DEVELOPMENT OF EFFICIENT REAL-FLUID MODEL IN SIMULATING LIQUID ROCKET INJECTOR FLOWS

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ABSTRACT

The characteristics of propellant mixing near the injector have a profound effect on the liquid rocket engine performance. However, the flow features near the injector of liquid rocket engines are extremely complicated, for example supercritical-pressure spray, turbulent mixing, and chemical reactions are present. Previously, a homogeneous spray approach with a real-fluid property model was developed to account for the compressibility and evaporation effects such that thermodynamics properties of a mixture at a wide range of pressures and temperatures can be properly calculated, including liquid-phase, gas-phase, two-phase, and dense fluid regions. The developed homogeneous spray model demonstrated a good success in simulating unielement shear coaxial injector spray combustion flows. However, the real-fluid model suffered a computational deficiency when applied to a pressure-based computational fluid dynamics (CFD) code. The deficiency is caused by the pressure and enthalpy being the independent variables in the solution procedure of a pressure-based code, whereas the real-fluid model utilizes density and temperature as independent variables. The objective of the present research work is to improve the computational efficiency of the real-fluid property model in computing thermal properties. The proposed approach is called an efficient real-fluid model, and the improvement of computational efficiency is achieved by using a combination of a liquid species and a gaseous species to represent a real-fluid species.

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It is found that the overall computational time can be reduced by one order of magnitude by avoiding the stiffness of inverting from the dependent variables (pressure and enthalpy) to independent variables (density and temperature) for multiple-species mixtures. The methodology of the proposed model and thermodynamics properties of some liquid species calculated from the model are reported herein. The accuracy and computational efficiency of the proposed efficient real-fluid model were evaluated by comparing to the numerical result of the developed real-fluid model tested previously.

INTRODUCTION

With the great demands and competitions for cheaper and safer launchers access to the space, the design of advanced reusable launching vehicles (RLV) is required to not only have higher payload-to-cost ratio, but also improve the reliability and thus extend the life of the reusable launching vehicle. The performance and hardware integrity of liquid rocket engines is greatly influenced by the propellant mixing near the injector. Understanding flow characteristics near the injector is thus very crucial in the advanced liquid rocket engine design. To obtain the information of flow phenomena near the injector, researchers have to rely on either the experimental study or numerical analyses. Conducting hot fire test of liquid injectors not only is too expensive and costly for all preliminary design concepts, but also encounters some technical problems in measuring multi-phase flow properties at the elevated pressure condition. Hence, most of the experimental tests were performed to measure chamber pressure and thrust of the engine. For the
The characteristics of spray combustion flows are multiple phases and chemical reactions. In order to properly account for the effect of phase change in spray combustion flows, a generalized equation of state (EOS) is required in order to accurately compute the thermal properties (such as density, enthalpy, speed of sound, and etc.) of the liquid propellant over a wide range of operating conditions. A typical pressure-density correlation for a given species can be plotted as shown in...
Figure 1, which consists of liquid, gas, two-phase, and dense fluid regimes. In our previous studies\textsuperscript{3-6}, a real-fluid model was developed and successfully predicted the compressibility effect of oxygen and nitrogen at an elevated pressure. In the developed real-fluid model, thermal and caloric equations of state, vapor pressure, heat of vaporization, surface tension, and transport properties are modeled with the equations of state proposed by Hirshfelder, et al\textsuperscript{5-16} (we term these the HBMS equations of state) and with conventional correlations\textsuperscript{17}, for the other properties. These correlations are explicit in density and temperature, and can be expressed as follows.

**HBMS thermal equation of state:**

\[
\frac{P}{P_c} = \sum_{j=1}^{4} T_{r,j}^{-2} \sum_{i=1}^{6} B_{ij} \rho_{r,i}^{-2} ; \quad T_r \equiv \frac{T}{T_c} ; \quad \rho_r \equiv \frac{\rho}{\rho_c}
\]

**HBMS caloric equation of state:**

\[
\frac{H - H_0}{RT} = Z_c \int_0^{\rho_r} \left[ \frac{P}{T_r} - \left( \frac{\partial P}{\partial T_r} \right) \right] \rho_r^2 d \rho_r + Z_c \frac{P}{\rho_r T_r} - 1
\]

where \( \rho_c, T_c, \) and \( P_c \) are the density, temperature, and pressure at the critical condition, while \( \rho_r \) and \( T_r \) are the reduced density and temperature which are normalized values with respect to the value at the critical condition. \( H \) and \( H_0 \) are the real-fluid enthalpy and ideal gas enthalpy of a given species. \( Z_c \) is the compressibility for a given species at the critical point. \( B_{ij} \) and \( R \) are the coefficients of the thermal property polynomial and the gas constant for a given species, respectively. However, for most of the multiple-species flow solvers either pressure and enthalpy are the primitive variables (pressure based), or the density and enthalpy are the primitive variables (density based). The inversion process from the dependent variables to the independent variables is very computationally intensive, especially for the chemically reacting flows where a mixture consists of multiple species and species concentrations of the mixture can change drastically (stiffness problem). The efficient real-fluid model is proposed to represent a real-fluid species \( (S) \) with a mixture of a liquid \( (S_l) \) and a gaseous \( (S_g) \) species, and can be expressed as

\[ S = (1 - f)S_l + fS_g \]

where \( f \) is the fraction of the gaseous species, and the split between \( S_l \) and \( S_g \) is defined by

\[ \rho = (1 - f)\rho_l + f\rho_g \]

The density \( \rho \) of the real-fluid species is obtained from the developed real-fluid model. One of the main features of the proposed efficient real-fluid model is that the density-temperature-pressure correlations of both the liquid and gaseous species are similar to the perfect-gas law such that the computational efficiency can be improved. Thus, the density of liquid \( (\rho_l) \) and gaseous \( (\rho_g) \) species can be explicitly calculated from pressures and temperatures. In addition, for the liquid species a compressibility factor \( (Z_{cl}) \), which is a function of temperature, and a fictitious molecular weight \( (M_{wl}) \) are employed to account for the compressibility effect. With a known pressure, the fictitious molecular weight, the compressibility factor, and the liquid density can be calculated as

\[ M_{wl} = \frac{\rho_o R_u T_o}{p} \]

where \( \begin{cases} T_o = T_c & \text{if } P \geq P_c \\ T_o = T_s & \text{if } P < P_c \end{cases} \)

\[ \rho_l(T) = \frac{pM_{wl}}{R_u Z_c T} \quad Z_c(T) = \frac{\rho(T)}{\rho_o} \]

\( R_u, T_s, \) and \( \rho_{s,l} \) are the universal gas constant, saturation temperature, and the saturation liquid density, respectively. The correlation of specific enthalpy between real-fluid species \( (h) \), liquid species \( (h_l) \), and gaseous species \( (h_g) \) can also be expressed as

\[ h = (1 - f)h_l + f h_g \]
The second main feature of the present model is that for a given pressure the specific heat \( C_{P,l} \) and the enthalpy \( H_l \) of the liquid species are polynomial functions of the temperature only similar to those of the gaseous species of the CEC code\(^{18} \), which can be shown as

\[
\frac{C_{P,l}}{R} = \sum_{n=1}^{5} A_n T^{n-1}; \quad \frac{H_l}{R} = A_6 + \sum_{n=1}^{5} A_n T^n
\]

\( A_n \) are polynomial coefficients of the liquid species, and can be obtained by curve fitting the real-fluid enthalpy for the temperature below either the saturation temperature (at subcritical pressure) or the critical temperature (at supercritical pressure). As a result, the effect of the heat of evaporation will be accounted for by increasing the fraction of gaseous species as the temperature increase. The last main feature of the present model is generating a look-up table for the speed of sound and the ratio of the specific heat based on the developed real-fluid model. The need for the speed of sound and the ratio of specific heat is to satisfy the correlation between the density and the pressure changes, which can be shown as

\[
\Delta \rho = \begin{cases} 
\frac{\Delta P }{\Delta t} \left( \frac{\partial (\rho)}{\partial P} \right)_T = \Delta P \frac{\gamma}{a^2} & : \text{both liquid and gas} \\
\frac{\Delta \rho M_w}{R_T} & : \text{ideal gas only}
\end{cases}
\]

This correlation can be applied to both density-based and pressure-based flow solvers, and is valid for liquid phase, gas phase, two-phase, and dense fluid regions. In order to apply the proposed effective real-fluid model to a flow solver, a preprocessor was constructed to generate the thermal properties of the liquid species for a given pressure. In the present model, the temperature is an explicit function of the specific enthalpy at a given pressure, and the fraction of the gaseous species and the density can be directly calculated based on the temperature as well. As a result, the computational time can be greatly reduced and the time marching step size can be increased because the matrix inversion for calculating mixture density and temperature from mixture enthalpy and pressure is avoided.

The proposed efficient real-fluid model was incorporated into the homogeneous spray methodology in the FDNS\(^{7-9} \) code to simulate the spray combustion problem. The framework of the FDNS code is an elliptic, finite difference Navier-Stokes flow solver, which employs a predictor plus multi-corrector pressure-based solution algorithm. Higher order upwind, total variation diminishing (TVD), or central difference schemes plus adaptive second-order and fourth-order dissipation terms are used to approximate the convection terms of the transport equations. Various matrix solvers, such as vectorized point implicit, conjugate gradient, and generalized minimal residual\(^{19} \) (GMRES), are provided in the code such that users can select one for a given transport equation. Since the FDNS flow solver is a structured code, multi-block, multi-zone grid topology was employed in the code so that problems with complex geometries can be analyzed efficiently. Since the flow solver is a pressure-based code, a pressure correction \( (P') \) equation is derived from the continuity equation and can be expressed as:

\[
\frac{\beta_p P'}{\Delta t} + \nabla \cdot \left( \bar{V}' \beta_p P' \right) = \nabla \cdot \left( \rho \frac{P'}{\Delta t} \right)
\]

\[= -\nabla \left( \rho \gamma \frac{V_i'}{a^2} \right) - \frac{P' - P^n}{\Delta t} \]

\[P^{n+1} = P^n + P' \quad \beta_p = \frac{\gamma}{a^2} \quad \bar{V}_i' = -D_p \nabla P'
\]

where the superscripts * and n denote the value at the intermediate and previous time steps, respectively. \( D_p \) is the inverse of the matrix of the coefficients of the convective terms in the finite-difference form of the inviscid equations of motion. For the homogeneous spray approach, the speed of sound \( (a) \), and the ratio of specific heat \( (\gamma) \) of a multi-component mixture can be calculated from the real-fluid properties of its constituents based on the additive volume method.

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where \( n_i, \alpha_i, \gamma_i, R_i, (C_p)_i, \alpha_i, \text{ and } M_{w_i} \) are the mole fraction, mass fraction, ratio of specific heat, gas constant, specific heat, speed of sound and the molecular weight of species "i", respectively.

### NUMERICAL RESULTS

In order to utilize the proposed effective real-fluid model, thermal properties of the liquid species as well as the split between gaseous and liquid species have to be generated beforehand. A pre-processor was constructed to generate those data needed by the present model based on the real-fluid model. The thermal properties of oxygen, hydrogen and RP-1 generated by the pre-processor are shown in Figures 2-13, respectively. It can be clearly seen that the thermal properties generated by the developed pre-processor accounts for the compressibility and heat of evaporation effects for these three species properly.

To examine the accuracy of the present model, a LOX/\( \text{GH}_2 \) uni-element shear coaxial injector, RCM-3 test case (Ref. 12), was simulated. Previously, the homogeneous real-fluid model was employed to simulate this test case, and good success was reported in Ref. 3 and 5. Thus, the accuracy and computational efficiency of the present model with the homogeneous spray approach can be evaluated comparing to the numerical result of the developed real-fluid model. As illustrated in Table 1, this is a super-critical spray combustion flow test case. Since surface tension is either zero or not well defined for super-critical conditions, drops either do not exist or are very unstable and do not survive very long. Therefore, the homogeneous spray model is an appropriate and effective approach for simulating this test case. The injector configuration and flow conditions for the RCM-3 test case are presented in Figure 14. A two-zone mesh system (61x39 and 301x101) was used to model the injector section and the combustion chamber.

As shown in our previous study\(^3\&5\), the numerical results of the equilibrium chemistry are almost identical to those of the finite-rate chemistry model because the reaction rate of the \( \text{H}_2/\text{O}_2 \) combustion at the elevated pressure is extremely fast. Moreover, the focus of the present study is to verify the accuracy of the proposed effective real-fluid model in predicting the thermodynamics properties over a wide range of temperatures. Therefore, it is more computationally efficient to utilize the equilibrium chemistry to simulate the super-critical \( \text{O}_2/\text{H}_2 \) combustion test case in the present study. The contours of predicted \( \text{OH} \) radical concentrations of both the present and the real-fluid models are shown in Figure 15. It is obvious the numerical results of both models are almost identical. In Figure 16, the oxygen concentration of the real-fluid model compares to the concentration of gaseous and liquid oxygen predicted by the present model. The sum of liquid and gaseous oxygen of the present model agrees very well with the oxygen concentration of the real-fluid model.

The radial temperature profiles predicted at several axial stations are shown in Figures 17-19, while the axial temperature profiles at several radial locations are shown in Figures 20-22. The agreement between the present model and the real-fluid model is excellent despite some small discrepancy at the location very close to the injector. This minor discrepancy is caused by the approximation that for the entire flow field all the property correlations of the present model are obtained based on a given pressure (chamber pressure in this case), whereas the pressure near the injector deviates substantially from the chamber pressure. This deficiency can be eliminated if the thermal properties are interpolated from property correlations of various pressures based on the local pressure. The thermal property interpolation for the proposed effective real-fluid model is being developed as part of this on-going research project. Nevertheless, for those multi-phase flow problems, where the pressures of the entire flow field do not differ too much from the value that the thermal properties for the liquid species were generated for, the fixed-pressure property approach is very efficient and effective. In addition to the model accuracy, more importantly the overall computational time is
reduced by one order of magnitude because the numerical simulation of the present model can be conducted with larger time marching step size (from 0.1 usec to 1µsec). This proves that the present model is able to relieve the stiffness problem by the utilization of two species representing a real-fluid species, as well as decoupling the process of computing the density and temperature.

CONCLUSIONS

A property pre-processor based on the present model was constructed to generate thermal properties for various liquid species. As can be seen from the generated thermal properties, the effects of compressibility and the heat of evaporation are taken into account by the developed property pre-processor. The present model does meet the goal of improving the computational efficiency of the real-fluid model. Meanwhile, the numerical result of the present model is almost identical to that of the real-fluid model. A minor discrepancy between the present model and the real-fluid model occurs near the injector, which is caused by the pressure deviation from the condition, which the thermal properties of the liquid species were generated for. This deficiency can be overcome by interpolating local thermal properties from a pre-generated property correlations based on the local pressure. The present study is just a proof of concept that the proposed model can be applied to simulate multiphase spray combustion flows. The variable-pressure version of the efficient real-fluid model is being developed as part of this on-going research activity. The result of this development will be reported in the future.

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REFERENCES


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Table 1. RCM-3 Test Case Operating Conditions

<table>
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<th>Conditions</th>
<th>H₂</th>
<th>O₂</th>
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<td>Mass flow rate</td>
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<td>Temperature</td>
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<td>Density</td>
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<td>12.34E-4 kg/m/s</td>
</tr>
</tbody>
</table>
Figure 1. Typical $P$-$p$-$T$ correlation for a given species

Figure 2. Comparison of oxygen density at various temperatures and pressures

Figure 3. Comparison of oxygen specific enthalpy at various temperatures and pressures

Figure 4. Comparison of oxygen speed of sound at various temperatures and pressures

Figure 5. Fractions of gaseous oxygen at various temperatures and pressures

Figure 6. Comparison of hydrogen density at various temperatures and pressures
Figure 7. Comparison of hydrogen specific enthalpy at various temperatures and pressures

Figure 8. Comparison of hydrogen speed of sound at various temperatures and pressures

Figure 9. Fraction of gaseous hydrogen at various temperatures and pressures

Figure 10. Comparison of RP-1 density at various temperatures and pressures

Figure 11. Comparison of RP-1 specific enthalpy at various temperatures and pressures

Figure 12. Comparison of RP-1 speed of sound at various temperatures and pressures
Figure 13. Fraction of gaseous RP-1 at various temperatures and pressures

Figure 14. Configuration and flow conditions for the RCM-3 test case

Figure 15. Comparisons of the OH concentrations near the injector face

Figure 16. Comparisons of the oxygen concentrations near the injector face

Comparisons of temperature profiles at X/D = 10 (RCM-3 test case)
Figure 18. Comparisons of temperature profiles at X/D = 20 (RCM-3 test case)

Figure 21. Comparisons of temperature profiles at R/D = 2 (RCM-3 test case)

Figure 19. Comparisons of temperature profiles at X/D = 30 (RCM-3 test case)

Figure 22. Comparisons of temperature profiles along the chamber wall (RCM-3 test case)

Figure 20. Comparisons of temperature profiles at R/D = 0 (RCM-3 test case)