Evaporation and dynamic characteristics of a high-speed droplet under transcritical conditions

Shichun Yang, Yanfei Gao, Cheng Deng, Bin Xu, Fenzhu Ji and Yongling He

Abstract
An evaporation and aerodynamic interaction model is developed for an isolated droplet introduced into transcritical and strong convective environments. The new numerical model takes into account variable thermophysical properties, gas solubility in the liquid phase, and vapor–liquid interfacial thermodynamics. The proposed model is verified by high-speed photography experiments carried out under different operating conditions. The influences of ambient conditions on the transcritical evaporation and aerodynamic interaction are investigated with the new model. The results indicate that (1) with increasing the liquid–gas relative velocity, the spatial temperature distribution becomes more nonuniform initially and then more uniform; (2) the drop drag increases rapidly with ambient pressure in the initial period and then significantly decreases; and (3) when the ambient temperature is lower than 1.5 times the fuel critical temperature, the droplet drag force decreased with the ambient temperature; otherwise, the drag force increased initially and then decreased with the ambient temperature.

Keywords
Transcritical, droplet, high speed, aerodynamic, evaporation

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Introduction
The problem of transcritical mixing attracts significant attention since numerous practical applications exist where the ambient pressure and temperature can approach or exceed the critical point of one of the fluid components (i.e. transcritical conditions).1,2 For the power systems such as aircraft jet engines, diesel engines, and gasoline direct-injection (GDI) engines, the transcritical mixing processes always occur. The liquid fuel is injected into the combustion chamber as a spray of droplets, which then undergo a sequence of physical processes including evaporation and breakup and mixing with the surrounding gas. During the processes, the heat and mass transfer as well as the aerodynamic forces control the droplet breakup. The resulted spray penetration and cone angle determine the spatial distribution of the equivalence ratio of the ignitable mixture formation and have a significant influence on combustion and formation of pollutants. Therefore, it is required to study the heat and mass transfer, interaction, and momentum exchange between the high-speed droplet and gas flow under convective transcritical conditions in detail.2

Several investigations on the whole spray and air–fuel mixing under subcritical or supercritical conditions

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have been presented in published literatures. As the chamber pressures approach the critical conditions, the atomization and fuel-air mixture formation exhibit a great sensitivity to pressures, temperatures, and local mixture concentrations. Tavlarides and Anitescu suggested that injecting fuels near the critical region into the engine cylinders is one way to increase engine efficiency and decrease emissions. Preheating the diesel upon injection provides better fuel-air mixing when this process is operated at the temperatures near the critical region. Segal and Polikhov investigated the effects of the ambient pressure and temperature on the jet breakup. They found that at subcritical conditions, the gas inertia and surface tension forces have the dominant effect on the formation of ligaments from which the materials break off and the drops form later; however, at supercritical conditions, only the reduced surface tension affects the jet surface behavior significantly. Polikhov and Segal found that the diffusion rate of oxygen into acetone in the transcritical and supercritical regimes is two orders of magnitude faster than that at low ambient pressures. Yin and Lu studied the effects of the injection temperature on the flow evolution. It was concluded that for supercritical injection temperatures, the jet surface becomes more unstable when the instability waves grow up, but for subcritical injection temperatures, the jet surface is nearly straight with the strong density stratification which suppresses the instability wave development. Rachedi et al. compared the jet behaviors of a hydrocarbon and a CO₂ supercritical fluid. The results showed that their behaviors are similar in most respects: the jet swirl number has a significant effect on cone angle, while the density ratio has a minor influence on it. Kim et al. conducted a computational analysis of four cryogen nitrogen jets at near-critical and supercritical pressures, with their computational fluid dynamics (CFD) code incorporated with two real-fluid equations of state and dense-fluid correction schemes. Roy et al. found that the droplet deformation occurs downstream beyond a 10 jet diameters distance from the nozzle, when a supercritical jet is injected into a subcritical environment at relatively low chamber temperatures.

However, all of the above studies are conducted from the macroscopic view. Down to the level of the fundamental element of spray (i.e. an isolated droplet), most of the existing researches for transcritical conditions concentrate on the drop evaporation in stagnant gas environments, without considering the nonideal fluid behavior under transcritical conditions, and on the transcritical droplet breakup. Little work has been done on the evaporation and dynamic characteristics of high-speed droplets under transcritical conditions.

The objective of this work is to develop an evaporation and aerodynamic interaction model for single droplets which are introduced into transcritical and strong convective environments, in order to gain a further understanding of the droplet evaporation and dynamic physics under extreme conditions. This model takes into account real-fluid property, high-pressure effects, and gas solubility in the liquid phase. Variable thermophysical properties for both liquid and gas phases is taken as functions of pressure, composition, and temperature. It also considers the spatial and temporal distribution of thermophysical properties inside the liquid-phase domain. Besides, an effective thermal conductivity is used for the liquid phase transfer process, which also reflects the liquid-phase internal circulation. The influences of ambient conditions on the heat and mass transfer and liquid-phase momentum exchange under convective transcritical conditions are investigated with the developed model. The high-speed photography experiments are carried out under different operating conditions in order to verify the effectiveness of the proposed evaporation and dynamic model for a high-speed droplet.

Model development

The developed evaporation and aerodynamic interaction model, for a high-speed droplet under transcritical and forced convective conditions, is described schematically in Figure 1. \( r \) stands for droplet radius, \( u_{rel} \) stands for the relative velocity between droplet and surrounding gas, \( m \) is droplet mass, and \( t \) represents time. \( x \) is the semi major axis of deformed droplet.

![Figure 1. Modeling of heat and mass transfer and droplet deformation under transcritical conditions.](image)
of the droplet’s equator from its equilibrium position) is taken into account for the calculation of aerodynamic forces.

The physical problem described here considers the heat and mass transfer and the interaction between an isolated evaporating droplet and a high-speed gas flow. The gas thermodynamics state is approaching the critical point. Near the critical point, the thermophysical properties of both vapor and liquid phases usually exhibit anomalous variations and are extremely sensitive to pressure and temperature, leading to a phenomenon commonly referred to as near-critical enhancement. The fluid has properties similar to both gases and liquids, for example, gas-like thermal properties and liquid-like densities.4 As one is approaching the critical point, the densities of both gas and liquid phases become approximately equal. The molecule net attraction in the interface region toward the dense phase is close to zero, namely, the metastable surface.17 At the critical point, many phenomena coexist near the critical point, for example, strengthened dissolution of gas phase in liquid phase, rapid decrease in evaporation enthalpy, and thermophysical property singularities. Due to the latter factor, the critical mixing point varies dynamically depending upon the mixture properties, potentially affecting the gas–liquid interface. Significantly decreased ratio of liquid density to gas density as well as weakened interface tension can lead to further enhanced aerodynamic interactions induced by the relative velocity between gas and droplet. All the above factors can affect the heat and mass transfer and aerodynamic interaction obviously. In this article, the heat transfer, mass diffusion, and aerodynamic interaction between the high-speed droplet and surrounding gas were studied. The gas atmosphere is nitrogen, and n-heptane is used as the fuel, which has a critical pressure $P_c$ of 2.74 MPa and a critical temperature $T_c$ of 540 K.

**Governing equations**

The developed model considers high-pressure effects, solubility of inert species into the liquid phase, real-fluid behavior of both liquid and gas phases, and the spatial distribution and temporal variation of thermophysical properties. Ambient gas is assumed to be dissolved only in a very thin layer of the gas–liquid interface and thus the gas diffusion into the liquid interior is ignored. Considering the forced convective heat transfer and mass diffusion in the gaseous boundary layer around the droplet, an effective conductivity is adopted based on effective film method, which also takes account of the liquid-phase internal circulation.18 The radiation heat transfer is negligible and considering small flow velocity in comparison with the acoustic speed, pressure keeps constant.

Energy conservation inside the droplet

\[ \frac{C_p}{\rho} \frac{dT}{dt} - \frac{1}{\rho r^2} \frac{\partial}{\partial r} \left( r^2 k^c c \frac{dT}{dr} \right) = 0 \]  

(1)

Continuity equation for liquid phase

\[ \frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \rho u \right) = 0 \]  

(2)

Liquid–gas phase energy balance

\[ k^c \frac{\partial T}{\partial r} \bigg|_{\text{sf}} = \left( \frac{H_{g, sf} - H_{l, sf}}{4\pi \cdot r^2} \right) \frac{dm}{dt} + \left[ h^*_g \left( T_{\infty} - T_{sf} \right) \right] \]  

(3)

Species conservation

\[ W_F = -\frac{dm}{dt} = 4\pi \cdot r^2 \cdot K_{FN} \cdot \frac{Y_{F, sf} - Y_{F, \infty}}{1 - \left( \frac{1 + w_c \cdot \rho_{sf}}{\rho_{F, sf}} \right) Y_{F, sf}} \]  

(4)

In the above equations, $r$ is the radial distance relative to droplet center, $u$ represents the radial velocity inside the droplet, $T$ is temperature, $\rho$ stands for density, $C_p$ indicates the constant pressure heat capacity, $k^c$ is the effective thermal conductivity, $H$ is enthalpy, $h^*_g$ and $K_{FN}$ are corrected heat transfer coefficient and mass diffusion coefficient, $Y$ stands for mass fraction in gas phase, $W$ indicates mass flow rate, subscripts $l$ and $g$ represent liquid and gas phases, subscripts $sf$ and $\infty$ are drop surface and infinite boundary, and subscripts $N$ and $F$ stand for nitrogen and fuel components, respectively.

In the research of C Crua et al.,19 the characterization of the initial stage of fuel spray is conducted using microscopic imaging that can measure droplet diameters with a high level of accuracy. However, they investigate the primary breakup process in which the spray turbulence is dominant, and we investigate the subsequent secondary breakup and mixture formation process in which gas–liquid interactions dominate the process. In the model of Ebrahimian and Habchi,20 the liquid-phase temperature is assumed to be uniform for liquid-phase balance equation, without considering the temperature inhomogeneity inside the droplet during the evaporation process. In addition, the mass and heat transfer coefficients have not been corrected for high heat and mass transfer. The method of Litchford and Jeng21 takes into account evaporation in the calculation of the boundary conditions and the effective thermal conductivity. It also considers the finite thermal conductivity, recirculation.

Therefore, we adopt the method (equation (4)) of Litchford and Jeng21 for species conservation. In addition, we use a uniform method to calculate both the gas and liquid thermodynamic parameters, by combining
the real gas state equation with the ideal gas specific heat capacity at constant pressure, and use the liquid vapor partial molar enthalpy difference to calculate the enthalpy of vaporization.

Nitrogen dissolution in the liquid phase is neglected in the droplet mass calculation. \( h_g \) is convective heat transfer coefficient and \( K_{FN} \) represents mass transfer coefficient. Heat transfer coefficient \( h_g \) for the gas mixture is calculated by

\[
h_g = \frac{k^c Nu}{2r_s} \tag{5}
\]

\[
Nu = \frac{2 + 0.555Re^{1/2}Pr^{1/3}}{\sqrt{1 + \frac{1.232}{RePr}}} \tag{6}
\]

\[
Re = \frac{2 \rho_g u_{rel} r_s}{\mu_g} \tag{7}
\]

\[
Pr = \frac{Cp_g \mu_g}{k^c} \tag{8}
\]

Mass transfer coefficient \( K_{FN} \) for the gas mixture can be written as

\[
K_{FN} = \frac{\rho_g D_{FN} Sh}{2r_s} \tag{9}
\]

\[
Sh = \frac{2 + 0.555Re^{1/2}Sc^{1/3}}{\sqrt{1 + \frac{1.232}{ReSc}}} \tag{10}
\]

\[
Sc = \frac{\mu_g}{\rho_g D_{FN}} \tag{11}
\]

where \( Nu \) represents Nusselt number, \( Re \) is Reynolds number, \( Pr \) is Prandtl number, \( \mu \) is viscosity, \( Sh \) stands for Sherwood number, and \( Sc \) represents Schmidt number. \( D_{FN} \) stands for mass diffusivity.

Mass conservation of droplet

\[
\frac{dm}{dt} = 4\pi r_s^2 \rho_l \frac{dr_s}{dt} + 4\pi r_s^3 \frac{d\rho_l}{dt} \tag{12}
\]

Surface tension

The mixture surface tension can be determined by

\[
\sigma_m = \left\{ \frac{[P_{i,N}]}{M_F} \left( \frac{\rho_{i,F} \times 10^{-3}}{M_F} \right) - \left[ \frac{P_{gmix}}{M_g} \right] \left( \frac{\rho_{gmix} \times 10^{-3}}{M_g} \right) \right\}^4 \times 10^{-3} \tag{13}
\]

\[
[P_{i,N}] = \sum_i \sum_{j,F,N} X_i^j X_j^i [P_j] = [P_F] \tag{14}
\]

\[
[P_{gmix}] = \sum_i \sum_{j,F,N} X_i^j X_j^i [P_j] \tag{15}
\]

\[
[P_j] = \frac{[P_i] + [P_j]}{2} \tag{16}
\]

where \( \rho_{i,F} \) is liquid fuel density, \( \rho_{gmix} \) is vapor mixture density, \([P_i]\) stands for parachor of pure component \(i\), \([P_j]\) represents parachor of pure heptane, \([P_N]\) stands for parachor of pure nitrogen, \(M_F\) and \(M_g\) are molecular weights of fuel and gas phase mixture, and \(X\) stands for molar fraction.

Droplet drag modeling

The drop drag force \( F_{drag} \) and the drag coefficient \( C_D \) can be calculated by

\[
F_{drag} = \frac{\rho_g u_{rel}^2 C_D A_f}{2} \tag{17}
\]

\[
C_D = \begin{cases} 
24/Re_g (1 + Re_g^{2/3})/6, Re_g \leq 1000 \\
0.424, Re_g > 1000 
\end{cases} \tag{18}
\]

where \( Re_g \) is the gas Reynolds number, and the drop deformation \( y (y = 2x/r_s) \) and frontal area \( A_f \) are calculated based on the droplet deformation and breakup (DDB) model.

Thermophysical properties

Critical mixing point. The fuel mass fractions of both the liquid phase and vapor phase are equal at the critical mixing point. In addition, surface tension and evaporation enthalpy decrease to zero, and the droplet surface disappears. For a binary mixture, the critical mixing point can be written as

\[
\left( \frac{\partial \ln \tilde{f}_F}{\partial X_F} \right)_{p,T} = 0 \tag{19}
\]

\[
\left( \frac{\partial^2 \ln \tilde{f}_F}{\partial X_F^2} \right)_{p,T} = 0 \tag{20}
\]

\[
\tilde{f}_F = PX_F \tilde{\phi}_F \tag{21}
\]

where \( \tilde{f} \) is fugacity, \( \tilde{\phi} \) stands for fugacity coefficient, and \( X \) stands for molar fraction.

Thermodynamic properties. In order to take into account real-fluid behavior, vapor–liquid phase equilibria, and high-pressure effects, the Peng–Robinson equation of state (EOS) is utilized for the gas phase and liquid phase mixture and can be written as
\[ P = \frac{RT}{v - b_m} - \frac{a_m}{v(v + b_m)} \]  
\[ (22) \]

where \( a_m \) and \( b_m \) stand for the EOS parameters corresponding to the fluid mixture, \( R \) stands for universal gas constant, and \( v \) is molar volume. The Peng–Robinson EOS can be used to calculate fugacity coefficients, specific enthalpy, and constant pressure heat capacity.

**Other physical properties.** Considering high density and pressure effects, the low-pressure model for thermal conductivities proposed by Chung et al. is modified with Chung et al. rules, and the liquid viscosity is calculated via the corrected method of Chung et al. The mass diffusion for binary systems is obtained from Wilke and Lee method, which utilizes Takahashi method for pressure corrections.

Thermodynamic properties in the gaseous boundary layer, such as \( T_g \) and \( X_g \), are estimated with \( 1/3 \) rule based on the average temperature and the average concentration, as expressed by equations (16) and (17)

\[ T_g = T_{sf} + \frac{(T_u - T_g)}{3} \]  
\[ (23) \]

\[ X_g = X_{F, sf} + \frac{(X_{F, u} - X_{F, sf})}{3} = \frac{2}{3} X_{F, sf} \]  
\[ (24) \]

where \( T \) stands for average temperature and \( X \) stands for average molar fraction of fuel components in gaseous film region.

**Boundary conditions**

At the drop center, the temperature gradient is assumed to be zero, and at the infinite boundary, all the variables remain at their initial values.

At the droplet surface, the vapor–liquid equilibrium is satisfied

\[ \tilde{\phi}_{F, g} X_{F, g} = \tilde{\phi}_{F, l} X_{F, l} \]  
\[ (25) \]

\[ \tilde{\phi}_{N, g} X_{N, g} = \tilde{\phi}_{N, l} X_{N, l} \]  
\[ (26) \]

**Solution procedure**

An efficient numerical algorithm based on iterative method is adopted to solve the governing equations. A central difference scheme is utilized regarding the numerical calculation of liquid-phase energy conservation, and a fully implicit scheme is adopted with regard to transient solution. A second-order one-sided difference is employed with a nonuniform grid system at the liquid–gas interface, considering extremely high gradients of thermophysical properties near the droplet surface. The non-dimensional time step size used in the simulation is \( 2 \times 10^{-5} \). Figure 13 in Appendix 2 is a program chart in order to explain the iterative method adopted for solving the governing equations.

**Experimental procedure**

In order to verify the effectiveness of the proposed evaporation and dynamic model for a high-speed droplet,
the high-speed photography experiments are carried out at room pressure and high temperature environments. The predicted and measured droplet trajectories are compared under different operating conditions in Table 1, where $d_{\text{init}}$ is the initial droplet diameter.

The high-speed imaging system for droplet motion measurement is shown schematically in Figure 2. At the right side, a gas nozzle with an inner diameter of 40 mm is included and enables continuous horizontal flows of nitrogen gas through the constant volume chamber. The gas velocity at the nozzle hole exit is determined from the air flow rate, which is monitored by a rotameter. A vertically mounted droplet generator is used to repeatedly produce monodisperse droplets with the diameter of 1 and 1.8 mm. The tip of the droplet generator is located, as close as possible to the gas nozzle outlet, at a horizontal distance of approximately 3 mm. Thus, the velocity at the gas nozzle outlet can be considered as that of the air flow surrounding the droplet. The working fluid is $n$-heptane, and the chamber is purged by injecting nitrogen gas, which replaces air inside the chamber in order to avoid combustion and oxidation processes and to observe the droplet movement. A cone-shaped ventline mounted at the left side of the chamber is utilized to eliminate the radial diffusion of the jet stream to some degree. Several T-type thermocouples are installed inside the chamber, the gas nozzle, and the droplet generator, in order to measure their internal fluid temperature in real time. The resistance heater with an electronic controller is used to heat the nitrogen gas to a desired temperature. An electric furnace is used to heat the fuel to required temperatures. The droplet generator tip is located as close as possible, in the vertical direction, to the horizontal air flow. The pressure inside the vessel is maintained at atmospheric pressure level.

A FASTCAM SA1.1 high-speed camera equipped with a 100-mm focal length macro lens, providing a $1024 \times 1024$ pixel resolution and a capture frame rate of 5400 frames/s, was used to image the backside illuminated droplets. Two quartz glass windows are installed oppositely on the chamber for optical accessibility. The droplet motion inside the gas flow is photographed through the high-speed camera. The resulting frames are recorded on data storage and then are analyzed to obtain temporal variations of droplet trajectories. The fuel collector is used to collect the falling droplets.

**Results and discussion**

**Model validation**

The ambient pressure is 0.1 MPa in the experiments and the critical properties of $n$-heptane are taken as a reference.

Figure 3 displays the consecutive images of fuel droplets with the initial diameter $d_{\text{init}} = 1.0$ mm (Figure 3(a)) and $d_{\text{init}} = 1.8$ mm (Figure 3(b)), which are introduced into the high-velocity gas flow. The initial droplet temperature and the chamber temperature are equal to 330 and 550 K (which corresponds to the reduced temperature $T/T_c$ of 1.02), respectively, and the relative velocity $u_{rel}$ is 48 m/s.

![Figure 3](image-url)
Figure 4 shows the comparisons between the predicted and measured droplet trajectories under different conditions. The initial droplet temperature and the chamber temperature are equal to 330 and 550 K. The ambient pressure is 1 bar and the relative velocity $u_{rel}$ is 48 m/s.

Heat transfer and mass diffusion coefficients

The non-dimensional time $\tau$ is defined as $\tau = t/\left(r_0^3 \rho_c C_{p_{ref}}/k_{ref}\right)$, where $r_0$ represents initial droplet radius, $\rho_c$ represents fuel critical density, and $C_{p_{ref}}$ and $k_{ref}$ stand for fuel specific heat capacity and thermal conductivity at room temperature, respectively. The non-dimensional heat transfer coefficient $h_{norm}$ and non-dimensional diffusion coefficient $K_{norm}$ are defined as $h_{norm} = h_{g}/(k_{ref}/r_0)$ and $K_{norm} = K_{g}/(k_{ref}/C_{p_{ref}}/r_0)$. $P_r (P_r = P/P_s)$ and $T_r (T_r = T/T_c)$ are the reduced pressure and temperature, respectively. In the following simulations, the ambient gas remains static and the fuel droplet initially is at subcritical state with a diameter of 40 μm and a temperature of 300 K.

Figures 5 and 6 show the effects of ambient temperature and pressure on transient heat transfer coefficient $h_{norm}$ and mass diffusion coefficient $K_{norm}$, with conditions $u_{rel} = 75$ m/s, $P_r = 1.0$ (in Figure 5), and $T_r = 1.0$ (in Figure 6). Figure 7 presents the temporal variations of heat transfer and mass diffusion coefficients at different $u_{rel}$ when both the reduced ambient pressure and reduced ambient temperature are equal to 1.0. As can be seen from Figures 5–7, when the relative velocity $u_{rel}$ keeps constant, the heat transfer and mass diffusion coefficients as well as their rising rates increase continuously as time elapses. The results indicate that the gas-phase dissolution in the liquid phase and the temperature rise of the liquid droplet during the transcritical evaporation process lead to reduced evaporation enthalpy and enhance the heat transfer from the gas to liquid and the mass diffusion of liquid in gas phase. The effects are especially obvious when the droplet temperature and the gas-phase dissolution increase. Figures 5 and 6 show that the heat and mass transfer coefficients vary more significantly with increasing ambient temperature or ambient pressure. This is due to the fact that the larger temperature gradient near the droplet surface accelerates the heat transfer from the ambient gas to the liquid, and the diminished evaporation enthalpy reduces the energy required for evaporation and makes the droplets evaporate more easily. When the $u_{rel}$ increases, the vapor mixture around the droplet surface is entrained much faster by the air flow, resulting in the improved gas–liquid mass and heat transfer.

Figure 4. Comparisons of predicted and measured droplet trajectories under different conditions. The initial droplet temperature and the chamber temperature are equal to 330 and 550 K. The ambient pressure is 1 bar and the relative velocity $u_{rel}$ is 48 m/s.

Figure 5. Temporal variations of heat transfer and mass diffusion coefficients at different ambient temperatures. The droplet temperature is 300 K and the $u_{rel}$ is 75 m/s.

Figure 6. Temporal variations of heat transfer and mass diffusion coefficients at different ambient pressures. The droplet temperature is 300 K and the $u_{rel}$ is 75 m/s.
exchange as shown in Figure 7. Compared with the results in Figures 6 and 7, Figure 5 shows that the ambient temperature initially has no effect on the mass diffusion and heat transfer coefficients during the convective and transcritical evaporation processes. It indicates that, when the pressure and the relative velocity \( u_{rel} \) remain constant, the temperature gradient near the droplet surface has no effect on the heat and mass transfer between the liquid and gas phases during the initial period.

**Temperature distribution inside the droplet**

Figure 8 presents the transient distribution of temperature inside droplet at different \( u_{rel} \) with conditions \( Pr = 1.0 \) and \( Tr = 1.0 \). The variation curves of temperature are much nonuniform initially because of the high temperature gradient. But the curves become much higher and more uniform as time progresses, which indicates that the internal circulation enhances heat conduction inside the droplet and the internal temperature of the droplet becomes more uniform. The temperature gradient increases progressively in the radial direction, indicating that less energy penetrates the droplet. Much of the heat transferred from the gaseous phase contributes to the evaporation of liquid fuel. Hence, the droplet surface regression rate changes much faster in comparison with the density decrease rate during the entire droplet lifetime. As can be seen in Figure 8, with increasing \( u_{rel} \), the spatial distribution of temperature becomes more nonuniform initially due to the higher temperature gradient, then becomes more uniform due to the enhanced internal circulation effect and the heat diffusion inside the droplet.

**Aerodynamic interaction between gas phase and liquid phase**

In the following simulations, different from the above-mentioned study where the \( u_{rel} \) keeps constant, the \( u_{rel} \) varies constantly over time due to the influence of aerodynamic force. The initial value of \( u_{rel} \) is 75 m/s.

The droplet drag and velocity determine the droplet breakup process, spray penetration, and cone angle, which directly affect the quality of the combustible mixture formation. Figures 9 and 10 give the temporal variations of \( u_{rel} \) and drag force at various ambient pressures, respectively. The reduced ambient temperature \( Tr \) is equal to 1.0, and the initial droplet velocity is 75 m/s. As shown in Figure 9, the \( u_{rel} \) decreases sharply initially and then varies more and more slowly as time progresses. This is because the drop drag and
gas–liquid momentum exchange are significant when the $u_{rel}$ is very high initially. In addition, the drop drag significantly decreases with the decrease in $u_{rel}$. Thus, the declining rate of the $u_{rel}$ decreases continuously in the process of gas–liquid momentum exchange. Figure 9 also shows that the velocity $u_{rel}$ decreases much more quickly as the pressure increases, but the effect of pressure on the $u_{rel}$ becomes weaker as time elapses. As shown in Figure 10, the drop drag significantly decreases as time progresses, with the rapid reduction of its variation rate.

This is due to the reduced $u_{rel}$. It can also be seen that, in the initial period, the drop drag increases rapidly with ambient pressure and the effect of pressure is very obvious. However, in the later stage, ambient pressure has an opposite effect, that is, the drop drag significantly decreases with ambient pressure. Thus, it can be concluded that the variations of thermodynamic and transport properties for gas phase and liquid phase, due to the temperature rise and the dissolution of ambient gas into droplet surface, can lead to the drop drag weakness obviously during the heat transfer and mass diffusion process.

Figures 11 and 12 depict the temporal variations of $u_{rel}$ and drag force at various ambient temperatures, respectively. The reduced ambient pressure $P_r$ is equal to 1.0, and the initial droplet velocity is 75 m/s. Figure 11 shows that the ambient temperature has almost no influence on the $u_{rel}$ when the ambient temperature $T/T_c$ is lower than 1.5. It indicates that the reduction of droplet drag force is equal to that of droplet mass, resulting in unchanged droplet acceleration. As can be seen from Figure 11, the $u_{rel}$ decreases with ambient temperature $T/T_c$ when the $T/T_c$ is higher than 1.5. It can be explained that the drag force increases initially with increasing ambient temperature (as shown in Figure 12). While the droplet evaporation rate and mass decrease rate become much faster than the drag force decrease subsequently, although the drag force decreases with increasing ambient temperature. Hence, the droplet drag acceleration always increases with ambient temperature during the entire process. The figure also shows that the influence of temperature on the $u_{rel}$ tends to weaken slowly as time progresses. It means that the reduced temperature gradient eliminates the influence of ambient temperature on drag acceleration to some degree.

Figure 12 shows that the drag force and its variation rate decrease gradually as time elapses, due to the $u_{rel}$ reduction. When the ambient temperature $T/T_c$ is lower than 1.5, the droplet drag force decreased with the ambient temperature. This is because the temperature rise results in the gas-phase density reduction, which attenuates the momentum exchange and interreaction between gas and liquid phases.
between the gas and the liquid. When the $T/T_c$ is higher than 1.5, the drag force increases with ambient temperature during the initial period of evaporation process but decreases with ambient temperature during the later stage. This is due to the fact that the thermodynamic and transport properties at high temperatures are more sensitive to the gas-phase and liquid-phase temperatures and the gas dissolution in the liquid, which enhances the effects of heat and mass transfer on the gas–liquid interaction and the drag force. Hence, the drag force exhibits a much steeper variation with time.

Conclusion

An evaporation and aerodynamic interaction model is developed for an isolated droplet introduced into transcritical and strong convective environments. The model is verified by comparing the calculation results and experimental results. The results are as follows:

1. The heat and mass transfer coefficients vary more significantly when the ambient temperature or the ambient pressure increases.
2. The ambient temperature has no effect on the mass diffusion and heat transfer coefficients initially.
3. With the relative velocity $u_{rel}$ increasing, the spatial temperature distribution becomes more non-uniform initially and then more uniform.
4. The drop drag increases rapidly with ambient pressure in the initial period and then significantly decreases.
5. When the $T/T_c$ is higher than 1.5, the $u_{rel}$ decreases with ambient temperature $T/T_c$; otherwise, the $u_{rel}$ remains unchanged.
6. When the ambient temperature $T/T_c$ is lower than 1.5, the droplet drag force decreased with the $T/T_c$; otherwise, the drag force increases initially and then decreases with $T/T_c$.

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Appendix 1

Notation

| Symbol | Description |
|--------|-------------|
| $a_m, b_m$ | EOS parameters |
| $A_f$ | frontal area of drop (m²) |
| $C_D$ | drag coefficient |
| $C_p$ | constant pressure heat capacity (J/(kg K)) |
| $C_p$ _ref | specific heat capacity of the liquid fuel at 293 K and 0.1 MPa (J/(kg K)) |
| $d_{init}$ | initial droplet diameter |
| $f$ | fugacity (Pa) |
| $F_{drag}$ | drop drag force (N) |
| $h_g$ | convective heat transfer coefficient (W/(m² K)) |
| $h_{norm}$ | non-dimensional heat transfer coefficient |
| $H$ | enthalpy (J/kg) |
| $k_{ref}$ | thermal conductivity of the fuel at 293 K and 0.1 MPa (W/(m K)) |
| $k_e$ | effective thermal conductivity (W/(m K)) |
| $K$ | model constant |
| $K_{FN}$ | mass transfer coefficient (kg/(m² s)) |
| $K_{norm}$ | non-dimensional diffusion coefficient |
| $m$ | droplet mass (kg) |
| $Nu$ | Nusselt number |
| $P$ | pressure (Pa) |
| $P_c$ | critical pressure of the fuel (Pa) |
| $P_r$ | reduced ambient pressure |
| $Pr$ | Prandtl number |
| $r$ | radial distance relative to droplet center (m) |
| $r_s$ | droplet radius (m) |
| $r_{so}$ | initial droplet radius (m) |
| $R$ | universal gas constant (J/(mol K)) |
| $Re$ | Reynolds number |
| $Sc$ | Schmidt number |
| $Sh$ | Sherwood number |
| $t$ | time |
| $T$ | temperature, initial droplet temperature (K) |
| $T_c$ | critical temperature of the fuel (K) |
| $T_{c,mix}$ | mixture temperature at the critical point (K) |
| $T_r$ | reduced temperature |
| $\bar{T}$ | average temperature in gaseous film region (K) |
| $u$ | radial velocity inside droplet relative to droplet center (m/s) |
| $u_{rel}$ | relative velocity between droplet and gas (m/s) |
| $v$ | molar volume (m³/mol) |
| $W$ | mass flow rate (kg/s) |
| $X$ | molar fraction |
| $\bar{X}$ | average fuel molar fraction in gaseous film region |
| $y$ | drop deformation |
| $Y$ | mass fraction in gas phase |
| $\mu$ | viscosity (Pa s) |
| $\rho$ | density (kg/m³) |
| $\rho_c$ | critical density of the fuel (kg/m³) |
| $\rho_l$ | average droplet density (kg/m³) |
| $\sigma_m$ | mixture surface tension (N/m) |
| $\tau$ | non-dimensional time |
| $\varphi$ | fugacity coefficient |
| $\nu$ | fuel component |
| $g$ | gas phase |
| $l$ | liquid phase |
| $N$ | nitrogen component |
| $sf$ | drop surface |
| $\infty$ | infinite boundary |
Figure 13. Program chart for the iterative method adopted for solving the governing equations.