Development of a Next-generation Spray and Atomization Model Using an Eulerian-Lagrangian Methodology

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Abstract
A next-generation spray and atomization model for high-pressure diesel sprays has been developed and implemented into an engine computational fluid dynamics (CFD) code (KIVA-3V), together with a nozzle flow cavitation model and an evaporation model for the Eulerian liquid phase. In contrast to the widely used Lagrangian atomization models that are based on liquid jet instability analyses, such as Kelvin-Helmholtz (KH) and Rayleigh-Taylor (RT) instability analyses, the new model is based on the assumption that high-pressure spray atomization under modern diesel engine conditions can be described by considering the turbulent mixing of a liquid jet with ambient gases. In the present study, several previously proposed techniques are used to correct for vortex stretching and compressibility effects in high-speed free jets. To describe the dispersion of the liquid phase into a gaseous medium, two transport equations based on the turbulent mixing assumption are solved for the liquid mass fraction and the liquid surface density (liquid surface area per unit volume). At an appropriate time, a switch from the Eulerian approach to the Lagrangian approach is made in order to benefit from the advantages of the traditional Lagrangian droplet treatment beyond the dense spray region near the nozzle. As in the existing ELSA (Eulerian-Lagrangian Spray and Atomization) model, the drop size, drop number and drop distributions are determined using the local liquid mass fraction and local liquid surface density. As an integral part of this study, a three-dimensional homogeneous equilibrium model (HEM) was developed to simulate the cavitating flow within diesel injector nozzle passages. The effects of nozzle passage geometry and injection conditions on the development of cavitation zones and the nozzle discharge coefficient were investigated. Vaporization in the Eulerian liquid phase is also accounted for with an equilibrium evaporation model, which was also developed and implemented in this study. Finally, the integrated spray and atomization models have been used to predict diesel spray development and atomization under various operating conditions, and the numerical results compare well with experimental data obtained from X-ray and other measurements.

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Introduction

High-speed diesel injection is an enabling technology for modern low-emission, high-efficiency diesel engines. Unlike low-speed liquid jets in the Rayleigh and first wind-induced jet breakup regimes [1], the atomization mechanisms for high-speed liquid jets are still not well-understood and knowledge is incomplete, even after more than one hundred years of study, both experimentally and numerically. For a typical spray in diesel engines, spray tip penetration, spray angle, droplet size and number density and their distributions have been the primary interests of investigations. With the advent of advanced experimental techniques, it is now possible to obtain more detailed spray information, such as the fine spray structure, spray momentum, and liquid volume (or mass) fraction distributions [2] [3] [4]. All these efforts have provided and will continue to provide new insights and motivations for the development of next-generation spray atomization models.

Lagrangian spray models based on KH-RT instability analyses [5] [6] have been most widely used for more than two decades. These numerical models have been successful because they are computationally efficient and at the same time provide reasonable agreements with experimental measurements, mostly in terms of penetration and spray angle, and in limited cases, also in terms of drop size, number density and their distributions.

Two-fluid methods with surface tracking or capturing, such as level set (LS) and volume of fluid (VOF) methods, are powerful tools for computing two-phase flows with propagating interfaces [7] [8]. In the LS method, a natural choice for the level set function is the signed distance to the interface, thus the interface is defined by locations where the level set function is zero. One of the advantages of the LS method is that it is easy to calculate curvatures of the interfaces, while a major drawback is that the LS method tends to lose or gain mass due to insufficient resolution [7] [9] [10]. The VOF method, on the other hand, has the advantage of mass conservation while it is difficult to compute accurate interface curvatures and normal vectors due to the discontinuity at interface [9]. In the VOF method, the interface is defined by locations where the liquid volume fraction is between 0 and 1. When applied to computations of high-speed liquid sprays, both the LS and VOF methods require a numerical mesh size of the order of a few microns in order to capture the smallest surface wave structures. This requirement either dramatically increases computational cost or significantly limits the extent of the computational domain.

Numerical methods based on potential flow theory have also been developed for spray atomization modeling purposes. Since the governing equation for these methods is the Laplace equation, only surface meshes of the liquid jet with a finite length are required. Researchers at Purdue University developed a non-linear atomization model based on the boundary element method (BEM) and boundary layer instability analyses [11] [12]. The model was intended for applications to two-dimensional axi-symmetric, inviscid and incompressible flows. By solving the governing equation for the velocity potential on the interface, nodal velocities were calculated and the surface evolution was tracked. Similar to the aforementioned two-fluid methods, a mesh size of the order of the smallest surface wavelength is required in order to achieve sufficient resolution. Evaluation of surface curvature is challenging for complex surface structures, and re-meshing of the moving surface requires certain reconstruction and smoothing algorithms. As also pointed out by Heister et al. [13], extending the two-dimensional axi-symmetric jet to the fully three-dimensional jet geometry is not practical in the present computation environment, due to prohibitive requirements for computation time and computer memory.

A three-dimensional source panel method based on potential flow theory, has been applied to model Lamb’s oscillating drop, a classical test problem for CFD code by Ning [14]. However, it was found that mass conservation is a difficulty due to insufficient resolution of the surface. One possible solution to alleviate this problem might be to use extremely fine panels and to adopt parallel computing to try to reduce computation times.

From this discussion it is clear that attempting to resolve the details of the liquid interface with either two-fluid or potential flow methods can be computationally prohibitive, even with the increased computer power now available. Furthermore, all these methods are based on the postulated breakup mechanism that considers surface wave evolution on an intact liquid core or a liquid jet of finite length. With ultra-high injection pressures (e.g., up to 300 MPa) proposed for modern diesel engines, the basic question of whether an intact core even exists for such high-pressure sprays is still under debate. New spray visualization techniques, such as X-ray absorption and ballistic imaging methods, suggest that no intact liquid core exists or that it is extremely short for high-pressure fuel injections under modern diesel engine conditions [2] [4].

The Eulerian-Lagrangian spray atomization method, also called the ELSA method, has been proposed and has been under development since 2001 [15] [16] [17]. It combines the Eulerian approach in the near-nozzle dense spray region with the Lagrangian approach in the dilute region downstream of the nozzle, and was intended for modeling high Reynolds number, high Weber number turbulent sprays. In this method, the spray is considered to be a single “effective” phase of liquid and gas mixture. The dispersion of the liquid
phase into a gaseous environment is described by the local liquid mass fraction and the local liquid surface density, which are solved from individual transport equations. Furthermore, a switch from the Eulerian approach to the Lagrangian approach is made in regions where the spray breakup process does not need to be resolved. It should be pointed out, however, that a complete Eulerian approach characterization of the spray is possible if desired. Under modern diesel engine spray conditions, where the extent of the liquid region near the nozzle is short due to fast breakup and vaporization, the Eulerian approach is particularly useful. An evaporation model for the Eulerian liquid phase can also be developed. In the present study, the ELSA method was combined with a Homogeneous Equilibrium Evaporation model and used for the development of a “next-generation” spray atomization model.

It is well recognized that the details of the internal nozzle flow have a strong impact on the spray and its atomization characteristics. This is particularly true when cavitation occurs within the nozzle passage. With increased injection pressure, nozzle flow models based on empirical correlations become increasingly inaccurate, and full three-dimensional nozzle flow solutions based on the governing Navier-Stokes equations are required. In numerical simulations of internal nozzle flow, two approaches are usually considered. Two-fluid nozzle flow models treat the liquid and vapor phases separately, i.e., two sets of governing equations, one for each phase are solved, and interactions between the phases is modeled by additional source terms [18]. On the other hand, continuum nozzle flow models consider the nozzle flow as a homogenous mixture of liquid and gases. The mixture density, which varies from the liquid density to the gas density to the cavitation density, indicates the fractions of liquid and gas in a given cell. These homogeneous equilibrium models (HEMs) are most widely used and have various forms, depending on how the equation of state and pressure are formulated [19]. In this study, a homogeneous equilibrium cavitating nozzle flow model has been developed and implemented into the KIVA-3V code [20].

Evaporation models for Lagrangian droplets are commonly available. However, for spray atomization models based on Eulerian or Eulerian-Lagrangian approaches, an evaporation model for the continuous liquid phase is needed. In this case, the local evaporation rate must be related to the local fuel vapor mass fraction, liquid surface density and local thermodynamic conditions. In the present study, an equilibrium evaporation model for the continuous liquid phase has been adopted for simplicity.

Numerical Models

Following the approach described above, an Eulerian-Lagrangian spray atomization (ELSA) model was implemented into the KIVA-3V code. In the ELSA model, the continuity, momentum, energy and turbulence equations are solved for a single phase turbulent flow. Transport equations for the liquid mass fraction and liquid surface density are also solved, which describe the liquid phase dispersion into the gaseous environment. In the transport equation for the liquid mass fraction, the turbulent diffusion flux of liquid is modeled using a gradient law. The production and destruction of liquid surface due to mean flow and turbulence stretching, collision and coalescence are accounted for with source terms in the transport equation for the liquid surface density. These source terms are subject to further validation and improvement. More details about these transport equations can be found in Blokkeel et al. [15] [16] [17].

In the ELSA method, high-pressure liquid injection is considered to be analogous to the turbulent flow of a liquid-gas mixture. Thus turbulence modeling is expected to have an important impact on the computational results. It has been found that the standard $k – \varepsilon$ model overestimates the spreading rate of circular jets while it predicts plane jet flows correctly. This has been confirmed by numerous experimental observations. Pope suggested that the stretching of vortex tubes by the mean flow leads to greater scale reduction and dissipation, less kinetic energy and a lower effective viscosity [21]. To correct for these effects, he introduced a non-dimensional invariant $\chi$ as a measure of vortex stretching, and assumed the dissipation rate, $\varepsilon$, to be a linear, increasing function of $\chi$, which leads to the following modified turbulence dissipation equation:

$$\frac{D \varepsilon}{Dt} = \frac{1}{\rho} \frac{\partial}{\partial x_i} \left[ \mu_t \frac{\partial \varepsilon}{\partial x_i} \right] + c_{\varepsilon} \frac{\mu_t}{k} \left[ \frac{\partial u}{\partial x_i} + \frac{\partial u}{\partial x_j} \frac{\partial u}{\partial x_k} \right] \frac{\partial u}{\partial x_k} - c_{\varepsilon} \frac{\varepsilon}{k} + c_{\varepsilon} \frac{\varepsilon^2}{\nu} \left( \frac{\partial \chi}{\partial x_i} \right) \left( \frac{\partial \chi}{\partial x_j} \right) \left( \frac{\partial \chi}{\partial x_k} \right)$$

(1)

where

$$c_{\varepsilon} = 0.79, \quad \chi = \omega_\theta \omega_\phi S_y$$

$$S_y = \frac{1}{2} \left( \frac{\partial u}{\partial x_i} + \frac{\partial u}{\partial x_j} \frac{\partial u}{\partial x_k} \right), \quad \omega_\theta = \frac{1}{2} \frac{\partial u}{\partial x_i} \frac{\partial u}{\partial x_j} \frac{\partial u}{\partial x_k}$$

(2)

In Equations (1) and (2), $k$ is the turbulent kinetic energy, $i$ is the time, and $i, j$ and $k$ are the indexes for the
three Cartesian directions, and \( \bar{u}_i \) and \( x_i \) are the velocity components and coordinates in the \( i \) direction respectively. \( \rho \) is the density, \( \mu_i \) is the dynamic turbulent viscosity, and \( c_{i1} = 1.44, c_{i2} = 1.92 \) and \( \sigma_i = 1.3 \) are the standard turbulence model constants.

The correction modification was explored in the present work to account for circular jet effects. Another important aspect relevant to high-speed spray modeling is the inclusion of compressibility effects. Variable density extensions of incompressible turbulence models, without explicit compressible terms, have failed to predict the significant decrease in the spreading rate [22]. It has been shown that in compressible turbulence, both the dilatational dissipation and the dilatational-pressure terms need to be modeled. Sarkar et al. [22] proposed a model for the compressible dissipation, based on an asymptotic analysis of the compressible Navier-Stokes equations and direct numerical simulations of the form:

\[
\frac{Dk}{Dt} = \frac{1}{\rho} \frac{\partial}{\partial x_i} \left[ \mu_i \frac{\partial k}{\partial x_i} \right] + \frac{\mu_i}{\sigma_i} \frac{\partial \bar{u}_i}{\partial x_i} \frac{\partial \bar{u}_i}{\partial x_i} - \epsilon \left( 1 + \alpha M_i^2 \right)
\]

(3)

where \( \sigma_i = 1.0 \) is a standard turbulence model constant, \( \alpha = 1.0 \) is a constant from this modification and \( M_i = \sqrt{2k/(\gamma RT)} \) is the turbulent Mach number. This model was also implemented in this study as an option. El Baz and Launder [23] proposed an alternative approach. They simply used a solenoidal (incompressible) dissipation rate equation that was sensitized to compressibility effects through the turbulent Mach number. These effects were accounted for through a modification to the decay coefficient \( C_{\epsilon_i} \):

\[
\frac{D\epsilon}{Dt} = \frac{1}{\rho} \frac{\partial}{\partial x_i} \left[ \mu_i \frac{\partial \epsilon}{\partial x_i} \right] + \frac{c_{i1} \mu_i \epsilon}{\rho} \left( \frac{\partial \bar{u}_i}{\partial x_i} \right)^2 \frac{\partial \bar{u}_i}{\partial x_i} - \frac{c_{i2} \epsilon^2}{1 + \beta_k M_i^2} k
\]

(4)

where \( \beta_k = 3.2 \) is a constant derived from calibration with direct numerical simulation (DNS) data. This model has also been implemented in this study. It can be easily shown, however, that the corrections in Equations (3) and (4) have equivalent effects on the turbulence diffusivity, i.e., with \( \alpha = \beta_k \), both correction methods have the same effects on computational results of high-speed free jets. This similarity has been further confirmed numerically for both liquid and gas jets by Ning [14].

It needs to be pointed out, however, that other techniques that target the turbulence length scale, viscous dissipation, and turbulent viscosity and wall boundary conditions have also been used by different researchers to correct for turbulence model effects. However, some of the model parameters are arbitrary and case dependent, thus those techniques were not adopted in the present ELSA model.

For the present nozzle flow simulations, isentropic nozzle flow is assumed, which leads to the following equation relating density and pressures [19]:

\[
\frac{DP}{Dt} = \frac{1}{a_i^2} \frac{DP}{Dt}
\]

(5)

where \( a_i \) is the isentropic sound speed varying from the gas sonic speed to the liquid sonic speed, depending on the void fraction. To be consistent with the phase calculations in the KIVA-3V code solver, the isentropic sound speed can be used to evaluate the kinematic volume change as [24]:

\[
\frac{\partial V}{\partial P} = -\frac{V}{\rho a_i^2}
\]

(6)

Finally, a pressure equation for the nozzle flow simulation is derived from the compressible continuity equation, combined with the isentropic relation in Equation (5) as:

\[
\frac{1}{a_i^2} \frac{\partial P}{\partial t} + \frac{\partial}{\partial x_i} \left( \rho \nabla P + \rho \nabla \cdot \mathbf{U} \right) = 0
\]

(7)

In the current nozzle flow simulations, both the reservoir (sac volume) and nozzle geometries were included in the computational domain. The pressure at the reservoir inlet was set to the injection pressure, while the pressure at the nozzle exit was set to the chamber pressure. Initially, both the reservoir and the nozzle were filled with static liquid fuel at the chamber pressure. The nozzle flow model could be improved in future to include the whole computational domain from the reservoir to combustion chamber for engine applications. However, for simplicity, the current approach was to extract flow information at the nozzle exit and to couple this information into the ELSA model as an inflow boundary condition for modeling the flow details outside the nozzle exit.

An equilibrium evaporation model for the Eulerian liquid phase was implemented, where the local vapor pressure is determined from the local temperature. The equilibrium fuel vapor mass fraction is then related to the vapor pressure and other physical conditions by:

\[
y_1^* = \frac{W_i}{W_i + W_v (p/p_v - 1)}
\]

(8)

where \( y_1^* \) is the local equilibrium fuel vapor mass fraction, \( W_i \) is the molecular weight of fuel vapor, \( W_v \) is the local average molecular weight of all gaseous species exclusive of fuel vapor, and \( p \) and \( p_v \) are the lo-
cal pressure and local vapor pressure, respectively. Given the local equilibrium vapor mass fraction, evaporation effects can be easily evaluated. This evaporation model is straightforward but can be updated to consider non-equilibrium evaporation effects in future.

**Results and Discussion**

The present implementation of the ELSA model was first applied to both liquid and gas jets to investigate turbulence model effects.

Figure 1 shows computational results for a helium gas jet which was injected into a nitrogen environment at the sonic speed (876.58 m/s). The injection pressure was 2.080e+5 Pa, chamber pressure was 1.013e+5 Pa, the orifice diameter was 0.279 mm and the temperature was 296 K. The computational domain for this gas jet was 40 mm x 60 mm. Figure 1(a) shows the density contour of the gas jet at t=4 ms after the start of injection, while Figure 1(b) compares experimental penetration data [25] with results from the present numerical simulations. In Figure 1(b), improvement in the accuracy of the numerical prediction was observed with the turbulence corrections described in “numerical models” section. Tests with other gas jets by Ning [14] have also shown that these modifications to the turbulence models are useful, although in some cases the improvements are marginal. Use of the model corrections is still preferred, because they provide a systematic and more physical way to account for deficiencies in the standard turbulence models, instead of the need for case-to-case calibrations.

![Density contour](image1.png)  
**Figure 1** Density contour at t=4 ms and spray tip penetrations for a helium gas jet injected at sonic speed

Figure 2 shows predicted liquid penetrations for two liquid jets using the present ELSA model, compared to experimental data of Siebers et al. [26], as well as predictions made using the standard KH-RT breakup model in the KIVA-3V code (e.g., see Beale and Reitz [6]). The injection pressure in Figures 2(a) and 2(b) was 142 MPa, and the chamber pressure in Figure 2(a) was 4.606 MPa and 11.25 MPa in Figure 2(b). The nozzle orifice diameter was 0.32 mm, the ambient gas was nitrogen at 300 K and the liquid was DF2 [20]. The spray penetrations calculated using the ELSA model in Figure 2 were based on a complete Eulerian approach, i.e., no switch from the Eulerian liquid phase to the Lagrangian droplet was made in these calculations. The good agreement with the experimental data confirms that the switch from the Eulerian to the Lagrangian approaches should not have a significant impact on the liquid spray penetrations. From the results shown in Figs 2(a) and 2(b), it is clear that the turbulence corrections in the present ELSA model significantly improve the predicted penetrations of the two Eulerian liquid sprays. Similar improvements have been observed for other non-vaporizing sprays tested by Ning [14].

![Liquid penetrations](image2.png)  
**Figure 2** Predicted liquid penetrations using the ELSA model (with and without turbulence corrections) for two non-vaporizing liquid sprays

The present ELSA model was further tested for non-vaporizing sprays by including the switch from the Eulerian to the Lagrangian approach. The numerical results from the ELSA model have been compared to available X-ray spray data of Malavé et al. [27]. The X-ray absorption method is a relatively new technique that allows visualization of the spray in the near-nozzle region. It was developed at the Argonne National Labora-
tory to make quantitative, time-resolved measurements of dense sprays. The fuel mass is measured from X-ray beam attenuation:

\[ \frac{I}{I_0} = \exp(-\mu_M \cdot M) \]  

where \( I \) is transmitted intensity, \( I_0 \) is incident intensity, \( M \) is fuel mass in the path of the X-ray beam and \( \mu_M \) is the absorption coefficient.

Figure 3 compares the drop size and drop distributions obtained from the ELSA model with those obtained using the KH-RT breakup models in the KIVA-3V code. In this non-vaporizing spray with diesel fuel injected into nitrogen environment at 300 K, the injection pressure was 95 MPa, the chamber pressure was 1.7 MPa and the orifice diameter was 0.13 mm. The computational domain for these calculations was 10 mm x 15 mm (only half of the domain is shown in Figure 3). For the ELSA calculations in Figure 3, the switch from the Eulerian approach to the Lagrangian approach was made when the local liquid volume fraction was greater than 10% but less than 99%. This criterion is subject to further improvement and validation, as part of the ongoing investigation of nozzle flow effects on the downstream spray atomization characteristics. From Figure 3 it is seen that the average drop size predicted by the ELSA model is smaller than that from the KH-RT breakup models. Note that the drop size in the ELSA model is determined using the predicted local surface area density. Assumptions are made about the role of surface tension and subgrid turbulence effects in the drop size model (Blokkeel [16]). Thus, a difference in drop size between the models is not unexpected, and model calibration using detailed drop size experimental data will be required. (The “drop size” in Figure 3 and other figures, where applicable, is drop radius in micron and SMD is Sauter mean diameter.)

Figure 4 Eulerian liquid phase and Lagrangian droplets computed from ELSA model for the same spray as in Figure 3 \((t = 100 \mu s)\)

Figure 4 displays the Eulerian liquid phase together with the Lagrangian droplet parcel locations at \(t = 100 \mu s\) for the same spray as in Figure 3. The “liq” contours in Figure 4 refer to liquid mass fraction, and a maximum value of 0.1 is used to highlight the spray structures. The liquid mass fraction in Figure 4 ac-
counts for both the Eulerian liquid phase and the Lagrangian droplets. Figure 5 further compares the liquid penetration predicted by the ELSA model with the experimental data from the X-ray measurements. It is observed that the penetrations predicted by the ELSA model are in good agreement with those from the X-ray measurements. In this figure, the liquid penetration includes both the Eulerian liquid phase and the Lagrangian droplets.

Figure 5 Liquid penetrations predicted by ELSA model vs. repeated X-ray measurements

In Figure 6, the liquid volume fractions computed from the ELSA model are compared to those from the X-ray measurements, for the same spray as in Figures 3 to 5. The resized domains in Figure 6 correspond to a 1.4 mm x 8 mm window in the actual test geometry, and the maximum liquid volume fraction in the domain is 0.5. In Figure 6(b), the ELSA model is seen to capture the spray structures in the dense spray region seen in the X-ray data of Figure 6(a), and the agreement is encouraging. The liquid volume fractions in Figure 6(b) also account for both the Eulerian liquid phase and the Lagrangian droplets.

Figure 6 Liquid volumetric fractions from ELSA model vs. X-ray measurement at t = 40 μs

A nozzle flow model has been developed in the present study to investigate the effects of nozzle internal geometry and injection conditions on the development of cavitation zones and the nozzle discharge coefficient. The nozzle flow model was first applied to the diesel sprays of Figs. 3 ~ 6, but with four slightly different nozzle passage geometries, i.e., cylindrical and converging nozzles with sharp and round nozzle entrances. Table 1 shows the nozzle flow simulation conditions, and Figure 7 compares the four nozzle geometries considered in the simulations. The K or KS factor of a nozzle is defined as \((ID - ED)/10\) where ID is the nozzle inlet diameter and ED is the nozzle exit diameter in microns. The K factor refers to nozzles with sharp inlets, while the KS factor refers to those with round inlets.

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Diesel</th>
</tr>
</thead>
<tbody>
<tr>
<td>Injection pressure</td>
<td>95 MPa</td>
</tr>
<tr>
<td>Chamber pressure</td>
<td>1.7 MPa</td>
</tr>
<tr>
<td>Chamber gas</td>
<td>Nitrogen</td>
</tr>
<tr>
<td>Temperature</td>
<td>296 K</td>
</tr>
<tr>
<td>Nozzle exit diameter</td>
<td>0.13 mm</td>
</tr>
<tr>
<td>Nozzle inlet diameter</td>
<td>0.13 mm (K or KS=0.0)</td>
</tr>
<tr>
<td>0.15 mm (K or KS=2.0)</td>
<td></td>
</tr>
<tr>
<td>Nozzle length</td>
<td>1.0 mm</td>
</tr>
</tbody>
</table>

Table 1 Nozzle flow simulation conditions

![Four geometries for nozzle flow simulations](image)

Figure 7 Four geometries for nozzle flow simulations
In the nozzle flow simulations, mesh sizes of 10 to 20 microns across the nozzle diameter were used. In Figure 7, 12 cells were used across the nozzle diameter and the radius of the rounded inlets was 30 microns. The diameter of the liquid reservoir above the nozzle inlet was set equal to 1.0 mm and its height was also 1.0 mm.

Figure 8 shows the transient cavitating flow development inside the cylindrical nozzle passage with a sharp nozzle inlet. The “vfrliq” in Figure 8 (and other figures, where applicable) refers to liquid volume fraction. The cavitation began to develop at the corner of the nozzle inlet at about $t = 5 \mu s$ and then evolved into a fully cavitating flow at $t = 20 \mu s$. In Figure 9, the steady state velocity and density distributions at the nozzle exit for the four nozzle passage geometries are compared. The results in Figure 9 suggest that the cylindrical nozzle passage with a sharp inlet ($K=0$) has the maximum cavitation, while the converging nozzle passage with a round inlet ($KS=2.0$) has the minimum cavitation. The velocity and density profiles at the nozzle exit were further applied to calculate the nozzle discharge coefficients.

Figure 10 compares the steady state nozzle discharge coefficients for the four nozzle passage geometries. It can be concluded from Figure 10 that converging nozzles (positive K or KS factor) lead to increased discharge coefficients, decreased cavitation. Rounded inlet nozzles increase discharge coefficients, and decrease cavitation. Figure 11 further displays the nozzle discharge coefficients as a function of time for the four nozzle passage geometries. From Figure 11, it is observed that steady nozzle flows are established at about $15 \sim 20 \mu s$ after the simulations began.
To further confirm the trends observed in the above nozzle flow simulations, the nozzle flow model was applied to another set of nozzle passage geometries under different operating conditions. In these nozzle flow simulations, the nozzle inlet and outlet diameters were either 0.241 mm or 0.257 mm, depending on whether it was a converging or diverging nozzle passage geometry. The sac reservoir above the nozzle inlet was cylindrical with a diameter of 1.02 mm and the sac volume was 0.7 mm$^3$. The length of the nozzle passage was 1.0 mm. Table 2 shows the operating conditions for these simulations, where \( \rho_a \) is the chamber gas density, \( P_{amb} \) is the ambient gas pressure and \( P_{inj} \) is the injection pressure. Figure 12 shows the four computational meshes used, and for each mesh, the 6 cases listed in Table 2 were considered.

Figure 13 shows the steady-state liquid volume fraction distributions within the four nozzle passage geometries for nozzle flow simulation Case 1 listed in Table 2. The legends for the liquid volume fraction in these pictures are the actual maximum and minimum liquid volume fractions in the domains. The results in Figure 13 indicate that converging nozzles tend to reduce cavitation while sharp inlets tend to increase cavitation, as expected.

Figure 14 further shows the effects of the nozzle passage geometries and injection conditions on the steady-state nozzle discharge coefficients for all cases listed in Table 2. It can be concluded from Figure 14, together with the results from Figures 9 to 11, that under the same injection conditions, converging nozzles (i.e., nozzles with positive K or KS factors) reduce cavitation and thus have larger discharge coefficients, compared to diverging nozzles. Compared to nozzles with rounded inlets, nozzles with sharp-edged inlets tend to increase cavitation and thus have smaller discharge coefficients. Finally, given the same pressure difference and nozzle geometry, a greater chamber pressure (or larger gas density) leads to less cavitation and thus a larger discharge coefficient.
The results from these nozzle flow simulations will be coupled with the ELSA model as inflow boundary conditions for modeling the flow details outside the nozzle exit in future simulations.

Finally, the equilibrium evaporation model developed for use with the present ELSA model has been applied to vaporizing sprays. Table 3 shows the injection conditions for three vaporizing sprays considered in these tests, and the predicted spray penetrations are shown in Fig. 15. It should be noted that in these vaporizing spray simulations, no switch from the Eulerian to the Lagrangian approaches is made - the purpose is to test the performance of the evaporation model as applied to the Eulerian liquid phase only.
Figure 15 shows the fuel vapor and liquid fuel penetrations calculated by the equilibrium evaporation model for the three gas densities listed in Table 3. The effects of gas density on both liquid and fuel vapor penetrations were simulated. The liquid penetration is seen to reach a maximum extent while the vapor phase continues to penetrate, consistent with experimental data of Siebers et al. [28] [29]. Given the simplicity of the equilibrium evaporation model for the Eulerian liquid phase, these results are very encouraging.

Figure 16 further shows the liquid and fuel vapor mass fractions at $t = 1 \text{ms}$ for the vaporizing spray Case 2 in Table 3. The maximum liquid mass fraction in Figure 16(a) was close to 1.0 at the nozzle inlet but the range was changed to 0.5 to highlight the spray structure. In Figure 16(b), the legend shows the actual maximum and minimum fuel vapor mass fractions in the domain. The computational domain in Figure 16 was $30 \text{mm} \times 60 \text{mm}$.

Figure 16 Predicted liquid fuel and fuel vapor mass fraction distributions at $t = 1 \text{ms}$ for Case 2 in Table 3

(a) Liquid mass fraction  (b) Fuel vapor mass fraction

Summary and Ongoing Work

A next-generation spray and atomization model for high-pressure diesel sprays has been developed and implemented into the KIVA-3V code. The major components of this model include an Eulerian-Lagrangian Spray and Atomization (ELSA) model, a three-dimensional nozzle flow cavitation model and an equilibrium evaporation model for the Eulerian liquid phase.

The ELSA model was first applied to non-vaporizing diesel sprays, using the complete Eulerian approach or the Eulerian-Lagrangian approach. It was found that the ELSA calculations are able to capture important spray characteristics, and comparisons of the numerical results from the ELSA model with those from the standard KH-RT breakup models and experimental measurements show encouraging agreements.

As part of the ongoing work in the present study, the numerical results from the nozzle flow simulations are being coupled into the ELSA model as inflow boundary conditions for modeling the spray and atomization details outside the nozzle exit. The numerical results, including the effects of nozzle flow cavitation physics are being compared with available experimental spray data.

In the present study a homogeneous equilibrium nozzle flow model has also been successfully applied to different nozzle injection conditions to investigate the effects of nozzle geometry and injection conditions on cavitation development and nozzle discharge coefficients. These effects are well captured by the model, and the predicted trends are consistent with those from experimental observations and theoretical analyses.

In particular, the effects of gas density on liquid fuel and fuel vapor penetrations in vaporizing sprays are well captured by the equilibrium evaporation model. The advantage of this evaporation model lies in its simplicity, and in the fact that it can account for the evaporation effects in the Eulerian liquid phase.

In the present model, the turbulent diffusion flux of liquid in the transport equation for liquid mass fraction was modeled by the gradient law, which leads to a standard diffusion term. This treatment could be improved in future to predict more realistic liquid dispersion in gaseous environment. Techniques have also been proposed to correct for effects of compressibility on the turbulence model in this study. The corrections have proven to be useful for both liquid and gas jets, and thus have been implemented into the present model.

Given the complexity of the liquid surface production and destruction mechanisms in atomizing high-speed diesel sprays, improvements of the source terms in the transport equation for the liquid surface density (which is used to determine the primary atomization drop size) will continue to be empirical in nature, i.e., the source terms will require calibration with available spray data.

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References


