although more accurate mixing rule might be required when LES or DNS with sufficiently fine grid is practical in future.

4. Conclusion

We have validated the CMR coupled with the SRK EOS using MD simulations against a model of a supercritical oxygen–hydrogen mixture fluid whose intermolecular interaction was given by the L–J potential with the modified L–B rules. Our results show that the thermodynamic variables from the MD simulations corresponded with those from the EOS employing the CMR within several percent even considering the statistical uncertainty of the present MD simulation. We also confirmed that the deviation of the thermodynamic variables in the SRK EOS employing CMR for the mixture increases little or does not increase compared with that for the single–component system. In the current framework of CFD based on RANS with incomplete turbulence models applied in the design or development stage, we conclude that the CMR cannot be a main factor to cause in–negligible errors in the CFD for liquid rocket engines. This is an important new information for the researchers and the users of CFD for combustion chambers in liquid rocket engines.

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