Prediction of the Impact of Nozzle Geometry on Spray Characteristics

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ABSTRACT: In the present paper, the formation and development of cavitation inside the nozzle of an atomizer with different geometrical characteristics have been studied numerically. Different shapes of inlet nozzles and different nozzle-length-to-diameter ratios have been investigated. The developed model has been built as a three-dimensional (3D) one, where the turbulence is modeled considering large eddy simulation. The obtained computational results showed good agreement with the reported experimental results. It has been found that the occurrence of cavitation depends on the amount of energy needed to overcome the viscosity and friction between the liquid layers. The mass flowing through the nozzle decreases with increasing cavitation. The intensity of cavitation depends on the nozzle entrance shape. Sharp edges cause cavitation to occur early in the nozzle, followed by an inclined shape, and then the curved entrance. The dissipative energy in the cavitation and bubble collapse result in an increase in the turbulent kinetic energy of the issuing liquid. This causes more liquid disintegration, leading to larger spray volume and smaller droplet size. The obtained results for spray droplet size distribution have been compared with experimental data developed by other researchers, and a good agreement has also been found.

1. INTRODUCTION

The characteristics of spray are controlled by the flow characteristics inside the atomizer nozzle.1 One of these characteristics is cavitation.2 The hydrodynamic pressure drop of the working fluid is the main reason for inception of this phenomenon, and this is often called hydrodynamic cavitation.3 Cavitation can be induced by both throttling effects and flow redirection.4 The regions at which recirculation occurs are characterized by liquid pressure reduction. This may lead to liquid vaporization in case the pressure goes below the liquid vaporization pressure at the corresponding temperature. Accordingly, the generated nuclei grow, causing cavitation. The development of the two-phase flow inside the nozzle passes through four stages. It starts with the onset of cavitation, followed by appearance of the cavity, its growth, and finally it ends with hydraulic flip.5 Ganippa et al. have experimentally shown that cavitation length also depends on the pressure ratio.5 The flow inside the injection nozzle is usually characterized by eddies and recirculation.7 Cavitation is sensitive to the change in the nozzle geometrical characteristics,8,9 which can be characterized by the entrance shape, the outlet shape, the ratio of the nozzle length (L) to its diameter (Dn), and the geometry of the nozzle internal passage (circular or rectangular, etc.). Also, the studies revealed that the change in the convergent angle has significant effects on flow characteristics and the generation of cavitation.10 Several experimental studies have examined the effect of the injector nozzle geometry on the characteristics of internal flow and consequently the issuing spray.11,12 Strong recirculation evolves due to the sudden contraction at the inlet flow passage to the nozzle. Ranz13 found that the initial disturbance of the injected liquid is caused by the nozzle entrance shape. Sou et al. experimentally studied the impact of nozzle design characteristics and consequently the inflow characteristics on the nozzle discharge coefficient.5 This verifies the computational findings, which shows that after cavitation occurred, the decrease in the discharge coefficient caused by the increase in the injection pressure becomes insignificant.14 Also, for a flow characterized by cavitation, the discharge coefficient is governed only by the cavitation number and it is almost constant.15 Nurick16 experimentally illustrated that cavitation depends on the ratio of entrance curvature (r) to nozzle diameter (Dn). He

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mentioned that the inception of cavitation decreases as larger inlet edge roundness is used. Cavitation inception is defined by Nurick as follows

$$C_{\text{indep}} = 1.9 \left( 1 - \frac{r}{D_{N,i,H}} \right) - \frac{1000}{Re}$$  \hspace{0.5cm} (1) $$

where $r$ is the curvature radius of the inlet to the nozzle and $D_{N,i}$ is the nozzle hydraulic diameter. Song et al.\textsuperscript{17} experimentally studied the effect of the nozzle ($L/D_{N}$) considering different entrance shapes of the injection nozzle on the inception of cavitation. For a sharp entrance edge, cavitation inception is observed early with a small $L/D_{N}$ ratio. Furthermore, cavitation was developed from inception to hydraulic flip at a low injection pressure ratio. Lichtarowicz et al.\textsuperscript{18} found that for short nozzles (e.g., $L/D_{N} < 2$), the reduction in the discharge coefficient due to the sudden contraction in the flow passage is more evident. They also found that the inceptioned cavitation approaches the vicinity of the exit of the nozzle. On the other hand, hydraulic flip instead of a cavitation film is formed, in the case of a low flow rate.\textsuperscript{19}

Regarding the passage geometry, the cavitation process in a nozzle with a two-dimensional (2D) cross section is the same as a nozzle with a circle cross section.\textsuperscript{12} The geometry of the nozzle passage regarding its shape of being constant, divergent, or convergent affects the flow velocity and its jet characteristic. It is defined by its degree of conicity ($k_{c}$), which is defined as follows\textsuperscript{20}

$$k_{c} = \frac{D_{N,i} - D_{N,o}}{10}$$  \hspace{0.5cm} (2) $$

where $D_{N,i}$ and $D_{N,o}$ are the inlet and outlet diameters, respectively, measured in microns. When $k_{c}$ increases, the flow accelerates in the nozzle, the spray tip penetration becomes longer, the spray cone angle decreases, and the droplet sizes become smaller.\textsuperscript{21} When the flow experiences transition from convergent to divergent sections, the flow is subjected to a high cavitation intensity.\textsuperscript{22} Nozzles with divergent holes are more sensitive to cavitation than nozzles with cylindrical nozzles.

Other design characteristics of the nozzle have an impact on the inception and development of cavitation inside the nozzle. For example, the size of the sac and the height of the needle also affect the inception as well as growth of cavitation.\textsuperscript{23}

On the one hand, appearance and growth of cavitation are also affected by different liquid properties such as density, viscosity, and surface tension. Liquids having less viscosity (the Reynolds number is higher) tend to have earlier cavitation.\textsuperscript{24} On the other hand, a higher liquid viscosity inhibits the inception of cavitation.\textsuperscript{25}

Cavitation influences the external flow out of the nozzle. The droplet size becomes smaller when the cavitation is stronger.\textsuperscript{26} Other factors too have an influence: the spray cone angle increases as the cavitation becomes intensive.\textsuperscript{27} Huh and Gosman\textsuperscript{28} suggested a correlation, which estimates the spray cone angle related to the turbulence intensity of the issuing flow from the nozzle. They assumed that the length scale ($L_{\lambda}$) and time scale ($t_{\lambda}$) of atomization could be combined to calculate the exiting radial velocity of the injected liquid. The correlation of the spray angle ($\theta$) with the aforementioned characteristics can be defined by the following expression:

$$\tan \left( \frac{\theta}{2} \right) = \frac{L_{\lambda}/t_{\lambda}}{U}$$  \hspace{0.5cm} (3) $$

where $U$ is the axial velocity of the bulk liquid velocity.

The present work aims at numerically investigating the internal flow behavior of diesel fuel in nozzles with different inlet geometries. It develops a numerical simulation for the flow inside nozzles, which have been experimentally tested by Park et al.\textsuperscript{29} This study goes beyond Park’s tested geometries. It includes other entrance geometries including inclined and rounded entrances. The paper investigates cavitation inception as a result of different entrance nozzle shapes. The developed numerical model links cavitation inception with the reduction in the mean value of mass flow. It extends to predict the issuing spray characteristics based on the cavitation intensity and pressure ratios.

2. RESULTS AND DISCUSSION

The validation of the developed numerical model was achieved using the experimental results developed by Park et al.\textsuperscript{29} Based on this simulation, the vapor fraction and turbulent kinetic energy are evaluated for different ratios of injection pressure ($P_{inj}$) and back-pressure ($P_{back}$). The cavitation inside the injection nozzle is studied considering different entrance geometries of the nozzle. Also, the relation between cavitation number and flow energy as well as Reynolds number ($Re$) is defined. Finally, the effect of cavitation on droplet size of the issuing spray is studied for different geometries of nozzle entrance.

2.1. Model Validation. Figure 1 shows the variation in the injection velocity with the change in the injection pressure ratio considering the experimental results of Park et al.\textsuperscript{29} according to Bernoulli’s equation (frictionless solution) and the predicted results. As shown in the figure, the value of the axial velocity in the nozzle increases nearly linearly with the increase in the pressure ratio of $P_{inj}/P_{back}$. The numerical model shows a good agreement with experimental results of Park et al.\textsuperscript{29} Both the experimental and numerical results are below the theoretical value of Bernoulli’s equation by almost 20%. This is attributed to the friction losses in the nozzle.

The buildup of cavitation can be indicated by the vapor fraction. Figure 2 depicts the vapor fraction inside the nozzle. Both the numerical simulation and experimental results have the same trends. There is no cavitation buildup when the pressure ratio is in the range from 1.3 to 1.9. Cavitation starts to appear at a pressure ratio of 2. With the increase in the pressure ratio, the cavitation increases and extends in the flow direction near the wall. For further increase in the pressure ratio up to 4, cavitation reaches the nozzle exit and the flow takes the form of a hydraulic flip.

Figure 3 defines different sections along the atomizer nozzle with a sharp edge entrance; it demonstrates the phase change of the diesel fuel throughout the nozzle. The cavitation inside the
nozzle depends on the pressure ratio and the nozzle geometry. As the pressure ratio increases, the liquid diesel tends to be subjected to cavitation. Cavitation occurs at the entrance edges as a result of the change in the flow direction due to the contraction in the flow passage. This is evident as the flow mainstream, which is not subjected to change in direction, does not experience cavitation (arrow no. 2 in Figure 3).

When the pressure ratio increases to 3, the quantity of vapor increases. The quantity of vapor reaches its highest value (nearly vapor fraction = 0.95) near the entrance edge. The vapor volume extends to the middle of the nozzle in the flow direction. After the nozzle middle, the vapor fraction decreases gradually. At a pressure ratio of 4, the vapor volume increases even until the liquid is wrapped at the existing edge and pushed with the liquid out of the nozzle.

Figure 4 demonstrates the turbulent kinetic energy and the vapor fraction inside a nozzle, with a sharp entrance edge, at a pressure ratio of 3. The curve can be divided into four zones, which represents the inflow behavior.

- Zone 1: It depicts the flow before entering the throttle area of the nozzle. In this zone, the flow does not
experience a phase change and the turbulent kinetic energy is minimum.

- Zone 2: When the flow goes through the throttle area, flow disturbances are developed. Accordingly, the vapor fraction and the TKE increase. The vapor volume fraction grows faster than the TKE. It reaches its maximum value earlier than the TKE.
- Zone 3: The turbulent kinetic energy grows to reach its minor peak. Moving downstream to the third zone, the vapor volume fraction declines, where the vapor bubbles collapse, leading to an increase in the TKE.
- Zone 4: In this zone, the vapor volume fraction becomes nearly constant and tends to zero. The turbulent kinetic energy decays due to the viscous effect of the flow, where the generation of TKE stops as the flow moves away from the zone where the bubbles collapse.

When the pressure ratio is increased to 3.5 as shown in Figure 5, the vapor fraction extends to a greater distance with the flow direction to the exit of the nozzle. The vapor is generated at the throttle area of the nozzle at \( X/L = 0 \). It sharply increases during the second zone at \( X/L = 0.2 \) and continues to increase gradually, reaching a maximum value at \( X/L = 0.4 \). The vapor bubbles begin to collapse in the third zone, and then, they sharply decrease as they approach the end of the nozzle in the fourth zone. On the other hand, the TKE increases in the direction of the flow and takes a semiconstant value for a very small distance around the distance \( X/L = 0.6 \). The TKE increases again during the third zone with the collapse of the vapor bubbles, and then, a relatively sharp increase is expressed in the fourth zone with a sharp decrease in the vapor fraction.

When the bubbles collapse, the vapor volume fraction decreases. The collapse of the traveling bubbles causes high local forces and frequency. These result in a high level of pressure fluctuations, leading to an increase in the turbulent kinetic energy.

2.2. Effect of Entrance Geometry of a Nozzle on the Inflow Characteristics. Figure 6 shows the exit velocity for different nozzle entrance geometries considered in this study. These include the sharp, inclined, and curved entrance edges. The exit velocity varies depending on the entrance geometry. The nozzle with a curved entrance gives the maximum axial velocity, followed by the inclined and then the sharp entrance. As a result, the kinetic energy at the curved entrance is a maximum and its value decreases in the case of the inclined entrance, while the lowest value is obtained in the case of a sharp entrance geometry.

In this section, the cavitation phenomenon was analyzed by a cavitation number \((Cn)\). The cavitation number in this work is defined as a relation between potential energy and kinetic energy as follows:

\[
Cn = \frac{2(P_{\text{back}} - P_r)}{\rho u_{\text{inj}}^2}
\]

where \( u_{\text{inj}} \) is the injected velocity, \( P_{\text{back}} \) is the ambient pressure, and \( P_r \) is the vapor pressure.

As shown in Figure 7, the cavitation number is affected by the shape of the entrance to the nozzle at the same pressure ratio. It was found that the kinetic energy is low and cavitation number increases when the nozzle has a low injection velocity.

On the other hand, cavitation inception is affected by the shape of the entrance to the nozzle, as shown in Figure 7. The cavitation inception is enhanced by the sudden change in the flow direction due to the sharp entrance at the pressure ratio \( P_r = 2 \). On the contrary, when the liquid is oriented, as in the inclined and curved entrance cases, the cavitation inception is delayed at pressure ratios \( P_r = 3 \) and \( 3.5 \), respectively.

For the inclined surface nozzle, the throttle area, “the contraction area”, has an inclined surface with an angle of 45°. This inclined surface has two edges. The presence of these edges at the contact between the inclined surface and the surface of the injector causes the separation of the boundary layer from the surface at the pressure ratio \( P_r = 3 \). This leads to the development of vortices. These vortices begin to form cavitation, which increases with the pressure ratio.

For a nozzle with a curved entrance “convex surface”, the contraction zone is characterized as a quarter of a circle with a radius of 3 mm. This shape allows for uniform flow through the throttle area. The streamline curvature effects on the pressure gradient in the boundary layer promote the risk of separation. Along a fair part of this section, there will be a positive pressure gradient. This positive pressure gradient may delay separation. In this case, cavitation occurs later compared with the inclined nozzle case. These vortices increase with increasing pressure ratios.
In general, the mass flow rate and the Reynolds number are affected by the entrance geometry due to the passage contraction regardless of its geometry. The real flow rate is lower than the flow rate calculated by the Bernoulli equation. This reduction is caused by the resistance to flow due to the energy dissipated by friction, eddies, and the buildup of cavitation.

Figure 8 demonstrates that the highest percentage in the mass flow rate reduction occurs in the nozzle with a sharp entrance edge followed by inclined and curved entrance edges, sequentially. The cavitation inception corresponds to zones A, B, and C for sharp, inclined, and curved entrance edges, respectively. Cavitation inceptions take place close to the mean value, which has a minimum moment around its mean flow value.

Regarding the effects of flow passage and injected liquid properties, Figure 9 presents a comparison among the Reynolds number values corresponding to the inception of cavitation according to some previous studies (Sou et al., Nurick, Park et al., and Suh et al.) together with the results from the developed model. These studies were selected as the nozzle geometries are characterized by a regular rectangular cross section with a sharp entrance edge. Different liquids were considered, including water, diesel fuel, biodiesel, and trichloroethylene, at room temperature, as shown in Table 1.

The Reynolds number is calculated based on the hydraulic diameter. The results are fitted by a linear relation, as shown in Figure 9. It can be noticed that point $b$, which corresponds to $1/Re = 0.6 \times 10^{-4}$, connects the two linear fittings with different slopes. Before point $b$, the linear fitting has a sharp slope of $52^\circ$; in contrast to that, after point $b$, the slope decreases to $5.7^\circ$.

By rewriting eq 4, it becomes as follows:

$$Cn = \frac{C_1}{Re_{b}} + C_2$$  \hspace{1cm} (5)

$$Cn = \frac{2D_e^2P_d}{Re_{b}o^2} - \frac{2D_e^2P_d}{Re_{b}o^2}$$  \hspace{1cm} (6)
Considering the similarity between the two relations eqs 5 and 6, the values of $C_1$ and $C_2$ are as follows.

$$C_1 = \frac{2D_h^2 P_f}{R_{ch}^2 v^2} \quad (7)$$

$$C_2 = -\frac{2D_h^2 P_f}{R_{ch}^2 v^2} \quad (8)$$

Cavitation inception is observed early in a nozzle with a sharp entrance edge at the $1/Re$ value of $0.7 \times 10^{-4}$ close to the line $bc$. When the entrance shape of the nozzle becomes inclined or has a curved entrance edge, cavitation inception becomes close to the line $ab$. For these cases, cavitation inception needs a high momentum to occur. Cavitation occurs at $1/Re$ values of $0.44 \times 10^{-4}$ and $0.39 \times 10^{-4}$ for inclined and curved entrances, respectively, as shown in Table 2.

### Table 2. Values of $1/Re$ and $Cn$ for Different Nozzle Entrances

| cases          | $1/Re$       | $Cn$ |
|----------------|--------------|------|
| sharp entrance | $0.7 \times 10^{-4}$ | 1.34 |
| inclined entrance | $0.65$       |      |
| curved entrance | $0.47$       |      |

A relation has been found between the cavitation number ($Cn$) at which there is an inception for cavitation inside the nozzle and the inverse of $Re$ of the issuing flow from the injection nozzle. Figure 9 shows this relation. According to eq 4, the cavitation number, $Cn$, depends inversely on the kinetic energy. In the meantime, $Re$ increases with an increase of the kinetic energy. As shown in Figure 9, the measurements carried out by many researchers show that the relation between $Cn$ corresponding to the inception of cavitation and $1/Re$ can be expressed as a linear relation, which has two ranges. For $Cn$ less than 1.3, the relation can be represented by the line $ab$, regardless of the type of injected liquid. On the other hand, when $Cn$ is greater than 1.3, the relation between $Cn$ and $1/Re$ is still linear, and yet, the slope becomes less, which is represented by the line $bc$. It is important to mention that this relation is applicable regardless of the geometry of the nozzle (sharp, inclined, or rounded), as shown by the model results, which fits with the proposed correlation, as shown in Figure 9.

This can be explained as follows: when $Cn$ is less than 1.3, this means a higher kinetic energy as well as inertia forces compared with both the pressure ($Cn$ is low) and the viscous force ($Re$ is high). This will enhance the tendency for the separation of boundary layers. This creates vortices, which stimulate early inception of the cavitation, leading to a higher slope of the line $ab$. On the contrary, as $Cn$ is higher than 1.3, both the pressure and the viscous force become higher compared with both the kinetic energy and inertia force. The two forces including the back-pressure and the viscous force will retard the tendency for the separation of the boundary layer, which will retard the inception of cavitation. Accordingly, the slope as presented by the line $bc$ becomes less.

Also, it is important to conclude that the inception of the cavitation for the rounded nozzle occurs at low $Cn$ and high $Re$. This is followed by the inclined nozzle. The inception cavitation number in the case of the sharp nozzle occurs at higher $Cn$ and lower $Re$ values, compared with the other geometries. This is consistent with the aforementioned explanation regarding the inception of the cavitation and its relation with the conditions leading to the separation of the boundary layers inside the nozzle.

The importance of Figure 9 is that it provides a simplified general correlation regardless of the type of injected liquid or the type of nozzle for a complicated phenomenon, which is inception of cavitation in nozzles.

To verify the results of the model for the issuing spray with experimental results, Figures 10 and 11 show a comparison between the predictions and experimental results of Park et al. for a nozzle with a sharp inlet edge. The comparison is carried out for average droplet sizes at sections from 40 mm up to 140 mm, with a step of 20 mm, downstream of the exit plane of the nozzle. Two cases are considered: the case characterized by noncavitating flow at a pressure ratio of 1.6, as shown in Figure 10, and the case characterized by cavitating flow at a pressure ratio of 3, as shown in Figure 11. The results show that the numerical predictions have a good agreement with experimental measurements of Park et al. In the case of noncavitating flow, the average of droplet sizes of the spray is 51 μm; as the flow evolves into a cavitation state, the average of the droplet sizes drops to 47 μm. This represents an average reduction in the droplet size of the spray by approximately 8%.

Using the developed model and considering different nozzle configurations at a pressure ratio of 1.6, all three nozzle configurations do not experience cavitation. Yet, at a pressure ratio of 3, the nozzle with an inlet sharp edge experiences vigorous cavitation, the inclined nozzle experiences mild cavitation, and the rounded inlet edge nozzle does not experience any cavitation.

Table 3 shows the outcome of the comparison defined by Figure 12. For a pressure ratio of 1.6, different levels of TKEs are generated inside the nozzle. This is due to the developed eddies as a result of the contraction of the flow inside the nozzle and the impact of the inlet edge configuration, regardless the inception of cavitation. This leads to different average droplet sizes from the different nozzle configurations, as shown in Table 3.

As the cavitation takes place in some nozzles at a higher pressure ratio of 3, TKE is enhanced for the cavitating cases (sharp and inclined edges) more than that for the noncavitating cases (rounded edge). As a result, this will lead to further
change with differt turbulent kinetic energy, which increases according to the bubble formation. The collapse of these bubbles produces value of mass developing from the noncavitation state to the cavitation state in inclined shape and then the curved entrance. When the cause cavitation to occur early in the nozzle, followed by an output results, it has been found that depending on the shape at 3. CONCLUSIONS

reduction in the average droplet sizes for the cavitating cases in comparison with the nozzle with no cavitation.

3. CONCLUSIONS

A comprehensive numerical simulation model has been developed in this paper, which predicts the characteristics of the nozzle inflow and correlated with the characteristics of the issuing spray. The model has been used to study the impact of the nozzle entrance geometry on both the flow inside the nozzle and the issuing spray. The model has been validated against experimental data published by Park et al. According to the output results, it has been found that depending on the shape at the inlet to the nozzle, the average velocity in the nozzle shall have different distributions. Also, the turbulence pattern will be different. The created vortices and eddies are the sources of bubble formation. The collapse of these bubbles produces turbulent kinetic energy, which increases according to the bubble dynamics. This energy causes more dispersion when the flow exits from the nozzle.

The local forces and intensities of the flow characteristics change with different nozzle entrance geometries. Sharp edges cause cavitation to occur early in the nozzle, followed by an inclined shape and then the curved entrance. When the flow develops from the noncavitation state to the cavitation state in the nozzle, cavitation inceptions take place close to the mean value of mass flowing reduction, which has a minimum moment around its mean flow value. Regarding the spray characteristics, as expected, the average droplet sizes decrease as the pressure ratio increases. Yet, it shows more decrease when cavitation happens at the same pressure ratio, which is highly linked with the inlet geometry to the nozzle. TKE is enhanced for the cavitating cases (sharp and inclined edges) more than that for the noncavitating cases (rounded edge), leading to further reduction in the average droplet sizes for the cavitating cases in comparison with the nozzle with no cavitation.

4. COMPUTATIONAL METHODS

In this section, the mathematical formulation for solving the flow inside the injection nozzle is introduced. This solution is extended to include the behavior of the flow issuing from the nozzle, such that it becomes possible to find out the impact of nozzle inflow on the characteristics of the issuing flow from the atomizer nozzle. If cavitation happens inside the nozzle such that churning flow or high turbulent flow emerges from the nozzle, the emerging flow shall experience disintegration, leading to spray formation. This disintegration is further enhanced due to the impact of the aerodynamic forces on the issuing flow, especially if the velocity of the issuing flow is high enough to stimulate these aerodynamic forces. Both the inflow and outflow can be specified as a two-phase flow, and yet, there is a substantial difference between the two flows. For the inflow, it starts as a one-phase liquid flow, and then, it may experience cavitation, such that it turns into a bubbly flow. These bubbles may persist, agglomerate, and turn into a slug or annulus flow, or they may collapse and turn the flow back into a highly turbulent single-phase flow. These depend on the flow conditions and the flow passage geometrical characteristics. On the other hand, the outflow experiences liquid disintegration, leading to the development of a liquid spray. For a liquid spray, the continuum phase is gas and the dispersed phase is liquid droplets. It usually passes through multiple stages from dense to diluted spray. A proper coupling is necessary to be defined between the two flows.

To solve this problem, this has been specified as a three-dimensional, turbulent, isothermal, two-phase flow problem. Based on this specification, the system of governing equations as well as the necessary submodels is defined. These submodels are different or need to be tuned, as in the case of turbulence modeling, for both the inflow and the outflow. This system of equations can be specified as simultaneous, nonlinear, partial differential equations, which are usually solved numerically. The finite difference technique will be used in this work to solve these equations. The flow consists of a spectrum of different eddies, varying from eddies the Kolmogorov length scale, up to large eddies. In this work, the large eddy simulation (LES) approach is considered to simulate this flow with such a spectrum of eddies. Accordingly, the governing equations are spatially low-pass-filtered, where the large eddies are solved directly from the equations, while the subgrid-scale eddies are modeled. The Taylor length scale is considered as the threshold between the two eddies’ length scales. Accordingly, the grid size is constructed to fulfill this requirement. Based on previous specifications, the governing equations as well as submodels can be illustrated as follows.

4.1. Nozzle Inflow Model. For the general case regarding whether the flow will experience cavitation or not, the phase continuity equation can be written as follows

$$\frac{\partial}{\partial t}(\rho q) + \nabla \cdot (\rho q \mathbf{v}) = m_{\text{net}}$$

(9)

where $q$ represents the phase (liquid or vapor). The source term $m_{\text{net}}$ represents the net phase change rate.

$$m_{\text{net}} = m^+ - m^-$$

(10)
The terms \( \dot{m}^+ \) and \( \dot{m}^- \) represent the effects of evaporation and condensation rates, respectively, as a result of the phase change, which is bubble formation due to cavitation or bubble collapse. The evaporation and condensation rates are derived from the bubble dynamics equation, which accounts for bubble growth and collapse. They can be calculated based on the Rayleigh–Plesset equation as illustrated in eqs 16 and 17.

Also, the sum of the phase’s volume fractions satisfies the physical constraint

\[
\sum_{q=1}^{n} \alpha_q = 1
\]  

(11)

Regarding the mixture flow continuity equation, it takes the following form

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0
\]  

(12)

where the mixture quantities are defined as follows

 densities

\[
\rho = \sum_{q=1}^{n} \alpha_q \rho_q
\]  

(13)

mass-averaged mixture velocity

\[
\vec{v} = \frac{1}{\rho} \sum_{q=1}^{n} \alpha_q \rho_q \vec{v}_q
\]  

(14)

Applying the filter on eqs 12 and 19, the mass and momentum balance equation becomes

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0
\]  

(22)

\[
\frac{\partial (\rho \vec{u})}{\partial t} + \frac{\partial}{\partial x_i}(\rho \vec{u} \vec{u}_i) = -\frac{\partial p}{\partial x_i} + \rho F_i + \mu \frac{\partial}{\partial x_j}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial \vec{u}}{\partial x_i}\right)
\]  

(23)

The SGS stress \( \tau_{sgs} = \rho \vec{u}_i \vec{u}_i - \rho \vec{u} \vec{u} \) is a new term appearing in LES equations. It accounts for resolved and subgrid-scale interactions. The main task of the SGS stress tensor model is to dissipate the energy transferred from turbulent large scales. It can be modeled as follows

\[
\tau_{sgs} = -2C_{k}\Delta \frac{\partial S_y}{\partial x_i}
\]  

(24)

where \( C_{k} \) is the subgrid-scale kinetic energy. It can be found by solving the kinetic energy transport equation.

\[
\frac{\partial \kappa_{sgs}}{\partial t} + \frac{\partial \kappa_{sgs}}{\partial x_i} = -r_{\kappa} \frac{\partial \kappa_{sgs}}{\partial x_i} - \epsilon_{sgs} + \frac{\partial}{\partial x_j}\left(\frac{\mu_{\kappa}}{\sigma_{\kappa}} \frac{\partial \kappa_{sgs}}{\partial x_j}\right)
\]  

(25)

where

\[
\mu_{\kappa} = C_{\kappa} \kappa_{sgs}^{3/2} \Delta, \quad \epsilon_{sgs} = C_{\epsilon} \frac{\kappa_{sgs}^{3/2}}{\Delta}, \quad \sigma_{\kappa} = 1 \text{ and } S_y
\]  

(26)
Here, \( C_k \) and \( C_v \) are dynamic constants that are defined, as illustrated in S2 (Appendix A).

### 4.2. Spray Model

Due to the effect of the expected cavitated flow inside the nozzle and the high emerging velocity of the flow in addition to the impact of the aerodynamic forces, the emerging flow is disintegrated into spray. Spray droplet diameters and velocities are defined stochastically according to a probability density function, which is taken as Rosen–Rammler in this work. The spray development is performed using the discrete droplet model (DDM). The injected liquid droplets are represented by parcels. These representative parcels move through the gaseous continuous phase. Droplet trajectories are calculated by a Lagrangian formulation that includes hydrodynamic drag, inertia, and gravity forces. This is also associated with droplet collision and breakup models. As the problem is isothermal, droplet evaporation has not been included.

The governing equations for this approach, represented in a vector form, can be summarized as follows.

#### 4.2.1. Gas Phase. Continuity equation

\[
\frac{\partial \rho_g}{\partial t} + \nabla \cdot (\rho_g \mathbf{u}_g) = 0
\]  

(Momentum equation)

\[
\frac{\partial (\rho_g \mathbf{u}_g)}{\partial t} + \nabla \cdot (\rho_g \mathbf{u}_g \mathbf{u}_g) = -\nabla p + \nabla \cdot \mathbf{T} + \mathbf{F}
\]  

where \( S_{\text{mom}} \) is a source term, which accounts for the momentum exchange due to the presence of droplets. It can be calculated according to eq 29.

\[
S_{\text{mom}} = m_d \left[ (u_{d,\text{in}} - u_{d,\text{out}}) + g \left( 1 - \frac{\rho_g}{\rho_0} \right) (t_{\text{in}} - t_{\text{out}}) \right]
\]  

where \( m_d \) is the mass flow rate of a droplet and \( t \) is the time; the quantities with subscripts in and out refer to the time instants that a droplet enters or leaves a computational control volume, respectively.

#### 4.2.2. Dispersed Phase. Droplet momentum equation

\[
\frac{d \mathbf{u}_d}{dt} = F_D (u - u_d) + g (\rho_g - \rho_d) \frac{u_{d}}{\rho_d} + F_e
\]  

where \( F_D (u - u_d) \) is the drag force per unit droplet mass.

\[
F_D = \frac{18 \mu}{\rho_d d_d^2} \frac{C_p R_e}{24}
\]  

Here

\[
R_e = \frac{\rho d_d |u_d - u|}{\mu}
\]  

where \( \mu \) is the molecular viscosity of the continuous phase, \( d_d \) is the droplet diameter, and \( R_e \) is the relative Reynolds number.

The drag coefficient can be taken as

\[
C_D = a_1 + a_2 \frac{R_e}{R_e} + a_3 \frac{R_e}{R_e}
\]  

where \( a_1, a_2 \) and \( a_3 \) are constants that apply to smooth spherical droplets over several ranges of \( Re \), given by Morsi and Alexander, as illustrated in S3 (Appendix B).

Regarding other forces, \( F_e \) is the force required to accelerate the fluid surrounding the droplet (force/unit particle mass), which can be represented as follows

\[
F_e = \frac{1}{2} \frac{\rho}{\rho_d} d^2 (u - u_d)
\]  

The turbulence is modeled using the LES approach similar to what has been carried out for the inflow. To predict the dispersion of droplets due to turbulence, the trajectories are solved as a stochastic tracking model and the fluid velocity in eq 30 is considered as the mean velocity. The random effect of turbulence on droplet dispersion is considered using the discrete random walk model.

Other models for droplet breakup and collision are also included. This includes the TAB model for droplet breakup as well as the droplet collision model as developed by O’Rourke. Both models are included in FLUENT software.

#### 4.3. Coupling Equations

To have a closure for the solution, a coupling between the inflow and outflow of the nozzle is needed. As aforementioned, the issuing flow is transformed into a spray, which follows a certain droplet size distribution. The distribution has been assumed to follow the Rosin–Rammler distribution. Yet, the status of this issuing flow and the effective area of the injection nozzle are key parameters in defining the droplet size spectrum, spatial distribution, and velocity. This is greatly affected by the intensity of cavitation, which is transformed into an increase in the turbulent kinetic energy of the issuing flow.

The droplet size distribution is defined by fitting the droplet size to the Rosin–Rammaller equation as follows

\[
m_{d,\text{e}} = e^\left( \frac{d}{d_{\text{m}}} \right)
\]  

where \( m_{d,\text{e}} \) is the mass fraction of droplets with diameter greater than the droplet diameter \( d_{\text{m}} \) and \( d_{\text{m}} \) is the mean diameter of droplets. Also, \( n \) is the spread parameter, which is defined as

\[
n = \frac{\ln(-\ln m_{d,\text{e}})}{\ln(d_{\text{m}}/d)}
\]  

To define the effect of the high turbulent kinetic energy on the breaking mechanism of the liquid into droplets, an analogy with the acoustic wave of ultrasonic atomizers is considered. This is used to find out the initial mean droplet size in eqs 35 and 36. It can be defined based on the surface tension, density, turbulent frequency, and the subgrid turbulent kinetic energy, as shown in the following equation.

\[
\overline{d_d} = C_\gamma \left( \frac{8 \pi S}{\rho \omega^2} \right)^{1/3}
\]  

where \( \omega = \frac{\rho \omega_k}{\rho} \) is the eddy frequency, calculated from the subgrid turbulent kinetic energy, and \( C_\gamma \) is the proportionality constant, which depends on the fluctuation intensity. It can take the value of 3.7 The initial maximum droplet size \( d_{\text{d,\text{max}}} \) is taken equal to the minimum value of either the large eddy scale or nozzle diameter as expressed in eq 38. On the other hand, the
initial minimum droplet size \( (d_{d,\text{min}}) \) is taken equal to the Taylor microscale, as shown in eq 39.

\[
d_{d,\text{max}} = \min \left\{ \left( C_{\mu} \frac{3}{2} \frac{k_{\text{sgs}}}{\varepsilon_{\text{sgs}}} \right)^{3/4}, D_N \right\}
\]

(38)

where \( C_{\mu} = 0.09 \) and \( D_N \) is the nozzle diameter.

\[
d_{d,\text{min}} = \left( \frac{10c_{\text{sgs}}}{\varepsilon_{\text{sgs}}} \right)^{1/2}
\]

(39)

When the liquid is pressurized with a pressure ratio equal to 3, it is found that the smallest droplet diameter equals to a value of the Taylor length scale. This is calculated from eq 39. The largest droplet diameter equals to the minimum value among the value of the largest length scale and the value of the hydraulic diameter of the injector (in this study, it is considered equal to the hydraulic diameter, which is calculated from eq 38). The diameter of the droplets ranges around a mean value, which is calculated by eq 37. Considering the aforementioned conditions and equations, the minimum, mean, and maximum diameters were 10, 43, and 300 \( \mu m \), respectively.

Regarding the droplet size distribution and considering the minimum, maximum, and mean droplet size, the size probability function can be constructed using the Rosin–Rammler distribution function for the spread parameter \( (n) \) of values 1, 2, 3, 4, and 5, as shown in Figure 13. When verified with SMD for spray, it is found that the spread parameter value of 3 is the value that gives the most suitable solution.

![Figure 13. Rosin–Rammler droplet size distribution. \( P_r = 3 \), with the characteristic sizes \( d_{d,\text{max}} = 300 \mu m \), \( d_{d,\text{min}} = 10 \mu m \), and \( d_d = 43 \mu m \). The spread parameter \( (n) \) has values 1, 2, 3, 4, and 5.](image)

The velocity of the droplet depends on the injection velocity, the effective nozzle area, and the mass flow rate, which results from the inflow model at the exit zone of the nozzle. The droplet trajectories are spatially randomly distributed, such that they do not go beyond the spray cone angle \( (\theta) \) in the solution domain.

Considering the experimental results of Park et al.\textsuperscript{29} for a nozzle that experiences cavitation, a correlation for the spray cone angle \( (\theta) \) can be developed and described by the following equation

\[
\theta = (Cr)^n (P_r)^m
\]

(40)

where \( P_r \) is the pressure ratio between the injection and back-pressure, \( n \) and \( m \) are constants, and their values are 0.7423 and 3.2417, respectively.

4.4. Computational Model. The current work simulates the atomizer nozzle that was used by Park et al.\textsuperscript{29} They used a nozzle with a sharp rectangular entrance shape and a length-to-width \( (L/W) \) ratio of 1.5, as shown in Figure 14.

![Figure 14. Nozzle dimensions.](image)

Commercial software (FLUENT) was used to solve the conservation equations. The solution was achieved by applying the boundary conditions and solver setup shown in Tables 4 and 5, respectively. The fuel properties are shown in Table 6.

### Table 4. Types of Boundary Conditions\textsuperscript{a}

| zone          | boundary conditions       |
|---------------|---------------------------|
| inlet         | pressure inlet            |
| wall          | no slip                   |
| outlet        | pressure outlet            |

\textsuperscript{a}Since an LES is used, the mesh is intensified near the wall to predict the effect of the velocity gradient due to the boundary layer at the wall.

### Table 5. Computational Model Solver Setup

| features of the problem | definitions                                      |
|-------------------------|--------------------------------------------------|
| solver                  | pressure-based, transient time, and space 3D    |
| viscous model           | multiphase mixture, viscous, large eddy simulation, kinetic energy |
| material                | diesel fuel                                     |
| inlet condition         | pressure inlet = 0.125–0.45 with step 0.025 (MPa) |
| temperature             | 293 (K)                                          |
| outlet condition         | pressure outlet = 0.1 (MPa)                     |

### Table 6. Fuel Properties

| fuel          | diesel |
|---------------|--------|
| density (kg/m\(^3\)) | 830     |
| surface tension (N/m)  | 0.026   |
| dynamic viscosity (Ns/m\(^2\)) | 0.00223 |
| vapor pressure (MPa)   | 0.00128 |

Regarding the accuracy of the computational solution, a grid refinement study is carried out based on the velocity at the nozzle exit. Three grids sizes are considered: fine, medium, and coarse grids. The grid refinement ratio \( (R_{iX}) \) is expressed as follows:

\[
R_{iX} = \frac{\Delta X_{\text{coarse}}}{\Delta X_{\text{medium}}} = \frac{\Delta X_{\text{medium}}}{\Delta X_{\text{fine}}} = 2
\]

(41)

Both the grid spacings and the predicted exit velocities are shown in Table 7.

According to, the convergence rate \( (CR) \) of the solution accuracy with the grid spacing can be expressed as follows
The solution error can be estimated by calculating the relative error for the finest grids to obtain an estimate of the value of the exit velocity at zero grid spacing, $Y_{ref}$. The Richardson extrapolation provides an estimation of the solution as

$$
Y_{ref} \approx \frac{R_i^{CR} \times Y(\Delta X_{fine}) - Y(\Delta X_{medium})}{R_i^p - 1}
$$

As shown in eq 46, the fine grid has a relative error of 0.044%, which is an acceptable error. The grid specifications for the computational domain in the present study are defined in Table 8.

Table 8. Grid Specification

| grid information | hexahedral cells | interior faces | nodes |
|------------------|-----------------|---------------|------|
|                   | 908 000         | 2 668 800     | 963 711 |

| Grid Quality | maximum cell squish | maximum aspect ratio | skewness |
|--------------|---------------------|----------------------|---------|
|              | 0.0                 | 1.732                | 0.0     |

To predict the spray characteristics, a uniform grid has been used as a solution domain. This grid has an aspect ratio of 1 and skewness of 0. The flow enters the solution domain with a velocity that is equal to the average exit velocity of the nozzle. This is defined based on the nozzle inflow model. All other fluid properties at the inlet to the spray model are the same as the fluid properties at the exit of the nozzle inflow model. The other boundary condition of the solution domain in the spray model is considered as the outflow type.

Regarding solution stability, which depends on the solution advancement time step ($\Delta t$), the stability analysis indicates that the solution is stable when the diffusion number ($dn$) is less than or equal to $3/2$. Accordingly, the solution can be advanced with $\Delta t$, which can be calculated from eq 47, as follows

$$
\frac{dn}{(\Delta x)^2} + \frac{\nu\Delta t}{(\Delta y)^2} + \frac{\nu\Delta t}{(\Delta z)^2} = 42
$$

where $\Delta x$, $\Delta y$, and $\Delta z$ are the minimum space steps in respective directions and $\nu$ is the kinematic viscosity ($m^2/s$).

**ASSOCIATED CONTENT**

**Supporting Information**

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsomega.0c05767.

C$_{d}$ and C$_{v}$ are coefficients which are determined dynamically by the test-scale and defined in Appendix A. The drag coefficient C$_{d}$ is defined in Appendix B (PDF)

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**Notes**

The authors declare no competing financial interest.

**NOMENCLATURE**

C$_{n}$ cavitation number
D$_{N}$ hydraulic diameter of the nozzle (m)

$dn$ diffusion number
d$_{d}$ droplet diameter (m)
d$_{d0}$ mean diameter of droplets (m)
d$_{d,max}$ initial maximum diameter, which is taken equal to the large eddy scale (m)
d$_{d,min}$ initial minimum droplet diameter, which is taken equal to the Taylor length scale (m)
F$_{b}$ body force (N)
F$_{a}$ additional acceleration (force/unit particle mass) term (N/kg)
F$_{D}$ drag force per unit particle mass (N/kg)
k$_{SG}$ dynamic subgrid-scale kinetic energy per unit mass ($m^2/s^2$)
L$_{n}$ length of the nozzle (m)
W width of the nozzle (m)
L$_{A}$ length scale (m)
m$_{d}$ mass fraction of droplets with the diameter greater than the droplet diameter (d$_{d}$)
$n$ spread parameter
P local pressure (Pa)
P$_{v}$ vapor pressure (Pa)
Greek Letters
\( \alpha \) phase volume fraction (dimensionless)
\( \beta \) probability (dimensionless)
\( \rho \) density (kg.m\(^{-3}\))
\( \rho_0 \) density of the droplet (kg.m\(^{-3}\))
\( \mu \) molecular viscosity (Pa.s)
\( \nu \) kinematic viscosity (m\(^2\).s\(^{-1}\))
\( \sigma_{ij} \) stress tensor due to molecular viscosity
\( \epsilon_{avg} \) subgrid dissipation rate
\( \tau_{ij} \) subgrid-scale stress

Subscripts
\( k \) phase
\( m \) mixture
\( l \) liquid
\( v \) vapor phase
\( \text{sat} \) saturation status
\( \text{t} \) turbulent
\( \text{in} \) inlet
\( \text{out} \) outlet
\( \text{ref} \) reference condition
\( \text{inj} \) injection parameter
\( \text{average} \) average value

Superscripts
- filtered script
- fluctuation script

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