Abstract
The fuel oil atomization is closely related to the combustion performance of the fuel in the internal combustion engine. However, during the oil atomization, the fast evaporating and moving oil droplets interact strongly with the surrounding gas, posing challenges towards the precise simulation of the combustion process. To precisely capture the interactions between fuel droplets and the surrounding gas, a new multi-droplets motion and evaporation model is deduced by introducing the local parameters surrounding the fuel droplets. The proposed model is validated comparing the simulation results against the experimental data of the containment spray process. Subsequently, the present model is adopted to simulate the fuel spray process in the typical constant volume bomb. The parameters evolution is presented during the course of the spray such as the gas temperature, droplet temperature, evaporating rate, velocity, radii variation, vapor concentration and air-fuel ratio. The analysis of the spray performance is conducted and the superiority of the new model is also discussed. The simulation analysis reveals that the spray droplets interact strongly with the surrounding gas; the developed droplet motion and evaporation model is advantageous in the simulation of the dense multi-droplets spray process.

Keywords: Constant volume bomb, Droplet evaporation, Fuel spray, Heat and mass transfer, Two-phase interaction

1. Introduction

During the course of the fuel oil combustion, the performance of the fuel oil atomization and evaporation is tightly linked to the efficiency of the internal combustion engine and the greenhouse gas emission. The thoroughly evaporating of the droplets is preferred and is beneficial for the fully burning. Therefore, it is necessary to investigate the evaporation characteristics of the fuel oil droplet during spray in the engine.

Many experimental studies have been conducted on the fuel spray process. Li et al. (2011) analyzed the droplet size distribution and evaporation characteristics of fuel spray of a swirl type atomizer by the laser diagnostic techniques and presented the influence of spray dynamics on the droplet size distribution. Sinha et al. (2016) experimentally studied the fuel droplet evaporation under forced convection using spray in the crossflow and analysis of the size and velocity of the evaporating droplet was conducted. Yan et al. (2016) measured the fuel evaporation ratio at different inlet conditions of cyclone separator and the evaporation characteristics were analyzed. Zhou et al. (2018) adopted two injectors with the diameters of 0.11 mm and 0.14 mm for scaling the fuel spray processes under the non-evaporating conditions and experimentally analyzed the spray characteristics. Ma et al. (2016) studied the effects of pentanol addition to diesel in different ratios on the spray and evaporation characteristics of the fuel in a constant volume chamber. In addition, there are a lot of experimental investigations about the evaporation, spray characteristics of liquid fuel at various cases (Hwang et al., 2015; Chen et al., 2016). However, the experiments are expensive and time-consuming, which restrict research process of the design and optimization of the internal combustion engine.
As to the numerical and modeling research, the present models can be mainly divided into two types including the homogeneous model and Euler-Lagrange model (Ding et al., 2017). The Euler-Lagrange method is more precise to track the interactions between the spray droplets and the surrounding gas due to the treatment of the spatially-dispersed phase. Most of the droplet evaporation models of Euler-Lagrange method are based on the droplet vaporization model proposed by Abramzon and Sirignano (1989). Chen et al. (2016) compared three heat and mass transfer models including the well-mixed model, the frozen evaporation model and the diffusion controlled model for multi-component droplet evaporation and combined the UNIFAC method with the heat and mass transfer models to account for the
non-linearity effect on fuel evaporation process. Sazhin (2017) reviewed the recent developments in the modeling of heating and evaporation of fuel droplets, identified the most important unsolved problems and pointed that the effects of non-spherical droplets, effects of the interaction between droplets, effects of the moving interface due to evaporation, development of advanced kinetic and molecular dynamics models and effective approximation of the kinetic effects were necessary. Al et al. (2015) developed a new approach to model the heating and evaporation of gasoline fuel droplets by replacing the components of gasoline with close chemical, thermodynamic and transport properties with characteristic components to reduce the number of the original composition of gasoline fuel. In addition, a number of researches have been conducted on the modeling of the droplet motion and evaporation as well as the interactions between the two phases (Dombrovsky and Sazhin, 2003; Sazhin et al., 2016). However, the mechanism of the interactions between the droplets and the surrounding gas are still not clear, especially for the dense droplet spray, where the evaporating droplets interact significantly with the surrounding gas and the interactions between droplets should be taken into account (Labowsky, 1980; Castanet et al., 2005; Castanet et al., 2016). And continuous investigations are necessary to figure out the droplet-gas two phases coupling mechanism.

Therefore, this paper aims to formulate the multi-droplets motion and evaporation model by introducing the local parameters surrounding the droplets and the more precise interactions between the fuel droplets and the surrounding gas can be tracked. Then, the model is utilized to simulate the fuel droplet spray process in the constant volume bomb to investigate the performance of the containment spray system. The parameters evolution is presented during the course of the spray such as the gas temperature, droplet temperature, evaporating rate, droplet velocity, radii variation, vapor concentration and air-fuel ratio. The analysis of the spray performance is conducted and the superiority of the new model is also discussed.

2. Theoretical model

As presented in Fig. 1, when a droplet evaporates in the gas, it will interact with surrounding gas. The evaporated vapor enters into gas flow field by diffusion, which will drive the gas surrounding the droplet to flow, mixing with each other. Consequently, the temperature and vapor concentration change accordingly. In addition, the influenced gas surrounding the droplet will have an impact on the droplet in return. Therefore, it is necessary to take into account the local parameters of both the droplet and the surrounding gas for more accurate simulation of the droplet-gas two-phase flow and heat and mass transfer, especially for the dense spray conditions.

Fig. 1. Schematic of the droplet evaporation.

Note: During the droplet evaporating in the gas, the evaporating droplet and the gas interact with each other within a specific region, with mass, momentum, energy and species exchange.

2.1 Hypothesis

In order to simplify the complex phenomena and formulate a precise droplet motion and phase change model, four hypotheses are present (Zhao et al., 2018) as follows: (1) The temperature within the droplet is uniform. As the radii of the spray droplets are usually less than 500 μm, the Biot number is below 0.1. Thus, the temperature gradient within the droplet can be neglected. (2) The droplet evaporation is spherically symmetrical. As the radii of the spray droplets are small, the droplets can be regarded as sphere with the evaporation proceeding due to the effects of the surface tension. (3) The radiative heat transfer can be neglected. Since the temperature difference between the droplet and the surface of the containment is sufficiently small, the radiative heat transfer is minute. (4) The Stefan flow is taken into account (Zhou et al., 2013). As the different species of the gas mixing within the containment can diffuse and mix with each
other, the Stefan flow should be considered during the process of the droplets spraying into the surrounding gas.

2.2 Droplet model

The entire mathematic model includes the droplet model and the gas equation, of which the droplet model is comprised of droplet motion model, evaporation equation and energy equation. The gas equation includes the continuous equation, momentum equation, energy equation and the species diffusion equation.

2.2.1 Droplet motion model

For the moving droplets carried by the surrounding gas in the containment, they will be affected by the gravity, additional mass force, buoyancy, drag force, Magnus lift force and Saffman lift force (Zhang et al., 2015; Zhao et al., 2018).

The whole droplet motion model includes the droplet displacement $x(t)$, rotation velocity $\omega(t)$ and velocity $v(t)$ equations (Zhang et al., 2016) and the expressions are as follows:

$$\frac{dx}{dt} = v. \tag{1}$$

$$I \frac{d\omega}{dt} = M. \tag{2}$$

$$m \frac{dv}{dt} = F_D + F_A + F_V + F_M + F_S. \tag{3}$$

Here, $I$ is the droplet moment of inertia, $I = 2mr^2/5$; $m$ is droplet mass, $m = 4/3 \pi r^3$; $M$ is rotation moment from the gas field, $M = -0.5 \rho_s C_M r^5 |\omega - \Omega/2| |\omega - \Omega/2|$; $F_D$ is the flow drag force; $F_A$ is the additional mass force; $F_V$ is the volume force, which is the resultant force of the gravity and buoyancy; $F_M$ is the Magnus lift force; $F_S$ is the Saffman lift force. The expressions of these quantities are presented in Ref (Zhao et al., 2018).

2.2.2 Droplet evaporation equation

Figure 1 presents the schematic of droplet evaporating in the gas, in which the droplet radius, temperature, surface pressure are $r$, $T_r$, $P_r$, respectively. The temperature and pressure of the surrounding gas are $T_{nr}$, pressure $P_{nr}$, respectively. It should be noted that $nr$ is the position of $n$ folds droplet radius from the droplet center. In the previous studies, the fluid parameters are usually considered to be the same as that of the free stream or at infinity (Abramzon and Sirignano, 1989), for example, the temperature and pressure at infinity, $T_\infty$, $P_\infty$. However, it is more reasonable and precise to take into account the local parameters of the surrounding gas at the position of $nr$ rather than at that at infinity, as the evaporating droplet is mainly affected by the local gas flow field within a specified influence region around the droplet, especially when there are plenty of droplets. Accordingly, the mass and heat transfer equation should be obtained by theoretical formula derivation (Zhao et al., 2018).

The derivation of droplet heat and mass transfer equation based on basic mass transfer theory is as follows:

The droplet mass vaporization rate based on mass transfer theory considering Stefan flow is (Zhang, 2011):

$$\dot{m} = 4\pi r^3 D_s \frac{d\rho}{dr} + Y_s \dot{m}. \tag{4}$$

Then, integrate Equation (4) from $r$ to $nr$ along the radial direction:

$$\dot{m} = \frac{n}{n-1} 4\pi r^2 D_s \ln(\frac{1-Y_s}{1-Y_{nr}}). \tag{5}$$

When taking into account the convection mass transfer, the mass transfer rate is expressed as:
Thus, the radius variation rate of the droplet can be obtained:

\[
\frac{dr}{dt} = \frac{n}{n-1} \frac{Sh \rho D_v}{2 \rho_d r} \left( \ln\left( \frac{1-Y_{\infty}}{1-Y_s} \right) \right) = \frac{n}{n-1} \frac{Sh \rho D_v}{2 \rho_d r} \ln(1 + B_M).
\]

where \( B_M \) is the Spalding mass transfer number, \( Sh \) is Sherwood number, \( Re \) is Reynolds number, \( Sc \) is Schmidt number, the expression of which are as follows:

\[
B_M = \frac{Y_{\infty} - Y_s}{1 - Y_s}, \quad Sh = 2.0 + 0.6 Re^{0.5} Sc^{1/3}, \quad Sc = \frac{V}{D_v}, \quad Re = \frac{2 \rho_v v r}{\mu}.
\]

Here, \( D_v \) is diffusion coefficient, which is calculated by empirical correlation of Fuller (Poling et al., 2001):

\[
D_v = \frac{1.43 \times 10^8 T^{1.75}}{p M_v^{1/2} \left( \Sigma_A \right)_A^{1/3} + \left( \Sigma_B \right)_B^{1/3}}, \quad M_{AB} = 2[(1/M_A) + (1/M_B)]^{-1}.
\]

where \( p \) is the local gas or vapor pressure, MPa; \( M_A \) and \( M_B \) are the molar mass of material A and B, respectively, g/mol; \( \Sigma_A \) and \( \Sigma_B \) are the molar volume of material A and B, respectively, cm\(^3\)/mol.

It should be noted that the above model is deduced from the typical hydrodynamic model (Abramzon and Sirignano, 1989). Actually the droplet evaporation model includes both the kinetic model and hydrodynamic model (Fujikawa et al., 2011; Kryukov et al., 2004). Both of two models can reflect the non-equilibrium phenomena. The difference is that the kinetic model is more capable of simulating the evolution of gas-liquid interface, especially when using Euler method, such as the VOF model. The hydrodynamic model is usually used under the framework of Lagrange method, which usually treats the droplet as a mass point. In addition, the evaporation progress is in the quasi-steady state and the Euler-Lagrange approach is adopted for the simulation, of which droplets are tracked by the Lagrange method, where the droplet is treated as a mass point. Hence, the shape of the droplet is not necessary to be considered in the present simulation. The interactions between the droplet and the gas phase are conducted by the mass, momentum and energy exchange. Therefore, in the present paper the droplet model adopts the hydrodynamic model.

### 2.2.3 Droplet energy equation

Accordingly the droplet energy equation can be deduced by the aforementioned ways. Hypothesis (1) indicates that the droplet remains spherical and evaporates uniformly, which reveals that the heat transfer between the droplet and the surrounding gas can be simplified as the heat conduction or convection through a spherical shell. In addition, the model is developed assuming that the droplet motion and evaporation process is in quasi-steady state. The gas phase is simulated by the Euler method. The droplets are tracked by the Lagrange method. The iteration method over time is adopted to solve these models. During every short time step, when calculating the parameters of the droplet, the gas phase parameters are taken as those of last time step and do not change within the time step. While for the iteration process, these parameters change with time. That is to say in the next iteration, the updated parameters of both the gas and the droplet are used. Thus, the droplet-gas two-phase flow and heat transfer process is in the quasi-steady state. And for the development of the droplet energy equation, the deducing method and the results based on steady state assumption can be adopted in the present model. Therefore, the differential equation of heat conduction without internal heat source is presented as (Yang and Tao, 2006):

\[
\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dT}{dr} \right) = 0.
\]
Integrate Equation (10) from $r_1$ to $r_2$ along the radial direction:

$$T = T_s + (T_1 - T_s) \frac{1}{r-1} \frac{1}{r_2} - \frac{1}{r_1-1} \frac{1}{r_2}.$$  \hfill (11)$$

Here, the temperature at the position of $r_1$ and $r_2$ are $T_1$ and $T_2$, respectively.

When $r_1=r$, $r_2=nr$, the heat transfer rate of $Q$ is obtained:

$$Q = \frac{4\pi\lambda(T_1 - T_w)}{1/r-1/nr} = \frac{n}{n-1} 4\pi r \lambda (T_1 - T_w).$$  \hfill (12)$$

If the convection heat transfer is taken into account, the heat transfer rate is expressed as:

$$Q = \frac{n}{n-1} 4\pi r^2 h(T_1 - T_w).$$  \hfill (13)$$

Then, the energy conservation equation of the droplet is presented as follows:

$$m_c \frac{dT}{dt} = \frac{n}{n-1} 4\pi r^2 h(T_1 - T_w) + \gamma m.$$  \hfill (14)$$

The variation rate of droplet temperature is obtained through simplification:

$$\frac{dT}{dt} = \frac{3}{\rho_c r} \left[ \frac{n}{n-1} h(T_1 - T_w) + \gamma \rho_d \frac{dr}{dt} \right].$$  \hfill (15)$$

Therefore, from the above equations, the basic droplet model can be summarized as follows:

$$\begin{align*}
\frac{dx}{dt} &= v, \\
\frac{d\omega}{dt} &= \lambda_C M \left[ \frac{\omega \cdot \Omega}{2} \right] \left[ \frac{\omega \cdot \Omega}{2} \right], \\
\frac{dv}{dt} &= \lambda_C D \left[ (u-v) \cdot (u-v) + \lambda_C M_a (u-v) \times (\omega \cdot \Omega) \right] + \\
&\quad \lambda_C S_a \left[ \Omega \right]^{0.5} \left[ (u-v) \times \Omega \right] + \lambda_C g, \\
\frac{dr}{dt} &= \frac{n}{n-1} \frac{Sh \rho_d D}{2 \rho_d r} \ln(1 + B_m), \\
\frac{dT}{dt} &= \frac{3}{\rho_d r} \left[ \frac{n}{n-1} h(T_1 - T_w) + \gamma \rho_d \frac{dr}{dt} \right].
\end{align*}$$  \hfill (16)$$

Here, $C_M$, $C_D$, $C_{Ma}$, $C_S$ are coefficients of the rotation moment, drag force, Magnus lift force and Saffman lift force, respectively (Zhang et al., 2015, 2016; Zhao et al., 2018). The expressions of Nusselt and Prandtl number are as
follows (Grant et al., 2000):

\[
Nu = 2.0 + 0.6Re^{0.5}Pr^{1/3}, \quad 0 \leq Re \leq 7 \times 10^4, \quad 0.6 \leq Pr \leq 400, \quad Nu = \frac{2hr}{\lambda}, \quad Pr = \frac{v}{\alpha}.
\]

(17)

It should be pointed that the local gas parameters at the position of \(nr\) surrounding the droplet rather than that at infinity are adopted in Equation (1)–(16), including the gas velocity, temperature, curl of flow field, etc. The gas parameters are calculated by \(k-d\) tree searching approach and the interpolation method (Zhang et al., 2015), by which the instantaneous changes of the local gas flow field and the instantaneous effects of the fluid field on the droplet can be tracked. For the value of the \(n\), it can be an integer between 5 to 10 (Zhao et al., 2018). The range of \(n\) is obtained based on the assumption “the pressure around the droplet varies exponentially to the radius”. The results of our previous work reveal that when the distance from the droplet center is larger than \((5r, 10r)\), the influence of the droplet on the gas parameters is little and the gas parameters change slightly. Thus, the position of \(nr\) \((5 \leq n \leq 10)\) can be taken as the specific gas boundary, where the gas parameters are taken as the characteristic parameters to calculate the droplet velocity, radius and temperature. The gas parameters at \(nr\) can be obtained by the query algorithm and interpolation method based on the calculated gas fluid field information (Zhang et al., 2015). Through this method, the local gas parameters change surrounding the droplet can be tracked. Especially, for the dense droplet-laden flow, it is more appropriate to use the local gas parameter surrounding the droplet. In the present paper, in order to obtain more precise simulation, the value of the \(n\) is specified as 10, which means that the gas parameters at the position of 10\(r\) distance from the droplet center are adopted for the calculation of the droplet velocity, radius and temperature.

### 2.2.4 Multi-droplets treatment

For the practical operation of the containment spray system, the droplets number is significantly large. Thus, it is fairly difficult to track every droplet. Therefore, as shown in Fig. 2 (a) and (b), the representative droplet \((X, V, r, T, P)\) is adopted and the whole droplets can be divided into several groups (Zhang et al., 2015). Here, the symbols of \(X, V, r, T\) and \(P\) are the droplet position, velocity, radius, temperature and pressure, respectively. The representative droplet is defined as a droplet with the parameters of \((X, V, r, T, P)\), that is equal to the average ones of the group of droplets. In addition, when the number of the groups is sufficiently large, these representative droplets can describe the large quantities of the droplets with high accuracy. Therefore, the independence verification of simulation results with the number of the groups should be conducted beforehand.

![Representative droplet schematic](image1.png)

(a) Representative droplet schematic.

![Droplet groups divided by representative droplet](image2.png)

(b) Droplet groups divided by representative droplet.

Fig. 2. Force schematic of the moving droplets carried by the surrounding gas.

Note: The representative droplet is proposed to stand for a group of droplets with the average parameters the same as the representative droplet. When the representative droplets are sufficient, they can represent all the droplets.

For detailed treatment of the divided groups, as shown in Fig. 2 (a) and (b), the representative droplet with \((X, V, r, T, P)\) is adopted. If dividing the droplet position \(X\), velocity \(V\), radius \(r\), temperature \(T\) and pressure \(P\) into \(N_X\), \(N_V\), \(N_r\), \(N_T\) and \(N_P\) groups uniformly, the distances between each group are \(\Delta X\), \(\Delta V\), \(\Delta r\), \(\Delta T\) and \(\Delta P\), respectively. Thus, the total droplets are classified into \(N\) groups, which can be expressed as \(N = N_XN_VN_rN_TN_P\). If \(w_i\) is the mass weight factor of the group \(i\), the behavior of the whole droplets can be obtained based on the characteristics of each group of representative droplet. Theoretically, the number of the droplets can be from one to hundreds of millions, as the representative droplet approach is adopted and the large number droplets can be divided into groups. Through this method, the computing requirement of the computer can be reduced significantly. The radii of representative droplets...
are between 1 μm to 1 mm, which is required to satisfy the hypothesis of the uniform temperature within the droplet and the droplet spherically symmetrically evaporating. For the droplet velocity, it can range from 0 m/s to hundreds approximately according to the practical conditions. The droplet temperature can be from 250 K to about 1400 K. The droplet pressure varies from 0.05 MPa to 8 MPa. Usually, for the practical process, only several parameters of $X$, $V$, $r$, $T$ and $P$ are different, which decrease the divided groups and is beneficial for the improvement of the calculation efficiency. For example, in the present paper, the temperature, radii, pressure and velocity of the spray droplets are similar. Thus, the groups are divided only based on the injection positions of the spray droplets as presented in Fig. 5.

2.3 Gas equations

The gas equation includes the mass conservation equation, momentum conservation equation, energy conservation equation and species conservation equation (Khatumria and Miller, 2003; Bovand et al., 2016):

\[
\frac{\partial p}{\partial t} + \nabla \cdot (\rho \vec{v}) = S_m, \tag{18}
\]

\[
\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot \vec{\tau} + \rho \vec{g} + \vec{F}. \tag{19}
\]

\[
\frac{\partial (\rho E)}{\partial t} + \nabla \cdot \left( \vec{v}(\rho E + p) \right) = \nabla \cdot \left( \frac{2}{\gamma+1} \nabla T - \Sigma h_j \vec{J}_j + (\vec{\tau}_{\text{eff}} \cdot \vec{v}) \right) + S_E. \tag{20}
\]

\[
\frac{\partial (\rho Y_j)}{\partial t} + \nabla \cdot (\rho \vec{v} Y_j) = -\nabla \cdot \vec{J}_j + S_i, \quad J_i = -\rho D_{ij} \frac{dY_j}{dx}. \tag{21}
\]

Here, the force imposed by the droplet on the gas, is just the reactive force acted by the gas on the droplet in Equation (3). Hence, the expression of $\vec{F}$ in Equation (19) is $-\sum (m_j - \vec{F}_j) / V_{cell}$. $S_m$, $S_E$ and $S_i$ are the mass source term, energy source term and species source term, respectively, which indicate the influence of the droplet on the gas fluid field. The according expressions are as follows:

\[
S_m = \sum_j \frac{m_j}{V_{cell}} = \sum_j \frac{n}{n-1} 2\pi r \rho_s \text{Sh ln}(1 + B_M) / V_{cell}. \tag{22}
\]

\[
S_E = \sum_j \frac{Q_j}{V_{cell}} = \sum_j \frac{n}{n-1} 4\pi r^2 h(T_j - T_{air}) / V_{cell}. \tag{23}
\]

\[
S_i = \sum_j \frac{m_j}{V_{cell}} = \sum_j \frac{n}{n-1} 2\pi r \rho_s \text{Sh ln}(1 + B_M) / V_{cell}. \tag{24}
\]

It should be pointed that water is the only one volatile component during the water droplet spraying in the air in the containment. Thus, the mass source term of $S_m$ is equal to species source term of $S_i$.

2.4 Numerical solution

For the droplet spraying in the constant volume bomb, the Euler-Lagrange approach is utilized for the simulation of the droplet-laden two-phase flow. The gas equation is solved using the software of FLUENT 16.0. The solution of the droplet motion and evaporation model is conducted by the four-step Runge-Kutta method through self-programming using C Language, which is integrated with FLUENT by User Defined Function (UDF) to introduce the interactions between the droplet and the surrounding gas.

It should be noted that the model is developed assuming the droplet motion and evaporation process is assumed to be in quasi-steady state. The iteration method over time is adopted to solve these models. During every short time step, when calculating the gas phase parameters, the droplet parameters are taken as those of last time step and do not change.
within the time step, and vice versa. For the simulation of the droplet, the slit-step algorithm is adopted, which means the calculation of the droplet evaporation and motion processes is separated during every short time step. That is to say when calculating the droplet moving, the droplet radius, mass and temperature are taken as those of last time step; when calculating the droplet evaporating, the droplet velocity and temperature are taken as those of last time step; and when calculating the droplet heating, the droplet radius, mass and velocity are taken as those of last time step. In the next iteration, the updated parameters of both the gas and the droplet are used. Therefore, in the manuscript, the left-hand side of equation (2) and (3) which should be expressed as \( \frac{d(I\omega)}{dt} \) and \( \frac{d(mv)}{dt} \) are simplified as \( I\frac{d(I\omega)}{dt} \) and \( m\frac{dv}{dt} \). It is the same to equation (10) and (14). Through this slit-step algorithm, the gas-droplets two-phase flow can be solved accurately and rapidly.

3. Numerical validation

As mentioned above, the two-way coupling between the droplet and the gas is intensive for the dense spray condition. Thus, the model is applied to the simulation of containment spray system and is validated comparing the predicted containment average temperature, pressure and vapor concentration with that of the benchmark experiments of the containment spray system obtained by Malet et al. (2005) and Porcheron et al. (2007) TOSQAN (TOnus Qualification ANalytique) (Porcheron et al., 2007) is an experimental program undertaken by the Institut de Radioprotection et de Sûreté Nucléaire (IRSN) to perform thermal hydraulic containment studies. The TOSQAN facility is a large enclosure devoted to simulate typical accidental thermal hydraulic flow conditions in nuclear-pressurized water reactor containment. Spray test 101 is performed in hot conditions to analyze the heat and mass transfer between spraying droplets and hot gas mixtures composed of air and steam. The following investigation in this paper is conducted based on the Spray test 101 to simulate the water droplet spraying in the gas mixtures composed of air and steam.

The TOSQAN facility presented in Fig. 3 consists of a closed cylindrical vessel (7 m$^3$ volume, total height of 4.8 m high, i.d.1.5 m) into which steam is injected through a vertical pipe located on the bottom vessel axis and droplet is sprayed through a vertical pipe located on the top vessel axis, 0.65 m from the top of the facility. The spray pipe inner diameter is 0.41 m. The walls of the vessel are thermostatically controlled by heated oil circulation to control the gas temperature inside the vessel. Optical accesses are provided by 14 overpressure resistant viewing windows permitting non-intrusive optical measurements along orthogonal enclosure diameters. The thermocouples are used to measure the gas temperature in the whole vessel. The particle image velocimetry technique (PIV) and laser Doppler velocimetry technique (LDV) are used to measure the droplets velocity. Raman spectrometry is adopted to measure the steam volume fraction. For the droplet motion and phase change model validation, this paper implements the same condition as the experiments, as shown in Tab. 1.

![Fig. 3. Schematic of the TOSQAN facility.](image)
with a spray angle of 55°. Thus, the spraying droplets are injected in a radial distribution during the simulation. As presented in Fig. 5, the injected droplets are divided into 20 groups according to the radial position to ensure the results independent on the group number. As for the droplet size distribution, the droplet radii are specified as 100 μm to agree with the measured results of the experiment, which means the droplet radii are in the mono-size distribution.

Table 1. Experimental parameters.

| parameter                     | value       |
|-------------------------------|-------------|
| \( r_0 / \mu m \)            | 100         |
| droplet initial velocity \( V_0 / m/s \) | 10~20       |
| droplet temperature \( T_d ^\circ C \) | 119.1~22.1 (0~1000 s), 22.1 (>1000 s) |
| air temperature \( T_g ^\circ C \) | 131         |
| wall temperature \( T_w ^\circ C \) | 131         |
| operating pressure \( P / MPa \) | 0.25        |
| spray mass rate \( g/s \)     | 29.96       |
| initial volume fraction of water vapor % | 59.1         |
| spray angle \( \theta \)      | 55          |

As mentioned above, the Euler-Lagrange approach is adopted for the simulation, of which the gas phase is simulated by the Euler method. And the droplets are tracked by the Lagrange method, where the droplet is treated as a mass point. Thus, both the gas and droplet boundary conditions should be implemented, respectively, as presented in Fig. 4. For the gas phase, as the TOSQAN facility is a closed cylindrical vessel, the boundary of the central vessel axis is set as axisymmetric and the other wall is set as the wall boundary with constant temperature. The two-dimensional axisymmetric model can transform the two-dimensional model to the three-dimensional when using FLUENT to simulate the droplet-gas two-phase flow. For the droplet phase, the side wall is set as wall-film boundary in FLUENT 16.0, which means that when the droplet collides with the solid wall, they will stick to the wall and the film will form accordingly. The water film can evaporate and change heat with the wall and the surrounding gas, which is conducted using the mathematical model in the software of FLUENT 16.0 (O’Rourke and Amsden, 1996). The boundary of the bottom sump is set as the wall-escape, as the droplet will be removed by the sump. The time step of the gas equation is taken as 0.01 s, while for the droplet motion and phase change model it is \( 10^{-6} \)~\( 10^{-5} \) s. The detailed time step for the droplet model is related to the droplet size and the velocity. When the droplet radius is smaller, the time step should be smaller accordingly. Among every time step of the gas equation, the droplet model is solved by iteration to update the mass, momentum and energy source.

The predicted gas average temperature, pressure and vapor mass fraction variation of the containment against experimental results are presented in Fig. 6 (a)–(c). Here, “numerical result” is the results obtained by the proposed model; “infinity model” is the results of the model adopting the gas parameters at infinity or that of the incoming flow, which neglects local parameters change during the course of droplet evaporation.

As presented in Fig. 6 (a)–(c), the numerical results agree well with the experimental ones, and the discrepancies are within ±15%, which indicates that the presented model is reasonable and can be applied to the simulation of
containment spray process. With time, the temperature decreases rapidly at the beginning, and then the decreasing rate becomes moderate until remaining stable. The pressure and the vapor mass fraction increase fast at the beginning, and then decrease gradually until remaining stable. That is mainly because the droplet temperature is lower than the gas one and the intensively evaporating droplets absorb a lot of energy, which results in the gas temperature decreasing continuously. At the beginning of the spray process, larger quantities of droplets are injected into the containment leading to the intensively evaporating of the droplets due to the large vapor concentration difference between the droplet surface and the surrounding air. Consequently, the vapor mass fraction increases rapidly and the pressure increases accordingly. With the process proceeding, the vapor mass fraction reduces gradually resulting from the vapor condensation due to the decreasing gas temperature and the decreasing temperature of the injected droplets. And the pressure decreases as well. Finally, the relatively stable status is reached as the temperature difference and the vapor concentration difference reduces continuously.

Fig. 6. Numerical average parameters of containment against experimental ones (Malet et al., 2005; Porcheron et al., 2007).

The temperature and vapor mass fraction distributions along the radial direction of the middle plane with height=2.4 m are presented in Fig. 7 (a) and (b), respectively. Fig. 6 and Fig. 7 indicate that the temperature and vapor mass fraction results of “numerical result” are below that of “infinity model”. Fig. 7 reveals that the difference between the numerical result and that of infinity model increases with time, especially in the central region where the droplets spray. That is because for “infinity model”, the gas parameters such as temperature, pressure and vapor mass fraction surrounding the droplets are considered to be equal to that at infinity or that of the incoming flow; and the values are taken as the average gas parameters of the whole fluid field; while for the model presented in this paper, the local gas parameters surrounding the droplets are introduced and the instantaneous variation of the local fluid field can be tracked and the transient influence of the fluid field on the droplet motion is considered. Therefore, the temperature of the gas surrounding the droplet is lower than the average temperature of the containment due to the cooling of the evaporating droplet; the local vapor mass fraction surrounding the droplet can be larger than the average one due to the droplet evaporation. Thus, the vapor concentration difference between the droplet surface and the surrounding gas is smaller and the droplet evaporates a bit slowly using the present model, consequently leading to the lower predicted vapor mass fraction, which agrees better with the practical process. In addition, the average temperature of the total containment will be lower due to the lower local temperature owing to the droplet cooling. All of the above influence leads to the underestimation of the average temperature, pressure and vapor mass fraction of the air. Therefore, the
present model is reasonable and precise to simulate the dispersed droplets flow as mentioned above.

Fig. 7. Temperature(a) and vapor mass fraction(b) distributions along the radial direction. (Height=2.4 m, middle plane)

4. Fuel spray simulation and results analysis

4.1 Fuel spray simulation in the constant volume bomb

The fuel spray simulation is conducted within a typical constant volume bomb based on the researches of Zhou et al. (2009, 2010) and Cao et al. (2011). The spray process of the tetradecane droplet is simulated. The constant volume bomb is a cylinder and the sizes are as follows: the height is 8 cm, the diameter is 2 cm and the diameter of the spray nozzle located on the top is 0.2 cm as presented in Fig. 8. As the focus of this investigation is on the fuel droplet evaporation characteristics during spraying, the generation process of the small droplets from the high-pressure nozzle is neglected for simplification. Instead, the spray droplets parameters including the initial position, velocity and radii are specified in the simulation.

The gas within the constant volume bomb is nitrogen with the density of 20 kg/m$^3$. The working pressure is 1.7 MPa and the temperature is 900 K. The component of the fuel droplet is tetradecane with the density of 818 kg/m$^3$. For the spray fuel droplets, the spray angle is 12°. The initial radii are specified as 20 μm, 30 μm and 50 μm, respectively, to analyze the characteristics of spray droplets with specified radius as shown in Table 2, which means that the droplet radii are in mono-size distribution. The radial distribution of droplets position is similar to that in Fig. 5. The initial temperatures are 600 and 700 K. The two-dimension axisymmetric model is adopted for the study of the three-dimension geometry. The boundary of the central axis is axisymmetric and the others are specified as wall conditions with a constant temperature of 900 K. The spray time is 2 ms and the time step is $2\times10^{-7}$ s with validation. The detailed simulation parameters are shown in Tab. 2. In addition, it should be noted that the cutoff radius in the simulation is specified as 2.5 μm, which means that when the droplet radius is below 2.5 μm, the droplet is considered to be thoroughly evaporated and the droplet radius turns to be zero directly.

![Fig. 8. Schematic of a typical constant volume bomb (Cao et al., 2011).](image)

(a) three-dimension model  (b) two-dimension axisymmetric model

Note: The constant volume bomb, a closed cylindrical vessel, total height 8 cm, inner diameter 2 cm, droplet spray nozzle, 0.2 cm from the top.
Table 2 The spray parameters in the constant volume bomb.

| Condition No | \( r_0 / \mu m \) | Droplet temperature \( T_{d0} / K \) | Droplet velocity \( V_0 / m/s \) |
|--------------|-----------------|----------------|-----------------|
| 1            | 50              | 600            | 70              |
| 2            | 50              | 700            | 70              |
| 3            | 30              | 600            | 70              |
| 4            | 30              | 700            | 70              |
| 5            | 20              | 600            | 70              |
| 6            | 20              | 700            | 70              |

4.2 Temperature analysis

The numerical temperature contours of both the gas and spray fuel droplet are shown in Fig. 9 and Fig.10, respectively. Due to the limited space, only the results of NO.1 and NO.3 are presented. The gas temperature contours within the constant volume bomb reveal that the gas temperature surrounding fuel droplets is lower and those far away from the droplets change slightly. With time, the gas temperature surrounding fuel droplets decreases at the beginning; subsequently, the gas temperature at the other positions reduces as well due to the droplet motion along the axis. It should be noted that the local supercooling phenomena occur due to the cooling of the low-temperature droplets, which reflects that the droplets influence the local surrounding gas. The lifetime of the fuel droplet is so short that the droplets cannot spread to the whole flow field. The penetration length of the fuel droplet hardly increases, which is because the droplets are thoroughly evaporated. Comparing NO.1 \((r_0=50 \, \mu m)\) and NO.3 \((r_0=30 \, \mu m)\), when other conditions are the same, the penetration length of the fuel droplet decreases significantly for the smaller droplets; and the surrounding gas temperature is much lower. That is because the smaller droplets evaporate faster and more heat are absorbed. The fuel droplet temperature contours within the constant volume bomb, as shown in Fig. 10, indicates that the droplet temperature increases within a distance from the spray inlet during the downward motion. After that, the droplet temperature maintains stable and the droplet evaporates continuously, the radius reduces until thoroughly evaporated.

![Fig. 9. The temperature contours of the gas within the constant volume bomb. (No. 1, No. 3)](image)

Note: Left column (denoted as “1”) shows the results of No. 1; the right column (denoted as “2”) presents the results of No. 3.

![Fig. 10. The temperature contours of the fuel droplet within the constant volume bomb. (No. 1, No. 3)](image)
4.3 Fuel droplet velocity and Evaporation rate analysis

The contours of the predicted evaporation mass rate of the fuel droplet at different time are presented in Fig. 11. Fig. 11 reveals that the fuel droplet evaporates continuously during the spray atomization process in the constant volume bomb until thoroughly evaporated. Fig. 11 indicates that the position distribution of the contours of the evaporation mass rate is in accordance with that of the temperature contours as shown in Fig. 10, which characterizes that of the distribution of the fuel droplet trajectories. In addition, the droplets surrounding the inlet evaporate fastest and the evaporation rate of the fuel droplets decrease with the increasing distance to the inlet along the axial direction. That is because on the one hand, the velocity of the droplet surrounding the inlet is the fastest and the convection heat and mass transfer are most intensive accordingly. On the other hand, with time, the fuel droplet evaporates continuously and the size of the droplet decreases during the downward motion. The mass evaporation rate of the smaller droplet becomes slower, which results in the total mass evaporation rate decreases accordingly. Comparing the conditions of NO.1 \((r_0=50 \mu m)\) and NO.3 \((r_0=30 \mu m)\), it reveals that the fuel droplet evaporates faster in the case of NO.3. Thus, the spray penetration is shorter and more heat is absorbed, which agrees with the temperature contours as shown in Fig. 9 and Fig. 10.

The droplet velocity contours of the fuel droplet during the spray atomization process in the case of NO.1 and NO.3 are presented in Fig. 12. Fig. 12 indicates that the droplet velocity decreases continuously until zero during the course of the downward motion after being ejected from the spray inlet. With time, the spray penetration increases accordingly until to become stable. The radial velocity distribution is in the form with a high middle and two low ends. The inertia of the droplet with larger radius is bigger as well. The droplet with larger radius is not easy to be affected by the surrounding flow field, and the spray penetration is longer. Therefore, the larger droplet can spread into much wider and farther scope of space in the constant volume bomb.

![Fig. 11. The evaporation rate contours of the fuel droplet. (No. 1, No. 3)](image)

Note: Left column (denoted as “1”) shows the results of No. 1; the right column (denoted as “2”) presents the results of No. 3.

![Fig. 12. The droplet velocity contours of the fuel droplet. (No. 1, No. 3)](image)

Note: Left column (denoted as “1”) shows the results of No. 1; the right column (denoted as “2”) presents the results of No. 3.

4.4 Fuel droplet radii analysis

In addition, the distribution of the dimensionless radius of the fuel droplets over time in different cases is
summarized as shown in Fig. 13. Fig. 13 indicates that the evaporation rate increases with the increasing initial temperature and radius of the fuel droplet. And the lifetime decreases significantly accordingly. That is the reason why both the temperature of the gas surrounding the droplet and the spray penetration decrease with the decreasing droplet radius. In addition, the droplet radius decreases continuously with time. And when the droplet radius decreases to one specific value, it turns to be zero directly. That is because as mentioned above, the cutoff radius in the simulation is specified as 2.5 μm, which means that when the droplet radius is below 2.5 μm, the droplet is considered to be thoroughly evaporated.

![Fig. 13. The fuel droplet dimensionless radii over time.](image)

Note: The droplet radius decreases continuously with time. And when the droplet radius decreases to one specific value, it turns to be zero directly. That is because the cutoff radius in the simulation is specified as 2.5 μm.

4.5 Fuel vapor mass fraction and air-fuel ratio analysis

During the course of the spray fuel droplet atomization and combustion in the internal combustion engine, the mixing performance of the air and the fuel vapor as well as the distribution of the fuel vapor are two important characteristics. The vapor mass fraction contours of the tetradecane droplet at different time in the case of No. 1 are presented in Fig. 14. Fig. 14 reveals that with time, the droplet evaporates continuously and the mass fraction of tetradecane vapor increases accordingly. For the distribution in the radial direction, the vapor mass fraction surrounding the central axis is the highest against to the other positions. The vapor mass fraction decreases with the increasing distance to the central axis. For the distribution in the axial direction, the vapor mass fraction surrounding the spray injection inlet is the highest against the other downward positions. That is because the spray droplet evaporates continuously during moving downwards and some droplets are thoroughly evaporated within a short trip. Thus, the remaining droplets that can travel to longer distance are fewer, which results in the decreasing vapor mass fraction.

As aforementioned, Fig. 14 presents the fuel vapor mass fraction contours. However, the air-fuel ratio is more preferred in the practical engineering. The air-fuel ratio is defined as the ratio of air mass against fuel vapor mass in the gas mixing in the internal combustion engine. Usually, the optimum air-fuel ratio for diesel fuel is about 14.3. It should be noted that in the present study, the nitrogen is utilized to take place of air as working media for simulation. Thus, the ratio of nitrogen to vapor mass is regarded as air-fuel ratio. The corresponding air-fuel ratio contours are presented in Fig. 13 through data processing using the software of Tecplot.

Figure 15 indicates that with time, the local maximum air-fuel ratio decreases continuously. The local minimum air-fuel ratio is 13.35 approximately at 0.5 ms as shown in Fig. 15 (a). However, the local minimum air-fuel ratio decreases to 5.14 at 2 ms as shown in Fig. 15 (d) due to the increasing spray droplets and the evaporation mass. The local air-fuel ratio at these positions far away from the spray inlet and the central axis is larger than that of the other
positions. That reveals that the appropriate air-fuel ratio can be obtained only at those positions with a specific distance to the spray inlet, where the fuel is easy to burn. That is in accordance with the fact that the burning flame is usually located at the position with a specific distance to the spray droplets (Luo et al., 2010). In order to capture the evolution of the average air-fuel ratio in the whole constant volume bomb, the average air-fuel ratio over time is presented in Fig. 16 through data processing.

Figure 16 reveals that with time, the fuel droplets evaporate fast and the evaporating mass of the fuel vapor increases rapidly accordingly. As the nitrogen mass within the constant volume bomb remains unchanged, the air-fuel ratio reduces rapidly. It should be noted that as the mass flow rate of the spray fuel oil is small, the optimum air-fuel ratio is not reached. The optimum air-fuel ratio can be obtained through increasing the mass flow rate of the spray fuel oil, i.e. about 4~5 times the original one.

![Fig. 14. The fuel vapor mass fraction contours. (No. 1)](image1)

![Fig. 15. The air-fuel ratio contours. (No. 1)](image2)

![Fig. 16. The average air-fuel ratio of the whole constant volume bomb over time.](image3)

Through the above analysis of the simulation results of the spray fuel droplet evaporation, it can be verified that the developed droplet motion and evaporation model with two-way coupling can be adopted to simulate of the fuel spray process. The proposed model has the advantage in tracking the motion and phase change characteristics of plenty of droplets and is superior to capturing the details of the two-way coupling and interactions, which is significant for the investigation of the coupling mechanism of the two phases. In addition, the aforementioned results reveal that the present model is applicable and can be extended to the other fields to study the detailed behavior of droplets-laden flow and heat and mass transfer, for example, the containment spray system, the fuel spray and atomization process and fire extinguishment process.

5. Conclusions

The multi-droplets motion and evaporation model is developed considering the local parameters surrounding the droplets. Through the proposed model, the detailed two-phase interactions between the droplet and the gas can be captured. Subsequently, the present droplet motion and evaporation model is utilized to reproduce the fuel spray process in the typical constant volume bomb. The parameters evolution is presented. The analysis of the spray
performance is conducted and the superiority of the new model is also discussed. Main conclusions have been made as follows.

1. The multi-droplets motion and evaporation model is developed considering the local parameters surrounding the droplets and the model is superior to capture the detailed interactions between the two phases.

2. The fuel droplet spray process in constant volume bomb is reproduced using the proposed model and the performance of the fuel spray system is analyzed including the evolution of the gas and droplet temperature, droplet velocity, evaporating rate, droplet radii, vapor mass fraction and air-fuel ratio.

3. The simulation analysis reveals that the spray droplets interact intensively with the surrounding gas and the developed model is advantageous in simulation of the dense multi-droplets spray process.

The proposed multi-droplets motion and evaporation model is capable of simulating discrete droplets motion and evaporation process in the surrounding gas and can be extended to investigate the two-phase interactions in the case of the containment spray system, fuel spray process and fire extinguishment process, and so on.

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