Numerical Modelling of Droplet Breakup for Flash-Boiling Fuel Spray Predictions

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Abstract

Flash-boiling of fuel sprays can occur under injection of superheated fuel into ambient pressure that is lower than the saturation pressure of the fuel and can dramatically alter spray formation due to complex two-phase flow effects and rapid droplet evaporation phenomena. Such phenomena exist in-cylinder at low-load in-city driving conditions where strict engine emission regulations apply, hence the need for faithful flash-boiling fuel spray models by engine designers. To enhance the current modelling capability of superheated fuel sprays, with focus on near-nozzle plume expansion, a flash-boiling breakup modelling approach was developed to introduce the thermal breakup mechanism of droplets caused by nucleation and bubble growth. This model was particularly aimed at sprays where levels of superheat introduced noticeable radial expansion of the plumes upon discharge from the nozzle orifice. The model was able to simulate droplet shattering by introducing Lagrangian child parcels at breakup sites with additional radial velocity components instigated by rapid bubble growth and surface instabilities. Combination of the flash-boiling droplet breakup model with a flash-boiling effective nozzle model that was used as boundary condition for the spray plumes offered a more complete modelling approach, where both in-nozzle phase change effects and near-nozzle flashing through droplet shattering were incorporated into the Eulerian-Lagrangian two-phase computational framework. Sensitivity studies were carried out to investigate important parameters which are inherently difficult to measure experimentally and offered valuable insight into modelling superheated sprays. The model was able to capture important flash-boiling spray characteristics and quantitative validation was achieved through comparison to experimental data in the form of penetration lengths and droplet sizes with a good level of agreement.

Nomenclature

Latin Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tr>
<td>$D_d$</td>
<td>Droplet diameter [µm]</td>
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<td>$Ec$</td>
<td>Eckert number</td>
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<td>$Fr$</td>
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<td>$Ja$</td>
<td>Jakob number</td>
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<tr>
<td>$kb$</td>
<td>Flash-boiling breakup criterion</td>
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<tr>
<td>$P_{inj}$</td>
<td>Injection pressure [Pa]</td>
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<tr>
<td>$P_{sat}$</td>
<td>Saturation pressure [Pa]</td>
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<td>$P_n$</td>
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<td>$X$</td>
<td>Rosin-Rammler scaling factor</td>
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1. Introduction

1.1. Flash-Boiling Fuel Sprays

Flash-boiling is a phenomenon which occurs when a liquid is discharged into an ambient gas with a pressure below that of the saturation pressure of the liquid. Several factors, such as the degree of superheat, can significantly change the way in which the injected fluid behaves. The ever-tightening tailpipe emission regulations within the context of direct-injection spark-ignition engines mean that understanding complex multiphase phenomena such as flash-boiling are crucial to developing cleaner combustion systems, especially at low-load in-city driving conditions where fuel spray formation and mixing can occur at sub-atmospheric in-cylinder pressures. Improved atomisation is a recognized consequence of flash-boiling in fuel sprays, driven mainly by rapid phase change mechanisms past the nozzle exit or even within the injector nozzle. It has been found by experimentation that it is the light fraction species in gasoline (like pentanes) that drive the general behaviour of gasoline sprays and their ‘collapse’ process past the nozzle exit at superheated conditions (van Romunde et al., 2007; van Romunde and Aleiferis, 2013), hence the need to be able to model flash-boiling sprays efficiently in the context of refinery stream fuels for advanced spark-ignition engines. Near-nozzle effects and phase change within the nozzle orifice have been experimentally documented and modelled previously by the current authors with various fuels (Serras-Pereira et al., 2010; Aleiferis et al., 2010; Price et al., 2015, 2016, 2018; Papadopoulos and Aleiferis, 2015). In-nozzle phase change can occur through heterogeneous wall nucleation and has been shown experimentally to reduce the effective nozzle diameter to around 40% of its nominal geometry (Wu et al. 2017a–b). At high levels of superheat, rapid phase change can continue past the nozzle exit, causing droplets and ligaments to shatter. Li et al. (2017) studied droplet shattering in a single ethanol droplet and documented a critical superheat degree of approximately $\Delta T = 25$ K. Droplet shattering has been labelled as one of the main contributors to the characteristic of plume expansion and increased atomisation under flash-boiling conditions (Oza and Sinnamon, 1983; Sovani et al., 2001; Lamanna et al., 2014; Kamoun et al., 2010). Particularly for multi-hole fuel sprays, a number of investigations into the near-nozzle region have been carried out and have documented the effect of flash-boiling on global spray characteristics under a wide range of fuel volatilities and thermodynamic conditions (van Romunde et al., 2007; Aleiferis and van Romunde, 2013; Moulaï et al., 2015; Wang et al., 2016). Specifically, van Romunde et al. (2007) and Aleiferis and van Romunde (2013) used magnified high-speed imaging to focus on the near-nozzle region and found that plumes can interact almost instantaneously upon discharge from the nozzle exit when considering multi-hole injectors. However, due to the minute length and time scales involved, as well as the complex two-phase flow of dense droplet field in the near-nozzle region, it has been extremely challenging to characterise the flashing process on an individual droplet scale. Moreover, compressibility effects which have been captured under extreme conditions (Simões-Moreira et al., 2002; Guo et al., 2019) are also thought to contribute to the rapid expansion of the spray under discharge, whereby under-expanded jet behaviour could exist. Optical nozzle studies allowing high-speed imaging of in-nozzle phase change have also been carried out in an attempt to understand and quantify phase change phenomena from both cavitation and flash-boiling and clearly documented the transition from subcooled to fully flashing sprays (Serras-Pereira et al. 2010; Aleiferis et al., 2010; Zhang et al., 2015). However, truly quantitative two-phase flow measurements both inside and just outside a real-size injector’s nozzle orifice
remain elusive, hence development and validation of modelling approaches of in-nozzle-out flash-boiling fuel injection is still a topic of on-going research efforts.

1.2. Present Contribution

The present work aims to advance the current modelling capability and understanding of flash-boiling sprays by developing and applying a new break-up model based on a Lagrangian Particle Tracking (LPT) approach. The method’s ability to automatically capture important flash-boiling spray characteristics was investigated. This was carried out by:

- Developing a breakup model approach which incorporated droplet shattering from nucleation and bubble growth within superheated liquid droplets. The model was implemented in such a way that new parcels could be introduced into the computational domain during breakup.
- Systematically investigating key model parameters to give insight into the sensitivity of the model and potential areas for optimisation by a step-by-step approach.
- Investigating the breakup model’s capability to improve near-nozzle predictions of curving of the plumes, downstream spray collapse and droplet sizes under flashing conditions.
- Comparing the predicted sprays to in-house spray experiments and quantitatively validate against penetration lengths and downstream droplet sizes.

The numerical breakup model presented here builds upon previous understanding and work carried out by the current authors. Initially, a parametric study was carried out to understand important parameters in the modelling of flash-boiling fuel sprays (Price et al., 2015) where it was found that in-nozzle phase change via wall-nucleation could be approximated quantitatively and then could be translated into numerical boundary conditions at the origin of the spray plumes by the form of a zero-dimensional flash-boiling effective nozzle model calculation to predict flash-boiling characteristics for a wide range of fuels and injectors (Price et al., 2016, 2018). This approach still holds and is discussed within the current work in conjunction with near-nozzle effects at full flash-boiling conditions. It is highlighted that the flash-boiling droplet breakup model presented in this paper is a contribution that has not been part of any of the previous papers by the current authors. Moreover, this flash-boiling droplet break-up model after introduction and initial assessment is also combined in this paper with our previously developed flash-boiling effective nozzle model to offer the potential for a more holistic approach to model flash-boiling fuel sprays that can be implemented relatively easily into in-cylinder engine spray simulations with a moving piston in the future.

2. Numerical Methodology

2.1. Computational Framework

A two-way coupled Lagrangian-Eulerian framework was used to model the dispersed multi-phase flow. The LPT technique was based on solving governing equations for individual parcels of the dispersed phase (liquid droplets). The continuous phase is expressed in Eulerian form and two-way coupled to the liquid droplets through the addition of source terms in the energy, mass and momentum transport equations of both phases. Turbulence was modelled using a Reynolds-Averaged Navier-Stokes (RANS) approach, specifically by the k-ε RNG (Re-Normalisation Group) model (Yakhot et al., 1992) previously shown to perform better in engine simulations than typical k-ε models (Han and Reitz, 1995, Malcolm et al., 2011, Xue et al., 2013). The governing equations were solved within the STAR-CD framework in addition to several supplementary flash-boiling models which were implemented by the current authors via user subroutines. The PISO pressure-velocity coupling algorithm (Issa, 1986) was used, with discretisation schemes for velocities, temperature, k and ε of second order in space and first order in time. The secondary breakup model of Reitz and Diwakar
(1986) was adopted and droplet-droplet collisions were modelled using the model of O’Rourke (1982) with the speed-up algorithm of Schmidt and Rutland (2004). A time step of 1 μs was used throughout. Temperature-dependent polynomial relationships for thermophysical properties were taken from the Yaws’ Property Database (Yaws, 2003) and implemented via user-coded subroutines. The fuel properties modelled in this manner include surface tension, viscosity, latent heat of evaporation, density, specific heat capacity, saturation pressure and thermal conductivity. Gas densities were modelled by the ideal gas law.

2.2 Flash-Boiling Droplet Breakup

In the case of flash-boiling conditions where droplets have been found to shatter (Oza, 1984; Peter et al., 1994; Kamoun et al., 2010) it is important to consider additional radial velocity components imposed on ‘child’ droplets through calculation of rapid bubble growth inside ‘parent’ droplets in order to capture the expansion of plumes upon discharge from the nozzle orifice.

The proposed breakup modelling approach works on the premise of introducing new parcels at breakup sites within the computational domain during injection. This approach allowed the code to introduce post-breakup child droplets, each with distinct properties (velocity, size, temperature, etc.). The flash-boiling breakup model works in parallel with the aerodynamic breakup model, whereby both parent and child droplets undergo aerodynamic breakup, although the flash-boiling breakup timescales are typically one order of magnitude smaller. The collision model also allowed both parent and child droplets to interact with surrounding numerical parcels post-breakup. The breakup model was implemented by incorporating not only the standard spray initialisation at injection with parcels but also the addition/removal of child/parent parcels at breakup sites throughout the domain. The flow chart in Figure 1 describes the algorithm used to model droplet breakup in flash-boiling sprays within user-coded subroutines.

![Figure 1. The flash-boiling droplet breakup model algorithm and implementation routine.](image-url)
The model works by iterating through all current parcels in the domain and determining whether the droplet properties meet the breakup criteria; if the criteria are met then the parcel will undergo breakup. As will be discussed in greater detail later, analytical models are solved to calculate child droplet properties for each specific parcel which has met the breakup criterion (child properties are a function of parent thermophysical properties, temperature, size and ambient pressure) and these child parcels are introduced with a relative position and velocity. The schematic displayed in Figure 1 demonstrates the breakup process in two-dimensions. The parent parcel is considered to carry initially no radial velocity from flashing and undergoes flashing breakup whereby parcels are introduced at the position \( x_p, y_p, z_p \) (subscript \( p \) represents ‘parent’) with velocities \( u_x + u_{xr}, u_y + u_{yr}, u_z + u_{zr} \) whereby subscripts \( x, y, z \) refer to the subsequent Cartesian components and subscript \( r \) refers to the additional radial component from flashing.

The implementation of child parcels with radial velocity components required a mathematical description of the breakup process to predict the radial velocity magnitude and child droplet sizes as a function of parent droplet properties. The approach was based on the studies of Zeng (2000) and Zeng and Lee (2001, 2002) by quantifying surface instabilities and internal bubble growth due to thermal non-equilibrium breakup. Breakup was assumed to occur when the instability wave amplitude equalled a characteristic length scale, in this case the film thickness. A schematic diagram is displayed in Figure 2 which displays the breakup process for a bubble-droplet system under thermal non-equilibrium. Initially, the bubble-droplet system consisted of a bubble with a radius determined from the balance between surface tension and pressure forces as described by Equation (1) (Plesset, 1954) with an initial surface instability of arbitrary amplitude (in this case 5% of the droplet radius).

\[
R_c = \frac{2\sigma}{P_{sat} - P_{\infty}}
\]  

(1)

The process of bubble and surface instability growth can be seen in Figure 2, whereby the reduction in liquid film thickness due to bubble growth competes with the growing surface instability. Child droplets were formed from the pinching off of the liquid film.

The size and velocity of the child droplets were dependent on the bubble and instability growth rates, which ultimately determined the film thickness at breakup as well as the radial velocity magnitude of child droplets. Zeng (2000) adopted a special case of the Rayleigh-Taylor instability analysis for a spherical interface (Sharp, 1984), where only the first order harmonics were considered to estimate the instability growth rate of a bubble-droplet system such as that of Figure 2.

Figure 2. A schematic showing the breakup of a bubble-droplet system under thermal non-equilibrium.

In the current work an extended model was adopted, based on the work of Lü et al. (2015), which incorporated the liquid viscosity terms through the Reynolds number. The viscosity terms were found to be an important addition to the model when large droplets at low superheats were adopted. The influence of these terms at the spray conditions of the current work was found to be very small. However, they are
included here for completeness and with the consideration for future implementation to other applications. Displayed in Equation (2) is the normalised growth rate equation documented in standard cubic form:

\[
\bar{\omega}^3 (\delta - \delta^2 - \Psi_0 \delta) + \bar{\omega}^2 \left(3 \delta W e_i^2 - \delta^2 3 W e_i^2 - \Psi_0 3 W e_i^2 - W e_o^2 + \delta 4 W e_i^2 + \Psi_0 W e_o^2 - \frac{4 \delta^3}{R e_2} W e_o^2 + \frac{4 \Psi_i (W e_i^1 W e_o^1)}{R e_2} W e_o^2 + \frac{4 W e_o^1}{R e_2} W e_o^2 \right) + \bar{\omega} \left(-3 W e_i^2 W e_o^2 + \delta^2 3 W e_i^2 W e_o^2 + \Psi_0 3 W e_i^2 W e_o^2 + 2 \delta^2 + 2 \delta^{-2} - 3 \Psi_i (M a_i^1 W e_i^1 W e_o^1) \delta^2 - \frac{4 \delta^3}{R e_2} 3 W e_i^2 W e_o^2 + \frac{4 \Psi_i (W e_i^1 W e_o^1)}{R e_2} 3 W e_i^2 W e_o^2 + \frac{4 W e_o^1}{R e_2} 3 W e_i^2 W e_o^2 + \frac{4 \Psi_o}{R e_2} 3 W e_i^2 W e_o^2 \right) + \left(2 \delta^2 3 W e_i^2 + 2 \delta^{-2} 3 W e_i^2 \right) = 0
\]

where:

\[
\bar{\omega} = \sqrt{\frac{\rho_i R_i^3}{\sigma}} \omega \quad (3), \quad \delta = \frac{R_o^2}{R_i^1} \quad (4), \quad M a_i = \frac{V_b}{c} \quad (5)
\]

\[
W e_o = \frac{\rho_i V_o^2 R_i}{\mu_o} W e_i = \frac{\rho_i V_o^2 R_i}{\mu_i} \quad (6)
\]

\[
R e_1 = \frac{\rho_o V_o R_o}{\mu_o}, \quad R e_2 = \frac{\rho_i V_i R_i}{\mu_i}, \quad \Psi_0 = \frac{\rho_g}{\rho_i}, \quad \Psi_1 = \frac{\rho_g}{\rho_i} \quad (8)
\]

Here, \(\bar{\omega}\) is the non-dimensional instability growth rate, \(\omega\) is the instability growth rate, \(R_1\) and \(R_o\) are the inner and outer radii, respectively, and \(V_o\) and \(V_b\) are the outer and inner surface velocities, respectively. \(c\) is the speed of sound and \(\rho_o\) and \(\rho_i\) refer to outer and inner gaseous densities, respectively. The cubic equation can be solved analytically and the largest real part of the three cubic roots was taken as the dominant instability growth rate. Secondly, the bubble growth rate was required to predict breakup properties. In the current work the bubble growth rate was taken to be described through the Rayleigh equation:

\[
V_b = \sqrt{\frac{2}{3 \rho_i (P_{sat} - P_{in})}} \quad (9)
\]

The Rayleigh equation was suited to rapid, early bubble growth regimes where cooling effects from evaporation and thermal diffusion to the bubble surface can be considered negligible (inertial dominated growth). This was incorporated into the Mikic bubble growth equation (Mikic et al., 1970) whereby for small timescales and inertia controlled growth the equation becomes close to that of Rayleigh. In the current work this assumption was deemed true for a bubble in a superheated droplet with diameter of between \(D_d=50\ \mu m\) and \(D_d=200\ \mu m\) with timescales from initiation to droplet breakup in the order of tens of microseconds.

### 2.3. Breakup Characteristics

#### 2.3.1. Breakup Criterion

A breakup criterion for bubble-droplet systems under thermal non-equilibrium was suggested by Zeng and Lee (2001) (Zeng, 2000, Lü et al., 2015) which is displayed in Equation (10):

\[
k_b(t_b) = \frac{\eta_o \exp(\omega t)}{R_o(t) - R_i(t)} \quad (10)
\]

where \(k_b(t_b)\) is the critical breakup criterion, a ratio between surface instability length scale and film thickness, \(\eta_o\) is the initial disturbance size (taken as \(\eta_o=0.05R_o(0)\)), \(t\) is time and \(R_o(t)\) and \(R_i(t)\) are the time varying outer and inner radius of the bubble-droplet system. The breakup criterion states that when the instability amplitude equals the film thickness, hence when \(k_b(t_b)=1\), the droplets pinch off and breakup
occurs. $kb(t_b)$ was proposed a potential parameter for model optimisation to take into account complexities found in real bubble-droplets, e.g. non-spherical droplets, multiple bubbles or external flow characteristics. However, due to obvious limitations in empirical data, a value of $kb(t_b)=1$ was assumed suitable as a first approximation within the context of the current work. The instability growth rate and bubble growth rate were used to calculate the properties of the bubble-droplet system at breakup as a function of operating conditions, fuel properties and breakup criterion. The transient behaviour of the breakup criterion and film thickness of a droplet-bubble system (with initial outer droplet diameter of 200 μm, equivalent to a typical nozzle hole diameter) can be seen in Figure 3.

$n$-Pentane was adopted for the calculations as it is the high volatility component in gasoline that drive the flash boiling and spray collapse process (van Romunde et al., 2007; van Romunde and Aleiferis, 2013). In Figure 3 the rapid increase in breakup criterion, $kb$ highlights the minute timescales associated with droplet shattering. A breakup timescale for each condition can be calculated, whereby at $T_d=383$ K and $T_d=323$ K the breakup timescales were $t_b=8.4$ μs and $t_b=24.2$ μs, respectively. This relates to a distance of around 0.84 mm and 2.42 mm, respectively for a droplet travelling at 100 m/s, a typical velocity found in multi-hole DISI injectors at the nozzle exit. The breakup length scales calculated bear a resemblance to the near-nozzle nature of flash-boiling witnessed in experiments (Aleiferis et al., 2010; Oza and Sinnamon, 1983). The sensitivity to an increasing fuel temperature on the breakup criterion of Figure 3 originates from an increase in surface instability and bubble growth rate, due to a reduction in surface tension and an increase in saturation pressure. An important property of the bubble-droplet system at the time of breakup was the film thickness which will be discussed next. Figure 3 also highlighted the rapid reduction in film thickness and the effect of liquid temperature which resulted in a film thickness at breakup ($kb=1$) of 5.7 μm and 8.0 μm at $T_d=383$ K and $T_d=323$ K, respectively.

2.3.2. Child Droplet Size

The size of the child droplets could be established from the bubble-droplet system properties at the time of breakup. The approach of Zeng (2000) was adopted which uses the conservation of mass and energy to determine child droplet size. The calculation of the Sauter Mean Diameter (SMD) is given by Equation (11):

\[
SMD = \frac{1}{2} \frac{R_2^2 + R_1^2}{R_3 - R_1^3} + \frac{3}{2} \frac{R_1^2(R_1^{-1} - R_2^{-1})}{R_3 - R_1^3} \frac{V^2}{2} \ \psi_l \ \frac{\rho_l}{\sigma} 
\]

(11)

Figure 3. The development of breakup criterion and film thickness over time. A breakup criterion equalling 1 is displayed via crosses. n-Pentane.

where $V_c$ is the child droplet velocity calculated in the following subsection. From here on child droplet sizes are stated in SMD for consistency. Displayed in Figure 4 is the calculated child droplet SMD for a parent
droplet size of \( D_d = 200 \, \mu m \). Ambient pressures of \( P_{\infty} = 1.0 \) bar and \( P_{\infty} = 0.5 \) bar were investigated along with a range of droplet temperatures. Here, SMD was plotted against the breakup criterion, \( k_b \).

![Figure 4. Child droplet size development plotted against breakup criterion. \( D_d = 200 \, \mu m \). \( n \)-Pentane fuel and ambient pressures of \( P_{\infty} = 1.0 \) bar and \( P_{\infty} = 0.5 \) bar](image)

Focusing on the SMD at breakup (when \( k_b = 1 \)), it was clear that with an increase in temperature droplet sizes reduced. This followed the trend expected and values of approximately SMD=17.5 \( \mu m \) at \( T_d = 383 \) K, \( P_{\infty} = 1.0 \) bar were in the range of downstream experimental SMD values of between 8–15 \( \mu m \) (Butcher \textit{et al.}, 2015; Aleiferis and van Romunde, 2013). The effect of reducing ambient pressure, particularly at lower temperatures was highlighted, \( e.g. \) SMD=17 \( \mu m \) at \( T_d = 383 \) K, \( P_{\infty} = 0.5 \) bar, 0.5 \( \mu m \) smaller than when \( P_{\infty} = 1.0 \) bar. The sensitivity to changing ambient pressure was slightly lower than one might have expected, however it was interesting to discover that the effect of both increasing temperature and decreasing pressure diminished due to the rate of film thinning reducing with time (see Figure 3). The fluctuation in SMD between \( k_b \) values of 0.1 and 0.4 is due to the second term in \textit{Equation (11)} diminishing with increasing \( k_b \). As the film thickness reduces and \( V_c \) increases towards \( V_b \), the calculation of SMD becomes dominated by film thickness.

The number of droplets required to conserve mass at conditions representative of those shown in Figure 4 were calculated for varying child droplet sizes. An outer parent diameter of \( D_d = 200 \, \mu m \) was adopted with a film thickness of 10 \( \mu m \) at breakup for simplicity. For child droplets of 10 \( \mu m \) the required number to conserve mass was approximately 260 droplets. At these diameters, the number of droplets required became quite sensitive to changes in droplet sizes, hence one should apply caution when adopting very small child droplets. Stochastic parcel sensitivity studies were carried out whereby the number of parent and child parcels were varied in the range 2000–8000 parent parcels and 10–50 child parcels. The results are not included here for the sake of brevity but it is noted that low sensitivity was observed and the number of parent and child parcels finally used were 6000 and 20 parcels/ms, respectively.

2.3.3. Child Droplet Radial Velocity Magnitude

A similar approach to that used to calculate child droplet sizes was adopted for the calculation of child droplet velocities. Here, conservation of mass and momentum before and after breakup were applied to predict the radial velocity of child droplets as a result of bubble growth and inertial shattering as shown in \textit{Equation (12)}:

\[
V_c = \frac{3R_i^2 V_b (R_o - R_i)}{R_o^3 - R_i^3}
\]  

(12)
where $V_c$ is the child droplet velocity magnitude and $V_b$ is the bubble growth rate as shown in Equation (9) for the Rayleigh growth regime (Plesset, 1954). $V_c$ was dependent on both film thickness and bubble growth. It was found that as the film thickness reduced to zero, $V_c$ asymptotically increased towards $V_b$. Child droplet velocity is plotted against breakup criterion, $kb$ in Figure 5 for n-pentane at a range of conditions.

The child droplet radial velocity, shown in Figure 5, ranges from 7.8 m/s to 27.8 m/s at $T_d=323$ K and $T_d=383$ K, $P_\infty=1.0$ bar, respectively. Reducing ambient pressure to $P_\infty=0.5$ bar increased radial velocity to 10.6 m/s and 28.9 m/s for $T_d=323$ K and $T_d=383$ K, respectively. The implementation of the breakup model to the LPT approach assumed that the mass exchanged between the liquid film and bubble was deemed negligible when compared to typical surface evaporation at high temperatures. For example, when the bubble reached $R_b=100$ µm the reduction in liquid mass would be 0.078%. The sensitivity of parent droplet size on child droplet velocity was investigated and the effect was found to be minimal, with a difference of around 2% between $D_d=200$ µm and $D_d=20$ µm. Irrespective of parent droplet size, the bubble growth rate ultimately determined child radial velocity. The small effects caused by changes in parent droplet size originate from the differences in film thickness at breakup (i.e. when $kb = 1$).

An attempt was made to validate the radial velocity components calculated. The limitations of direct measurement of radial velocity components within droplets very close to the nozzle exit by typical optical techniques like Phase Doppler Anemometry (PDA) are well known (Aleiferis and van Romunde, 2013, Behringer et al., 2014; Butcher et al., 2015). Therefore, here, an estimation of the radial velocity component magnitude caused by flash-boiling was made from high-speed experimental images of full sprays at a range of conditions. In order to calculate the radial velocity component from flash-boiling alone, cone angles were measured at approximately 10 and 12.5 nozzle diameters downstream for subcooled and superheated sprays from single hole injectors. High-speed images of Aleiferis et al. (2010) and Postrioti et al. (2015) were adopted and cone angle measurements were taken at 10 nozzle diameters downstream. Radial penetration data of Allocca et al. (2014) were also adopted at the earliest spray measurement time of 45 µs after first sign of liquid which corresponded to an axial distance of around 12.5 nozzle diameters. The radial velocity component from flash-boiling was estimated based on the increase in cone angle when moving from a subcooled spray to a flash-boiling spray. The increase in cone angle/radial penetration along with axial velocities allowed an estimation of the radial velocity component introduced through flash-boiling. The resultant radial velocity components can be seen in Figure 6, whereby a number of liquid fuels were used.
Figure 6. A comparison between radial velocity components as a function of superheat degree for a range of fuels. Radial velocity estimated from experimental high-speed images and compared to analytical calculations.

The experimental data of Aleiferis et al. (2010) and Allocca et al. (2014) are comparable to the analytical model predictions, with radial components in the range 7–34 m/s and a similar gradient between varying superheats. The sensitivity of radial velocity magnitude and plume expansion under flashing conditions was obvious, as previously documented by Zeng et al. (2012), and also suggested radial velocity magnitude as an area of optimisation within the model due to uncertainties in phenomena outside the current modelling scope, such as near-nozzle compressibility effects. The sensitivity to fuel properties on the radial velocity component can also be seen in Figure 6. For a specific superheat, n-pentane produced a higher radial velocity component when compared to iso-octane and n-heptane, a result also of lower density, surface tension and viscosity. Considering the limitations in capturing experimentally with high-resolution such data using high-speed optical techniques and the general scatter in measurements, the prediction is considered sufficiently acceptable. More to the point, it is noted that the trend and range shown in Figure 6 was also found in good agreement with recent ultra-high speed (million-frame/s) imaging studies of flash-boiling liquid jets by Alghamdi et al. (2019).

The bubble growth rates and breakup timescales within fully flashing sprays are considered to remain mostly within the inertia controlled growth regime (Razzaghi, 1989). Plesset (1954) stated that under rapid bubble growth conditions, the change in bulk liquid temperature within the droplet is negligible. This assumption was applied to the current breakup model whereby parent and child droplet temperatures were assumed equal. It should be noted that surface evaporation and convective heat transfer models remained active.

2.4. Flash-Boiling Effective Nozzle Model

For completeness a brief overview of a flash-boiling effective nozzle zero-dimensional model is given here which offered a predictive method in determining initial droplet sizes at the nozzle exit. This modelling methodology was developed recently by the current authors (Price et al., 2016, 2018) and offered a normalised approach to predict the level of flash-boiling within high-pressure gasoline injectors. Specifically, a drift flux model based on heterogeneous nucleation was adopted to predict phase change within the nozzle orifice at superheated conditions (based on studies by Janet et al., 2015) which was then translated into an initial droplet diameter at the nozzle exit within the LPT framework. The reduction factor applied to the initial
droplet diameter can be seen in Figure 7 which was normalised against a non-dimensional parameter containing the Weber, Eckert, Jacob, Froude (and/or Eötvos) numbers and a non-dimensional temperature parameter $T^* = (T - T_{sat})/T_{sat}$ for a range of single component fuels at conditions representative of DISI engines.

Figure 7. Normalised initial droplet diameter reduction factor predicted by the flash-boiling effective nozzle model for a range of single-component fuels at different ambient pressures (Price et al., 2018).

This effective nozzle model, suggesting initial droplet diameters in the order 20 μm gave good agreement to experimental flash-boiling spray formation, where characteristics such as plume merging and spray collapse were captured. If the flash-boiling breakup model is applied to parent droplet sizes of $D_d = 20$ μm, the child droplet size reduced to SMD=2.5 μm at $T_d = 393$ K. Another aspect of the effective nozzle model was the near-nozzle region, where significantly large cone angles can occur due to flash boiling, hence the need to combine the diameter reduction factor with an empirical superheated cone angle relationship. However, such empirical relationships may not always work well over a range of conditions and fuels (Price et al. 2016, 2018). Therefore, an optimised link between in-nozzle phase change by the effective nozzle model and near-nozzle droplet shattering by the breakup model was expected to offer a more complete solution to predicting superheated fuel sprays in terms of capturing droplet sizes and curving of the plumes by incorporating near-nozzle radial expansion effects.

2.5. Injector and Grid

A 6-hole asymmetric injector was adopted throughout the current work. The injector under study has been extensively characterised experimentally by van Romunde et al. (2007), van Romunde and Aleiferis (2009), Aleiferis and van Romunde (2013) and Butcher et al. (2013, 2015) and a large database exists for direct comparison over a broad range of conditions. A mass flow rate of 0.12 mg/ms was adopted at an injection pressure of $P_{inj} = 150$ bar (Butcher et al., 2013, 2015). The current computational framework has been validated quite extensively through comparison of penetration lengths, droplet sizes and spray formation at subcooled, low superheats and highly superheated fully flashing sprays over a wide range of fuels (Price et al., 2015, 2016, 2018). For the exact nozzle hole geometry see Butcher et al. (2013, 2015). As previously mentioned, n-pentane fuel was adopted in the current work due to its ability to flash-boil under typical engine operating conditions and drive gasoline sprays’ collapse (van Romunde et al., 2007; Aleiferis and van Romunde, 2013; Serras-Pereira et al., 2007, 2008). This was highlighted numerically in Price et al. (2018). To replicate a quiescent environment comparable to experimental studies and maintain focus for future adaptation to full engine simulation, a Cartesian mesh with cell size 1 mm$^3$ was used to mesh a cubic domain.
of 80 mm$^3$ representing the size of a typical automotive cylinder bore. A mesh dependency study was carried out and documented in a previous publication (Price et al., 2015) where cells of between ~0.5 and 3 mm$^3$ were studied. 1 mm$^3$ cell size gave reasonable accuracy whilst adhering to a typical in-cylinder engine simulation cell size of 0.8–1 mm$^3$ (Malcom et al., 2011) and within reasonable computing times. A time step of 1 µs was adopted which again represented the requirement for future engine simulation applications and corresponded to approximately 0.01 crank angle degrees at 1500 RPM. Currently, the industry standard for engine simulation is a Cartesian or ‘trimmed’ mesh, hence the importance of studying a Cartesian mesh whilst some well-known mesh artefacts may present themselves, stemming primarily from the droplet collision sub-models drawing parcels away from cell boundaries when the injector axis is in parallel with continuous mesh boundaries (found mostly in uniform grids), causing areas with no parcels along cell boundaries (Post and Abraham, 2002; Schmidt and Rutland, 2004). Therefore, complete suppression of such effects was not pursued here since the focus was on the behaviour of the new breakup model itself and not on collision submodelling that was handled by parallel sensitivity studies. For example, using a polyhedral grid or rotating the Cartesian mesh (i.e. ensuring that none of the plumes is aligned with mesh lines) can minimize such effects but may lead to some extreme spray collapse in some cases, especially for a polyhedral mesh, as has been discussed by Price et al. (2018) in some detail and not elaborated further on here for the sake of brevity.

3. Results and Discussion

3.1. Initial Studies

The breakup model was implemented through user-coded subroutines whereby parcels were introduced at specific locations within the computational domain referring to droplet breakup sites calculated for each parent droplet. A simple example of a single-hole spray which incorporated the breakup model with reduced parent parcels for illustration purposes can be found in Figure 8. The droplet shattering mechanism can be seen in Figure 8, whereby the parent droplets (in red) shatter into a number of child droplets (in blue) with additional radial velocity components. The child droplets are ejected radially perpendicular to the parent droplet trajectory. A number of approaches were investigated, including completely randomised ejection angles, but little sensitivity was found.

Figure 8. A simple example of spray which incorporated droplet shattering (reduced number of parcels is used here for illustration purposes).

From here on all studies refer to the multi-hole injector of Aleiferis and van Romunde (2013). A series of sensitivity studies were undertaken to investigate the capabilities of the flash-boiling droplet breakup model at a range of thermodynamic conditions. This was to provide insight into the effect of important parameters and, where possible, to make direct comparisons with experimental data including spray formation from images, plume penetration and droplet sizes. Specifically, four operating conditions were studied, namely a subcooled one with fuel temperature $T_{\text{inj}}=293$ K at ambient pressure $P_{\infty}=1.0$ bar, and three superheated ones with fuel temperature $T_{\text{inj}}=363$ K at ambient pressure $P_{\infty}=0.5$ bar, $T_{\text{inj}}=393$ K at $P_{\infty}=1.0$ bar and $T_{\text{inj}}=393$ K at
$P_\infty=0.5$ bar. High-speed $n$-pentane and gasoline images are displayed at 777 µs ASOI (including an injector driver delay of around 300 µs as quantified by van Romunde and Aleiferis, 2009).

The subcooled spray at 293 K, 1.0 bar is shown in Figure 9. This produced three distinct plume pairs with no inter-plume interactions and ‘linear’ trajectories. The Reitz and Diwakar (1986) secondary breakup model coefficients were optimised according to Price et al. (2018) for the same injector. At the flash-boiling conditions of 363 K and 393 K, the flash-boiling droplet breakup model was found to be able to capture the typical multi-hole flash-boiling spray structures which include plume interaction/merging and droplet entrainment into the central low pressure region. The right-hand side plumes interacted forming a combined single plume with a large degree of droplet recirculation at the plume tips. All plumes were seen to favour the inner central region with a noticeable curvature in comparison to the more ‘linear’ plumes of the subcooled spray.

![Figure 9](image)

Figure 9. Spray formation at subcooled condition of $T_{inj}=293$ K at $P_\infty=1.0$ bar and three flash-boiling conditions of $T_{inj}=363$ K at $P_\infty=0.5$ bar, $T_{inj}=393$ K at $P_\infty=1.0$ bar and $T_{inj}=393$ K at $P_\infty=0.5$ bar, $n$-Pentane. Experiments by Aleiferis and van Romunde (2013), $n$-Pentane.

At the highest superheat case of $T_{inj}=393$ K at $P_\infty=0.5$ bar the plumes were noticeably wider than at the lower temperature condition of 363 K, 0.5 bar (about 40%, with the space between plumes narrowing accordingly), highlighting the ability of the model to automatically predict a widening of the plume angle near the nozzle. In the above sprays the initial parent droplet diameter was kept constant, equal to the nozzle diameter ($D_d=200$ µm) in an attempt to understand the model’s ability to capture flashing characteristics whilst adopting the ‘blob’ method for simplicity, i.e. as shown in the subcooled spray with only aerodynamic breakup mechanisms.

Liquid penetration lengths and downstream droplet SMD were quantitatively compared to experimental data at flash-boiling conditions, which are shown in Figures 10–11. The SMD value was calculated 25 mm downstream of plumes 1 and 6 replicating that obtained by PDA measurements by Aleiferis and van Romunde (2013). The liquid penetration displayed in Figure 10 matched the experiment but the heated fuel cases were found to be over predicted, especially in the later stages of spray after around 550 µs ASOI, suggesting initial
injection velocity matched experiment but droplet sizes or breakup severity could be improved. The SMD data shown in Figure 11 at the steady state condition (after 500 μs) was 11.4 μm and 10.6 μm at 393 K, 1.0 bar and 393 K, 0.5 bar, respectively within a few microns of the experimental SMD of 8.4 μm and 7.1 μm, respectively (i.e. within about 30%). This confirms that droplet shattering can contribute quite significantly to reducing droplet sizes at flash-boiling conditions. Considering the complexity of the droplet shattering mechanism and the implementation of the breakup methodology with no detailed calibration at this stage, a reasonable prediction of breakup through flash boiling was achieved. It is worth highlighting that the over-prediction in SMD in the order 4 μm will have contributed to the over-prediction in penetration lengths and also would have affected the momentum exchange between phases and ultimately the level of spray collapse which has been shown previously to be quite sensitive to droplet sizes (Price et al., 2015). The highest superheated case of 393 K, 0.5 bar was in the order 1–2 μm smaller agreeing with the directionality of physical data (although one is reaching the limit of experimental accuracy at this stage). Optimisation was initially sought by studying the child droplet velocities and sizes in the next section.

Figure 10. Liquid penetration at $T_{\text{inj}}=293$ K at $P_{\infty}=1.0$ bar, $T_{\text{inj}}=363$ K at $P_{\infty}=0.5$ bar, $T_{\text{inj}}=393$ K at $P_{\infty}=1.0$ bar and $T_{\text{inj}}=393$ K at $P_{\infty}=0.5$ bar, n-Pentane. Symbols: Experiments by Aleiferis and van Romunde (2013), n-Pentane.

Figure 11. SMD at $T_{\text{inj}}=363$ K at $P_{\infty}=0.5$ bar, $T_{\text{inj}}=393$ K at $P_{\infty}=1.0$ bar and $T_{\text{inj}}=393$ K at $P_{\infty}=0.5$ bar, n-Pentane. Symbols: Experiments by Aleiferis and van Romunde (2013), n-Pentane.
3.2. Child Radial Velocity Magnitude and Size

Droplet momentum is certainly one of the dominant factors affecting the level of spray collapse and interaction with the gaseous phase. In an attempt to understand the potential for model optimisation through child droplet properties, child droplet velocity and size was systematically varied from the default model prediction. Child droplet diameters of 8.2 µm, 16.4 µm (analytical model solution) and 32.8 µm were studied along with two child radial velocity magnitudes of 31.8 m/s (analytical model solution) and 63.6 m/s. Resultant spray formation can be seen in Figure 12.

![Figure 12. Spray formation at $T_{inj}=393$ K at $P_{\infty}=1.0$ bar, $n$-Pentane with varying child droplet velocity and child droplet diameter. Sprays plotted at 777 µs ASOI including injector driver delay. Experiments by Aleiferis and van Romunde (2013), n-Pentane.](image)

The default model spray (16.4 µm and 31.8 m/s) showed plumes being drawn into the central region. The near-nozzle expansion was somewhat captured, however experiments showed outer spray envelope cone angles as high as 160°–180° very close to the nozzle orifice. When child droplets were reduced to 8.2 µm, droplets were drawn into the central axis narrowing individual plumes. When child radial velocity magnitude was increased, e.g. 8.2 µm and 63.6 m/s, the predicted near-nozzle angle increased slightly and plumes were found to curve towards the central region, suggesting that even though child droplets were being ejected radially at a higher velocity, an increased degree of collapse was present. At larger child droplet diameters of 32.8 µm air entrainment was limited which resulted in droplets continuing on their nominal trajectory unlike that of experiment. This suggested that child droplet sizes above ~30 µm were outside of a ‘terminal momentum’ where air entrainment can encourage spray collapse.

The liquid penetration lengths and SMD for each case can be found in Figures 13–14. The penetration lengths of Figure 13 showed that large radial velocity components and a larger degree of plume spreading reduced penetration lengths closer to experimental values. The case of 16.4 µm, 63.6 m/s showed better overall agreement in terms of penetration. A small reduction in SMD was also produced as the radial velocity magnitude increased for fixed initial child droplet size, a result of a larger plume footprint interacting with the gaseous phase. The difference in SMD between droplet sizes was somewhat reduced due to the aerodynamic breakup sub-model and evaporation causing droplets to converge towards a stable droplet diameter. The case of 16.4 µm, 63.6 m/s showed an intermediate level of agreement with the droplet sizing experiments, despite its matching the penetration the closest. Therefore, the degree of potential optimisation through child droplet breakup properties was clear, whereby sensitivity existed in each aspect.
of the spray including spray formation, the collapsing mechanism, droplet sizes and penetration lengths. It is noted that 16.4 µm, 31.8 m/s were the values used for the simulations in the rest of the paper as this is what the breakup analysis predicted. However, further sensitivity analysis is shown in the next section on parent droplet diameters and later by an optimisation parameter for expansion velocities, building upon the results of the current section and associated understanding.

Figure 13. Liquid penetration for varying child velocity size and radial velocity magnitude at $T_{inj}=393$ K at $P_{∞}=1.0$ bar, $n$-Pentane. Symbols: Experiments by Aleiferis and van Romunde (2013), $n$-Pentane.

Figure 14. SMD for varying child velocity size and radial velocity magnitude at $T_{inj}=393$ K at $P_{∞}=1.0$ bar, $n$-Pentane. Symbols: Experiments by Aleiferis and van Romunde (2013), $n$-Pentane.

3.3. Parent Droplet Diameter

Aleiferis et al. (2010) and Li et al. (2015) are among those who have experimentally established in-nozzle phase change from superheated effects and it has been well documented that the initial droplet size at the nozzle orifice can be dramatically affected by flash-boiling and greatly influence spray formation. The use of the 'blob' method at flash-boiling conditions was deemed an over-simplification due to a reduction in effective nozzle hole size from the two-phase flow within. Reducing the initial droplet diameter was previously found to be an effective way of introducing flash-boiling characteristics into the LPT framework (Price et al., 2015). In the previous sub-section, the flash-boiling breakup model attempted to replicate this enhanced atomisation through downstream breakup alone, whilst incorporating an automatic calculation of plume expansion through radial shattering. In reality, a combination of both in-nozzle and near-nozzle effects
would occur under fully flashing operating conditions. By reducing initial droplet diameter, to take into account the reduction in effective nozzle diameter, the subsequent droplets which undergo thermally driven breakup will intrinsically be smaller. Although some optical nozzle experiments are available for qualitative validation, the exact flash-boiling mechanism is still under intense study. An attempt was made to find a best-practice approach which adhered to available experimental data. The aim of capturing flashing characteristics with a focus on downstream droplet sizes over a range of conditions was investigated.

Displayed in Figure 15 is the spray formation of n-pentane at $T_{inj}=393$ K, $P_{\infty}=1.0$ bar and $T_{inj}=393$ K, $P_{\infty}=0.5$ bar for various initial droplet diameters, ranging from the nozzle orifice diameter of $D_d=200$ µm, 100 µm and 50 µm.

Parent droplet sizes of both $D_d=200$ µm and $D_d=100$ µm showed qualitatively similar spray formation to experiment with a degree of droplet recirculation at the plume tips. The near-nozzle expansion was under-predicted, which suggested that larger radial velocity magnitudes may have been present and could be due to under-expanded jet-like behaviour and the collision model may have also been over-predicting near-nozzle droplet collisions (see Schmidt and Rutland (2004) who discussed limitations with the current collision modelling technique). It should be highlighted that as the parent sizes start to reduce to values quite lower than 100 µm, e.g. down 50 µm as also included in Figure 15, one begins to reach a feasible limit where a significant portion of droplets can evaporate completely and current numerical models operate far from their designed limits.

To quantitatively understand predicted child droplet properties at varying parent droplet sizes, the downstream droplet SMD was calculated at 25 mm downstream of the nozzle orifice and is displayed in Figure 16. The SMD was compared to the experimental data of Aleiferis and van Romunde (2013) at the same spatial location. Figure 16 shows again that with initial $D_d=200$ µm the droplet SMD downstream was over-predicted. When parent droplet sizes were reduced to $D_d=100$ µm SMD values fell to within 2 µm of experiment for both operating conditions. Parent droplet sizes of $D_d=50$ µm generally under-predicted SMD even when considering the amount of coalescence visible within the plumes in Figure 15, where droplets in the order 25–35 µm existed, particularly at the plume tips and periphery. It is interesting to note that for all cases, the sensitivity of downstream droplet sizes to parent droplet size was smaller than first expected. However, it was clear from Figure 15 that the sensitivity of spray formation and global spray pattern is considerably greater and initial droplet sizes can play an important role in predicting the severity of spray collapse. It was also clear that this parameter offered great potential for model optimisation, agreeing with
The flash-boiling effective nozzle model documented in Price et al. (2016 and 2018) was developed on the basis of in-nozzle vapour generation as a number of experiments have documented this phenomenon (Wu et al., 2017a–b; Li et al., 2015; Aleiferis et al., 2010; Butcher et al., 2013).

The effect of in-nozzle phase change should be limited as to not under-predict droplet sizes downstream of droplet shattering and not lead to spray plume structures unrealistically thin not matching experimental observations. Parent droplets in the order 20 μm produced child droplets in the range 1–3 μm which were considered overly small in comparison with test data. Wu et al. (2017a), using optical nozzle experiments with n-pentane fuel, found that a limit in bubble volume fraction within the nozzle was reached at fully flashing conditions, due to choking of the flow. This occurred because two-phase flows are thought to choke at significantly lower velocities than single-phase flows (Sovani et al., 2001) and such phenomena have been documented in the case of flash-boiling sprays (Bar-Kahony and Sher, 2004; Gopalakrishnan and Schmidt, 2008) where sonic conditions and resultant shock waves have been visualised by Vieira and Simões-Moreira (2007) using Schlieren imaging. In the work of Wu et al. (2017a) flow choke produced a bubble volume fraction limit for the optical slit-nozzle studied, where increasing the superheat had no further effect on the amount of vapour within the orifice. Through observation, the effective nozzle diameter or width of the liquid phase within the optical nozzle was seen to reach a limit of approximately 30% of the nominal nozzle diameter. Gopalakrishnan and Schmidt (2008) were also able to capture the ‘vapour lock’ phenomenon observed by Reitz (1990) whereby the orifice became saturated with vapour, limiting the vapour generation rate and significantly reducing mass flow rates. Experimental spray work and analysis by Lacey et al. (2017) using propane and iso-octane fuels has also highlighted that injector throat Mach numbers for single-phase and two-phase flows determined whether the injector was choked and that the pressure at which the nozzle choked was meaningful in characterising the injection process and near-nozzle spray behaviour than just considering the saturation pressure of the fuel in the rail. Choked conditions were estimated for the current injector setup using an analytical technique for the calculation of sonic velocity in a two-phase mixture. Although calculating correctly sonic velocities in two-phase mixtures is not trivial, an approximation by the following equation was used (Brennen, 2009):

\[
\frac{1}{c} = \frac{\alpha}{kP_n} \left[ \rho_l (1 - \alpha) + \rho_g \alpha \right]
\]

where \(c\) is the sonic velocity, \(\alpha\) is the vapour volume fraction, \(P_n\) is the nozzle pressure and \(k\) can be considered unity as first approximation in the current work (representing isothermal bubble behaviour). The
sonic velocity of the two-phase flow can be estimated for a varying degree of volume fraction, whereby at a volume fraction of $\alpha=0.5$ the lowest two-phase sonic velocity was calculated. The sonic velocity was plotted against volume fraction for $n$-pentane at $T_{\text{inj}}=363$ K with varying pressure and can be found in Figure 17. Pressure was varied in order to understand its effect on the resultant sonic velocity as the pressure within the nozzle orifice drops rapidly over the nozzle orifice length.

![Image](image_url)

Figure 17. Sonic velocity of two-phase mixture of $n$-Pentane with varying nozzle pressure at $T_{\text{inj}}$ of 363 K and 393 K.

Figure 17 highlights the dramatic reduction in sonic velocity as the flow becomes a two-phase mixture of liquid and vapour. At $P_h=5.0$ bar, the sonic velocity was reduced to around 60 m/s for a volume fraction of $\alpha=0.5$, a condition which, if accurate, could lead to choking with injection velocities in the order 90–120 m/s depending on temperature. At the further reduced pressure of $P_h=1.0$ bar, the sonic velocity at $\alpha=0.5$ is as low as 27 m/s. The in-nozzle pressure can arguably remain higher than the downstream ambient pressure, with a sudden reduction at the nozzle orifice, especially under choked conditions (Sovani et al., 2001). The flow also tends to be asymmetric and inhomogeneous (Aleiferis et al., 2010), hence it is difficult to accurately calculate the degree of choking and subsequent effects within the nozzle. However, from the calculation of Figure 17, it can be concluded that a degree of choking is possible within the nozzle under fully flashing conditions. Hence, it is reasonable to assume a limit of in-nozzle vapour fraction under flashing conditions, as also documented by Wu et al. (2017a–b).

Based on the above reasoning, a lower parent droplet size limit can be estimated for the current numerical framework and through a calibration exercise produce downstream droplet sizes comparable to experimental data. A droplet reduction factor limit of 0.5 was suggested for the current work based on informed analysis of the droplet reduction factor and lowest sonic velocity calculation. This limit will produce an initial droplet size with mean value of $D_d=100$ µm with the current injector at fully flashing conditions, however the complex relationship between the in-nozzle and near-nozzle flashing mechanisms still remains as an area of focus for further research into the flashing phenomenon. The combination of the flash-boiling effective nozzle model documented in Price et al. (2016 and 2018) and the breakup model documented in the current work, offers the potential to provide a more holistic flash-boiling modelling approach within the LPT framework. In-nozzle phase change and the subsequent reduction in effective nozzle diameter would be predicted by the zero-dimensional flash-boiling effective nozzle model. The near-nozzle flashing mechanism causing plume radial expansion and curving would be captured through the breakup model via droplet shattering. The link between both models would therefore take into account both aspects of flash-boiling
sprays, theoretically producing appropriate droplet sizes with an automated calculation of additional radial velocity and increased cone angle instead of having to rely on empirical near-nozzle spray plume cone angle adjustments. From here on a limit of 0.5 in the normalised initial droplet diameter reduction factor from the flash-boiling effective nozzle model was applied to all simulations which adopted the flash-boiling breakup model.

### 3.4. Droplet Size Distribution

The size of parent droplets undergoing breakup as previously investigated in Figure 15 proved an important aspect in capturing downstream droplet sizes as well as spray formation. As well as parent droplet sizes, another important aspect was the distribution of parent droplet sizes, which in turn influenced child droplet characteristics and global spray properties. Here, a range of parent droplet size distributions were investigated with the flash-boiling breakup model. The distributions adopted can be found in Figure 18 and included a Rosin-Rammler distribution with shape factors of $q=4.0$, 3.2 and 2.6 (within the range stated by Beck and Watkins, 2002) with a scaling factor $X=100 \, \mu m$ and a normal distribution with standard deviations 5, 10 and 15 $\mu m$ (within the range measured by Behringer et al., 2014 and Butcher et al., 2015) about a mean of 100 $\mu m$. Child droplet sizes were calculated using a Rosin-Rammler distribution with shape factor $q=3.2$ (Beck and Watkins, 2002).

**Figure 18.** Parent droplet size distributions using the Rosin-Rammler distribution function and a normal distribution function.

The resultant spray formation can be found in Figure 19 for each distribution case for n-pentane at $T_{inj}=363$ K and $P_{\infty}=0.5$ bar. The global spray formation showed slight differences with varying parent droplet distribution. The case of Rosin-Rammler with a shape factor $q=2.6$ (i.e. the widest distribution function) the curvature of the plumes towards the central region was somewhat eliminated, due to the number of large droplets existing within the plumes. As the distribution was narrowed ($q=4.0$) plumes seemed to show a more qualitative representation to experimental images. The normal distribution was comparable to the constant parent droplet size case due to the narrow distribution of droplet sizes being introduced at the nozzle exit.

The percentage droplet count was measured at a resolution of 0.5 $\mu m$ at 25 mm vertically downstream and compared to the experiments of Butcher et al. (2015) in Figure 20. This illustrates a good comparison, whereby the peak value matched experiments at approximately 7 $\mu m$. The Rosin-Rammler distribution with $q=2.6$ showed that small droplets of around 2–3 $\mu m$ were introduced into the spray, however this resulted in an under-prediction of droplets in the range 6–9 $\mu m$. The overall comparison to experiments showed good agreement with a droplet count within ~1.5% of experiment for droplets greater than ~2 $\mu m$. From hereon, the Rosin-Rammler distribution with $q=3.2$ was adopted.
Figure 19. Spray formation with varying parent droplet size distributions using Rosin-Rammler with $q=4.0$, $3.2$, $2.6$, $X=100$ µm and a normal distribution function with mean $100$ µm, standard deviations $5$, $10$, $15$ µm, $n$-Pentane. Experiments by Aleiferis and van Romunde et al. (2013), $n$-Pentane. $T_{in}=363$ K, $P_{in}=0.5$ bar.

Figure 20. Predicted droplet size distributions using Rosin-Rammler parent droplet size distributions with $q=4.0$, $3.2$, $2.6$, $X=100$ µm and a normal distribution with mean $100$ µm, standard deviations $5$, $10$, $15$ µm, $n$-Pentane. Experiment by Butcher et al. (2015), Gasoline.

3.5. Nozzle Hole Spacing and Model Optimisation

The flash-boiling breakup model has proven an effective method in predicting child droplet sizes, hence producing flash-boiling sprays with downstream droplet sizes within reasonably matched range to those of experiments and globally similar collapsed spray structures and matched spray tip penetrations. These data were obtained by initially assuming that all plumes originated from the same spatial location for simplicity. Such a single injection point was deemed suitable to the LPT methodology as initial approximation due to injected parcels becoming active $1$ time step downstream of the nozzle orifice hence no real interaction between holes occurred numerically at the single point. However, as next step and in an effort to reduce the near-nozzle collisions and enhance near-nozzle droplet expansion, the distance between injector nozzle holes in the simulation setup was matched to nozzle-hole spacing data obtained for this injector by silicon castings and subsequent electron microscope analysis (Butcher et al., 2013 and 2015). The separation of holes was measured to be in the range of $0.2$–$0.3$ mm. It is also noted that Khan et al. (2017) identified nozzle-hole spacing as an effective method in reducing near-nozzle interaction and somewhat preventing unrealistic
collision model behaviour. This was especially attractive with the breakup model whereby the number of collisions was significantly more than in the case of more traditional approaches, naturally due to the droplet shattering in the dense spray area.

The spray formation with increased nozzle hole spacing in Figure 21 showed a more relaxed collision behaviour in the near-nozzle region and resulted in a wider downstream cone angle. The ‘End view’ image highlighted the collapsing nature of the multi-hole spray with a clear curvature of the plumes inwards towards the central region. The area at the bottom of the spray remained free from droplets and showed a convincing likeness to experiment. Spacing nozzle holes appropriately may offer an immediate method to partially overcome limitations and numerical artefacts stemming from typical droplet collision models, as documented previously (Schmidt and Rutland, 2004; Price et al., 2018). A new sophisticated approach to improve current collision models when applied at extreme conditions like those presented here would be beneficial. The ‘Base View’ image clearly shows that a collapsing mechanism was present in more than one plane, where plumes 1 and 6 (left hand side) showed signs of entrainment towards the central axis, similar to that seen in the experimental images, although a degree of separation remained due to aforementioned artefacts.

\[ D_{\text{d}} \mu m \]

\[ T_{\text{inj}} = 393 \text{ K}, P_{\infty} = 0.5 \text{ bar} \]

Gasoline \hspace{1cm} n-Pentane \hspace{1cm} Gasoline \hspace{1cm} Gasoline

Figure 21. Effect of injector nozzle-hole spacing, n-Pentane. Experiments by van Romunde et al. (2007) and Aleiferis and van Romunde (2013), n-Pentane and Gasoline.

In a further sensitivity analysis to understand spray formation at flash-boiling conditions, it was decided to apply an empirical constant to the child radial velocity component magnitude as \( C_c \times V_c \) with an initial value of \( C_c = 1.5 \) to cover a wider area of expansion velocities like those reported recently by Alghamdi et al. (2019). This was also done to represent any additional forces acting on the jet exiting the nozzle, such as expansion due to compressibility effects and under-expanded jet behaviour at high superheat degrees, as well as other uncertainties in the real physical mechanism of the predicted velocity magnitude. An attempt at fundamentally understanding and implementing this is being carried out by the current authors using under-expanded jet simulations (Hamzehloo and Aleiferis, 2016). However in the present work due to remaining limitations in quantification of such effects, it was assumed that forces acting on the liquid phase from under-expanded jet expansion effects were somewhat considered in the additional radial velocity component and could have been responsible for the need to fine tune velocity components. To conserve child droplet momentum, child droplet size was reduced to account for the increasing velocity. The optimised model properties showed better agreement to the experiments compared to the default model child droplet properties as displayed in Figure 22. This figure also displays predictions by the flash boiling effective nozzle coupled to a superheated cone angle empirical relationship according to Price et al. (2016 and 2018).
Figure 22. Spray breakup with increased expansion velocity. Results from the flash-boiling effective nozzle model also shown with superheated cone angle relationship. Experiments by van Romunde et al. (2007) and Aleiferis and van Romunde (2013), n-Pentane and Gasoline.

The optimised model properties showed a better general comparison to experiment compared to the default model child properties, whereby a more severe plume curvature was seen and a larger degree of recirculation was present at the low ambient pressure condition. The ‘Base view’ highlighted a more severe collapsing mechanism and showed complete merging of plumes 1 and 6. Plumes 2, 3, 4 and 5 showed similarities to
experiment where complete merging of plumes was present. The increase in the near nozzle cone angle from the larger child droplet radial velocity magnitude seemed to enhance the collapsing mechanism through stronger jet tip vortices and a more severe air entrainment mechanism, which showed that greater near-nozzle expansion can promote spray collapse. It was obvious that optimisation through child droplet properties was available and that the complex interactions between the dispersed phase, continuous phase, as well as interactions between the plumes themselves meant that further fine tuning of model parameters could be beneficial. It is also noted for completeness that some mesh artefacts related to droplet collision modelling effects, as mentioned in earlier section of this paper, can be observed. For example, in the region between plumes for the breakup model, small droplets may appear aligned vertically leaving some gaps instead of dispersed more uniformly. As already mentioned, such effects can be eliminated by manipulation of the orientation of grid lines with respect to the spray but it was decided to leave the grid formulation identical at all conditions and for all models in the current paper. The reader is referred to Price et al. (2018) for a more detailed discussion of such issues.

The penetration, SMD and droplet size distributions are displayed in Figure 23, Figure 24 and Figure 25, respectively. The penetration for both the default and optimised breakup model was within ~3.5% and 1% at 1000 μs ASOI showing good agreement over the entire injection duration. The downstream SMD was again slightly over-predicted for the default breakup model but reduced to within 1 μm at steady state conditions once the radial velocity was increased. The droplet size distribution was included for completeness and showed that the higher superheated case resulted in a narrower distribution of droplets. The larger SMD found for the breakup model in comparison to the flash-boiling effective nozzle model can be seen within the droplet size distributions shown in Figure 25 whereby a greater degree of larger droplets than 7 μm existed. It is also interesting to see that there are a larger number of smaller droplets than 3 μm. This showed that the model was able to produce a larger range of droplet sizes, a result of child droplet size being a function of parent droplet size which is dependent on the initial droplet size distribution.

Figure 23. Liquid penetration under flash-boiling conditions with a breakup model setup of increased expansion velocity $V_c$. Compared to the flash-boiling effective nozzle model with empirical superheated cone angle applied as boundary conditions at the point of injection. Symbols: Experiments by Aleiferis and van Romunde (2013), $n$-Pentane.
Figure 24. SMD under flash-boiling conditions with a breakup model setup of increased expansion velocity $V_c$. Compared to the flash-boiling effective nozzle model with empirical superheated cone angle applied as boundary conditions at the point of injection. Symbols: Experiments by Aleiferis and van Romunde (2013), n-Pentane.

Figure 25. Downstream droplet count under flash-boiling conditions with a breakup model setup of increased expansion velocity $V_c$. Compared to the flash-boiling effective nozzle model with empirical superheated cone angle applied as boundary conditions at the point of injection.

4. Summary and Conclusions

A breakup modelling approach was developed and aimed at capturing the droplet shattering mechanism present in flash-boiling fuel sprays. The shattering process was incorporated through the introduction of child parcels at breakup sites with individual properties (e.g. a radial velocity component, size and mass), which were calculated using linear stability analysis, bubble growth and the conservation laws. A number of sensitivity and parametric studies were carried out in an attempt to overcome limitations in employing empirical functions for near-nozzle cone angle effects and the flash-boiling breakup model was used in addition to a previously developed flash-boiling effective nozzle model (Price et al., 2016, 2018) in order to predict effects from the contribution of both in-nozzle phase change and near-nozzle expansion through bubble growth and droplet shattering. A multi-hole injector was studied at a range of conditions using n-pentane and compared to n-pentane and gasoline spray images and associated experimental data.
quantitatively through penetration lengths and downstream droplet sizes. Qualitative assessment was also achieved through comparison to spray formation phenomena captured by high-speed optical imaging techniques. The main conclusions from the current work can be summarised as follows:

- Use of linear stability and bubble growth analysis proved to be an efficient approach in predicting fuel droplet shattering properties with a good degree of sensitivity to thermodynamic conditions typically found in direct-injection spark-ignition engines.
- The developed breakup model was able to predict important flash-boiling spray characteristics such as plume merging, spray collapse and droplet recirculation through the breakup of droplets near the nozzle exit.
- The introduction of an additional radial velocity component near the nozzle orifice allowed an increasing cone angle to be predicted automatically. Dramatic near-nozzle expansion was somewhat limited by effects related to increased severity of droplet-droplet collisions close to the nozzle orifice.
- Initial droplet ‘blob’ size was found to be a central parameter in predicting flash-boiling fuel spray behaviour. In-nozzle phase change was accounted for through a zero-dimensional flash-boiling effective nozzle model with a maximum contribution of 50% reduction in effective nozzle diameter and initial blob size. This was within the range documented in several publications which associated a limit with compressibility effects and vapour locking.
- Downstream droplet distributions were compared to experimental data and showed good agreement at 0.5 bar, 363 K. Peak values were ~7 µm diameter for both computational and experimental data and sizes of >2 µm were captured to within approximately 1–2% of droplet sizing experiments.
- Optimisation of the breakup model through incorporation of nozzle-hole spacing details and child droplet radial velocity tuning was also investigated. Distinct curvature of plumes became more prominent and resultant droplet sizes were within 2 µm of experiment and penetration lengths matched to within 1% over the flash-boiling conditions studied.

Some suggestions for future improvement in the numerical framework’s ability to deal with flash-boiling sprays can be put forward. There is scope for optimising the degree of contribution from the flash-boiling droplet breakup model and flash-boiling effective nozzle model by application to other injection systems. Focus could also be directed towards the droplet collision model and related criteria of various modes of collision (Aleiferis et al., 2014), including mesh sensitivity and resultant artefacts. This would offer further progress towards a code capable of modelling sprays holistically at subcooled and superheated conditions. Although a number of studies have been carried out in an attempt to overcome collision modelling issues at typical conditions (e.g. Munnannur and Reitz, 2007; Schmidt and Rutland, 2004), no detailed data analysis exists at flash-boiling operation since one would also require new high-resolution experiments of binary droplet collisions at some extreme thermodynamic conditions. For completeness, it is also noted that although matching spray parameters like penetration and droplet sizes gives strong confidence in the validation of certain submodels and presents a modelling framework that is considered sufficient for application to engine design at realistic operating conditions, there are remaining thermophysical processes that warrant both experimental and modelling attention with high-resolution techniques for further fundamental understanding of the behaviour of fuel flash boiling injection. For example, effects related to choked flow and jet under-expansion at the nozzle exit may require a dedicated parallel study.

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