Large-eddy simulation on the effects of fuel injection pressure on gasoline spray characteristics

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Gothenburg, Sweden 2019
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ABSTRACT

Increasing the injection pressure in gasoline direct injection engines has a substantial potential to reduce emissions while maintaining high efficiency in spark ignition engines. Present gasoline injectors operate at pressures of 20 to 30 MPa. However, the use of higher-pressure fuel injection (40 to 60 MPa or more) could potentially reduce emissions and increase fuel efficiency. To fully exploit the capabilities of high-pressure fuel injection technology, a fundamental understanding of gasoline spray characteristics and behavior at such high injection pressures is vital. Such an understanding could also be used to further model development and facilitate the integration of advanced injection systems into future gasoline engines.

This work presents numerical simulation studies on gasoline sprays formed at fuel injection pressures between 40 and 150 MPa. Three nozzle hole shapes (divergent, convergent, and straight) with different configurations (6 or 10 holes) were considered in the simulation to determine how a nozzle geometry affects spray formation. The numerical calculations were performed in a constant volume spray chamber under non-vaporizing conditions to best match the experimental setup. The gas flow was modeled using a large-eddy simulation (LES) approach, while a standard Lagrangian model was utilized to describe the liquid fuel spray. Spray atomization was modeled using the Kelvin Helmholtz – Rayleigh Taylor (KH-RT) atomization model, with the droplet size distribution being assumed to follow a Rosin-Rammler distribution function. Simulation results for the spray liquid penetration length are validated with experimental findings under different fuel injection pressures. Afterwards, an arithmetic mean droplet diameter (D10) and a Sauter mean droplet diameter (D32) as a function of pressure are compared against the measured droplet diameters. Simulated drop size distributions are presented and compared with measured droplet sizes. The results indicate that high fuel injection pressures increase the liquid penetration length and significantly reduce droplet sizes, and that nozzle shape significantly affects spray characteristics and spray formation.

In addition, raising the injection pressure from 40 to 150 MPa with a divergent nozzle was predicted to reduce the SMD from 13.4 to 7.5 µm while increasing the probability of observing droplet diameters of 5-10 µm from 40% to 72%. Similar results were obtained for the other nozzle shapes.

Keywords: High pressure fuel-injection, LES, GDI engine, Spray characteristics
LIST OF PUBLICATIONS

This thesis is based on the work contained in the following publication:

Publication A Sandip Wadekar, Akichika Yamaguchi, and Michael Oevermann "Large-eddy simulation on the effects of fuel injection pressure on the gasoline spray characteristics" in SAE 2019- International powertrains fuels and lubricants meeting, San Antonio, USA.

Other related publications:

Publication B Sandip Wadekar, Michael Oevermann, and Andrei Lipatnikov, 'Large Eddy Simulation of Stratified Combustion in Spray-Guided Direct Injection Spray-ignition engine' in WCX™18: SAE world congress experience, Detroit, MI, USA.

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Last but not the least I cannot conclude without acknowledging my parents, my brother and my lovely wife for their endless support.
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1 Introduction

Combustion has been a key technology for transportation since the last century. Despite its central role in improving living standards, it has had significant adverse environmental impacts. Notably, the CO2 emissions it produces have contributed greatly to global warming. In addition, combustion creates noise and produces pollutants that reduce air quality in urban areas. Consequently, legislatures around the world are introducing increasingly strict regulations requiring the automotive sector to reduce its emissions. For instance, the European Union has implemented legislation limiting the fleet average CO2 emissions of vehicles to 130 g/km (depending on vehicle weight) [1]. This limit is expected to be reduced to 95 g/km in 2021 and then to between 68 and 78 g/km in 2025. Similar regulations have been or will be implemented in other countries. To meet these requirements, vehicle manufacturers are exploring a range of strategies to reduce emissions, including geometrical improvement (downsizing), advanced combustion modes (direct-injection, charge stratification, and lean combustion), turbo-charging, and variable valve timing. However, these techniques increase the complexity of vehicle engines and typically offer only marginal benefits.

An alternative approach would be to replace emission-generating internal combustion engines with battery electric power-trains, which emit no harmful pollutants directly. This could be a viable solution if the electricity used to power the vehicles was generated from renewable sources. However, the capacity and working lifespan of currently available batteries are very limited, and the environmental friendly disposal of used batteries is challenging. Therefore, the complete replacement of internal combustion engines with battery electric power-trains is not currently a promising general solution to the environmental problems associated with transportation.

1.1 Motivation

Future legislation requirements for fuel consumption and emissions have prompted efforts to develop new spark ignition (SI) engine technologies. This has resulted in extensive research on Gasoline-Direct Injection (GDI) systems because of their potential to reduce fuel consumption and exhaust emissions. The present injection system needs to provide an improved spray characteristic such as spray penetration length, fuel atomization, droplet sizes and droplet size distribution to enhance a combustion system efficiency. Spray characteristics have a huge influence on the combustion system efficiency because the spray directly controls the dynamics of the combustion process.

To meet the demand of better spray characteristics, fuel injection pressures in GDI systems have been increasing continuously since their introduction to the market in the late 1990s [2]. In the beginning, first-generation fuel injection systems used injection pressures of 5-10 MPa and supported stratified combustion. The spray generated by these injectors are very sensitive to the engine’s operating and thermodynamic conditions; high chamber
pressures reduce the spray angle and penetration [3]. The second drive for increase in fuel injection pressures was the need to improve atomization and mixture formation, which was achieved using second-generation spray-stratified combustion systems in 2006 [4]. Over the last decade, maximum fuel injection pressure has increased from 200 to 250 bar, and more recently, injection pressure up to 300 bar has utilized, achieved through a common rail-system and smaller nozzle. Looking into the potential of high fuel injection pressure, it is expected that fuel injection pressure will increase to 400 bar by 2020 and, 600 bar by 2025. The injection pressure will keep increase, together with related injector modifications such as changes in nozzle geometry and design which could increase fuel efficiency by as much as 4 % [5].

1.2 Challenges

Two major factors controlling fuel/air mixing in GDI engines are the fuel injection system and the nozzle geometry. The evolution of the spray in the injection system begins as the fuel exits the nozzle. The near-nozzle flow typically consists of a liquid core (dense spray) and a dilute spray region. At the boundaries of the liquid core region, the spray breaks up into droplets. This process, known as primary breakup, is poorly understood because it involves a number of complex phenomena. Experimentally, it is difficult to isolate all the physical processes. This complexity becomes even greater at high injection pressures because the relevant events occur on such short characteristic timescales. These problems are exacerbated by the limited optical accessibility of the near-nozzle region, which restricts the scope for experimental determination of spray characteristics.

In the dilute spray region, the liquid core breaks up further into smaller droplets in a process known as secondary breakup, which governs the transition from the dense to the dilute spray regimes. Secondary breakup is crucial for combustion engines because efficient atomization increases the spray’s surface area, enabling faster vaporization under realistic engine conditions.

Spray dynamics are complex multi-scale physical phenomena that are highly sensitive to the injector nozzle geometry (cavitation), nozzle exit conditions (turbulence), and fuel injection pressure. These conditions can change the atomization behavior and course of physical processes of the spray after the nozzle exit. As noted above, the measurement techniques have some limitations (for instance optical accessibility) to incorporate all the physical processes. Also, it is very challenging to isolate all the physical process. On the other hand, Computational fluid dynamics (CFD) simulations offer an alternative way of studying these processes, and are becoming increasingly reliable and effective tools for studying phenomena such as spray injection and its subsequent development. On the other hand, the simulation techniques are becoming an increasingly reliable and effective tool for the detailed study of insight phenomena including spray injection and its subsequent processes. However, due to different scales are involved to address the atomization process and nozzle flow, it is challenging to consolidate the entire phenomenon (atomization and nozzle flow) in single CFD frame work.
At present, direct numerical simulation (DNS) is the only computational method capable of resolving all length scales involved in the atomization process [6]. Unfortunately, its high computational cost largely restricts its use to academic test cases. An alternative method with lesser computational costs, the large-eddy simulation (LES) technique, has been widely used to simulate unsteady multiphase phenomena. LES can accurately capture intrinsically time- and space-dependent phenomena because it directly resolves large-scale turbulent structures and uses a model to describe sub-grid scale structures. Some recent studies [7, 8, 9] clearly highlights the capabilities of LES for the spray atomization. In both commercial and non-commercial CFD codes, LES simulations are commonly performed using a Lagrangian particle tracking (LPT) approach to model the dispersed spray droplets. In this approach, bunches of droplets with identical properties are represented as parcels (numerical particles) that are tracked by the Lagrangian method. This method represents the multi-dimensionality of fuel sprays exceptionally well. However, its accuracy depends strongly on the number of parcels per second in the simulated injection; large numbers of parcels are required to describe spray dynamics well.

In this work, the LES-LPT approach was used to model fuel sprays consisting of discrete sets of computational parcels whose evolution depends on the exchange of mass, momentum, and energy with the continuous gas phase, which was modeled using an LES approach. Additional sub-models were used to describe the processes of liquid jet atomization, droplet breakup, droplet dispersion, and transfers of momentum and kinetic energy. Internal nozzle flow is not simulated since the focus is away from the nozzle.

1.3 Objective and thesis outline

The objective of this work is to quantify the effects of fuel injection pressure on the characteristics of sprays formed at high pressures in a constant volume spray chamber rig. Numerical simulations with three different nozzle hole geometries (divergent, convergent, and straight) were performed to understand how nozzle geometry influences the spray characteristics at such high injection pressures, and compare with the experimental data. The comparison of the measurement data with the numerical model allows, on the one hand, the validation of the models at such higher-pressure injection conditions and facilitate the integration of such advanced injection systems into future gasoline engines, on the other hand, it helped to enlighten over the reliability of the measurement preformed.

This thesis is divided into five sections. This introductory section is followed by section 2, which describes the modeling strategy in more detail. Section 3 explains the simulation set-up, including the studied nozzle types and operating conditions, mesh generation procedure, and numerical setup. Section 4 presents results relating to spray penetration, spray shape, droplet size and distribution, breakup point correlations, and spray velocities. Finally, section 5 summarizes the conclusions that were drawn.
2 Modeling approach

In CFD, three well-established fundamental methods are available with their own strengths and weaknesses. First is the Reynolds-Averaged Navier-Stokes (RANS) technique, which has been used extensively in spray simulations [10, 11, 12]. This technique resolves the time-averaged Navier-Stokes and provides an access to the time averaged mean quantities with considerable computational cost. Its time averaging nature limits its use for global predictions only, and therefore, it cannot be used to investigate the transient behavior. Second method is the DNS, which resolves all length scales involved in a spray development. However, DNS is computationally very expensive. Finally, a less computationally demanding technique is large-eddy simulation (LES), which solves large-scale structures but models small-scale structure. The ability of each technique to resolve the length scale involved the typical flow is shown in figure 2.1.

![Figure 2.1: Length scales resolved and modeled by different numerical techniques.](image)

2.1 Fluid motion

Spray modeling is complex because it requires simultaneous treatment of the liquid and gas phases and the interactions between these two phases. The gas phase is usually modeled using a Eulerian approach, while the liquid phase is handled using the Lagrangian particle tracking (LPT) method. The interaction between both phases are accounted for by using an additional source term in the Eulerian gas phase conservation equation. The numerical simulations presented here were conducted using the LES method, in which the flow is described using the following governing equations for mass (2.1), momentum (2.2) and energy (2.3):

\[ \text{(Equation 2.1)} \]

\[ \text{(Equation 2.2)} \]

\[ \text{(Equation 2.3)} \]
\[
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial (\bar{\rho} \bar{u}_j)}{\partial x_j} = S_{ev}, \tag{2.1}
\]

\[
\frac{\partial (\bar{\rho} \tilde{u}_i)}{\partial t} + \frac{\partial (\bar{\rho} \tilde{u}_i \tilde{u}_j)}{\partial x_j} = \frac{\partial \bar{\tau}_{ij}}{\partial x_j} + \frac{\partial \tau_{ij}^{sgs}}{\partial x_i} - \frac{\partial \bar{p}}{\partial x_i} + S_{i,m}, \tag{2.2}
\]

\[
\frac{\partial (\bar{\rho} \tilde{h})}{\partial t} + \frac{\partial (\bar{\rho} \tilde{h} \tilde{u}_j)}{\partial x_j} + \frac{\partial (\bar{\rho} K \tilde{u}_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \alpha_{eff} \frac{\partial \tilde{h}}{\partial x_j} \right) + \frac{\partial (\bar{\rho} \tilde{u}_j)}{\partial x_j} + S_h. \tag{2.3}
\]

Here, overline denote Reynolds averaged and tilde show Favre filter quantities, with relation \( \tilde{q} = \bar{p} \bar{q} / \bar{\rho} \). Within the governing equations, \( \rho \) denotes the density, \( u_j \) is flow velocity vector, \( p \) is pressure, \( K \) is kinetic energy, and \( \tau_{ij} \) is the viscous shear stress. The effective diffusivity \( \alpha_{eff} \) is calculated by addition of laminar and turbulent thermal diffusivity. In the mass conservation equation, the source term \( S_{ev} \) is added for the fuel evaporation, however, present study is based on non-evaporative spray, so \( S_{ev} \) is neglected. The momentum source term \( S_{i,m} \) represents the force that the droplets strives on the gas phase, while the heat transferred from the liquid phase is accounted for by the energy source term \( S_h \). The unresolved sub-grid stress \( \tau_{sgs} \) is modeled using the standard Smagorinsky model [13], expressed as:

\[
\tau_{ij}^{sgs} = -2 \bar{\rho} \nu_T (\tilde{S}_{ij} - \frac{1}{3} \delta_{ij} \tilde{S}_{kk}), \tag{2.4}
\]

\[
\nu_T = C_s^2 \Delta^2 \sqrt{2 \tilde{S}_{ij} \tilde{S}_{ij}}, \tag{2.5}
\]

\[
\tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right). \tag{2.6}
\]

Here, \( \nu_T \) is the turbulent viscosity, \( \delta_{ij} \) is the Kronecker delta, and the Smagorinsky constant \( C_s \) is set to 0.2. The grid size \( \Delta \) was calculated using the cubic root of the cell volume. The Sutherland law was used to calculate the dynamic viscosity, and the state of the gas was computed using the relations for an ideal gas:

\[
\bar{\rho} = \bar{\rho} R \bar{T}, \quad C_v = \frac{R}{\gamma - 1}, \quad C_p = C_v + R. \tag{2.7}
\]

The specific heat capability at constant pressure and constant volume are indicated by \( c_p \) and \( c_v \), respectively.
2.2 Droplet motion

A real spray contains very large number of droplets, and solving the equations of motion for each droplet would be very expensive. Therefore, multiple droplets with identical properties are grouped together into a single term ‘parcel’. In parcel approach, each parcel represents an average droplet/particle at a given point, therefore, it can handle very large number of droplets with a reasonable computational power.

In the simulations, liquid fuel parcels are injected at very high injection pressures into a quiescent gas environment, then the liquid parcels start to be decelerated by interactions (drag) with the gas phase. This results in an exchange of momentum between the gas and liquid phases, mainly due to their different relative velocities. This exchange of momentum is evaluated by assuming that the drag force acting on a liquid parcel is:

\[
\frac{1}{6} \rho_p \pi d^3 \frac{du_p}{dt} = \frac{1}{2} (u_g - u_p)(u_g - u_p) \rho_g C_D \frac{\pi d^2}{4},
\]

where, \(d\) is the droplet diameter, \(\rho_p\) is the particle density, \(u_p\) is the particle velocity, \(\rho_g\) is the gas density. The gas velocity \(u_g\) is interpolated to the particle position from the adjacent cells, and \(C_D\) is the coefficient of drag force acting on a droplet, defined as:

\[
C_D = \frac{24}{Re_p} \left(1 + \frac{1}{6} Re_p^{2/3}\right) \text{ for } Re_p < 1000,
\]

\[
C_D = 0.424 \quad \text{for } Re_p > 1000.
\]

The Reynolds number of the particle is calculated using the viscosity of the gas \(\nu_g\), as:

\[
Re_p = \frac{|u_g - u_p| d}{\nu_g}.
\]

The position of parcels \(x_p\) with respective to time \(t\) is updated by \(dx_p/dt = u_p\).

2.3 Droplet break-up model

Spray atomization can be divided into two main steps: primary break-up of the liquid jet and secondary break-up of the droplets and ligaments. In this work, primary break-up is described using the blob method [14], in which blobs of diameter equal to the nozzle diameter are injected and the number of droplets injected per unit time is calculated based on a predicted mass flow rate profile. In this way, a detailed simulation of near-nozzle phenomena is replaced by the injection of large spherical droplets that break-up into smaller droplets during secondary break-up. A schematics of the blob injection method is shown in figure 2.2.
For the secondary break-up, the well-known Kelvin-Helmholtz Rayleigh-Taylor (KH-RT) model [15, 16] is chosen based on the fact that a spray of high-pressure fuel injection lies in a break-up regime of a high Weber number. This model combines both Kelvin-Helmholtz (KH) and Rayleigh-Taylor (RT) instabilities. Schematics of the KH and RT breakup is shown in figure 2.3.

In KH instability, the breakup of fuel injected at higher velocities is independent of initial radius of the liquid jet, and the unstable growth of perturbations at the liquid-gas interface is attributed to shearing between the fluids. The break-up is calculated based on the wavelength of the fastest growing instabilities due to aerodynamic forces. The fastest growing wave ($\Lambda_{KH}$) and growth rate ($\Omega_{KH}$) are expressed numerically as:

$$\Lambda_{KH} = 9.02 \frac{r_d(1 + 0.45 \, Oh^{1/2})(1 + 0.4 \, Ta^{0.7})}{1 + 0.865 \, We^{1.67}},$$

(2.12)

$$\Omega_{KH} = \frac{(0.34 + 0.038 \, We^{3/2})}{(1 + Oh)(1 + 1.4 \, Ta^{0.6})} \sqrt{\frac{\sigma}{\rho_d \, r_d^3}},$$

(2.13)
Where, $We = \rho_g |u_d - u_g|^2 r_d / \sigma$ is the Weber number, $Oh = \sqrt{We/Re}$ is the Ohnesorge number, $Ta = Oh \sqrt{We}$ is the Taylor number, $r_d$ is the droplet radius, $u_d$ is the droplet velocity, and $\sigma$ is the surface tension of liquid droplet. After the KH breakup, the critical droplet radius $r_{\text{crit}}$ is the size of new droplets, which is assumed proportional to the wavelength of the fastest growing or most probable unstable surface wave $\Lambda_{KH}$, such as:

$$r_{\text{crit}} = B_0 \Lambda_{KH},$$

where $B_0$ is a breakup constant. The breakup time $\tau_{KH}$ controls the breakup rate and is a function of the growth rate ($\Omega_{KH}$) and the fastest growing wave ($\Lambda_{KH}$), such as:

$$\tau_{KH} = \frac{3.76 B_1 r_d}{\Lambda_{KH} \Omega_{KH}},$$

where $B_1$ is a breakup constant. The change of radius of the original droplets can be calculated using the following expression:

$$\frac{dr_d}{dt} = -\frac{r_d - r_{\text{crit}}}{\tau_{KH}}.$$

Rayleigh-Taylor instability waves originate from acceleration normal to the droplet-gas interface on the surface of droplet. The RT breakup occurs, if the fluid is accelerated in a direction different to that of the density gradient. When liquid ligaments are decelerated by drag in the gas phase, instability may grow on trailing edge of the droplet. Therefore, RT breakup is controlled by the rate of disturbance growth on the surface of the droplet. The fastest growing wave ($\Omega_{RT}$) and wavelength ($\Lambda_{RT}$) are given by:

$$\Omega_{RT} = \sqrt{\frac{2 |g_t(\rho_l - \rho_g)|^{1.5}}{3\sqrt{3\sigma} (\rho_l - \rho_g)}}, \quad \text{with}$$

$$g_t = (g - \frac{du_d}{dt}) \cdot \frac{u_d}{|u_d|},$$

$$\Lambda_{RT} = 2\pi c_0 \sqrt{\frac{3\sigma}{|g_t(\rho_l - \rho_g)|}}.$$

Here, $g$ is the gravitational force and $c_0$ is a modeling parameter. Two criteria determine the outcome of RT breakup: if the wavelength of the fastest growing wave is smaller than the droplet diameter and perturbations are allowed to grow for some time, the droplet will be replaced by a parcel of smaller droplets when the growth time exceeds the typical RT time. The RT breakup time is given by:

$$\tau_{RT} = \Omega_{RT}^{-1}.$$
For KH breakup, the stripped mass of parcels will be allocated to a new parcel (with a radius of $r_{crit}$) when the total stripped mass exceeds some proportion of the original mass of parcel. For RT breakup, the number of parcels will be unchanged, but the post-breakup parcels will contain more and smaller identical droplets.

In the simulations, droplet breakup is occurs via the mechanism that predicts the shortest breakup time. The Kelvin-Helmholtz mechanism usually dominates near the nozzle exit, while the Rayleigh- Taylor mechanism becomes dominant further downstream. The model is described in more detail elsewhere [17]. The model parameters used in this work are summarized in table 3.4.
3 Computational set-up

3.1 Nozzle type and operating condition

In this work, three axisymmetric nozzle configurations were considered in the simulations: divergent, convergent and straight, with exit hole diameters of 380, 148, and 114 µm, respectively. Despite their different geometries and exit diameters, all three nozzles are designed for same mass flow rates (15 mg/ms at 20 MPa). The internal nozzle flow was not considered in the simulations, but the effect of nozzle geometry was accounted for in the simulation setup. Details of the nozzle geometries are presented in table 3.1.

<table>
<thead>
<tr>
<th>Hole shape</th>
<th>Injector-1</th>
<th>Injector-2</th>
<th>Injector-3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nozzle shape</td>
<td>Divergent</td>
<td>Convergent</td>
<td>Straight</td>
</tr>
<tr>
<td>Exit hole diameter</td>
<td>380 µm</td>
<td>148 µm</td>
<td>114 µm</td>
</tr>
<tr>
<td>Flow rate</td>
<td>15 mg/ms at 20 MPa</td>
<td>15 mg/ms at 20 MPa</td>
<td>15 mg/ms at 20 MPa</td>
</tr>
<tr>
<td>L/D ratio</td>
<td>5.5</td>
<td>5.5</td>
<td>5.5</td>
</tr>
</tbody>
</table>

Table 3.1: Specifications of the injector nozzles considered in the simulations and experiments.

Simulations of injections at pressures between 20 and 150 MPa were performed for all three nozzles. The operating conditions considered in the simulations are summarized in table 3.2.
<table>
<thead>
<tr>
<th>Fuel</th>
<th>n-heptane</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chamber gas</td>
<td>air</td>
</tr>
<tr>
<td>Chamber temperature [K]</td>
<td>293</td>
</tr>
<tr>
<td>Chamber pressure [MPa]</td>
<td>0.1</td>
</tr>
<tr>
<td>Fuel injection pressure [MPa]</td>
<td>40, 60, 80, 100, 120, 150</td>
</tr>
<tr>
<td>Injection duration [ms]</td>
<td>≈ 3</td>
</tr>
<tr>
<td>Injection mass [mg]</td>
<td>54</td>
</tr>
</tbody>
</table>

Table 3.2: Operating conditions considered in the simulations.

Figure 3.1: (a) Top view and, (b) 3D view of cylinder mesh.

3.2 Computational mesh

Spray simulations using LES turbulent modeling require high quality meshes. Moreover, mesh-induced errors, numerical instabilities, and numerical dissipation should be minimized to obtain an accurate numerical solution. The complete meshing work was performed using the OpenFOAM meshing tool blockMesh. The computational domain was a closed cylinder of length 120 mm and diameter 180 mm. The spray chamber grid consisted of almost equidistant hexahedral cells. The total number of parcels and grid resolution were determined based on previous parcel and grid sensitivity studies [18, 19, 20]. The total mass of the liquid fuel (about 54 mg) was injected via 4e7 parcels in the simulations. The average grid cell size of the central-square zone inside the chamber was 0.5 mm. The grid size then increased to 1.0 mm towards the chamber surface, resulting in a total number of cells equal to 24 million. The fuel is injected from the center of the top-plane (the x,y-plane) of the domain in the z-direction. A top view of the spray chamber, and a 3D view of the full cylinder mesh is shown in figure 3.1 (a) and 3.1 (b), respectively.
3.3 Numerical set-up

All the simulations were performed using OpenFOAM-2.2.x [21]. An implicit, second-order backward scheme is applied for the time discretization. The convective scalar fluxes of momentum were treated with a second-order accurate central differencing scheme. Zero-gradient boundary conditions were applied for all scalar quantities at walls. In all simulation cases, liquid fuel (n-heptane) is injected into the constant volume spray chamber under atmospheric conditions (T=293 K and p=0.1 MPa). Initially, there was no gas-phase flow inside the chamber. Gas-phase recirculation zones and turbulence were created through the momentum transfer from the liquid jet to the gas-phase. The injected mass through the nozzle for all injection pressure cases was taken from experimentally determined mass flow rate profiles. For all cases, the number of parcels injected per second was set to 4e7, and the coefficient of discharge and half cone spray angle varied with the nozzle geometry, as suggested by experimental spray images for the studied injection pressures. The numerical spray set-up parameters are summarized in the table 3.3.

<table>
<thead>
<tr>
<th>Nozzle</th>
<th>Divergent</th>
<th>Convergent</th>
<th>Straight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Discharge Coef.</td>
<td>0.95</td>
<td>0.7 to 0.9</td>
<td>0.7 to 0.9</td>
</tr>
<tr>
<td>Parcel per sec.</td>
<td>4e7</td>
<td>4e7</td>
<td>4e7</td>
</tr>
<tr>
<td>Spray angle (half cone angle)</td>
<td>Constant</td>
<td>Variable</td>
<td>Variable</td>
</tr>
<tr>
<td>8.8°</td>
<td>5 to 9°</td>
<td>5 to 9°</td>
<td></td>
</tr>
</tbody>
</table>

Table 3.3: A summary of numerical spray set-up parameters.

<table>
<thead>
<tr>
<th>Type</th>
<th>Model</th>
<th>Constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>Injector</td>
<td>Multi-hole injector</td>
<td>6 holes, $D_0 = 380 \mu m$</td>
</tr>
<tr>
<td>Primary break-up</td>
<td>Uniform droplet size</td>
<td>$380 \mu m$</td>
</tr>
<tr>
<td>Secondary break-up</td>
<td>KH-RT</td>
<td>$B_0 = 0.61, B_1 = 40, C_0 = 1, C_1 = 0.1, n=3$</td>
</tr>
<tr>
<td>Droplet distribution</td>
<td>Rosin-Rammler</td>
<td></td>
</tr>
<tr>
<td>Dispersion model</td>
<td>Stochastic dispersion</td>
<td></td>
</tr>
</tbody>
</table>

Table 3.4: Sub-models used in the simulation.

All of the simulated sprays were non-reactive and non-evaporating. The sub-models used in the simulations are summarized in table 3.4. A multi-hole injector with all nozzles (either 6 or 8 nozzles) was simulated. Primary break-up and secondary break-up were modeled using the blob injection model and KH-RT model, respectively. Large blobs of diameter equal to the nozzle exit diameter were injected at the start of each simulation. The Rosin-Rammler distribution function [22] was used to describe the droplet distribution inside the spray jet, and a stochastic dispersion model was used to account for turbulent fluctuations in droplet trajectories. The spray model was tuned for one case (100 MPa for each nozzle) by varying the value of discharge coefficient ($C_d$) and spray jet angle, in
such a way that it accurately reproduces the experimental spray penetration length.
4 Results and Discussion

In the present study, the results of spray characteristics under higher fuel injection pressures were compared with the experimental findings. In particular, the computed liquid penetration length, spray structure, droplet size and distribution, and spray velocity were presented under the operating conditions summarized in table 3.2.

4.1 Spray penetration

Figure 4.1 compares the measured and calculated spray penetration for the three nozzles as a function of the time for fuel injection pressures of 40, 100, and 150 MPa. The spray penetration length is defined here as the distance between the nozzle tip and the farthest point of the spray tip along the injector axis (vertical axis of spray chamber). Experimentally measured spray penetration length is estimated from optical images by applying a post-processing technique based on a pixel-based threshold filter. Each measured data point shown in figure 4.1 represents an average of 20 injection shots; the shaded band shows the standard deviation of the experimental data. The spray model was tuned only for one case (100 MPa) for each nozzle in such a way that it accurately reproduces the experimental spray penetration length.

Simulations at the other injection pressures of each nozzle followed the same tuned values, only the different mass flow rate profile was provided. The calculated spray penetration lengths for all nozzle and injection pressures were in good agreement with experiment. This indicates that the exchange of momentum between the liquid and gas phases was modeled accurately. It also demonstrates that the aerodynamic forces acting on the droplets, which strongly influence the atomization process, were also well described. Overall, the spray-tip penetration results clearly indicate that increasing the fuel injection pressure increases spray penetration and reduces injection duration.

The divergent nozzle shows the gradual rise of penetration for all the injection pressure, which indicates that the spray has gone through the secondary breakup. However, in the convergent and straight hole nozzle, penetration curve looks very steep. This suggested that the spray has not sufficiently gone through the secondary breakup and indicates the presence of strong liquid core.

4.2 Spray shape

Figure 4.2 compares high-speed camera images of spray formed at two time points (0.318 and 0.53 ms) after start of injection (aSOI) and the corresponding calculated spray shapes for all three nozzles at injection pressures of 40, 100, and 150 MPa. The measured images are the averaged images of 20 shots. All spray jets were taken into account for the appropriate comparison with experimental images. The computed results show that the overall spray shape is well predicted by the model.
Figure 4.1: Comparison between experimental (dots) and simulated (solid lines) for three different nozzles at injection pressures of 40, 100 and 150 MPa. The filled areas indicate the experimental standard deviations.

It should be noted that the gas in the chamber initially is at rest. The spray demonstrates strong transient behavior as it penetrates into this quiescent environment. The flow is mainly driven by the momentum of the droplets. Larger droplets stay longer in the center of the jet due to their inertia, while smaller droplets are more dispersed to the sides. The near-nozzle region of the spray looks very dense, but the jet becomes dilute further.
downstream. The simulated spray shape also indicated that the droplets are randomly distributed around the spray jets and spray tip region. Moreover, when the droplets are injected, a recirculation zone is created by momentum exchange between the gas and liquid phases.

Figure 4.2: Comparison between measured and calculated spray images for divergent, convergent and straight hole nozzles at 0.318 and 0.53 ms aSOI at injection pressures of 40, 100, and 150 MPa.

Sprays generated with the divergent hole nozzle appear to be wider and to have more radially disperse tips than those for the other nozzles. This may be because the divergent nozzle generates a higher and more stable spray-jet angle. In experimental images, near spray tip zone of divergent nozzle appear to be rather blunt, which suggested the extensive radial dispersion of droplets. This radial dispersion of droplets appears to increase steadily and survive for a long time as the spray progresses downstream. However, the numerical model predicts a narrower spray tip than was observed experimentally.

The convergent and straight hole nozzles produced comparatively narrow spray jets because both nozzles have smaller nozzle exit diameters than the divergent nozzle. The simulation result shows that the liquid droplets are decelerated, particularly near the spray tip region, which could possibly induce the small vertex like structures. This deceleration of droplets results in an enhancement of radial dispersion of droplets, causing the spray near the tip become wider in shape compared to the spray of previous time as well as
spray jet of divergent nozzle of respective time. The radial dispersion of the droplets is increased with the injection pressure. The simulation also shows the similar radial dispersion of droplets at around spray jet.

It is interesting to see the spray jet structure looks different at the same time for each nozzle with respect to the injection pressure. The possible reason is the different spray jet angle for each nozzle. The injection pressure appears to affect the spray penetration length more than the spray structure; the convergent and straight nozzles appear to yield significantly higher penetration than the divergent nozzle at any given injection pressure.

### 4.3 Droplet size and distribution

Figure 4.3 compares measured and calculated droplet sizes in terms of the arithmetic mean droplet diameter (D10) and Sauter mean diameter (SMD or D32) for all three nozzles and injection pressures. The measured mean diameters shown are the time-averaged droplet diameters at the probe location (80 mm downstream of the injector tip). In general, the numerical model accurately captures the mean diameters for all nozzles at all injection pressures.

![Figure 4.3: Comparison between measured and calculated mean diameter for three different nozzle at all considered injection pressures, right: arithmetic mean diameter (D10), left: Sauter mean diameter (D32).](image)

The results clearly demonstrate that the size of the fuel droplets decreases by increasing the fuel injection pressure, irrespective of nozzle shape. Moreover, the droplet diameters (both D10 and D32) for the divergent nozzle exceed those for the other nozzles, irrespective of injection pressure. However, the arithmetic mean droplet diameter (D10) varies less at higher injection pressures than the SMD. This is probably because at high injection pressures, droplets more quickly reach to saturation state with sufficiently small diameter, when their diameter is so small that they are stable and do not show further secondary break-up. However, the Sauter mean diameter (D32) significantly reduces at higher the
injection pressures. The SMD is very sensitive in nature to the presence of larger droplets. This means higher injection pressure drastically reduces the larger droplets comes from initial stage. The decrease in SMD value means large contact surface area of the droplets, and thus faster evaporation under real engine conditions. The simulation result shows the

Figure 4.4: Comparison between measured and calculated droplet size distributions for the three nozzles at injection pressures 40, 100, and 150 MPa.

higher values of the mean droplet diameters (D10 and D32) in the very beginning (not shown) because of the primary atomization which is modeled by the assumption of the
initial droplet diameter being equal to the nozzle exit diameter. Moreover, during the initial stage of the atomization process, the aerodynamic interactions between the air and fuel are relatively weak.

Besides the droplet mean diameters, the droplet size distribution within a spray is of crucial importance for the atomization process. In this work, the local droplet size distribution was measured experimentally in a cross-section of two intersecting lasers beams 80 mm downstream of the injector tip. The measurements were acquired when the injector needle was fully open, so the contribution of the large initial droplets was not accounted. In the simulation, nearly same sampling point with a radius of 2 mm is considered. Figure 4.4 presents a quantitative comparison of local droplet size distributions for the sprays by all nozzle at different fuel injection pressures. Reasonably well agreement between experimental and simulated size distributions is observed for all injection pressures.

For all three nozzles, the droplet size distribution curves at 150 MPa injection pressure indicated that the highest probability of smaller droplets ranging between 3 to 7 µm. At this injection pressure, the droplet size distributions profile also look very narrow towards the smaller droplets compared to the droplet distributions at other injection pressures. The distribution profiles confirm the previously reported finding that the droplet sizes decrease as the fuel injection pressure increases, irrespective of nozzle shape. Accordingly, the proportion of smaller droplets in the 100 MPa case is lower than in the 150 MPa case but higher than in the 40 MPa case. Furthermore, the droplet size distributions at pressures 40 MPa shows comparatively higher probability of large droplets. The droplet size distribution curves look more widely distributed and are biased towards large droplet sizes (right side).

The droplet size distributions for the divergent nozzle indicate that it produces higher droplet diameters than the convergent and straight hole nozzles at the same injection pressures. At this point, this very hard to explain this phenomenon. Moreover, the droplet size distributions for the convergent and straight hole nozzles at injection pressures of 100 and 150 MPa are quite similar, which indicates that raising the injection pressure above 100 MPa may not result in further improvements to spray atomization. It may possible that the droplet size reached to the saturation at 100 MPa, and all the energy gained from the injection pressure would be converted into horizontal velocities, which is clearly visible in the spray structure.

4.4 Breakup point correlation

For the divergent nozzle, the development of the spray penetration length can be divided into two phases that are distinguished by a change of the slope, as described by Hiroyasu [23]. Figure 4.5 illustrates the estimation of break-up point. The first phase starts at the beginning of injection ($t = 0$, needle starts to open) and ends when the liquid jet emerging from the nozzle hole begins to break ($t = t_{break}$). Because of the small needle lift and the high mass flow in the beginning of injection, the first jet breakup need not always occur
immediately after the liquid leaves the nozzle. During this time, penetration increases linearly over time. During the second phase ($t > t_{\text{break}}$) the spray tip consists of smaller droplets, and the tip velocity is smaller than in first phase. The spray tip continues to penetrate the gas with high kinetic energy, with slower droplets at the tip due to high exchange of momentum with the gas. Note that needle movement was not considered in the simulations. Figure 4.6 shows the calculated breakup time for the divergent nozzle at different injection pressures.

![Figure 4.5: The estimation of break-up point as suggested by Hiroyasu [23].](image)

For the convergent and straight hole nozzles, the spray penetration length was almost linear for all injection pressure, straight hole with 40 MPa case is exceptional. This behavior indicates the presence of strong liquid core with sufficiently high velocity.

![Figure 4.6: Comparison between measured and simulated breakup times for the divergent nozzle at different injection pressure.](image)
4.5 Spray-induced velocities

Numerical calculation usually needs the experimental data for the validation. Unfortunately, no experimental spray velocity measurements data were available for the investigated nozzles. Figure 4.7 shows the spray-induced axial velocity of the spray jet for all injector nozzles at injection pressure of 40, 100, and 150 MPa. Note that the axial velocity is calculated in the spray direction at the fully developed stage.

The axial velocity for the divergent nozzle appears to be almost constant throughout the spray. At 100 MPa injection pressure, the axial velocity is almost similar to that at 150 MPa injection pressure case. It might be based on the fact that the droplet size in both cases are very similar.

Figure 4.7: Axial velocity of the spray jet for different nozzle at different injection pressure.

On the other hand, velocity induced by the convergent nozzle spray exhibited more curious behavior. At all injection pressures, it show a very steep axial velocity gradient in the near-nozzle region. A similar trend was observed for the straight hole nozzle spray. The higher velocity in the beginning part indicates that the spray jet has a strong liquid core with very high velocities. This is also demonstrated by the spray penetration length curves for the convergent and straight hole nozzles.

Figure 4.8 shows the spray-induced radial velocity of the spray jet for all injector nozzles at 40, 100, and 150 MPa injection pressure at locations 20 and 50 mm downstream of the nozzle tip. The velocity profiles for the divergent nozzle appear to be wider than those for the other nozzles, keeping in mind the divergent nozzles has larger spray-jet angle (not shown). The velocities observed at the two measurement locations were very similar.

In contrast, the velocities for the convergent nozzle were almost twice those for the divergent nozzle at the same injection pressure. Moreover, the velocity profiles of convergent nozzle show a narrow radial distribution compared to divergent nozzle. The magnitude of
the radial velocity in the convergent case was lower further downstream, as also observed for the axial velocity. Similar observations were noted for the straight hole nozzle. It is worth noting that the radial velocity profiles for the convergent and straight hole nozzles were similar at all injection pressures.
5 Summary/conclusion

The main aim of this work was to investigate and understand the impact of gasoline sprays formed at injection pressures of 40 to 150 MPa by studying spray characteristics such as the penetration length, spray shape, droplet mean diameter, and droplet size distribution using an LES-LPT simulation model. An additional goal was to evaluate the predictive accuracy of the model. The LES simulation results were compared to experimental data, yielding the following conclusions:

- The model accurately predicts the spray tip penetration length for all investigated injection pressures. It correctly predicts an increasing penetration length with increasing injection pressure. The droplet break time moderately influenced by the higher injection pressure.

- The numerical model accurately reproduced the global spray shapes observed experimentally. Different nozzle geometries produced distinct spray structure at diverse injection pressures. As the injection pressure increased, smaller droplets became more widely distributed in the computational domain and shows more radial dispersion for all the nozzles.

- The predicted D10 and D32 values agreed well with experiment for all nozzle types. The SMD is significantly reduced by increased pressure compared to the arithmetic mean diameter values. Additionally, the convergent and straight hole nozzles exhibited steeper reductions in droplet diameter than the divergent nozzle.

- The simulated droplet size distributions agreed well with experiment and confirmed that droplet size decreases as the injection pressure increases. The droplet breakup time is considerably reduced when compare the lowest pressure to highest investigated pressure.

- The divergent nozzle exhibited a uniform velocity profile along the spray axis. In contrast, the convergent and straight hole nozzles produced very high velocities near the injector nozzle that decreased on moving towards the spray tip. This indicates the presence of a strong liquid core in the spray.
6 Future work

The overall objective of the present ongoing work is to investigate the potential of high-pressure fuel injection to improve of the fuel-air mixing in the engine cylinder through the Large-eddy simulation method. In the first phase, the impact of high pressure injection on spray characteristics through the different nozzle geometry type is investigated. The next steps of the project are as follows:

- **Investigation of spray-induced turbulence and entrainment**: In this part, investigation will be done to quantify the impact of high pressure injection in terms of spray-induced turbulence and air entrainment in the spray.

- **Investigation of mixture formation in a GDI engine**: In this part, cold flow LES simulation will be performed with spray injection at different pressure on the optical research engine. The focus will be on the fuel-air mixture formation.

- **Full cycle LES simulation with spray and combustion**: In this part, based on fuel-air mixture formation study, LES simulation will be performed to investigate the behaviour of the combustion process.
Bibliography


