Secondary Atomization Modelling of High Pressure Electrostatically Charged Diesel Fuel Sprays

G. H. Amine-Eddine∗, J. S. Shrimpton, and A. Kourmatzis†
Energy Technology Research Group
University of Southampton
Southampton, UK

Abstract
Electrostatic atomization presents itself as a novel way to improve fuel spray characteristics and dynamics prior to combustion. Pertinent to high pressure fuel injection systems typically employed within automotive and marine sectors, potential improvements include the creation of finer spray droplets through the promotion of secondary atomization, increased droplet dispersion due to electrostatic repulsion forces, and as a consequence, increased spray evaporation rates when subjected to elevated engine temperatures. These improvements are particularly advantageous for achieving combustion efficiency and reducing soot emissions. However, to evaluate the impact of electrostatic fuel atomization on the design, development, and optimization of high pressure fuel injection systems, there is the need for a cost-effective and reliable CFD methodology that can predict charged high pressure spray behaviour.

In this paper, a 2D Eulerian-Lagrangian code is used to evaluate a numerical methodology designed for the simulation of high pressure electrostatically atomized Diesel fuel sprays. A secondary atomization model, modified to include the effects of electrical charge on droplet deformation and breakup mechanisms, is examined through simulations and validated in relation to spatial statistics obtained from experimental phase Doppler anemometry measurements.

Spray dispersion rates examined qualitatively during the transient initial injection period were observed to increase in charged sprays at the cost of decreased spray penetration rates. Droplet diameter PDFs sampled at centreline downstream locations within computed uncharged sprays, show a distinct evolution from a bi-modal, to uni-modal droplet size distribution as spray injection velocities increase. For computed charged sprays, PDFs sampled at the same locations are all uni-modal, with a single peak for droplet diameters present within the range 0.1-0.25D/d_{inj}. Droplet axial velocity profiles from simulated charged sprays show reasonable agreement with corresponding experiments, with average percentage errors between profiles ranging from 16.2% to 27.5%.
Introduction

Fuel spray behaviour, including the dynamics of breakup, dispersion and penetration all have a strong influence on the performance, and efficiency of combustion processes. High pressure fuel injection systems typically employed within automotive, aerospace, and marine sectors, have existing capabilities in benefiting these combustion processes. However, with rising costs of fuel and the tightening of emissions legislation, comes an increasing demand for engine manufacturers to seek technologies that help to reduce fuel consumption and harmful air pollutants in their newly developed engines. One solution, is the use of charged injection technology, which via the process of electrostatic atomization, presents itself as a novel way to improve fuel spray characteristics and dynamics prior to combustion.

When electrically insulating dielectric liquids are subjected to charged injection at high hydrodynamic pressures, the increase in flow-rate allows for greater levels of charge to be imparted to the spray. Recent experiments by Kourmatzis et al. [1] have reached spray specific charge levels of $6 \text{C/m}^3$, at elevated injection pressures ranging 15-35bar, which corresponds to injection velocities of 40-50m/s for a nozzle orifice of diameter 125$\mu$m. At these elevated injection conditions, spray processes such as secondary atomization start to dominate. This process is promoted further by the high levels of charge on droplets, acting to decrease their stability and increase their likelihood of breakup.

Despite these potential benefits, there yet exists a reliable CFD methodology that can successfully predict the behaviour of charged high pressure sprays. In this paper, we present a methodology that achieves this aim.

Experimental Spray Characteristics

In order to make reliable CFD predictions of charged high pressure sprays, we need to be certain about the accuracy of numerical methodologies used. To achieve this, simulated CFD sprays are set-up to reflect the conditions present in selected experimental sprays from the investigation presented by Kourmatzis et al. [1]. A summary detailing the operating conditions of these experiments are listed in Table 1, along with liquid properties for the Diesel fuel used listed in Table 2.

The primary investigation of Kourmatzis et al.[1] was to assess the electrical and atomization performance of a plane-plane type, charge injection atomizer illustrated in Figure 1, at pump pressures ranging from 15 to 35 bar. Such pressures correspond to injection velocities of up to 50m/s, and due to these high injection velocities present, spray specific charges up to $6 \text{C/m}^3$, were successfully injected into the spray. Spay specific charges at such a level had never been achieved previously, with implications considered significant in terms of advancing electrostatic atomization technology towards industrial application within existing high pressure spray systems.

<table>
<thead>
<tr>
<th>Case</th>
<th>$U_{inj}$ (m/s)</th>
<th>$\dot{m}$ (kg/s)</th>
<th>$Q_v$ (C/m$^3$)</th>
<th>$Re_j$</th>
<th>$We_j$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1P</td>
<td>37</td>
<td>0.38</td>
<td>6</td>
<td>1943</td>
<td>5750</td>
</tr>
<tr>
<td>2P</td>
<td>40</td>
<td>0.41</td>
<td>6</td>
<td>2100</td>
<td>6720</td>
</tr>
<tr>
<td>3P</td>
<td>48</td>
<td>0.49</td>
<td>5.5</td>
<td>2520</td>
<td>9677</td>
</tr>
</tbody>
</table>

Table 1. Operating conditions for charged high pressure spray cases from experiments of Kourmatzis et al. [1]. For all spray cases Diesel fuel was used, the orifice diameter was $d_{inj} = 125\mu$m, and the surrounding gas density throughout the spray was 1.184kg/m$^3$.

<table>
<thead>
<tr>
<th>Property</th>
<th>Diesel</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density, ($\rho_d$) $kgm^{-3}$</td>
<td>840</td>
</tr>
<tr>
<td>Dynamic Viscosity, ($\mu_d$) $kgm^{-1}s^{-1}$</td>
<td>0.002</td>
</tr>
<tr>
<td>Surface Tension, ($\sigma$) $Nm^{-1}$</td>
<td>0.025</td>
</tr>
<tr>
<td>Relative Permittivity, ($\epsilon_r$)</td>
<td>2.0</td>
</tr>
<tr>
<td>Electrical Conductivity, ($k$) $pSm^{-1}$</td>
<td>5.0</td>
</tr>
</tbody>
</table>

Table 2. Properties of Diesel fuel at 293K unless otherwise stated.
ments taken along the spray centreline. On this matter, a bi-modal PDF was present at locations closer to the nozzle exit orifice, for both cases 1P and 2P of Table 1. With further downstream displacements, the bi-modal PDF peaks for case 1P remained relatively unchanged, whereas for case 2P, the peak density present at larger droplet diameters gradually diminished whilst the peak density present at smaller droplet diameters increased. For case 3P, a uni-modal PDF was observed with a single peak present at small droplet diameters for all sampled downstream displacements. These observations demonstrate how secondary atomization is an ongoing process, with characteristics unique to the spatial and temporal development of the spray plume.

Regions of Droplet Deformation and Secondary Atomization

The non-dimensional parameters that characterise deformation and breakup processes of liquid droplets, are the Weber and Ohnesorge numbers defined as,

$$W_e = \frac{\rho_0 u_{rel}^2 D_0}{\sigma} \quad (1)$$

$$Oh = \frac{\mu_d}{\sqrt{\rho_0 \sigma D_0}} \quad (2)$$

Here the surface tension $\sigma$ is responsible for the cohesiveness properties of the liquid droplets surface, and the dynamic viscosity $\mu_d$ responsible for the dampening of unstable perturbations. An increase in viscosity essentially corresponds to a slowing down of the droplet deformation process. This allows time for drag forces to react, reducing relative velocities and the potential for the droplet to breakup. If the Weber number for a given droplet exceeds a critical Weber number $W_{e, crit}$, only then will the droplet undergo breakup. According to the review of Faeth [2], the critical Weber number may be taken as $W_{e, crit} = 12$ for $Oh < 0.1$, where the effect of dynamic viscosity is negligible. For $Oh > 0.1$, the correlation reported by [3] may be used.

$$W_{e, crit} = 12(1 + 1.077Oh^{1.62}) \quad (3)$$

Qualitatively, prior to the onset of secondary atomization for $We < W_{e, crit}$, the droplet experiences a deformation that may be approximated as a thin disc-like shape normal to the flow direction.

Here we introduce the diameters $D_0$, $D_{cro}$ and $D_{min}$, corresponding to the initial spherical droplet diameter, the cross-stream diameter normal to the flow direction, and the minimum diameter parallel to the flow direction respectively.

Zhao et al. [4] showed that at the onset or secondary atomization, droplet deformation was related to the Weber number of the surrounding fluid such that,

$$\left( \frac{D_{cro}}{D_0} \right)_{max} = \left( \frac{D_{min}}{D_0} \right)^{-1/2} - 1 + 0.20We^{0.56}(1 - 0.48Oh^{0.49}) \quad (4)$$

For $Oh > 0.1$, the maximum deformation of the droplet at a given Weber number decreases due to slowing of the rate of deformation, which subsequently reduces the droplets relative velocity [4]. In equation (4), $(D_{cro}/D_0)_{max}$ represents the maximum possible deformation which occurs at the onset of secondary atomization. Considering the effects of droplet deformation on drag characteristics, we utilise the correlation by Liu et al. [5], which approximates drag of a deformed droplet as a linear function of deformation.

$$C_D = C_{D, Sphere}(1 + 2.632y) \quad (5)$$

Here $y = 1 - (D_0/D_{cro})^2$ is the non-dimensional displacement of the droplet equator, and $C_{D, Sphere}$ the co-efficient of drag for a sphere.

$$C_{D, Sphere} = \begin{cases} \frac{24}{Re} \left( 1 + \frac{1}{6} Re^{2/3} \right) & ; Re \leq 1000 \\ 0.44 & ; Re > 1000 \end{cases} \quad (6)$$

To take into account the time-varying properties of droplet deformation, we assume that the ratio
$D_{cr0}/D_0$ varies according to a half normal distribution with a mean of unity and a standard deviation equal to $\frac{1}{2}(D_{cr0}/D_0)_{\text{max}}$.

For $We > We_{\text{crit}}$, different droplet breakup regimes may be identified [6]. These breakup regimes are typically identified for $Oh < 0.1$ as follows.

- Bag, $12 < We < 20$
- Multi-mode, $20 < We < 80$
- Stripping, $80 < We < 800$
- Catastrophic, $We > 800$

Many authors have reported different ranges of Weber numbers classifying the aforementioned breakup regimes. However, regardless is the fact that as droplet Weber numbers increase, different breakup mechanisms occur. The reader is referred to the comprehensive review of Guildenbecher et al. [7] for details regarding the characteristics of droplet breakup within these regimes.

**Time-scales of Secondary Atomization**

Most secondary atomization processes occur over a finite period of time. Experimentally measured time-scales for these processes are typically made non-dimensional using the characteristic droplet deformation time-scale derived by Ranger and Nicholls [8].

$$\tau^* = \frac{D_0}{u_{rel}} \left( \frac{\rho_d}{\rho_f} \right)^{1/2} \tag{7}$$

The duration for initial droplet deformation $t_{\text{ini}}$ is typically a constant $1.6\tau^*$ [9]. Beyond such a duration, the droplet is said to undergo breakup that lasts for a finite period of time. Following a survey on hydrodynamic fragmentation, Pilch and Erdman [10] devised a set of correlations that characterised the total breakup time of droplets, spanning a wide range of Weber numbers.

\[
\frac{t_b}{\tau^*} = \begin{cases} 
6 (We - 12)^{-0.25} & ; 12 < We < 18 \\
2.45 (We - 12)^{0.25} & ; 18 < We < 45 \\
14.1 (We - 12)^{-0.25} & ; 45 < We < 351 \\
0.766 (We - 12)^{0.25} & ; 351 < We < 2670 \\
5.5 & ; We > 2670
\end{cases}
\tag{8}
\]

For high pressure cases examined in this study, it is unlikely for uncharged spray droplets to exceed Weber numbers greater than $\approx 45$. However, for charged spray droplets, the presence of charge would act to decrease the effective surface tension, resulting in much higher Weber numbers than one would otherwise expect for an uncharged spray.

**Stable Droplet Diameters following Secondary Atomization**

During breakup, the size of unstable droplets is assumed to vary continuously in time according to equation (9), reflecting the finite time required for the breakup mechanisms to result in a stable droplet with diameter $D_{\text{stable}}$.

$$\frac{dD}{dt} = -\frac{(D_0 - D_{\text{stable}})}{t_b} \tag{9}$$

The stable droplet diameter $D_{\text{stable}}$ is subsequently evaluated using the following correlations.

For $12 < We < 18$,

$$D_{\text{stable}} = \frac{D_0}{D_{32}} \frac{0.32We^{2/3}}{\left[ \frac{4.1}{(We - 12)^{1/4}} \right]^{2/3}} \frac{\sigma}{\rho_g u_{rel}^2} \tag{10}$$

for $18 < We < 45$,

$$D_{\text{stable}} = \frac{D_0}{D_{32}} \frac{0.32We^{2/3}}{\left[ \frac{2.45(We - 12)^{1/2} - 1.9}{(We - 12)^{1/4}} \right]^{2/3}} \frac{\sigma}{\rho_g u_{rel}^2} \tag{11}$$

for $45 < We < 100$,

$$D_{\text{stable}} = \frac{D_0}{D_{32}} \frac{0.32We^{2/3}}{\left[ \frac{12.2}{(We - 12)^{1/4}} \right]^{2/3}} \frac{\sigma}{\rho_g u_{rel}^2} \tag{12}$$

and for $We > 100$,

$$D_{\text{stable}} = We_{\text{crit}} \frac{\sigma}{\rho_g u_{rel}^2} \left(1 - \frac{V^*_{c}}{u_{rel}} \right)^{-2} \tag{13}$$

In equation (13), $V^*_c$ is the velocity of the fragment cloud post-breakup, and is calculated via,

$$V^*_c = u_{rel} \left( \frac{\rho_f}{\rho_d} \right)^{1/2} \left( B_1 \tau^*_\text{crit} + B_2 \tau^*_b \right) \tag{14}$$

where co-efficients $B_1$ and $B_2$ are chosen to fit experimental data [11], and their values taken typically as 0.375 and 0.236 respectively\(^1\).

\(^1\)It should be noted here that according to Pilch and Erdman [10], co-efficients $B_1$ and $B_2$ differ depending on whether
Correlations defined by equations (10)-(12) were based on improved estimates for average fragment droplet sizes produced in the bag and multi-mode breakup regimes [12]. Furthermore, we employ the use of the relation \( D_{0,5}/D_{32} = 1.2 \) which relates the mass median to the Sauter mean diameter of the droplet fragment cloud post breakup [13]. We found these improved correlations overcome the pitfalls in \( D_{stable} \) prediction for \( W_e < 100 \) originally noted by Pilch and Erdman [10]. Figure 3 illustrates the variation of \( D_{stable}/D_0 \) as a function of \( W_e \) predicted by these improved correlations. Selected and most recent experimental observations on stable droplet diameters produced in the bag and multi-mode breakup regimes are included in Figure 3 for reference [4][14][15][16].

![Graph](image)

**Figure 3.** Influence of \( W_e \) on \( D_{stable}/D_0 \) predicted by correlations (10)-(13)

**Accounting for Electrical Charge on Droplets**

**Charge Mobility During Breakup**

An experimental study by Guildenbecher and Sojka [17] noted that breakup is not only a function of charge level, but also dependant on the rate of charge movement [18]. It was therefore assumed that similar dependencies exist within the principles of secondary atomization. To account for this, all fluids possess an electrical resistivity, resulting in a finite rate of charge movement characterised by the charge relaxation time.

\[
\tau_Q = \frac{\varepsilon_0 \varepsilon_r}{k}
\]  

(15)

Here \( \varepsilon_r \) is the relative permittivity of the liquid and \( k \) is the electrical conductivity of the liquid. This charge relaxation time can be made non-dimensional using (7), yielding the conductivity number \( k^* \) [17].

\[
k^* = \frac{\varepsilon_0 \varepsilon_r u_{rel} D_0}{k \left( \frac{\rho_f}{\rho_d} \right)^{1/2}}
\]  

(16)

The conductivity number allows us to compare the time-scale of charge movement throughout the droplet to the characteristic breakup time of a droplet undergoing secondary atomization. Therefore, when \( k^* \ll t_{rel}^* \), the rate of charge movement is much faster than the rate of deformation such that the charge will re-distribute itself quickly throughout the droplet, by migrating and spreading uniformly across the droplet surface to achieve a distribution that minimizes electrostatic stresses [17]. Alternatively, when \( k^* \gg t_{rel}^* \), the rate of charge movement is assumed to be frozen throughout the breakup process. Therefore, any droplet deformation whether it be prior to, or during secondary atomization should result in a faster breakup process. Guildenbecher and Sojka [17] examined this effect, but found no significant impact on either the initial breakup times, nor total breakup times of charged droplets undergoing secondary atomization. This is not to say a role does not exist, but rather the effect is hidden within the inevitable existing experimental uncertainty and the dominant mechanisms of aerodynamic fragmentation. For high pressure sprays examined in this study, \( k^* \approx O(10^{-5}) \), which indicates that charge is effectively frozen throughout breakup processes.

**Maximum Rayleigh Limit Charge**

Assuming an isolated, electrically conducting spherical droplet, the maximum charge held is defined by the droplets Rayleigh limit.

\[
Q_{ray} = 4\pi \sqrt{0.5 \varepsilon_0 \sigma D_0^3}
\]  

(17)

In reality, this Rayleigh limit is rarely ever reached, due to the fact that either electrical or aerodynamic forces act to deform the droplet away from the perfect electrical, and physical symmetry conditions assumed. This typically limits the maximum charge level to be \( \approx 80\% \) of the Rayleigh limit [19].

**Charged Droplet Fission**

Charged droplets that exceed their Rayleigh limit undergo a process known as Coulomb fission, whereby a stream of sibling droplets, each carrying with them a fraction of the parents mass and charge, eject from the surface of the parent droplet [19][20][21]. For evaporating droplets whereby mass is lost without any loss of charge from the surface, modelling the Coulomb fission process is essential to ensure that total spray evaporation rates are predicted as accurately as possible. Evaporation rates are promoted in sprays by the increase in number.
of small droplets, and the subsequent increase in total spray surface area, relative to a spray containing the same volume of liquid across larger droplet sizes. Although evaporation does not occur for high pressure sprays investigated in this study, we found that approximately 2% of droplets exceed their Rayleigh limits after aerodynamically induced secondary atomization. We therefore include the modelling of Coulomb fission processes, only for completeness of the numerical method.

Theoretical analysis performed on charged droplet fission processes have predominately relied upon the minimization of Gibbs free energy technique [22][23][24], using knowledge of parent droplet parameters, and assumptions relating to the formation of a stream of ejected sibling droplets. To model Coulomb fission, we utilise the relationship [25][26],

\[
\frac{f_q}{f_m} = C \sqrt{\frac{\rho_d D_0^3}{8\sigma}} \frac{k}{\epsilon_0 \epsilon_r} \quad (18)
\]

Here, \( f_q = \Delta Q/Q_d \) and \( f_m = \Delta m/m_d \) denote the fractional charge and mass lost from the parent to sibling droplets. The empirical constant in equation (18) was calculated to be \( C \approx 14.78 \). This value was found following numerical tests of equation (18) with input parameters from known experimental observations [19][20][21], predicting that parent droplets typically lose between 10-18% of their charge, and 1-2.3% of their mass [21]. Any number between \( n_p = 7-30 \) of sibling droplets may eject from the parent droplet during fission [27], each with a diameter \( \approx 10\% \) of their parents original droplet diameter prior to fission [21]. Assuming identical sibling droplets and a uniform variation of \( \Delta Q, \Delta m, \) and \( n_p \) within experimentally observed ranges, one can subsequently calculate the size, and the charge held by sibling droplets produced during the fission process.

**Effective surface tension**

To account for electrically charged droplets, one may equate a force balance between the surface tension restorative forces of a spherical droplet, and the disruptive forces of electrostatic charge. One may then obtain an equation for the effective surface tension,

\[
\sigma^* = \sigma - \frac{Q_d^2}{8\pi^2 \epsilon_0 D_0^3} \quad (19)
\]

valid within the limits, as \( Q_d \to 0, \sigma^* \to \sigma, \) and \( Q_d \to Q_{ray}, \sigma^* \to 0. \) Subsequently, equation (19) may be used in place of \( \sigma \) appearing in (1) and (2), to yield corresponding electrostatic \( We_{e-} \) and \( Oh_{e-} \) numbers. Usage of \( \sigma^*, We_{e-}, \) and \( Oh_{e-} \) is then incorporated within the aforementioned deformation and secondary atomization models relating to uncharged spray droplets.

**Impact on Weber, Ohnessorge and Breakup Time-scales**

An increase in surface charge density leads to increased \( We_{e-} \) and \( Oh_{e-} \) numbers. At elevated \( Oh_{e-} \) numbers, \( We_{crit} \) also increases. However, the observed breakup modes for droplets that exceed \( We_{crit} \) within a given Weber number range remains the same [7]. With a predicted increase by \( Oh_{e-} \) in the dampening of unstable perturbations, there is yet a greater influence of droplet charge on \( We_{e-} \) numbers, subsequently promoting secondary atomization. This was validated during an experimental study performed by Guildenbecher and Sojka [28], who showed that for highly conductive liquids, use of equation (19) leads to an increased agreement with the Pilch and Erdman [10] breakup correlations governing total droplet break-up times.

**Spray Discretisation**

The CFD code used to simulate our charged high pressure sprays was originally developed as part of theoretical, computational and experimental studies on mechanisms governing electrostatic atomization of hydrocarbon oils [29]. The code was later extended during a previously published CFD study evaluating a numerical methodology suitable for simulating low pressure electrostatically atomized dielectric liquid sprays [30], where specific details regarding the numerical methods may be found.

In this section, we present only details relevant to the specification of initial discrete phase conditions.

**Initial Conditions of the Discrete Phase**

Due to the large injection velocities present within high pressure sprays, there is an inherent difficulty faced by experimentalists in measuring mean jet breakup lengths. Based on previous work regarding charged low pressure sprays [30], we can justify the use of equations (20), (21), and (22) below to specify jet breakup lengths for all our charged high pressure sprays.

\[
l_j = U_{inj} \tau_j \quad (20)
\]

\[
\tau_j = \frac{\epsilon_0 \epsilon_r}{\kappa Q_v} \quad (21)
\]

\[
\kappa = A \mu_d^{-1} \quad (22)
\]

Here \( A \) is taken as a constant equal to \( 4 \times 10^{-11} \) [30]. These equations were found to be far more re-
liable in predicting finite mean jet breakup lengths than classical models governing laminar and turbulent jets. These classical models failed in their predictive capabilities when their jet Weber and Ohnesorge numbers were modified to account for electrical charge using an effective surface tension derived for a round cylindrical jet [1].

The initial velocity of droplets is specified by both mean and fluctuating components of the injection conditions, assumed at the atomizer orifice plane.

\[ U_{d,t=0} = U_{inj} + U' \times RAN_G \]  
\[ V_{d,t=0} = V_{inj} + V' \times |RAN_G| \]

Here \( RAN_G \) is a random number taken from a Gaussian distribution with zero mean and unit variance. We assume that the initial axial velocity of droplets is equal to the bulk mean injection velocity \( U_{inj} \), plus a fluctuating component where \( U' \) was taken to be equal to 40% of \( U_{inj} \). Furthermore, we assume droplets have a mean radial velocity component \( V_{inj} = 0 \), with a fluctuating radial component \( V' \) determined via the half-spray cone angle \( \theta/2 \). For charged sprays, the half-spray cone angle is a difficult quantity to measure experimentally, mainly due to the fact that charged droplets tend to follow parabolic paths. However, if we assume that all spray droplets originate at, or near the centreline of the liquid jet, we may utilise the following correlations to determine the half-spray cone angle [31][32].

\[ \tan(\theta/2) = \frac{4 \pi}{A} \left( \frac{\rho_f}{\rho_d} \right)^{0.5} \frac{\sqrt{3}}{6} \]

\( A \) is taken as a constant dependent on the nozzle design, or approximated using,

\[ A = 3.0 + 0.28 \left( \frac{l}{d_{inj}} \right) \]

These correlations were chosen for their suitability across most modern Diesel injectors.

The next part of the injection procedure requires specification of the initial droplet size distribution. Due to the presence of secondary atomization, it is unreliable to use measured PDFs obtained from experimental PDA data. This is because measured PDFs are functions of transient secondary atomization processes, exhibiting themselves as spatially dependent characteristics within the spray plume. Initial PDFs are therefore assumed to take the form of a normal distribution, chosen such that the mean diameter equals the orifice diameter, with a standard deviation equal to \( \frac{1}{3} d_{inj} \). This yields a normally distributed diameter PDF, with diameters spanning the range \( \approx 0.2 \times d_{inj} \), aimed to reflect the theory whereby diameters of droplets produced from the largest unstable wavelength on a liquid jet, are equal to \( 1.89 d_{inj} \) [33][34].

For initial specification of droplet charges, we use the modelled Q-D method as employed in previous computational studies [35][36].

\[ \frac{Q_{d,k}}{Q_{d,k+1}} = \left( \frac{D_k}{D_{k+1}} \right)^m \]

Here the constant \( m \) is taken as 1.8 [36]. This allows the total charge injected during any time interval \( Q \Delta t \), to be expressed in terms of a conserved injected current \( \dot{Q}(t) \) such that,

\[ \dot{Q} \Delta t = \sum_{k=1}^{K_p} N_{d,k} Q_{d,k} = \sum_{k=1}^{K_p} N_{d,k} \left( \frac{D_k}{D_1} \right)^m \]

where \( K_p \) is the total number of parcels injected during the time interval, and \( N_d \) the number of real droplets contained within each injected parcel. Charge is then defined conservatively without explicitly constraining it to obey any limits. Furthermore, we include a variation in charge based on typical values determined from experiments, for the standard deviation of charge levels across different diameter classes. From experiments of Rigit and Shrimpton [37], standard deviations of charge levels are approximately 10% of droplet Rayleigh limits.

Critically, mass is conserved throughout the injection process by adjusting the number of real droplets contained within each injected parcel. Similarly, charge is conserved by adjusting the relative droplet charge levels across all injected parcels.

**Results**

Statistics were post-processed from simulated CFD sprays in a similar manner to statistics processed from experimental PDA measurements. Sample control volumes from CFD and experimental measurements were taken at the same downstream and radial locations away from the atomizer orifice. This allows for an accurate assessment of model performance and the CFD procedures employed.

Figures 4 and 5 show the initial spray development for the uncharged and charged, case 3P high pressure sprays respectively. Results show how the charged spray penetrates less downstream over the 5ms interval than the uncharged spray. Due to
the presence of Lorentz forces acting on charged droplets, there is an increase in radial dispersion, more so than what is typically observed for uncharged sprays. In agreement with theory suggesting that the presence of charge on droplets increases the tendency for droplets to breakup, results show evidence of an increased abundance of small \((D/d_{inj} < 1)\) droplets within the charged spray. In relation to findings of previous researchers, Kayhani et al. [38] stated that atomization to rapid leads to inadequate spray penetration. Furthermore, Kwack et al. [39] who performed experiments examining electrostatic dispersion of Diesel fuel jets at high back pressures, observed a rapid breakup of the spray jet without any presence of large droplets within the spray core. Our results agree well with these previous findings, giving confidence in the methods used to model secondary atomization within charged high pressure sprays.

Figure 6 compares droplet diameter PDFs obtained from computed sprays, with available PDFs obtained from experimental spray measurements. With regards to uncharged computed sprays, a distinct evolution from a bi-modal to uni-modal droplet size distribution is observed with increasing spray injection velocity, relative to fixed downstream sample locations. For charged computed sprays, droplet size distributions are predominantly uni-modal, with a single peak for droplet diameters occurring in the range 0.1-0.25\(D/d_{inj}\). Furthermore, the tails in these distributions in the direction of increasing droplet diameters tend to show reduced probabilities as spray injection velocities increase. Comparison of PDFs between computed and experimental charged sprays only show reasonable agreement for case 3P. For case 1P, computed results show a uni-modal PDF, whereas the experimental PDF remains bi-modal. A similar behaviour is observed for case 2P, the only difference being an increase in smaller droplet probability within the bi-modal experimental PDF. These discrepancies are most likely caused by weaknesses in the modelling of dispersion for charged high pressure sprays.

Figure 7 shows mean axial velocity profiles of charged droplets compared between spray simulations and experiments. Profiles computed for high pressure sprays all show reasonable agreements with experiments, with the exception being case 3P where the computed profile exceeds the experimental profile near the spray centreline by nearly a factor of 3. To explain this behaviour, one can observe in Figure 7 that as spray injection velocities increase, the mean velocity of droplets sampled at the spray centreline decreases. An increase in spray injection velocity therefore leads to greater dispersion which adds a radial component to droplet velocities. Our computed profiles do not show evidence of this behaviour. Instead, there is a tendency for computed profiles to exceed experimental profiles near the spray centreline. Nevertheless, for increasing \(r/d_{inj}\), the computed profiles show reasonable consistency in their agreement with experimental profiles.

Figure 7 also includes an experimental mean axial velocity profile for a 34\(\text{m/s}\) low pressure spray, originally presented as spray (ii) by Shrimpton and Yule [40], and its computed corresponding profile taken from a recently published CFD study [30]. Comparing case 1P to spray (ii) up to \(r/d_{inj} = 100\), experimental profiles show reasonable agreement with each another. Furthermore, the computed profile for case 1P agrees well with its own experiment, and that of spray (ii). This gives us confidence that the method used to model secondary atomization within charged high pressure sprays, accounts reasonably well for charged spray behaviour existing in sprays where secondary atomization is not a dominant process.

Lastly, the average percentage errors between computed and experimental mean velocity profiles were calculated to be 19.5\%, 16.2\%, and 27.5\% for spray cases 1P, 2P, and 3P respectively.

**Conclusions**

A numerical methodology is presented, suitable for predicting characteristics of high pressure electrostatically charged Diesel fuel sprays. Most importantly, the methodology is reliable at predicting secondary atomization processes for both uncharged and charged sprays.

Qualitative examination between selected uncharged and charged high pressure sprays show how radial dispersion in charged sprays is increased significantly over uncharged sprays. This increase in charged spray radial dispersion comes with the cost of decreased spray penetration rates.

For uncharged computed sprays, sampled droplet diameter PDFs measured between cases show a distinctive evolution from a bi-modal to unimodal droplet size distribution as spray injection velocity is increased. For charged sprays, droplet diameter PDFs are predominantly uni-modal, with a single peak in droplet diameters present within the range 0.1-0.25\(D/d_{inj}\).

For the fastest charged high pressure spray, the droplet diameter PDFs between computed and experimental sprays show excellent agreement. Furthermore, droplet axial velocity profiles from computed charged high pressure sprays show reasonable
agreement with corresponding experimental spray profiles, with average percentage errors ranging from 16.2% to 27.5%.

The results from this investigation highlight the suitability of the CFD methodology presented, for simulating high pressure electrostatically charged fuel sprays, at elevated injection conditions typically employed within automotive and marine sectors.

Further work aims to apply this CFD methodology within the context of a large marine Diesel engine application.

Acknowledgement
This work was supported by an ESPRC Doctoral Training Centre grant EP/G03690X/1

References


**Figure 4.** Initial spray development and penetration of the uncharged 3P high pressure spray. Time snapshots of spray droplets taken at a) 3ms, b) 4ms, c) 5ms after start of injection.

**Figure 5.** Initial spray development and penetration of the charged 3P high pressure spray. Time snapshots of spray droplets taken at a) 3ms, b) 4ms, c) 5ms after start of injection.
Figure 6. Histogram PDF measurements obtained from post-processed CFD simulation data for uncharged (i) and charged (ii) high pressure sprays; a) Case 1P, b) Case 2P, and c) Case 3P. Overlaid profiles correspond to experimental spray PDFs. PDFs were sampled along the spray axis downstream from the atomizer at 17 cm for Case 1P, 15 cm for Case 3P, and at 12.5 cm and 17.5 cm for the uncharged and charged Case 2P respectively.
Figure 7. Mean droplet axial velocity profiles for charged high pressure cases 1P, 2P, and 3P, as well as spray (ii) from Shrimpton and Yule [40].