

# Numerical Modelling of Fuel Spray Formation and Collapse from Multi-Hole Injectors under Flash-Boiling Conditions

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## Abstract

Flash-boiling of fuel sprays can occur when the fuel enters a metastable superheated state, which is common in direct-injection spark-ignition engines operating at low in-cylinder pressures and/or hot fuel temperatures. The effect of flash-boiling on the resultant spray formation can be both detrimental and advantageous to engine operation, hence numerical modelling capability is essential in future engine optimisation and design. A recently-developed new model by the current authors that can be applied as zero-dimensional boundary condition for multi-hole flash-boiling fuel spray predictions was investigated over a wide range of injection systems, focusing on the model's ability to quantify in-nozzle phase change effects and automatically predict important global spray characteristics such as spray collapse, droplet recirculation and plume merging within a Lagrangian particle tracking framework. Mesh-type sensitivity was highlighted using a uniform Cartesian and a non-uniform polyhedral mesh. The model was also normalised through a dimensionless parameter for a wide range of single component fuels. The model was validated both qualitatively and, where possible, quantitatively against experimental data. The model's ability to deal with a wide range of injection configurations and operating conditions was confirmed and a number of limitations are highlighted and discussed with respect to future work.

## 1. Introduction

Flash-boiling is a rapid phase-change process which occurs when a liquid is discharged into an ambient environment with a pressure below that of the fuels saturation pressure, causing the fuel to enter a metastable superheated state. The sudden increase in superheat of liquid fuels in direct-injection is partly due to the extremely small timescales associated with the depressurisation across the nozzle orifice, whereby latent heat cannot be consumed through typical boiling. However, nucleation and rapid bubble growth can occur in the available timescales, promoting atomisation [1] which can significantly affect spray formation and in turn alter in-cylinder mixing, combustion and emissions.

Flash-boiling in Direct-Injection Spark-Ignition (DISI) engines is likely to occur when the engine is operating hot at part-load or aggressive valve profiles are adopted such as Early Intake Valve Closure, producing a partial in-cylinder vacuum during injection. Flash-boiling of fuel sprays in multi-hole injectors is an important area due to the possibility of fuel sprays behaving unlike that of the designed spray characteristics. Typically, individual spray cone angles increase, droplet sizes reduce and vapour concentrations increase [2, 3], all naturally leading to plume-plume interactions and a collapsing mechanism in multi-hole sprays. This mechanism has been seen to both reduce and increase liquid penetration, depending on the severity of superheating and collapse [4]. An increase in penetration can promote unwanted phenomena such as wall wetting and can result in higher unburnt hydrocarbon emissions from incomplete combustion. However, flash-boiling can also enhance in-cylinder mixture formation due to the rapid atomisation, smaller droplets and increased vaporisation which can promote a more homogenous distribution of fuel. The reader is guided to [3] and [5] for in-depth reviews of flash-boiling.

Nucleation and bubble growth are phase change mechanisms which yield the flash-boiling process, whereby bubble nuclei appear on interfaces such as geometrical boundaries, dissolved gas or impurities in the fuel (heterogeneous nucleation). If the thermophysical conditions allow, these nuclei form vapour bubbles which grow rapidly through an initially inertia controlled period moving towards a thermally controlled slower growth phase

via a transitional period in-between where the effect of surface tension becomes proportional to the effect of pressure forces and heat diffusion [6, 7]. The introduction of the gaseous phase in, at or outside of the nozzle orifice significantly influences the behaviour of the liquid phase, promoting atomisation at the very early stages of injection, as opposed to the less violent aerodynamically induced breakup which requires the interaction between ligaments/droplets and the surrounding ambient gas [8]. The gaseous phase in the nozzle exit, introduced through rapid phase change, may exit the nozzle as an under-expanded jet, suddenly expanding and drawing the liquid phase radially outwards forming a wider plume cone angle (see [9] for simulations of under-expanded jets from mm-size nozzles). A secondary flash-boiling process is inertial shattering, a process which may occur when rapid bubble growth occurs outside of the nozzle exit. Liquid droplets shatter under the forces applied from rapid bubble growth, ejecting secondary droplets with additional radial momentum [10], contributing to the widening of plumes close to the nozzle orifice to angles as wide as  $180^\circ$  [11].

The quantification of flash-boiling fuel sprays is notoriously difficult, due to the limitations associated with the minute timescales ( $\sim 1\text{--}100\ \mu\text{s}$ ) and length-scales of high-pressure gasoline injectors (typical nozzle diameter of  $\sim 100\text{--}250\ \mu\text{m}$  with length to diameter ratios of 1–5). However, a number of attempts have been made. Sher and Elata [12] were among the first to try and quantify the flashing process in terms of downstream spray characteristics. Binary mixtures of toluene and Freon 22 were used in a pressure can apparatus, which in turn were used to derive a mathematical model to predict downstream droplet sizes over a range of experimental pressures and temperatures. A second important study on the measurement of flash boiling sprays was carried out in [2], where an Infrared Extinction/Scattering method was used to measure the fuel vapour concentration in *n*-Pentane sprays under superheated conditions. It was found that under flash-boiling conditions there was a significant increase in vapour concentration and the vapour footprint was seen to increase dramatically. A more recent experimental contribution to the understanding of flash-boiling sprays was conducted [13] whereby the effect of nozzle configuration on global spray characteristics was carried out by investigating nine nozzle tip configurations. It was found that an injector with a large number of holes caused a more pronounced collapsing mechanism, due to the closer proximity of plumes. Other examples of recent experimental characterisation of flash-boiling include that of [14] and [15] who found that, among other variables, the ratio of ambient pressure to saturation pressure was an essential parameter in predicting the onset of flash-boiling. It is clear that many factors influence flash-boiling fuel sprays, from fuel properties, nozzle configurations, operating conditions to the dynamics of the overall injection system.

Flash-boiling sprays have been studied using pure Eulerian frameworks (such as [16, 17]) and also techniques based on the Lagrangian particle tracking framework. The latter has many advantages over a purely Eulerian simulation, foremost being the relatively light computational power requirement allowing full engine spray and mixture formation simulations to be run with a practical turnaround. Previous work by the current authors [18] investigated the Lagrangian modelling capability with respect to fully flashing multi-hole sprays, whereby a superheat evaporation model based on the heat transfer coefficient of [2] was implemented to improve modelling accuracy. It was concluded that the Lagrangian framework was able to capture important global spray characteristics such as spray collapse, plume merging and droplet recirculation if appropriate boundary conditions are used (representing enhanced atomisation close to the nozzle exit). In a secondary study [19] a new model was developed to automatically predict appropriate spray boundary conditions at the nozzle exit as fuel superheat is increased, with respect to previous conclusions. This, in combination with the superheated evaporation submodel, led to capturing important spray characteristics for a specific 6-hole injector.

## 2. Present Contribution

The aim of the current work was to further develop and apply a flash-boiling spray model to a two-phase Lagrangian/Eulerian framework and validate its ability to predict both qualitative and quantitative flash-boiling characteristics over a wide range of injector nozzle multi-hole geometries and a variety of single-component fuels. This was carried out by:

- Understanding the sensitivity of the flash-boiling model to single-component fuel properties, and normalising all fuels through a dimensionless parameter at the nozzle exit.
- Applying the model through user-coded subroutines to a range of fuels under sub-cooled and superheated flash-boiling conditions.

- Investigating the model's ability to predict flash-boiling spray characteristics such as plume merging, spray collapse and droplet recirculation from a wide range of multi-hole injector nozzle geometries, including both symmetric and asymmetric configurations.
- Comparing computational sprays to experimental data and where possible making quantitative comparisons to liquid penetration and droplet sizes, as well as fuel vapour concentration and droplet temperatures.

The paper highlights predictive improvements and discusses various challenges in view of further developments and application to in-cylinder mixture formation simulations.

### 3. Numerical Methodology

A two-way coupled Lagrangian-Eulerian framework was used to enable numerical modelling of a dispersed multi-phase flow. The Lagrangian particle tracking 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 through the addition of source terms in the energy, mass and momentum transport equations of both phases. The system of equations was solved by the numerical code STAR-CD. The PISO pressure-velocity coupling algorithm was used [20] with STAR-CD's temporal discretisation scheme with an accuracy in between that of first and second order. Second-order discretisation of momentum, turbulence and temperature was achieved using the Monotone Advection and Reconstruction Scheme (MARS). The conservation of Lagrangian quantities (velocity, position, size, density and temperature) were solved using first-order ordinary differential equations. Turbulence was modelled using a Reynolds-Averaged Navier-Stokes (RANS) approach, specifically the  $k$ - $\epsilon$  RNG (Re-Normalization Group) model [21] previously shown to perform better in engine simulations than typical  $k$ - $\epsilon$  models [22, 23, 24]. The default turbulence model constants were adopted. The Reitz-Diwaker secondary breakup model [8] was adopted and droplet-droplet collisions were modelled using the model of [25] where a speed-up algorithm has also been adopted [26]. A time step of 1  $\mu$ s was used throughout. Temperature dependent polynomial relationships for the thermo-physical properties of fuels were taken from the Yaws' Property Database [27] and implemented via user coding. The fuel properties modelled in this manner include: surface tension, viscosity, latent heat of vaporization, density, specific heat capacity, saturation pressure and thermal conductivity. Vapour and gas densities were modelled by the ideal gas law.

#### 3.1 Flash-Boiling Atomisation Model

A superheat evaporation model was implemented by user coding in order to add flash-boiling modelling capability in terms of surface evaporation from a superheated liquid droplet. This has been documented in a previous publication by the current authors [18] and is based on the work of [28] and [29]. The heat transfer coefficient relationship of Adachi distinguishes three different regimes dependent on the degree of superheat. In order to quantify the phase change mechanism of flash-boiling through wall nucleation inside of the nozzle orifice and implement this as a spray boundary condition, a zero-dimensional model based on the wall nucleation study [30] was developed and implemented through user coding. This has been documented recently in detail [19], however an overview of the model's formulation and approach is given here for completeness. Specifically, the model relies on the prediction of phase change through heterogeneous wall nucleation by calculating the bubble number density, departure frequency and bubble departure size. From this, a total volumetric flow rate per surface area can be calculated and then applied to specific nozzle geometries. The volumetric flow rate of vapour is then translated into an equivalent droplet diameter at the nozzle exit (where mass is conserved through an increase in droplet count), representing in-nozzle liquid atomisation triggered by flash-boiling induced phase change. Firstly, nucleation site density per unit surface area is calculated based on a dimensionless nucleation site density function as well as a property function dependent on the liquid to gas density ratio as displayed in Equation (1):

$$N_{nuc} = \frac{1}{D_b^2} N_{nuc}^* F(\rho^*) \quad (1)$$

where the dimensionless nucleation density,  $N_{nuc}^*$  is given as:

$$N_{nuc}^* = \left[ \frac{D_b (T_{inj} - T_{sat}) \rho_g H_L}{2\sigma T_{sat}} \right]^y \quad (2)$$

Here  $\sigma$  is the surface tension coefficient,  $T_{sat}$  the saturation temperature of the fuel,  $D_b$  the bubble departure diameter,  $T_{inj}$  the fuel injection temperature,  $\rho_g$  the fuel vapour density and  $H_L$  the latent heat of vaporisation. The exponent,  $\gamma$  displayed in Equation 2 was suggested as an appropriate parameter for model refinement [31], this was investigated in [19] and was found to greatly enhance the applicability of the current methodology to a wide range of fuels and conditions. In the current work this is not optimised for individual test cases as this is seen to lie outside of the current scope. Secondly, the bubble departure diameter is calculated as follows [32]:

$$D_b = 2.64 \cdot 10^{-5} \theta_c \left( \frac{\sigma}{g \Delta \rho} \right)^{0.5} (\rho^*)^{0.9} \quad (3)$$

where  $\theta_c$  is the contact angle,  $g$  the acceleration due to gravity,  $\Delta \rho$  the dimensional density ratio ( $\rho_l - \rho_g$ ) and  $\rho^*$  the property density function. The contact angle, which represents the angle between the tangent of the bubble surface and boiling surface, can be set to a value of  $45.78^\circ$ , as previously adopted in [17]. This was originally derived in [33] using the theory of capillarity to calculate the bubble diameter at departure representing a balance between body forces and surface tension which subsequently determines the bubble geometry. The property density function and dimensionless density are defined in Equation (4) and (5), respectively.

$$F(\rho^*) = 2.157 \cdot 10^{-7} (\rho^*)^{-3.12} (1 + 0.0049 \rho^*)^{4.13} \quad (4)$$

$$\rho^* = (\rho_l - \rho_g) / \rho_g \quad (5)$$

where  $\rho_l$  is the liquid density. Finally the bubble departure frequency is calculated as follows:

$$f = \frac{1.18}{D_b} \left[ \frac{\sigma g (\rho_l - \rho_g)}{\rho_l^2} \right]^{0.25} \quad (6)$$

The nucleation site density, departure frequency, bubble diameter and specific nozzle inner-orifice area can be used to calculate a vapour volume flow rate which is then converted into a void fraction based on the ratio of volumetric flow rate of liquid and vapour. To translate the degree of phase change to a reduction in droplet diameter, representing in-nozzle/near-nozzle atomisation, the void fraction in the nozzle is translated into a droplet diameter based on the maximum possible height for the liquid phase when the liquid is assumed to reside at the bottom of the nozzle unmixed with the gaseous phase, which can be seen in the schematic diagram displayed in Figure 1. The asymmetry adopted here has been documented in experimental work in [34] and represents asymmetry caused by cavitation in the upper surface region and mechanically driven flow favouring the lower portion of the nozzle orifice. Two different methods of translating void fraction into droplet diameter were investigated in [19] including a symmetrical vapour film and linear translation. Mass is conserved through an increase in droplet count within each stochastic parcel. Note that a lower droplet diameter limit of  $14 \mu\text{m}$  was applied at extreme conditions, which previously displayed reasonable predictions of highly flashing sprays and prevented instability.

The model was validated against the optical slit-nozzle experimental data of [35], which is displayed in Figure 2; values of exponent  $\gamma$  of Equation (2) of both 4.4 and 4.05 are shown. The area percentage of vapour predicted lies within the range of experimental data, particularly in the superheat region of  $P_\infty/P_s = 0.1\text{--}0.3$  where the majority of flash-boiling test cases used within the current work reside. This evaluation displays that the model is able to predict in-nozzle phase change within a reasonable degree of accuracy. Fine tuning of model constants for each case is proposed, to take into account difficult to measure properties such as boiling surface and fuel impurities, however in the current work this is not carried out.

### 3.2 Cone Angle Relationship

Throughout the current work the initial plume cone angle was investigated using a constant cone angle taken from the subcooled spray images (typically  $\theta = 15^\circ$ ), and at fully flash-boiling cases a cone angle relationship taken from the work of [36] is adopted. The work of [36] developed a dimensionless relationship based on the underlying assumption that the cause for a widening cone angle stems from the bubble nucleation and shattering mechanism, which was translated into a cone angle for specific operating conditions and fuels. The following parameter was used to predict the widening of the plume at superheated conditions for a range of single-component hydrocarbon fuels and water.

$$\theta = \log \left( \frac{R_p^2 \theta^3}{m_a^2} \right) \quad (7)$$

where  $R_p$  is the pressure ratio between  $P_{sat}$  and  $P_\infty$ ,  $m_a$  the atomic mass of the fuel,  $\theta$  the dimensionless surface tension defined as  $\theta = \frac{a_o \sigma}{k_b T_{inj}}$  where  $a_o$  is the molecular surface area,  $k_b$  the Boltzmann constant and  $T_{inj}$  the injection temperature. The resultant individual plume cone angle is applied as an initial boundary condition to highly flash-boiling sprays in the current work and documented to the nearest degree.

### 3.3 Simulation Set-up

A number of injectors were modelled in the current work, each injector configuration is displayed in Table 1 along with important injection data, and injector directionality is documented in the Appendix.

Both symmetric and asymmetric injectors were modelled with varying numbers of holes and plume angles. The mass flow rates used in the current work (unless otherwise stated) were estimated from experimental data of similar injection systems. *n*-Pentane, and *iso*-Hexane were investigated as surrogate single component fuels in the case of experiments using multi-component gasoline fuel blends on the basis that high-volatile components in gasoline, like Pentanes and Hexanes, drive the flashing mechanism. Work documented in [41, 42, 43] have shown that *n*-Pentane can produce similar spray characteristics and provide a good level of evaluation especially in terms of the collapsing mechanism. *n*-Hexane was also investigated with the sole purpose of highlighting the trend seen as one moves from a high volatile fuel (*n*-Pentane) through *iso*-Hexane towards a lower volatile fuel, and was not expected to represent gasoline fuel accurately.

To replicate a quiescent environment comparable to experimental studies and maintaining focus for future adaptation to full engine simulation, a cubic mesh with cell size  $1 \text{ mm}^3$  was used to mesh a cubic domain of  $80 \text{ mm}^3$  representing the size of a typical automotive cylinder bore. A mesh dependency study was carried out and documented in a previous publication [18] where cells of between  $\sim 0.5$  and  $3 \text{ mm}^3$  were studied. However,  $1 \text{ mm}^3$  cell size gave reasonable accuracy whilst adhering to a typical engine simulation cell size of  $0.8\text{--}1 \text{ mm}^3$ . In an attempt to understand mesh artefacts found in the current study, particularly in the case of symmetrical injectors at flashing conditions (due to droplet trajectories aligning with cell boundaries passing through the entire domain) a polyhedral mesh with a  $1.5 \text{ mm}$  base size was adopted for fully flashing cases. An internal section view of each mesh is displayed in Figure 3. Currently, the industry standard for engine simulation is a Cartesian or ‘trimmed’ mesh hence the importance of studying a Cartesian mesh whilst well-known mesh artefacts remain [26, 44]. A time step of  $1 \mu\text{s}$  was adopted which again represents the requirement for future engine simulations and represents approximately  $0.01$  crank angle degrees at  $1500 \text{ RPM}$ .

## 4. Results and Discussion

### 4.1 Subcooled Sprays

A subcooled spray was modelled and compared to the experimental data of [43]. Model optimisation of the Reitz-Diwaker secondary breakup model [22] was investigated. The breakup model contains a stable droplet diameter derived from Weber number and breakup timescale, including model constants,  $C_{b1}$ ,  $C_{s1}$ ,  $C_{b2}$ ,  $C_{s2}$  which are displayed in Equations (8)–(11); Equations (8) and (9) bag breakup, Equations (10) and (11) stripping breakup.

$$We \equiv \frac{\rho_l |u_g - u_d|^2 D_d}{2\sigma} \quad \tau_b = \frac{C_{b2} \rho_d^{1/2} D_d^{3/2}}{4\sigma_d^{1/2}} \quad \frac{We}{\sqrt{Re_d}} \geq C_{s1} \quad \tau_b = \frac{C_{s2}}{2} \left( \frac{\rho_d}{\rho} \right)^{1/2} \frac{D_d}{|u_g - u_d|} \quad (8, 9, 10, 11)$$

$C_{s2}$  has been shown in [45] to vary quite significantly between  $\sqrt{3}$  and 20. Here the value of  $C_{s2} = 8$  was used as adopted in [46] to promote breakup. Reitz and Diwaker [8] stated that values of  $C_{b1}$  have been shown in literature to vary between  $C_{b1} = 3.6\text{--}8.4$  and in a previous study by the current authors [18] values of  $C_{b1}$  and  $C_{s1}$  of 2.0 and 0.1 showed a reduction in global Sauter Mean Diameter (SMD) of around 65%. In an attempt to improve SMD predictions at subcooled conditions, the breakup model constants were optimised. The resultant sprays displayed in Figure 4 show the effect of enhanced breakup through model constant optimisation ( $C_{b1} = 3.0$ ,  $C_{s1} = 0.2$ ,  $C_{b2} = 1.5$ ,  $C_{s2} = 8.0$ ). It is noted that the injector has been tilted by  $19^\circ$  in reference to the plume directionality listed in the Appendix. Figure 5 shows the time varying SMD and liquid penetration at the subcooled condition of *n*-Pentane at  $P_\infty = 1 \text{ bar}$  and  $T_{inj} = 293 \text{ K}$ . The reader should be aware that the computational results have been modified to incorporate the injection delay of experiment by including the injector driver's delay duration (typically around  $300 \mu\text{s}$ ) to the computational results.

Initial droplet sizes smaller than the nozzle orifice diameter are known to occur from cavitation effects [47]. The reduction in theoretical nozzle diameter due to cavitation was previously estimated for the current injector for a range of liquid temperatures [19] in the range of 10%, which suggests the blob-method, whereby initial droplet sizes are equal to the geometrical nozzle orifice diameter [48] is viable and the flash-boiling nozzle model was applied directly to the nozzle diameter. It was clear that the breakup model constants can be tuned to achieve a reasonable match of both SMD and penetration to experimental data using the current framework. From here on the optimised model constants were used throughout and subcooled sprays were included to highlight the complete transitioning from subcooled to fully-flashing sprays.

## 4.2 Model Normalisation

An attempt was made to generalise the model for a large range of single component hydrocarbon fuels, including alkane, alcohol and aromatic groups. Displayed in Figure 6 is the droplet diameter reduction factor, which is the boundary condition parameter calculated by the model from the degree of phase change within the nozzle (injection system of [40]) at ambient pressure conditions and applied as a reduction factor to initial droplet diameter with a nominal size equal to the nozzle orifice diameter. It can be seen that fuel properties largely affect the degree of phase change, with significant differences in droplet diameter reduction factor for a specific superheat degree ( $\Delta T = T_{inj} - T_{sat}$ ). Each fuel behaved correspondingly to molecular structure, where lighter components such as butane ( $C_4H_{10}$ ) required a smaller superheat than heavier components such as Octane ( $C_8H_{18}$ ) to reach the same reduction factor, and this trend was seen through each fuel group. The most influential parameter found, due to the large variation between fuels, was the latent heat of evaporation. With alcohols typically having a large latent heat of evaporation (for Ethanol  $0.850 \times 10^6$  J/Kg in comparison to *n*-Pentane's  $0.306 \times 10^6$  J/Kg at 363 K, 1 bar), the nucleation site density was found to increase with higher latent heat causing a larger degree of nucleation for a given superheat. The aromatics on the other hand showed a shallow gradient corresponding, in part, to their relatively low latent heat of evaporation. Fuel densities also considerably influenced model behaviour; Equations (1), (3) and (6).

Due to the buoyancy force vs. surface tension force determining the departure bubble diameter, surface tension was another important fuel property. A normalisation parameter was derived (derivation displayed in Appendix) to normalise droplet diameter reduction factor for all fuels. The normalisation parameter denoted  $\eta$  in this instance is displayed in Equation (12).

$$\eta = \frac{\rho_g^{0.1}(\rho_l - \rho_g)^{0.4} H_L T^*}{\sqrt{g\sigma}} \quad (12)$$

where  $T^*$  is the dimensionless superheat as follows:

$$T^* = \frac{T_l - T_{sat}}{T_{sat}} \quad (13)$$

It was found that the density term in Equation 12 can be simplified as follows:

$$\eta = \frac{\sqrt{\rho_g} H_L T^*}{\sqrt{g\sigma}} \quad (14)$$

The normalisation parameter of Equations (12) and (14) can be re-written using well-known dimensionless quantities as:

$$\eta = \frac{\sqrt{We} Fr T^*}{Ec Ja} \quad (15)$$

where the Weber number has been defined as:

$$We = \frac{[\rho_g^{0.1}(\rho_l - \rho_g)^{0.4}]^2 U^2 D_b}{\sigma} \quad \text{and} \quad We = \frac{\rho_g U^2 D_b}{\sigma} \quad (16)$$

for Equations 12 and 14 respectively, the Froude number is  $Fr = \frac{U}{\sqrt{g D_b}}$ , the Eckert number is  $Ec = \frac{U^2}{\Delta T C_p}$  and the

Jakob number is  $Ja = \frac{C_p \Delta T}{H_l}$ . Equation (15) suggests a relationship between mechanical and thermal forces exists.

Mechanical forces include inertia vs. surface tension in the form of the Weber number as well as buoyancy forces associated with Froude number. Thermal forces comprise of thermal dissipation with respect to the flows kinetic

energy and latent heat effects from the Eckert and Jakob number, respectively. It should be noted here that the Weber number stated above has been simplified from the more complex Weber number derived directly from Equations (1)–(6). Due to this simplification having small effect, the typical form of  $We$  was favoured in Equation (15). It is also noted that the normalisation parameter can also be expressed in terms of the Eötvös number ( $Eu$ ) instead of Froude by suitable rearrangement.

Figure 7 displays all fuels plotted against the normalisation parameter of Equation (15) at ambient pressure conditions ranging from  $P_\infty = 0.3$  bar to  $P_\infty = 1.0$  bar. It is clear that all fuels collapsed closely onto a single curve by this approach, hence easy to implement in a code to account for a range of fuels when performing in-cylinder mixture formation simulations; the averaged curve is also displayed in Figure 7. The range of pressures investigated ( $P_\infty = 0.3$ – $1.0$  bar) was typical of that found at throttled intake-stroke conditions when fuel is injected directly into the cylinder to increase mixture homogeneity at ignition timing. The authors provide a word of caution for pressures residing significantly far from these shown.

### 4.3 Flashing Sprays of Injectors with Asymmetric Nozzles

#### 4.3.1. 6-Hole Asymmetric Injector [40]

In order to investigate the model's ability to automatically predict flash-boiling spray formation for a wide range of injector configurations and fuels, multiple injectors were investigated over a range of ambient pressures and injection temperatures. Firstly, both alkane and alcohol fuels were applied to a 6-hole asymmetric injector which has been characterised experimentally [40]. The resultant spray formation is displayed in Figures 8, 9 and 10 for alkanes and alcohols, respectively. The driver delay found in experiment (typically 300  $\mu$ s) was added to the computational sprays.

An important observation in [40] was the comparison between single and multi-component fuels at flashing conditions. The lighter components of gasoline are what drive the flash-boiling process, and single-component fuels such as *n*-Pentane showed reasonable comparisons to multi-component gasoline in regards to spray formation for fully flashing sprays [41–43]. *n*-Pentane sprays were able to capture flashing characteristics at the highest superheated case of  $T_{inj} = 393$  K and  $P_\infty = 0.5$  bar in Figure 8, such as the complete plume merging and droplet recirculation close to the plume tips as well as a degree of curvature of the plumes. At  $T_{inj} = 393$  K and  $P_\infty = 1.0$  bar the model predicted a similar flashing mechanism for *n*-Pentane which was also present in experiment. *iso*-Hexane captured the entire transition from subcooled to fully-flashing sprays when compared to gasoline. The transitioning spray shows the plumes beginning to merge, and the reader should be aware that droplet display techniques usually hide some of the smaller droplets due to droplet-size scaling. *n*-Hexane demonstrated the effect of fuel volatility on the model's behaviour and subsequent spray formation. At the most extreme case, *n*-Hexane began to flash-boil.

Displayed in Figure 9 is the most extreme condition visualised from the 'front view' which can be seen in Table 1. The Cartesian mesh cases both showed good qualitative agreement with experiment, capturing a degree of collapse whilst maintaining definition between plumes either side of the central axis. The polyhedral mesh case however displayed a more uniform fully merged plume, which was found to be a common theme throughout all injectors investigated. The severity of spray collapse when using the polyhedral mesh diminished variations stemming from differences in injector configurations. Although the central region remained without droplets in the experimental images, replicating that of the computational spray, the polyhedral mesh was investigated for completeness. It can be seen that for the polyhedral mesh, the collapsing mechanism was over-predicted, whereby all plumes merge into a single large cone angled plume. In the case of *n*-Pentane, good agreement was seen in terms of qualitative characteristics, however the over-prediction of collapse suggested the current available collision model could be vastly improved in the case of flash-boiling sprays [49]. Also displayed for *n*-Pentane fuel in Figure 8 is a spray with the cone angle scaling relationship of [36], Equation (7) resulting in an initial plume cone angle of 102°. Qualitatively, the wider cone angle was comparable to that seen in experiment, specifically in the near nozzle region.

Volatility was not the only important parameter in predicting the onset of flash-boiling. Ethanol, which has a higher boiling point than both Hexanes, was shown to collapse completely at the same conditions in Figure 10, a result of the Ethanol's steep gradient in droplet reduction factor (see Figure 6). In contrast, *n*-Butanol, an alcohol that is also considered as a future fuel for internal combustion engines but has much lower volatility than Ethanol, demonstrates very different behaviour in Figure 10.

Liquid spray penetration for *n*-Pentane, *n*-Hexane and *iso*-Hexane sprays is compared to experimental data in Figure 11. At subcooled conditions, penetration was predicted accurately due to breakup model optimisation. At superheated conditions, the penetration was typically over-predicted when using a small cone angle ( $\theta = 15^\circ$ ) but reduces to closely match experiment when the cone angle was increased. It should be noted that injection velocities increase at higher temperatures to account for the reduction in liquid density at fixed mass flow rate.

In order to understand the computational framework's ability to predict flash-boiling of lower volatility fuels, an extreme case was investigated, specifically  $T_{inj} = 453$  K,  $P_\infty = 0.3$  bar using *n*-Butanol. A comparison was made to the experiments of [40] in Figure 12. The polyhedral grid was again added to highlight the sensitivity of the collision model at such conditions. If the model was pushed to extreme temperatures, even for low volatility fuels, a fully collapsing spray was achieved. Here, at such conditions, it is worth noting that evaporation models are likely to stray from the designed operating window and can become the dominant process controlling droplet behaviour. The polyhedral mesh showed a similar trend with an increased severity of spray collapse. This was seen throughout and highlights the conclusion of [26] that droplets are drawn away from cell boundaries which limit collapse in the case of the Cartesian mesh.

Along with liquid penetration lengths, droplet sizes were also compared to experiments. Time varying SMD values were calculated at a position 20 mm downstream of the nozzle exit within a 2mm wide volume and are displayed in Figure 13. At subcooled conditions for *n*-Pentane the SMD value was calculated at  $\sim 20$   $\mu\text{m}$  at steady-state conditions, whereas experiment showed a value of  $\sim 12.5$   $\mu\text{m}$ . The aerodynamic breakup model could have easily been optimised to match SMD perfectly, however a trade-off with penetration lengths would exist. Here, the focus lies with superheated sprays and at both conditions for *n*-Pentane, the SMD was within 2  $\mu\text{m}$  once a steady measurement was acquired (typically after 450  $\mu\text{s}$ ). When compared to the increased cone-angle cases, a further reduction in SMD was seen, a result of a larger spray footprint interacting with surrounding gas over a larger area. *n*-Hexane and *iso*-Hexane typically should have a larger SMD. This was highlighted in the case of *n*-Hexane at  $T_{inj} = 393$  K,  $P_\infty = 0.5$  bar which did not enter the fully flashing regime, hence the droplet sizes were around 10  $\mu\text{m}$  larger than those of *n*-Pentane and *iso*-Hexane.

#### 4.3.2. 7-Hole Asymmetric Injector [39]

A 7-hole asymmetric injector taken from the work of [39] was investigated and displayed in Figure 14. An injection delay of around 400  $\mu\text{s}$  was added to the computational sprays. The majority of sprays modelled in Figure 14 were either subcooled or contained a low degree of superheat as shown by  $P_\infty/P_{sat} > 1$  (subcooled) or having a value of between  $P_\infty/P_{sat} = 0.4$  and 1. Spray structures at  $P_\infty = 1$  bar showed similar characteristics such as the non-uniformity at the spray tip as well as plume merging from droplet breakup and aerodynamic drag. At  $T_{inj} = 353$  K and  $P_\infty = 0.5$  bar *n*-Pentane showed a complete collapsing spray with increased penetration length. The wider cone angled spray ( $100^\circ$  angle) highlighted mesh artefacts present which resided on the vertical linear mesh boundary, which was overcome by using a polyhedral mesh. Both Hexane isomers contained very low degrees of superheat resulting in initial droplet sizes remaining close to the nozzle orifice size.

To quantify the model's ability to predict spray characteristics for varying ambient pressure and fuel temperature, the liquid penetration was compared to that of [39] in Figure 15. The injection delay period from rising edge of injection pulse to fuel seen at the nozzle tip was about 400  $\mu\text{s}$  and has been accounted for. A small under-prediction of liquid penetration was found for the ambient pressure conditions, with an accuracy of  $\sim 10\%$  at 1000  $\mu\text{s}$ . At  $P_\infty = 0.5$  bar the penetrations were predicted to within  $\sim 3\%$  at 1000  $\mu\text{s}$  and highlighting the framework's ability to capture the increased penetration caused by spray collapse. It is re-iterated here that the basic breakup model constants were optimised only for one of the injectors at subcooled conditions, as explained earlier, and these were purposely fixed and applied to all other injectors of the current study. Therefore, the under-predicted penetration of this injector at atmospheric conditions was likely caused by a combination of this and the fact that flow rate experimental data for this injector were available only for gasoline at a single condition and not for the more volatile pentane and hexane components over a range of conditions. This injector could be associated with stronger coupling between in-nozzle phenomena and downstream plume interaction because of the closer proximity of the nozzle holes and much narrower outer envelope spray angle in comparison to the injector used for original tuning, hence the breakup constants could be further optimised to eliminate this under-prediction.

To further understand the sprays quantitatively, SMD was compared to experimental data. The SMD was calculated within a 2 mm wide plane normal to the central plume 25 mm downstream of the nozzle exit and averaged over the injection event. At the subcooled conditions of  $T_{inj} = 293$  K,  $P_\infty = 1.0$  bar and  $P_\infty = 0.5$  bar for *n*-

Pentane the SMD was predicted within 10  $\mu\text{m}$  and 55  $\mu\text{m}$  of the experiment, respectively. The Reitz-Diwakar breakup model [8] relies on ambient gas density to calculate a stable droplet diameter. For example, halving ambient pressure and consequently halving gaseous density (within ideal gas law assumptions), stable droplet diameter doubles and bag-breakup timescales increase (see Equations 8–11). The work of [46] found a similar trend at 20 mm downstream of the nozzle exit, here an increase in ambient pressure displayed a significant reduction in droplet diameter from 60  $\mu\text{m}$  at 11.0 bar to 30  $\mu\text{m}$  at 30 bar back pressure, and breakup timescales were seen to reduce. This behaviour is not seen in the experiment and the breakup model needs to be re-optimised to account for the effects associated with spray formation under reduced pressures. It should also be noted that variations in injection velocity between temperatures are likely to influence downstream SMD measurements. At superheated conditions, the evaporation rates became significant and the initial droplet sizes were reduced, allowing the SMD to be predicted within  $\sim 3$   $\mu\text{m}$  and 7  $\mu\text{m}$  at  $T_{inj} = 353$  K,  $P_{\infty} = 1.0$  bar and  $T_{inj} = 353$  K,  $P_{\infty} = 0.5$  bar respectively. *n*-Hexane and *iso*-Hexane led to significantly higher SMD for the low pressure high-temperature case due to lack of flash-boiling (*n*-Hexane and *iso*-Hexane had a small degree of superheat of  $T^* = 0.1$  and  $0.129$  and  $P_{\infty}/P_{sat} = 0.356$  and  $0.275$ , respectively) and non-optimised basic breakup parameters at sub-cooled conditions for individual injectors.

### 4.3.3. 2-Hole and 6-Hole Asymmetric Injector [38]

To investigate this further, two additional multi-hole asymmetric injectors were investigated for a range of single-component fuels, one 2-hole and another 6-hole asymmetric nozzle pattern characterised experimentally [38]. The flow rate adopted here was derived from a similar type of solenoid injector used in [40]. The work of [50] also characterised another similar type of injector for varying injection pressure and showed a reduction in mass flow rate of approximately 10% when moving from  $P_{inj} = 150$  bar to 100 bar. Hence the flow rate adopted is 3.6 and 10.8 mg/ms for the 2-hole and 6-hole injectors respectively (see Table 1). Firstly, the 2-hole injector configuration was studied for  $T_{inj} = 413$  K and  $P_{\infty} = 0.4$ –1.0 bar. *n*-Pentane, *n*-Hexane and *iso*-Hexane were compared to Mie scattering spray images of multi-component gasoline fuel. The superheated cone angle relationship of [36] giving an individual plume cone angle of  $107^\circ$  and a polyhedral mesh were also studied for the most extreme superheated *n*-Pentane spray (minor differences were found between mesh types at subcooled/non-flashing conditions). It should also be noted that both experimental injectors were rotated through  $10^\circ$  (in comparison to nominal plume data in the Appendix) and this was replicated in the computational set-up. The predicted spray formation is compared to experiments in Figure 16.

Theoretically the entire range of conditions can be dealt with using the current computational framework. At subcooled conditions the aerodynamic breakup model dominated, reducing droplets from the nozzle orifice diameter to one tenth of that value within 20 mm of the nozzle exit. In the transitioning regime, the flash-boiling model and breakup model worked together, whereby initial droplet sizes remained above the breakup criterion. At fully flashing conditions, the model introduced small initial droplets which evaporated rapidly, these resided below the breakup criterion hence the aerodynamic breakup model became obsolete (droplet coalescence could produce droplets which meet this criterion).

The computational sprays of *n*-Pentane contained a significant degree of superheating, even at  $P_{\infty} = 1.0$  bar. This produced a collapsed spray for all flash-boiling cases of *n*-Pentane and *iso*-Hexane, although *iso*-Hexane contained larger droplets. *n*-Hexane, being the least volatile of the three fuels, lagged behind in terms of predicting the onset of flash-boiling, and only collapsed fully at pressures less than  $P_{\infty} = 0.7$  bar. This trend highlighted the influence of volatility on spray characteristics, a similar trend was documented in [51, 52] whereby *n*-Hexane produced smaller droplets and penetration when compared to lower volatile fuels *n*-Heptane and *n*-Decane. Due to the plume axis located away from the vertical cell boundaries mesh effects could be seen on the inner edge of the plume which followed the cell mesh line. At the lowest ambient pressure conditions of  $P_{\infty} = 0.4$  bar, the collapsed single plume showed less curvature when compared to the higher pressure cases. The lower gas density at reduced ambient pressures resulted in weaker interaction with droplets and hence less air entrainment. The polyhedral case showed a more uniform spray structure, with equal amounts of recirculating droplets either side of the main plume. An important aspect of flash-boiling sprays is the expansion in the near-nozzle region. This expansion can reach angles as high as  $180^\circ$  immediately after the nozzle exit as seen in optical nozzle experiments [34]. The computational spray with increased cone angle of  $107^\circ$  significantly increased the liquid footprint, and also captured severe curvature of the plume into the central region. Nevertheless, it is also clear that the cone angle scaling relationship can be improved and as a result this could also improve the downstream spray formation predictions.

The 6-hole version of the above injector [38] was also studied and displayed in Figure 17 for the same ambient pressures but lower injection temperatures of  $T_{inj} = 368$  K. Again, the model predicted automatically critical flash-boiling spray characteristics. The transition from non-collapsing to a collapsing spray could be seen in the case of *n*-Pentane, where plumes started to curve inwards and eventually formed a fully-collapsed spray. The curvature of the right-hand side plume seen in experiment at subcooled conditions ( $T_{inj} = 293$  K and  $P_{\infty} = 1.0$  bar) suggested that the close proximity of plumes encouraged spray collapse. This could be seen at  $T_{inj} = 368$  K and  $P_{\infty} = 1.0$  bar for all fuels, whereby plumes began to merge even at low superheat degrees in the case of *n*-Hexane. Further increasing the superheat showed a more severe collapsing mechanism as well as a significant degree of plume tip recirculation in the case of *n*-Pentane, a characteristic which was found in experiment. At the lowest pressure operating condition, *n*-Pentane collapsed and penetrated further than all other conditions, replicating experiment. A large number of small droplets (8–15  $\mu\text{m}$ ) resided in, and travelled parallel along the cell boundaries and produced a mesh artefact for the Cartesian mesh case. This caused an area free of droplets in the central region (as shown by [26]), however the overall spray shape represented that of experiment in terms of a fully collapsed spray with similar trajectory. The polyhedral mesh was also adopted for this case and could be seen to overcome this issue as shown in previous injectors but penetration lengths were under predicted in comparison to experiments. Here a single unbroken plume was developed with significant droplet recirculation. The smaller-droplet representation bottom-up view highlighted that asymmetries existed within the bulk spray similar to the more defined plumes seen in the comparable experimental image.

A quantitative comparison was made to liquid penetration and can be seen in Figure 18. For all fuels at both  $P_{\infty}$  of 1 bar and 0.7 bar the penetration was predicted to within 2% and 6% at 800  $\mu\text{s}$ , respectively. At the fully-flashing condition, the complete collapse of the *n*-Pentane spray showed little influence on penetration length when compared to non-flashing *n*-Hexane and *iso*-Hexane. Although droplet sizes differed significantly along with spray shape, the low ambient pressure dampened these effects (due to drag forces diminishing with gaseous density). The large cone angle spray test case (angle of  $104^{\circ}$ ) displayed a severe curvature of the plumes close to the nozzle exit, an important property of highly flashing sprays. However, simply increasing the cone angle was an oversimplification which highlighted the importance of being able to model the momentum exchange between radial and axial droplet momentum components by a more explicit formulation. The polyhedral mesh reduced penetration due to significant droplet recirculation increasing the amount of momentum exchange between leading droplets and gas.

## 4.4 Flashing Sprays of Injectors with Symmetric Nozzles

Two symmetrical multi-hole injectors were investigated. Due to the nozzle symmetry alongside the uniform Cartesian mesh, a greater degree of mesh sensitivity was expected originating from the collision model.

### 4.4.1. 6-Hole Symmetric Injector [37]

Firstly, a symmetric 6-hole injector, adopted in the work of [37] was studied. Here an ambient pressure of  $P_{\infty} = 0.3$  bar was used throughout and a fuel temperature of  $T_{inj} = 373$  K. *n*-Pentane, *n*-Hexane and *iso*-Hexane were again used to compare with experimental data of gasoline. It is noted here that the experimental data included a total injection delay in the range 600–1500  $\mu\text{s}$  from start of rising edge of the trigger signal, including a capacitance delay of 300–1200  $\mu\text{s}$  and a mechanical delay of 300  $\mu\text{s}$  [53]. Considering the long duration of this delay and related uncertainties due to approximate values given, direct comparison to experiments in terms of exact timing was not straightforward. Figure 19 shows sprays at 600  $\mu\text{s}$  ASOI (stated as 2000  $\mu\text{s}$  ASOI in [37] – and considering a delay of 1400  $\mu\text{s}$ ). The same test case was also studied on a polyhedral mesh which is also shown in Figure 19.

At the flash-boiling condition of  $T_{inj} = 373$  K and  $P_{\infty} = 0.3$  bar of *n*-Pentane, a significant transformation in spray structure was predicted. Plumes merged to form a concentrated plume with high axial momentum, as also seen in experiments. The numerical spray formation showed a significant amount of droplet recirculation, which was also visible in experiments to a degree, and represented by the lighter shade of grey surrounding the bulk liquid. *iso*-Hexane showed a lesser degree of spray collapse as expected and helped demonstrate the process of spray collapse, *i.e.* larger droplets penetrated further radially and required more time to collapse. Although the spray formation for the flash-boiling Cartesian mesh spray of *n*-Pentane captured realistic characteristics, it contained signs of numerical mesh phenomena as documented previously by [26, 44]. These mesh artefacts stemmed from the collision model's ability to draw parcels away from cell boundaries when the injector axis was in parallel with continuous mesh boundaries (found in uniform grids), causing areas with no parcels along cell boundaries.

The polyhedral mesh removed mesh artefacts, whereby a solid single plume was predicted for *n*-Pentane. Although convergence criterion was met a degree of asymmetry was introduced, possibly caused by the non-uniformity within the mesh. The *iso*-Hexane spray case displayed a smaller influence from the polyhedral mesh when compared to the Cartesian mesh, due to the larger and fewer droplets present. This was even more so in the *n*-Hexane case where negligible differences were seen. Using a smaller parcel representation in post-processing highlighted asymmetry in parcel distribution, like that seen in experiment where a star shape was produced. Limitations in the current collision model were highlighted in the case of symmetric injectors aligned with mesh boundaries and may require refinement especially when taking into consideration the increased vapour concentration surrounding droplets, rapid evaporation forces, *etc.* which are likely to cause the collision criteria to change [44]. A quantitative comparison was made to experiments through liquid penetration, and is displayed in Figure 20. The penetration curves showed that the current simulation set-up somewhat over-predicted penetration lengths at subcooled conditions. This was expected since optimisation of the atomisation submodel parameters of [45] at subcooled conditions was only done for the 6-hole asymmetric injector of [40] as discussed early on in this paper. However, it can be seen that both cases came within 15%, a result of increased evaporation competing with an increased injection velocity for higher temperature cases. The collapsing mechanism seen for *n*-Pentane caused an increase in penetration, the same trend as experiment.

#### 4.4.2. 8-Hole Symmetric Injector [4]

A second symmetrical injector configuration was investigated, albeit with 8 holes this time. The experimental work was carried out by [4] and studied the effect of flash-boiling on Ethanol fuel. An injection temperature of  $T_{inj} = 363$  K was studied at ambient pressures that ranged from  $P_{\infty} = 0.2$  bar to 1.0 bar. Similarly to the previous 6-hole symmetrical injector of [37] the cloverleaf mesh artefact presented itself at flash-boiling conditions, where the probability of droplet-droplet interaction was increased with an increasing number of smaller droplets. Hence, the polyhedral mesh was also adopted to provide insight into the effects of mesh type for the most extreme operating condition. The predicted sprays can be seen in Figure 21 where comparisons were made to Mie-scattering spray images.

Due to Ethanol having large latent heat of evaporation the gradient of the droplet diameter reduction factor (Figure 6) was significantly steeper than alkanes and aromatics. This caused a sudden reduction in droplet size when moving from  $P_{\infty}/P_{sat} = 0.256$  to 0.128. At low ambient pressures in the case of the Cartesian mesh, the clover-leaf artefact became prevalent, where 8 original plumes collapsed into four, with trajectories diagonal relative to the cell boundaries. This exact effect was described in [26] and was caused by the collision model calculating a larger probability of collisions for parcels with large relative velocity. Hence, droplets moving at 90° to each other have the highest chance to coalesce, this phenomenon draws droplets away from cell boundaries and results in trajectories favouring a diagonal path due to the exchange of momentum between collector and donor parcels. Although this phenomenon was clearly evident, the outer cone angle is seen to reduce following experimental trends. It was apparent that mesh type had very little affect at non-flashing conditions, where collisions are at a minimum. However, as the operating condition moved towards the fully flashing spray, the effect became noticeable. At  $P_{\infty}$  of 0.2 bar, the mesh artefacts were eliminated for the polyhedral mesh case and important spray characteristics are captured including complete plume collapse, and a curvature of the bulk liquid towards the central region, an effect of increased air entrainment due to stronger jet tip vortices associated with flashing sprays [54]. In this specific case, it was clear that improvements were achieved by adopting a polyhedral mesh. However, due to limitations in engine modelling, and as highlighted in previous injector studies this improvement was exaggerated in this case due to the symmetrical nature of both injector and positioning within the mesh.

### 4.5 Fuel Vapour and Liquid Temperature

#### 4.5.1. Single-Hole Injector Evaporation

In an attempt to validate the heat and mass transfer models, a single-hole injector study was carried out and compared to the Planar Laser-Induced Fluorescence (PLIF) experimental data of [55] with Ethanol fuel injected through a 3-mm diameter nozzle hole with 10 bar injection pressure. Spray formation and droplet temperatures are displayed in Figure 22 and quantitative measurements of liquid temperature on the central axis of the plume are displayed in Figure 23.

The liquid temperatures predicted were close to the temperatures measured, at 312 K vs. 309 K and 301 K vs. 301 K at 10 mm downstream for  $P_\infty = 0.4$  bar and  $P_\infty = 0.2$  bar respectively. The near-nozzle region ( $< 2$  mm) where droplets were averaged over a volume of  $0.2 \times 0.2$  mm in the central axis showed a more rapid heat loss process when compared to experiments. However, it is noted that temperature PLIF measurement are well-known for their complexity in calibration, especially when applied to flows with large temperature gradients. The complex multiphase phenomena at the nozzle exit are adding to uncertainties that are not easy to quantify, like in the near-nozzle region of the case under study here. The work of [55] quoted total uncertainty of the order 6–10 K at temperatures in the range 340–380 K which can also justify the differences between simulation and experiments in the near-nozzle region.

#### 4.5.2. Multi-Hole Injector Evaporation

To further understand the framework's ability to predict heat and mass transfer at both subcooled and superheated conditions, a direct comparison was made to the experimental work of [56] whereby the Laser-Induced Exciplex Fluorescence (LIEF) technique was adopted to quantify vapour concentrations in a 8-hole symmetric injector using *n*-Hexane fuel with 9.5% vol. of additives, specifically 90.5% vol. *n*-Hexane, 0.5% vol. fluorene (FB), 9% vol. diethyl-methyl-amine (DEMA), where FB was the monomer and DEMA was the Exciplex-forming molecule. Injection pressure was set to 100 bar with 9.15 mg injected over 1.2 ms. This validation approach required good accuracy across many spray parameters including liquid and vapour penetrations, droplet sizes, spray structure and collapsing mechanism, as well as heat and mass transfer effects. Hence, one has to apply caution to quantitative comparisons, especially when also considering the complexity of calibration involved with LIEF techniques and the dependence of the signal on various parameters when applied to realistic spray injection studies at challenging conditions of combined heat and mass transfer.

Vapour concentrations for  $T_{inj} = 298$  K and  $T_{inj} = 328$  K at  $P_\infty = 0.4$  bar are displayed in Figure 24 at 0.7 ms after the fuel first emerged through the orifice of the nozzle. One can see comparable trends between simulations and experiments and it is also noted that the experimental images do not come with a scale since these were not shown in calibrated form [56]. By means of qualitative comparison, vapour remained in the vicinity of two distinct plumes for  $T_{inj} = 298$  K, whereas vapour was drawn into the central region for the hotter case of  $T_{inj} = 328$  K whilst maintaining some vapour as distinct plumes. The polyhedral mesh case was included for completeness and shows smaller peak values in concentration than the Cartesian one.

Vapour concentration in [mg/mL] for *n*-Hexane in each computational cell was obtained 20 mm downstream of the nozzle exit and compared to the experiments at these conditions. The vapour concentrations displayed in Figure 25 showed peak values of  $1.2 \times 10^{-2}$  mg/mL,  $3.1 \times 10^{-2}$  mg/mL, and  $3.9 \times 10^{-2}$  mg/mL for experiment, polyhedral and Cartesian mesh respectively at  $T_{inj} = 298$  K. At  $T_{inj} = 328$  K the vapour concentrations increased to peak values of  $4.4 \times 10^{-2}$  mg/mL,  $6.2 \times 10^{-2}$  mg/mL, and  $10.5 \times 10^{-2}$  mg/mL, respectively. The vapour concentration predicted by the numerical framework for the transitioning case ( $T_{inj} = 328$  K,  $P_\infty = 0.4$  bar) shown in Figure 25, predicted three distinct peaks whereas the experiment showed a more uniform distribution of vapour. The difference was partially caused by the sensitivity of measuring vapour concentrations at a specific distance downstream. This technique showed high sensitivity especially for the transitioning case where the vapour concentration varied significantly in the central region over a small axial distance. In the case of the experimental data, the central vapour region was found to penetrate further and hence the measurement technique (20 mm downstream) picked up the more even distribution of vapour, which can be found at a slightly higher position within the numerical sprays. Although an over-prediction was found for the numerical vapour concentrations, the effect of spatial distribution, penetration lengths as well as droplet sizes and spray formation will have contributed to the differences seen.

A higher temperature case was also investigated, specifically  $T_{inj} = 358$  K at  $P_\infty = 0.4$  bar. The resultant vapour distribution on the vertical central plane and vapour concentration along the radial co-ordinate 20 mm below the nozzle tip are displayed in Figures 27 and 28, respectively. At this condition, apart from the standard Cartesian mesh and polyhedral one, a Cartesian mesh which has been rotated through two axes by  $45^\circ$  to show the effect of mesh orientation was also included in the simulations. As the temperature and superheat were increased to  $T_{inj} = 358$  K a larger amount of vapour was present spatially in Figure 26. However, the experiment showed a much narrower vapour area than the simulations and also than the experiments at the earlier lower superheat of Figure 24. It also showed much larger vapour concentration along the central axis than Figure 24. From Figure 26 and Figure 27 it is also clear that the Cartesian mesh introduced again some mesh artefact producing a lack of vapour

within the central region downstream of the bulk vapour. By rotating the mesh through  $45^\circ$  this was eliminated and the vapour concentration was closer to the experiment, with a peak value of 0.32 as opposed to the experimental value of 0.22. By rotating the mesh, artefacts seen in the standard Cartesian mesh were reduced and the vapour distribution became more evenly distributed, similar to the polyhedral mesh case. This resulted in a vapour concentrations being in-between that of the standard Cartesian mesh and polyhedral mesh case which were found to under-predict and over-predict concentrations, respectively. This suggests that the polyhedral mesh over-predicts the collapsing mechanism for the vapour phase as well as the liquid phase (highlighted throughout the current work for each injector studied).

## 5. Conclusions

The current work adopted a Lagrangian computational framework alongside a flash-boiling boundary condition nozzle exit and enhanced droplet heat transfer model in an attempt to automatically capture important flash-boiling spray characteristics. Furthermore, automatic adjustment of the cone angle for each spray plume was studied according to the relationship provided by [36]. Six different injectors were studied to investigate the model's capability and sensitivity to plume angles and plume proximity. Each study investigated a range of operating conditions, including subcooled, transitional low superheats, moderate flashing sprays and highly superheated sprays. These were achieved through both high temperature fuel (as hot as  $T_{inj} = 453$  K) and low ambient pressures (as low as  $P_\infty = 0.2$  bar). High volatility single-components fuels like *n*-Pentane, *n*-Hexane, *iso*-Hexane and Ethanol were primarily modelled because it is the high volatility components in gasoline that drive the flash boiling process. A lower volatility alcohol, *n*-Butanol was also modelled. The main conclusions are summarised as follows:

- The flash-boiling nozzle exit boundary condition model was successfully normalised through a dimensionless parameter of the  $We$ ,  $Ja$ ,  $Ec$  and  $Fr$  (or  $EO$ ) numbers for a wide range of single component fuels, including alcohols, alkanes and aromatics, over a pressure range of  $P_\infty = 0.3$ – $1.0$  bar. A single curve of droplet diameter reduction factor vs. the dimensionless relationship can be used to predict automatically the degree of initial atomisation at the nozzle exit that leads to downstream spray development effects.
- The modelling approach was able to capture important flash-boiling spray characteristics, such as plume merging, collapse and an increased degree of droplet recirculation for all injector geometries studied, particularly at high superheat degrees.
- Transitional flash-boiling and subcooled spray modelling was enhanced through secondary breakup submodel optimisation, which encouraged plume merging and improved penetration lengths as well as enhancing SMD predictions.
- Liquid spray penetration was calculated and where possible compared to experimental data. An example includes the comparison made with the in-house studies of [40] and [39] for 6- and 7-hole asymmetric injectors which displayed a good match, typically within 2–8% depending on the degree of superheat. The comparison to the work of [38] with the 6-hole asymmetric injector predicted penetration lengths within 2–5% even at high superheats. At the highest superheat that led to extreme spray collapse into a single high momentum plume with fast penetration, the results highlighted the necessity for further improvements to capture extreme radial and axial droplet momentum balance transfer effects for some injector geometries.
- Droplet sizes were compared to experimental data for the 6- and 7-hole asymmetric injectors of [40] and [39]. At flashing conditions the model was able to predict SMD values close to experiments.
- Automatic adjustment of the cone angle for each spray plume displayed some improvement for specific spray cases, where a significant expansion at the nozzle exit is seen. This is still one of the limitations of the model however and highlights the importance of modelling the initial widening of the plume cone angles at increased superheats more accurately.
- An important conclusion for future implementation into full engine simulations is the effect of uniform Cartesian mesh structure on flash-boiling spray formation. When a uniform mesh structure was used at flashing conditions and plumes were injected along cell boundaries (commonly seen in symmetric injectors) the well-known 'clover leaf' artefact was produced. A polyhedral mesh was also investigated and this was seen to prevent mesh artefacts especially in the case of symmetric injectors when plumes travel through the domain at angles parallel to cell boundaries. However, the polyhedral mesh over-predicted the collapsing

mechanism for some injectors, suggesting that even though the Cartesian mesh produces mesh artefacts the global spray characteristics remained closer to experiments at most cases. The polyhedral mesh was also found to diminish effects from varying injector configurations at flash-boiling conditions, whereby a uniform single plume was produced for all injectors investigated. The current work also highlights limitations in current droplet collision models, where standard collision regimes and criteria based on droplet  $We$  number and cell-based collision detection methodologies originally designed at subcooled conditions become questionable.

- Heat and mass transfer rates were investigated through comparisons to single-hole and multi-hole injector PLIF and LIEF experiments from the literature. Single-hole injector tests provided evidence that droplet temperatures are predicted to within  $\sim 5$  K downstream of the nozzle exit. The multi-hole injector study provided evidence that the vapour phase was drawn into the central axis as superheat increases. Considering experimental uncertainties and many important simulation parameters, direct quantitative comparisons to vapour concentration and droplet temperatures near the nozzle were not straightforward. However, the predictions were broadly comparable to experimental data when one also takes into account the relative simplicity of the proposed modelling approach that was intentionally aimed for.

It is noted that the basic breakup parameters at subcooled conditions were optimised initially to match the experimental data for one of the injectors only and then fixed throughout for the rest of the injectors, therefore, there is clearly scope for individual injector optimisation. More importantly though, on the basis of the conclusions above, current work of the authors is focused on the near-nozzle region at superheated conditions. Here liquid ligaments and droplets can shatter under nucleation and bubble growth, introducing additional radial momentum at the initial stages of spray formation. This physical process is currently being investigated in the development of a new breakup model where the inertial shattering is incorporated.

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## References

- [1] Reitz, R. (1990). A photographic study of flash-boiling atomization. *Aerosol Science and Technology*, 12, pp. 561–569. DOI: 10.1080/02786829008959370.
- [2] Adachi, M., Tanaka, D., Hojyo, Y., Marwan, A., Senda, J. & Fujimoto, H. (1996). Measurement of fuel vapor concentration in flash boiling spray by infrared extinction/scattering technique. *JSAE Review*, 17, pp. 231–237. DOI: 10.1016/0389-4304(96)00025-2.
- [3] Sher, E., bar-Kohany, T. & Rashkovan, A. (2008). Flash-boiling atomization. *Progress in Energy and Combustion Science*, 34, pp. 417–439. DOI: j.pecs.2007.05.001.
- [4] Zeng, W., Xu, M., Zhang, G., Zhang, Y. and Cleary, D.J. (2012). Atomization and vaporization for flash-boiling multi-hole sprays with alcohol fuels. *Fuel*, 95, pp. 287–297. DOI: 10.1016/j.fuel.2011.08.048.
- [5] Witlox, H. W. M. & Bowen, P. J. (2002). Flashing liquid jets and two-phase dispersion: a review prepared by Det Norske Veritas Ltd for the Health and Safety Executive, London HMSO, ISBN 0717622509.
- [6] Mikic, B.B., Rohsenow, W.M. & Griffith, P. (1970). On bubble growth rates. *International Journal of Heat and Mass Transfer*, 13, pp. 657–666. DOI: 10.1016/0017-9310(70)90040-2.
- [7] Lee, H.S. and Merte, H., (1996). Spherical vapor bubble growth in uniformly superheated liquids. *International Journal of Heat and Mass Transfer*, 39, pp. 2427–2447. DOI: 10.1016/0017-9310(95)00342-8.
- [8] Reitz, R. & Diwakar, R. (1986). Effect of drop breakup on fuel sprays. SAE Technical Paper 860469. DOI: 10.4271/860469.
- [9] Hamzehloo, A. & Aleiferis, P. G. (2016). Numerical modelling of transient under-expanded jets under different ambient thermodynamic conditions with adaptive mesh refinement. *International Journal of Heat and Fluid Flow*, 61, pp. 711–729. DOI: 10.1016/j.ijheatfluidflow.2016.07.015.

- [10] Oza, R. & Sinnamon, J. (1983). An experimental and analytical study of flash-boiling fuel injection. *SAE Technical Paper 830590*. DOI: 10.4271/830590.
- [11] Aleiferis, P. G., Serras-Pereira, J., Augoye, A., Davies, T. J., Cracknell, R. F. & Richardson, D. (2010a). Effect of fuel temperature on in-nozzle cavitation and spray formation of liquid hydrocarbons and alcohols from a real-size optical injector for direct-injection spark-ignition engines. *International Journal of Heat and Mass Transfer*, 53, pp. 4588–4606. DOI: 10.1016/j.ijheatmasstransfer.2010.06.033.
- [12] Sher, E. & Elata, C. (1977). Spray formation from pressure cans by flashing. *Industrial & Engineering Chemistry Process Design and Development*, 16, pp. 237–242. DOI: 10.1021/i260062a014.
- [13] Aori, G., Hung, D. L. S. & Zhang, M. (2016). Effect of nozzle configuration on macroscopic spray characteristics of multi-hole fuel injectors under superheated conditions. *Atomization and Sprays*, 26, pp. 439–462. DOI: 10.1615/AtomizSpr.2015011990.
- [14] Araneo, L. & Donde, R. (2017). Flash boiling in a multihole G-DI injector – Effects of the fuel distillation curve. *Fuel*, 191, pp. 500–510. DOI: 10.1016/j.fuel.2016.11.104
- [15] Lacey, J., Poursadegh, F., Brear, M. J., Gordon, R., Petersen, P., Lakey, C., Butcher, B., Ryan, S. (2017). Generalizing the behavior of flash-boiling, plume interaction and spray collapse for multi-hole, direct injection. *Fuel*, 200, pp. 345–356. DOI: 10.1016/j.fuel.2017.03.057.
- [16] Gopalakrishnan, S. & Schmidt, D. P. (2009). A computational study of flashing flow in fuel injector nozzles. *SAE int. J. Engines*, 1, 160–170. DOI: 10.4271/2008-01-0141.
- [17] Janet, J. P., Liao, Y. & Lucas, D. (2015). Heterogeneous nucleation in CFD simulation of flashing flows in converging-diverging nozzles. *International Journal of Multiphase Flow*, 74, pp. 106–117. DOI: j.ijmultiphaseflow.2015.04.005.
- [18] Price, C., Hamzehloo, A., Aleiferis, P. G. & Richardson, D. (2015). Aspects of numerical modelling of flash-boiling fuel sprays. *SAE Technical Paper 2015-24-2463*. DOI: 10.4271/2015-24-2463.
- [19] Price, C., Hamzehloo, A., Aleiferis, P.G. & Richardson, D. (2016). An approach to modelling flash-boiling fuel sprays for direct-injection spark-ignition engines. *Atomization and Sprays*, 26, pp. 1197–1239. DOI: 10.1615/AtomizSpr.2016015807.
- [20] Issa R. I. (1986). Solution of the implicitly discretised fluid flow equations by operator-splitting. *Journal of Computational Physics*, 62, pp. 40–65. DOI: 10.1016/0021-9991(86)90099-9.
- [21] Yakhot, V., Orszag, S.A., Thangam, S., Gatski, T.B., Speziale, C.G. (1992). Development of turbulence models for shear flows by a double expansion technique. *Physics of Fluids*, 4(7), pp. 1510–1520. DOI: 10.1063/1.858424.
- [22] Han, Z. & Reitz, R. D. (1995). Turbulence modeling of internal combustion engines using RNG  $\kappa$ - $\epsilon$  models. *Combustion Science and Technology*, 106, pp. 267–295. DOI: 10.1080/00102209508907782.
- [23] Malcolm, J.S., Behringer, M.K., Aleiferis, P.G., OudeNijeweme, D. & Mitcalf, J. (2011). Characterisation of flow structures in a direct-injection spark-ignition engine using PIV, LDV and CFD, *SAE Technical Paper 2011-01-1290*.
- [24] Xue, Q., Som, S., Senecal, P. K., Pomraning, E. (2013). Large eddy simulation of fuel-spray under non-reacting IC engine conditions. *Atomization and Sprays*, 23, pp. 925–955. DOI: 10.1615/AtomizSpr.2013008320.
- [25] O'Rourke, P. (1981). Collective drop effects on vaporizing liquid sprays. PhD Thesis, United States: Princeton University.
- [26] Schmidt, D. P. & Rutland, C. J. (2004). Reducing grid dependency in droplet collision modeling. *J. Eng. Gas Turbines Power*, 126, pp. 227-233. DOI: 10.1115/1.1564066.
- [27] Yaws, C.L., Yaws' handbook of thermodynamic and physical properties of chemical compounds: physical, thermodynamic and transport properties for 5,000 organic chemical compounds, Knovel, Norwich, NY, 2003.
- [28] Spalding, D. B. (1953). The combustion of liquid fuels. Symposium (International) on Combustion, 4, pp. 847–864. DOI: S0082-0784(53)80110-4.

- [29] Adachi, M., McDonell, V. & Tanaka, D. (1997). Characterization of fuel vapor concentration inside a flash boiling spray. *SAE Technical Paper 970871*. DOI: 10.4271/970871.
- [30] Riznic, J. R., and Ishii, M. (1989). Bubble number density and vapor generation in flashing flow. *Int. J. Heat and Mass Transfer*, 32(10), pp. 1821-1833. DOI: 10.1016/0017-9310(89)90154-3.
- [31] Kocamustafaogullari, G. & Ishii, M. (1983). Interfacial area and nucleation site density in boiling systems. *International Journal of Heat and Mass Transfer*, 26, pp. 1377-1387. DOI: 10.1016/S0017-9310(83)80069-6.
- [32] Kocamustafaogullari, G. (1983). Pressure dependence of bubble departure diameter for water. *International Communications in Heat and Mass Transfer*, 10, pp. 501-509. DOI: 10.1016/0735-1933(83)90057-X.
- [33] Fritz, W. (1935). Maximum volume of vapor bubbles. *Physikalische Zeitschrift*, 36, pp. 379-384.
- [34] Serras-Pereira, J., van Romunde, Z., Aleiferis, P. G., Richardson, D., Wallace, S. & Cracknell, R. F. (2010). Cavitation, primary break-up and flash boiling of gasoline, *iso*-octane and *n*-pentane with a real-size optical direct-injection nozzle. *Fuel*, 89, pp. 2592-2607. DOI: 10.1016/j.fuel.2010.03.030.
- [35] Li, S., Zhang, Y. & Xu, B. (2015). Correlation analysis of superheated liquid jet breakup to bubble formation in a transparent slit nozzle. *Experimental Thermal and Fluid Science*, 68, pp. 452-458. DOI: j.expthermflusci.2015.04.023.
- [36] Kamoun, H. Lamanna, G. & Weigand, B. (2010). High-speed shadowgraphy investigations of superheated liquid jet atomisation. ILASS-Americas 22<sup>nd</sup> Annual Conference on Liquid Atomization and Spray Systems, Cincinnati, USA.
- [37] Mojtabi, M., Wigley, G. & Helie, J. (2014). The effect of flash boiling on the atomization performance of gasoline direct injection multistream injector. *Atomization and Sprays*, 24, pp. 467-493. DOI: 10.1615/AtomizSpr.2014008296.
- [38] Yang, S., Key, S., Road, W., Song, Z., Wang, T. and Yao, Z. (2013). An experiment study on phenomenon and mechanism of flash boiling spray from a multi-hole gasoline direct injector. *Atomization and Sprays*, 23, pp. 379-399. DOI: 10.1615/AtomizSpr.2013007539.
- [39] Behringer, M., Aleiferis, P. G., OudeNijeweme, D. & Freeland, P. (2014). Spray formation from spark-eroded and laser-drilled injectors for disi engines with gasoline and alcohol fuels. *SAE Int. J. Fuels Lubr.* 7, pp. 803-822. DOI: 10.4271/2014-01-2745.
- [40] Aleiferis, P. G. & van Romunde, Z. R. (2013). An analysis of spray development with *iso*-octane, *n*-pentane, gasoline, ethanol and *n*-butanol from a multi-hole injector under hot fuel conditions. *Fuel*, 105, pp. 143-168. DOI: 10.1016/j.fuel.2012.07.044.
- [41] van Romunde, Z. Van, Aleiferis, P. G., Cracknell, R. & Walmsley, H. (2007). Effect of fuel properties on spray development from a multi-hole DISI engine injector. *SAE Technical Paper 2007-01-4032*. DOI: 10.4271/2007-01-4032.
- [42] van Romunde, Z. & Aleiferis, P. G. (2009). Effect of operating conditions and fuel volatility on development and variability of sprays from gasoline direct-injection multihole injectors. *Atomization and Sprays*, 19, pp. 207-234. DOI: 10.1615/AtomizSpr.v19.i3.10.
- [43] Aleiferis, P. G., Serras-Pereira, J., van Romunde, Z., Caine, J. & Wirth, M. (2010b). Mechanisms of spray formation and combustion from a multi-hole injector with E85 and gasoline. *Combustion and Flame*, 157, pp. 735-756. DOI: 10.1016/j.combustflame.2009.12.019.
- [44] Post, S. & Abraham, J. (2002). Modeling the outcome of drop-drop collisions in diesel sprays. *International Journal of Multiphase Flow*, 28, pp. 997-1019.
- [45] Reitz, R. (1987). Modeling atomization processes in high-pressure vaporizing sprays. *Atomisation and Spray Technology*, 3, pp. 309-337.
- [46] O'Rourke, P. & Amsden, A. (1987). The TAB method for numerical calculation of spray droplet breakup. *SAE Technical Paper 872089*. DOI: 10.4271/872089.

- [47] Desantes, J. M., Payri, R., Salvador, F. J. & De La Morena, J. (2010). Influence of cavitation phenomenon on primary break-up and spray behavior at stationary conditions. *Fuel*, 89(10), pp. 3033–3041. DOI:10.1016/j.fuel.2010.06.004.
- [48] Perini, F. & Reitz, R. D. (2016). Improved atomization, collision and sub-grid scale momentum coupling models for transient vaporizing engine sprays. *International Journal of Multiphase Flow*, 79, pp. 107–123. DOI: 10.1016/j.ijmultiphaseflow.2015.10.009.
- [49] Pischke, P., Kneer, R. & Schmidt, D. P. (2015). A comparative validation of concepts for collision algorithms for stochastic particle tracking. *Computers and Fluids*, 113, pp. 77–86. DOI: 10.1016/j.compfluid.2015.01.018.
- [50] Gandhi, A. H. & Meinhart, M. (2009). Fuel Injector Flow Rate Analysis for the Duratec 35 EcoBoost Engine. *SAE Technical Paper 2009-01-1505*. DOI:10.4271/2009-01-1505.
- [51] Zigan, L., Schmitz, I., Flügel, A., Knorsch, T., Wensing, M. & Leipertz, A. (2010). Effect of fuel properties on spray breakup and evaporation studied for a multihole direct injection spark ignition injector. *Energy and Fuels*, 24, pp. 4341–4350. DOI: 10.1021/ef1003914.
- [52] Zigan, L., Schmitz, I., Flügel, A., Wensing, M. & Leipertz, A. (2009). Influence of fuel properties on spray formation and evaporation measured on a piezoelectric injector for the 2nd generation gasoline direct injection. In *Institution of Mechanical Engineers – Injection Systems for IC Engines Conference*, pp. 193–202.
- [53] Motjabi, M. (2011). Optical analysis of multi-stream GDI sprays under various engine operating conditions, PhD Thesis, Loughborough University.
- [54] Zhang, M., Xu, M., Zhang, Y., Zhang, G., and Cleary, D. J. (2013). Flow-field investigation of multihole superheated sprays using high-speed piv. part ii. axial direction. *Atomization and Sprays*, 23, pp. 119–140. DOI: 10.1615/AtomizSpr.2013007454.
- [55] Vetrano, M. R., Simonini, A., Steelant, J. & Rambaud, P. (2013). Thermal characterization of a flashing jet by planar laser-induced fluorescence. *Experiments in Fluids*, 54, pp. 1573. DOI 10.1007/s00348-013-1573-8.
- [56] Zhang, G., Hung, D. L. S. & Xu, M. (2014). Experimental study of flash boiling spray vaporization through quantitative vapor concentration and liquid temperature measurements. *Experiments in Fluids*, 55, pp. 1804. DOI: 10.1007/s00348-014-1804-7.

## Appendix

The derivation of the normalisation parameter is displayed here. The model is based on the calculation of a volumetric flow rate of vapour within the nozzle orifice, which is then translated into a theoretical reduction in droplet size at the nozzle exit. The volumetric flow rate of vapour is described as follows:

$$\dot{V}_{vap} = N_{nuc} f V_b S_{nozzle} \quad (A.1)$$

Where  $N_{nuc}$  is the nucleation site density,  $f$  the departure frequency,  $V_b$  the bubble volume at departure, and  $S_{nozzle}$  the inner surface area of the nozzle orifice.  $N_{nuc}$  was found to be very sensitive to changes in operating conditions, varying between  $9.55$  and  $5.51 \times 10^{13}$  at  $310$  K and  $410$  K respectively using  $n$ -Pentane at  $P_{\infty} = 1$  bar.  $N_{nuc}$  is displayed in Equation A.2.

$$N_{nuc} = \frac{1}{D_b^2} N_{nuc}^* F(\rho^*) \quad (A.2)$$

The large variation in  $N_{nuc}$  originates from the dimensionless nucleation site density,  $N_{nuc}^*$  which ranges from  $2.12 \times 10^6$  to  $3.00 \times 10^{14}$  at  $310$  K and  $410$  K.  $D_b^2$  and  $F(\rho^*)$  have a significantly smaller effect, in the range  $5.14 \times 10^{-8}$  to  $2.34 \times 10^{-10}$  and  $2.31 \times 10^{-13}$  to  $4.29 \times 10^{-11}$  at  $310$  K and  $410$  K respectively. Also, due to  $V_b$  being proportional to  $D_b^3$ ,  $f$  being proportional to  $D_b^{-1}$  and  $N_{nuc}$  being proportional to  $D_b^{-2}$  within the calculation of  $\dot{V}_{vap}$ ,  $\frac{1}{D_b^2}$  within  $N_{nuc}$  can be neglected. Hence, an attempt was made to normalise the model through  $N_{nuc}^*$  displayed in Equation A.3.

$$N_{nuc}^* = \left[ \frac{D_b (T_{inj} - T_{sat}) \rho_g H_L}{2 \sigma T_{sat}} \right]^y \quad (A.3)$$

Expanding  $D_b$  in Equation A.3 gives:

$$N_{nuc}^* = \left[ \frac{2.64 \times 10^{-5} \theta_c \sigma^{0.5} (\rho_l - \rho_g)^{0.9} (T_{inj} - T_{sat}) \rho_g H_L}{g^{0.5} (\rho_l - \rho_g)^{0.5} \rho_g^{0.9} \sigma T_{sat}} \right]^y \quad (A.4)$$

Hence:

$$N_{nuc}^* = \left[ \frac{\rho_g^{0.1} (\rho_l - \rho_g)^{0.4} H_L T^*}{g^{0.5} \sigma^{0.5}} \right]^y \quad (A.5)$$

Where:

$$T^* = \frac{T_l - T_{sat}}{T_{sat}} \quad (A.6)$$

The parenthesis of  $N_{nuc}^*$  showed a good degree of normalisation of different fuels at different pressures and temperatures. Hence the normalisation parameter becomes:

$$\eta = \frac{\rho_g^{0.1} (\rho_l - \rho_g)^{0.4} H_L T^*}{\sqrt{g \sigma}} \quad (A.7)$$

It was found that the density term can be simplified without significantly effecting the normalisation of droplet diameter reduction factor as displayed in Equation A.8.

$$\eta = \frac{\sqrt{\rho_g H_L T^*}}{\sqrt{g \sigma}} \quad (A.8)$$

The well-known non-dimensional numbers were substituted into Equation A.8 as follows:

$$\eta = \frac{\sqrt{We Fr T^*}}{Ec Ja} \quad (A.9)$$

where the Weber number has been defined as  $We = \frac{\rho_g U^2 D_b}{\sigma}$ , the Froude number is  $Fr = \frac{U}{\sqrt{g D_b}}$ , the Eckert number is  $Ec = \frac{U^2}{\Delta T C_p}$  and the Jakob number is  $Ja = \frac{C_p \Delta T}{H_L}$ . The Weber number displayed in Equation A.10 would need to be adopted if Equation A.7 was used.

$$We = \frac{[\rho_g^{0.1} (\rho_l - \rho_g)^{0.4}]^2 U^2 D_b}{\sigma} \quad (A.10)$$

The non-dimensional parameter can also be expressed on terms of the Eötvös number ( $Eu$ ) instead of Froude by suitable rearrangement.

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## Nomenclature

### Latin Symbols

|                 |                                            |
|-----------------|--------------------------------------------|
| $a_o$           | Molecular surface area [ $m^2$ ]           |
| $C$             | Droplet count                              |
| $C_p$           | Specific heat capacity [ $J/kg \cdot K$ ]  |
| $D_b$           | Bubble departure diameter [ $m$ ]          |
| $Ec$            | Eckert number                              |
| $Eo$            | Eötvös number                              |
| $f$             | Frequency of bubble departure [ $s^{-1}$ ] |
| $Fr$            | Froude number                              |
| $F(\rho^*)$     | Property function                          |
| $g$             | Acceleration due to gravity [ $m/s^2$ ]    |
| $H_L$           | Latent heat of vaporisation [ $J/kg$ ]     |
| $Ja$            | Jakob number                               |
| $R_p$           | Pressure ratio                             |
| $S_{nozzle}$    | Inner-nozzle surface area [ $m^2$ ]        |
| $T^*$           | Dimensionless superheat degree             |
| $T_{inj}$       | Injection temperature [ $K$ ]              |
| $T_l$           | Liquid temperature [ $K$ ]                 |
| $T_{sat}$       | Saturation temperature [ $K$ ]             |
| $P_\infty$      | Ambient pressure [ $Pa$ ]                  |
| $P_{sat}$       | Saturation pressure [ $Pa$ ]               |
| $m_a$           | Atomic mass [ $kg$ ]                       |
| $N_{nuc}$       | Nucleation site density [ $m^{-2}$ ]       |
| $N_{nuc}^*$     | Dimensionless nucleation site density      |
| $U$             | Flow velocity [ $m/s$ ]                    |
| $u_d$           | Droplet velocity [ $m/s$ ]                 |
| $u_g$           | Gas velocity [ $m/s$ ]                     |
| $V_b$           | Volume of bubble [ $m^3$ ]                 |
| $\dot{V}_{vap}$ | Volumetric flow rate of vapour [ $m^3/s$ ] |
| $We$            | Weber number                               |
| $\gamma$        | Nucleation site density exponent           |

### Greek Symbols

|              |                                        |
|--------------|----------------------------------------|
| $\Delta\rho$ | Dimensional density ratio [ $kg/m^3$ ] |
| $\Theta$     | Non-Dimensional surface tension        |
| $\theta_c$   | Contact angle [ $^\circ$ ]             |
| $\theta$     | Cone angle [ $^\circ$ ]                |
| $\eta$       | Normalisation Parameter                |
| $\rho^*$     | Dimensionless density function         |
| $\rho_g$     | Density of gas [ $kg/m^3$ ]            |
| $\rho_l$     | Density of liquid [ $kg/m^3$ ]         |
| $\sigma$     | Surface tension [ $N/m$ ]              |

**Table 1.** Spray test cases.

| Author<br>(Year)                                  | Injector Data                                                                                                                                                                                         | Fuel<br>(CFD fuel if<br>different)                                                                         | Operating<br>Conditions                                                                                    | Injector Configuration<br>(front view) (top view)                                                                                                                          |                                                                                                                                                                            |
|---------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Mojtabi<br><i>et al.</i><br>(2014)<br>[37]        | <ul style="list-style-type: none"> <li>6-hole symmetric</li> <li>Outer spray angle 60°</li> <li>Nozzle diameter 0.17–0.28 mm (0.2mm adopted) [53]</li> <li><math>\dot{m} = 18</math> mg/ms</li> </ul> | Gasoline<br>( <i>n</i> -Pentane<br><i>n</i> -Hexane<br><i>iso</i> -Hexane)                                 | $P_{\infty} = 0.3$ bar<br>$T_{\infty} = 298$ K<br>$P_{inj} = 120$ bar<br>$T_{inj} = 273$ – $373$ K         |                                                                                         |                                                                                         |
| Zeng <i>et al.</i> (2012)<br>[4]                  | <ul style="list-style-type: none"> <li>8-hole symmetric</li> <li>Outer spray angle 60°</li> <li><math>\dot{m} = 12.5</math> mg/ms* [50]</li> </ul>                                                    | Ethanol                                                                                                    | $P_{\infty} = 0.2$ – $1.0$ bar<br>$T_{\infty} = 298$ K<br>$P_{inj} = 50$ bar<br>$T_{inj} = 298$ – $363$ K  |                                                                                         |                                                                                         |
| Yang <i>et al.</i> (2013)<br>[38]                 | <ul style="list-style-type: none"> <li>2- and 6-hole asymmetric</li> <li><math>\dot{m} = 3.6</math> mg/ms (2-hole)</li> <li><math>\dot{m} = 10.8</math> mg/ms (6-hole)* [50]</li> </ul>               | Gasoline<br>( <i>n</i> -Pentane<br><i>n</i> -Hexane<br><i>iso</i> -Hexane)                                 | $P_{\infty} = 0.4$ – $1.0$ bar<br>$T_{\infty} = 293$ K<br>$P_{inj} = 100$ bar<br>$T_{inj} = 293$ – $413$ K | <br> | <br> |
| Behringer<br><i>et al.</i><br>(2014)<br>[39]      | <ul style="list-style-type: none"> <li>7-hole asymmetric (laser drilled injector)</li> <li><math>\dot{m} = 14</math> mg/ms</li> </ul>                                                                 | Gasoline<br>( <i>n</i> -Pentane<br><i>n</i> -Hexane<br><i>iso</i> -Hexane)<br>Ethanol<br><i>n</i> -Butanol | $P_{\infty} = 0.5$ – $1.0$ bar<br>$T_{\infty} = 298$ K<br>$P_{inj} = 120$ bar<br>$T_{inj} = 293$ – $353$ K |                                                                                        |                                                                                       |
| Aleiferis<br>and van<br>Romunde<br>(2013)<br>[40] | <ul style="list-style-type: none"> <li>6-hole asymmetric</li> <li><math>\dot{m} = 12</math> mg/ms</li> </ul>                                                                                          | Gasoline<br>( <i>n</i> -Pentane<br><i>n</i> -Hexane<br><i>iso</i> -Hexane)<br>Ethanol<br><i>n</i> -Butanol | $P_{\infty} = 0.5$ – $1.0$ bar<br>$T_{\infty} = 298$ K<br>$P_{inj} = 150$ bar<br>$T_{inj} = 293$ – $393$ K |                                                                                       |                                                                                       |

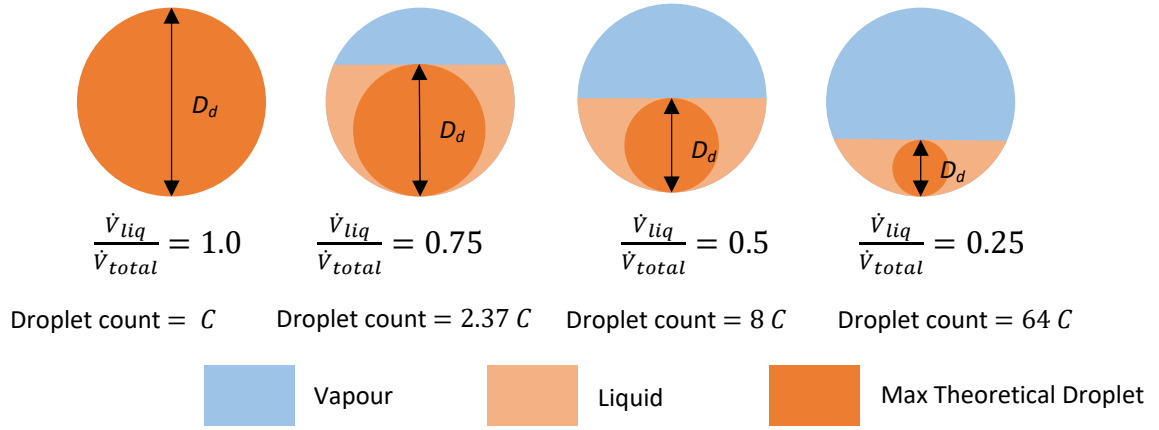
\* Estimated data from similar injection systems

**Table A1.** Fuels normalised through the dimensionless relationship in Figure 7.

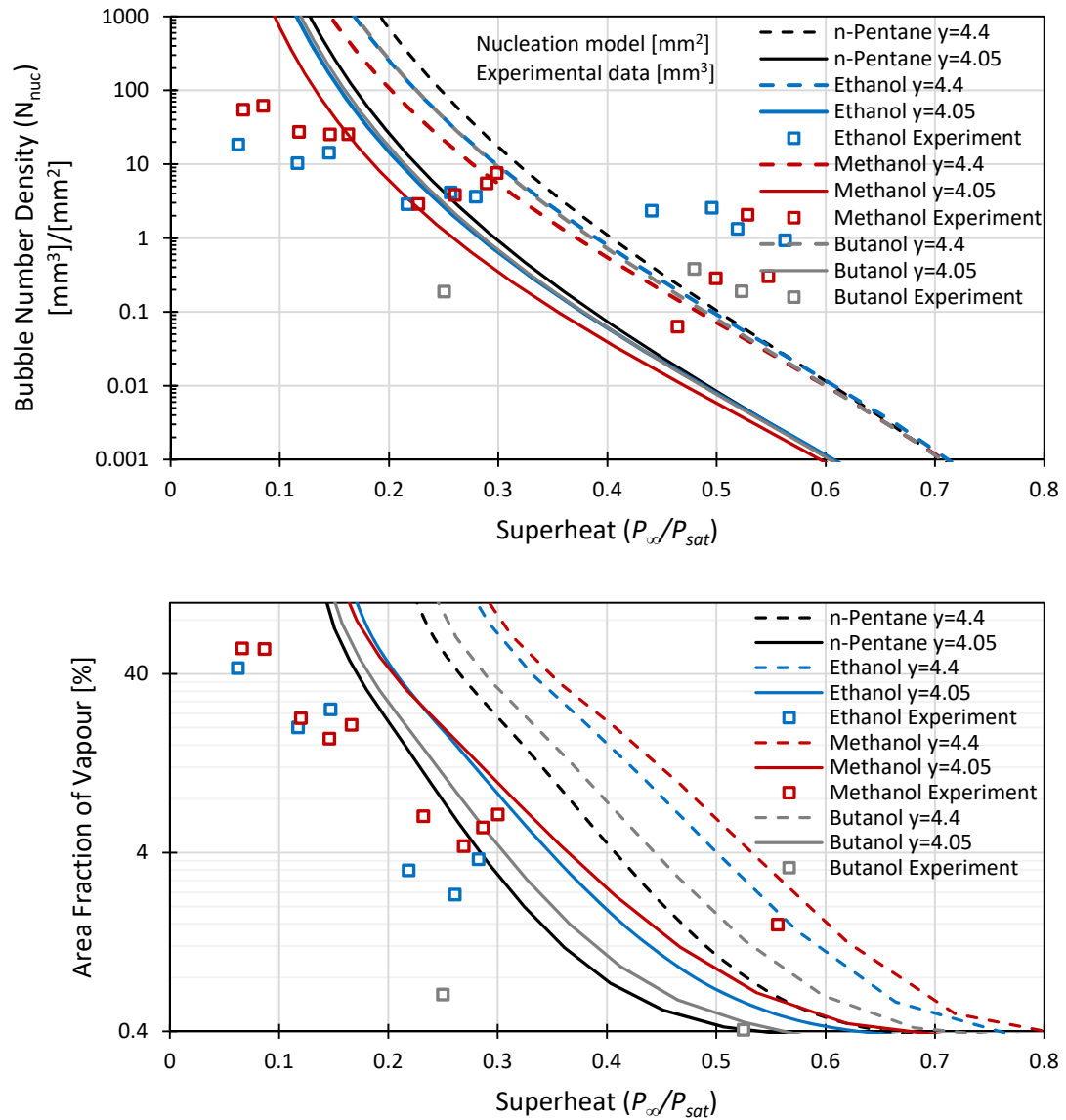
| <b>Fuel</b>         | <b>Chemical Formula</b>           | <b>Molecular Weight [g/mol]</b> | <b>Boiling Point at 1.0 bar [K]</b> |
|---------------------|-----------------------------------|---------------------------------|-------------------------------------|
| <i>Alkanes</i>      |                                   |                                 |                                     |
| <i>n</i> -Butane    | C <sub>4</sub> H <sub>10</sub>    | 58.12                           | 272.2                               |
| <i>n</i> -Pentane   | C <sub>5</sub> H <sub>12</sub>    | 72.15                           | 309.1                               |
| <i>n</i> -Hexane    | C <sub>6</sub> H <sub>14</sub>    | 86.17                           | 341.5                               |
| <i>iso</i> -Hexane  | C <sub>6</sub> H <sub>14</sub>    | 86.17                           | 333.0                               |
| <i>n</i> -Heptane   | C <sub>7</sub> H <sub>16</sub>    | 100.21                          | 371.4                               |
| <i>neo</i> -Heptane | C <sub>7</sub> H <sub>16</sub>    | 100.21                          | 352.0                               |
| <i>n</i> -Octane    | C <sub>8</sub> H <sub>18</sub>    | 114.23                          | 398.0                               |
| <i>iso</i> -Octane  | C <sub>8</sub> H <sub>18</sub>    | 114.23                          | 372.3                               |
| <i>Alcohols</i>     |                                   |                                 |                                     |
| Methanol            | CH <sub>3</sub> OH                | 32.04                           | 337.7                               |
| Ethanol             | C <sub>2</sub> H <sub>6</sub> O   | 46.06                           | 351.4                               |
| Propanol            | C <sub>3</sub> H <sub>8</sub> O   | 60.09                           | 370.0                               |
| <i>n</i> -Butanol   | C <sub>4</sub> H <sub>10</sub> O  | 74.12                           | 390.0                               |
| <i>n</i> -Pentanol  | C <sub>5</sub> H <sub>11</sub> OH | 88.15                           | 410.7                               |
| <i>Aromatics</i>    |                                   |                                 |                                     |
| Benzene             | C <sub>6</sub> H <sub>6</sub>     | 78.11                           | 352.1                               |
| Toluene             | C <sub>7</sub> H <sub>8</sub>     | 92.14                           | 383.4                               |
| <i>o</i> -Xylene    | C <sub>8</sub> H <sub>10</sub>    | 106.16                          | 417.0                               |
| <i>m</i> -Xylene    | C <sub>8</sub> H <sub>10</sub>    | 106.16                          | 412.0                               |
| <i>p</i> -Xylene    | C <sub>8</sub> H <sub>10</sub>    | 106.16                          | 411.2                               |

**Table A2.** Injector directionality in Cartesian form.

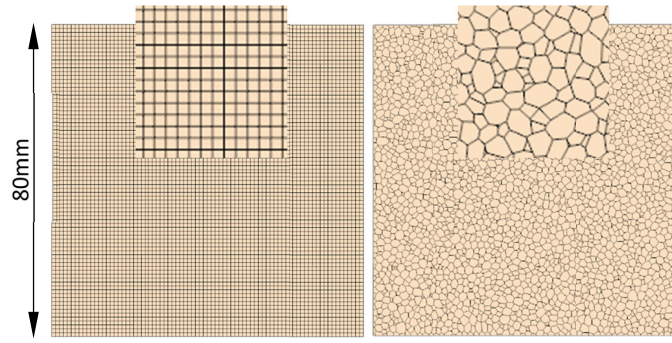
| <b>Aleiferis and van Romunde (2013) [40] – 6-Hole (Asymmetric)</b> |          |          |
|--------------------------------------------------------------------|----------|----------|
| <i>X</i>                                                           | <i>Y</i> | <i>Z</i> |
| 1.551                                                              | 0.578    | -1.000   |
| 1.551                                                              | -0.578   | -1.000   |
| 0.106                                                              | 0.380    | -1.000   |
| 0.106                                                              | -0.380   | -1.000   |
| -0.355                                                             | 0.274    | -1.000   |
| -0.355                                                             | -0.274   | -1.000   |
| <b>Behringer <i>et al.</i> (2014) [39] – 7-Hole (Asymmetric)</b>   |          |          |
| <i>X</i>                                                           | <i>Y</i> | <i>Z</i> |
| 0.052                                                              | 0.227    | -1.000   |
| 0.052                                                              | -0.227   | -1.000   |
| 0.268                                                              | 0.319    | -1.000   |
| 0.268                                                              | -0.319   | -1.000   |
| 0.510                                                              | 0.137    | -1.000   |
| 0.510                                                              | -0.137   | -1.000   |
| 0.364                                                              | -0.000   | -1.000   |
| <b>Yang <i>et al.</i> (2013) [38] – 2-Hole</b>                     |          |          |
| <i>X</i>                                                           | <i>Y</i> | <i>Z</i> |
| -0.141                                                             | 0.577    | -1.000   |
| 0.141                                                              | 0.577    | -1.000   |
| <b>Yang <i>et al.</i> (2013) [38] – 6-Hole (Asymmetric)</b>        |          |          |
| <i>X</i>                                                           | <i>Y</i> | <i>Z</i> |
| 0.151                                                              | -0.088   | -1.000   |
| -0.151                                                             | -0.088   | -1.000   |
| -0.462                                                             | 0.465    | -1.000   |
| 0.462                                                              | 0.465    | -1.000   |
| -0.141                                                             | 0.577    | -1.000   |
| 0.141                                                              | 0.577    | -1.000   |
| <b>Mojtabi <i>et al.</i> (2014) [37] – 6-Hole (Symmetric)</b>      |          |          |
| <i>X</i>                                                           | <i>Y</i> | <i>Z</i> |
| 1.000                                                              | -1.732   | 0.000    |
| -1.000                                                             | -1.732   | 0.000    |
| 0.500                                                              | -1.732   | 0.866    |
| -0.500                                                             | -1.732   | 0.866    |
| -0.500                                                             | -1.732   | -0.866   |
| 0.500                                                              | -1.732   | -0.866   |
| <b>Zeng <i>et al.</i> (2012) [4] – 6-Hole (Symmetric)</b>          |          |          |
| <i>X</i>                                                           | <i>Y</i> | <i>Z</i> |
| 0.397                                                              | 0.787    | -1.000   |
| -0.397                                                             | 0.787    | -1.000   |
| 0.262                                                              | -0.155   | -0.676   |
| -0.262                                                             | -0.155   | -0.676   |
| 0.189                                                              | -0.480   | -0.572   |
| -0.189                                                             | -0.480   | -0.572   |
| <b>Zhang <i>et al.</i> (2014) [56] – 8-Hole (Symmetric)</b>        |          |          |
| <i>X</i>                                                           | <i>Y</i> | <i>Z</i> |
| 0.700                                                              | 0.000    | -1.000   |
| 0.495                                                              | 0.495    | -1.000   |
| 0.000                                                              | 0.700    | -1.000   |
| -0.495                                                             | 0.495    | -1.000   |
| -0.700                                                             | 0.000    | -1.000   |
| -0.495                                                             | -0.495   | -1.000   |
| 0.000                                                              | -0.700   | -1.000   |
| 0.495                                                              | -0.495   | -1.000   |



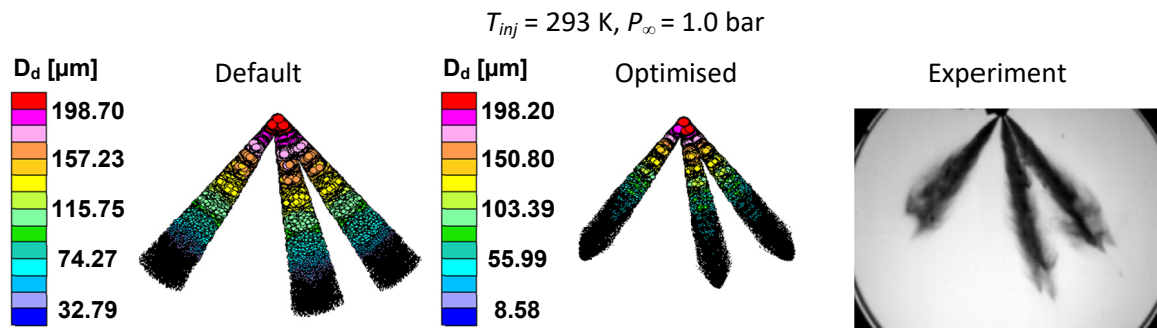
**Figure 1.** A schematic showing the translation of void fraction to droplet diameter through an asymmetric vapour film method.



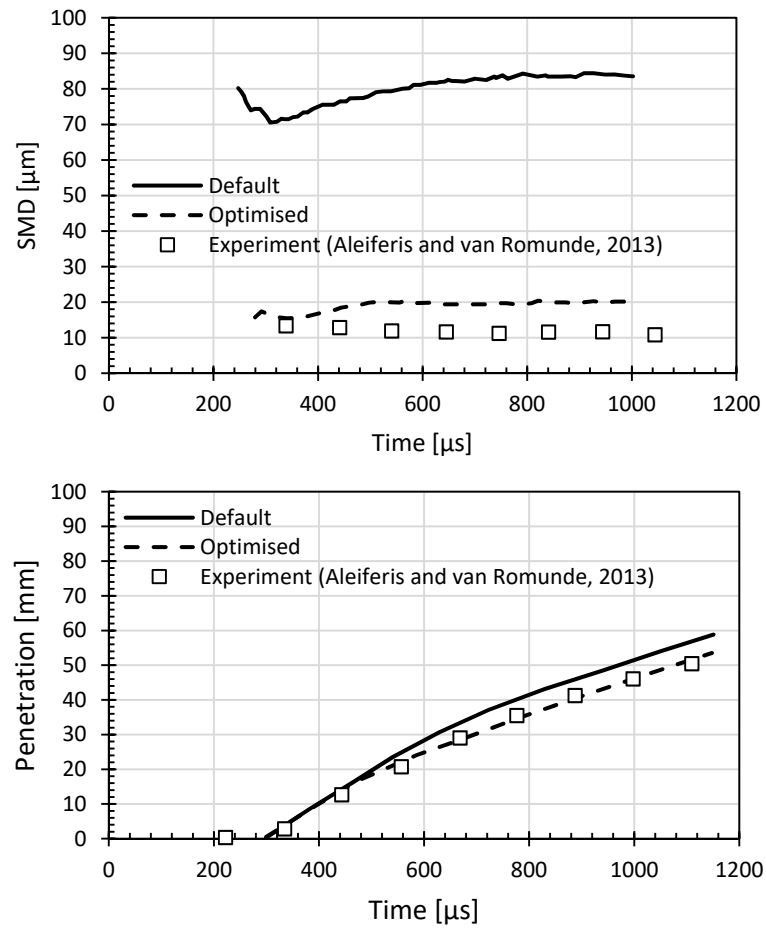
**Figure 2.** In-nozzle bubble number density (top) and area fraction of vapour (bottom) plotted against normalised superheat degree compared to experimental data of [35].



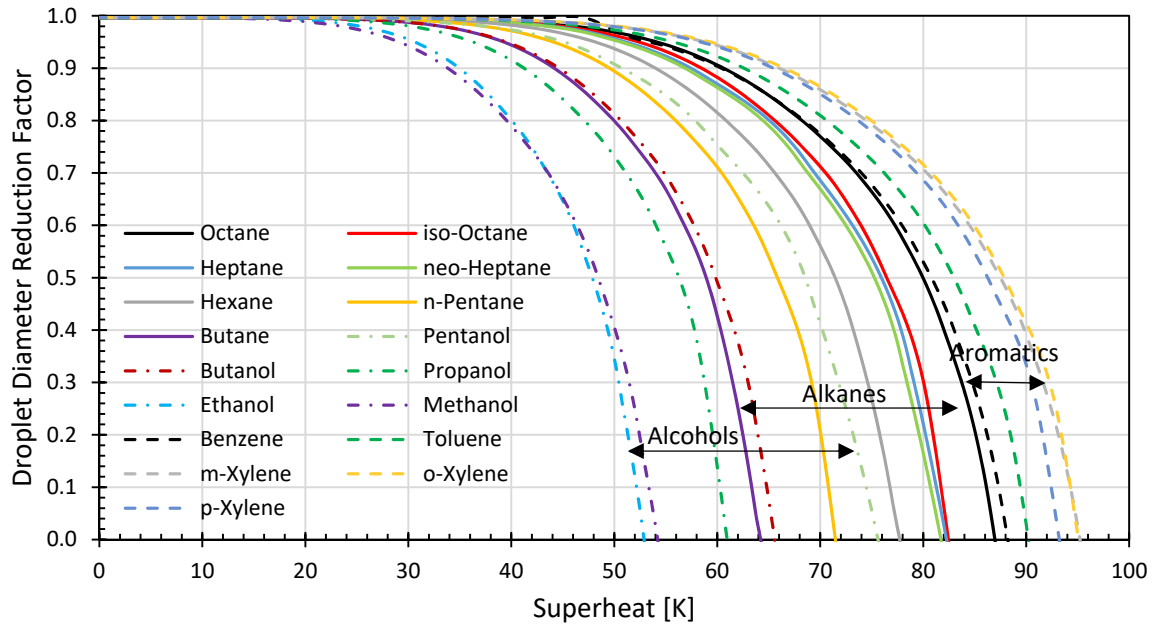
**Figure 3.** Cartesian (left) and polyhedral (right) meshes adopted in the current computational work.



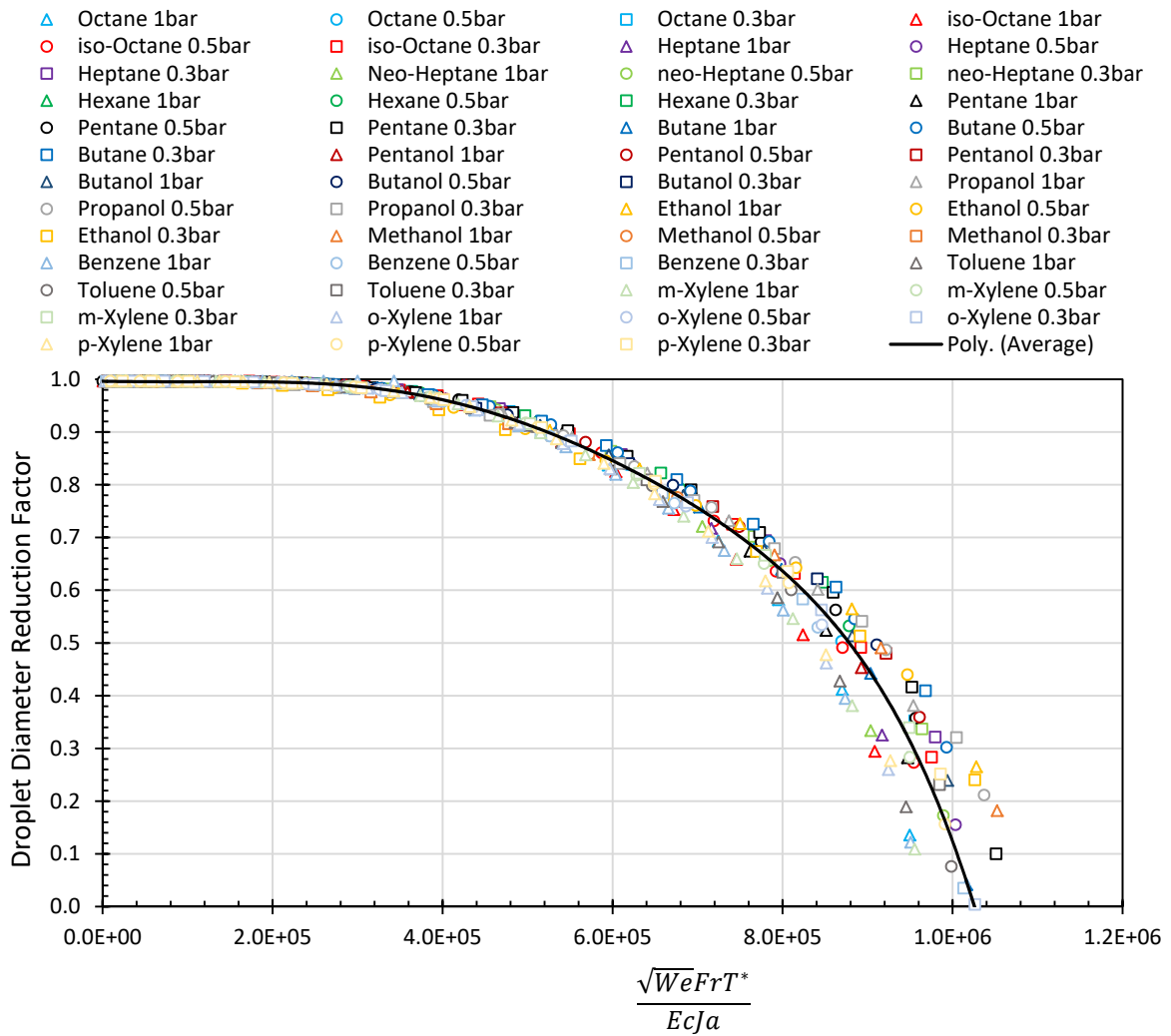
**Figure 4.** Spray formation at subcooled conditions using default and optimised secondary breakup model constants compared to experiments which can be found in [41], *n*-Pentane.



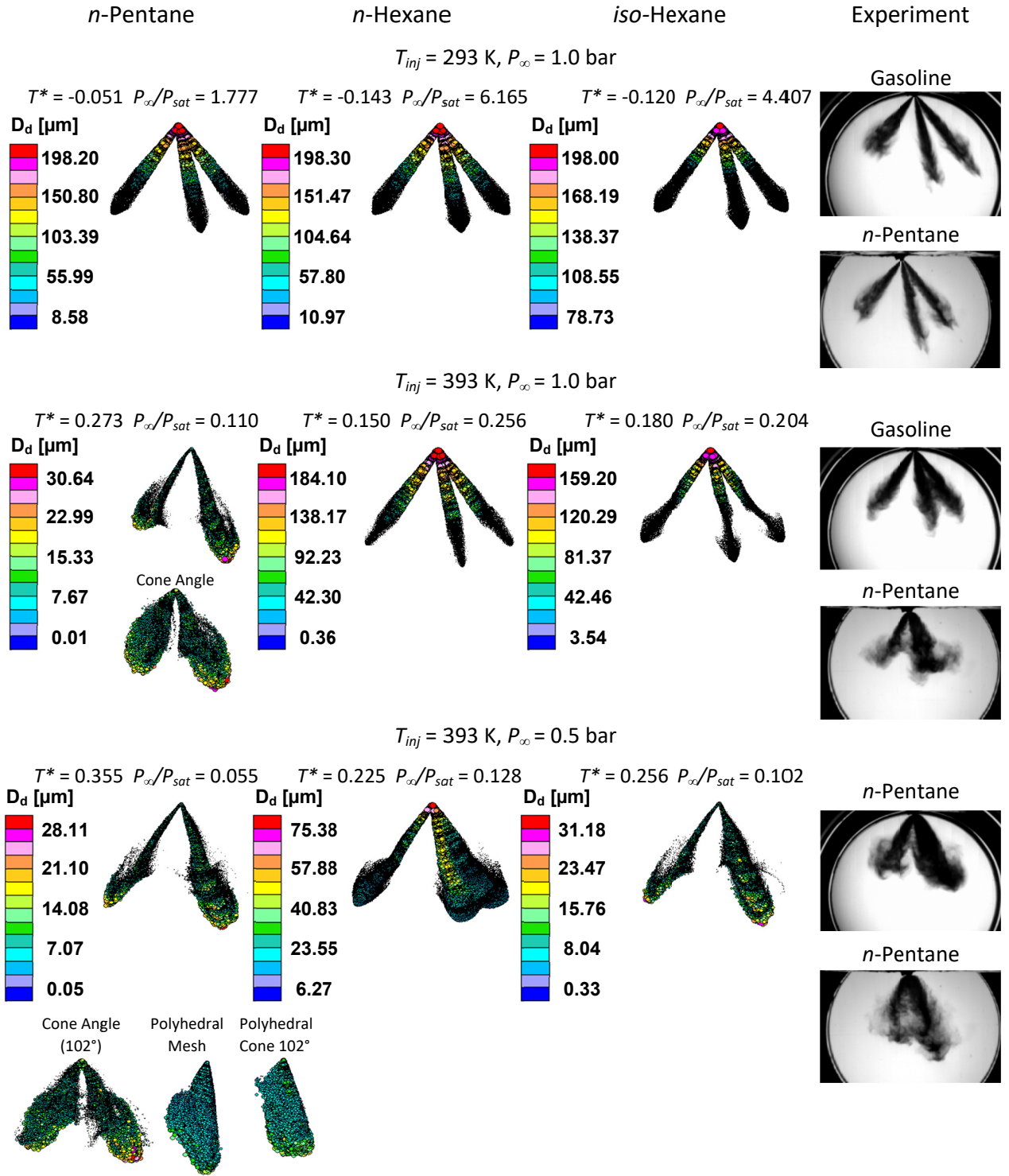
**Figure 5.** SMD and liquid penetration at subcooled conditions using default and optimised secondary breakup model constants compared to experiments which can be found in [40], *n*-Pentane.



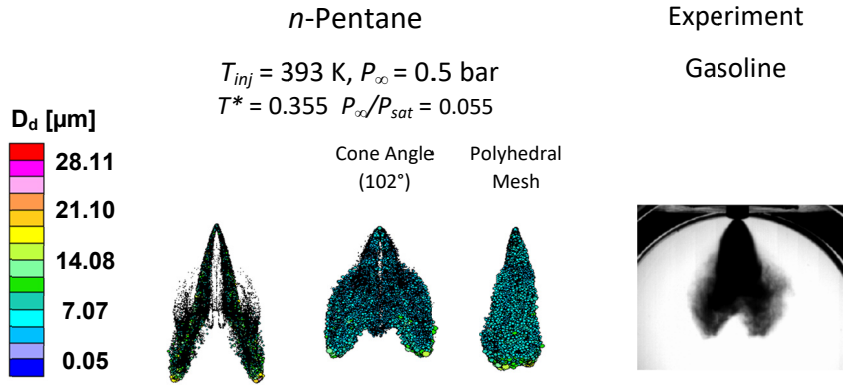
**Figure 6.** Droplet reduction factor for a range of single-component fuels plotted against superheat.



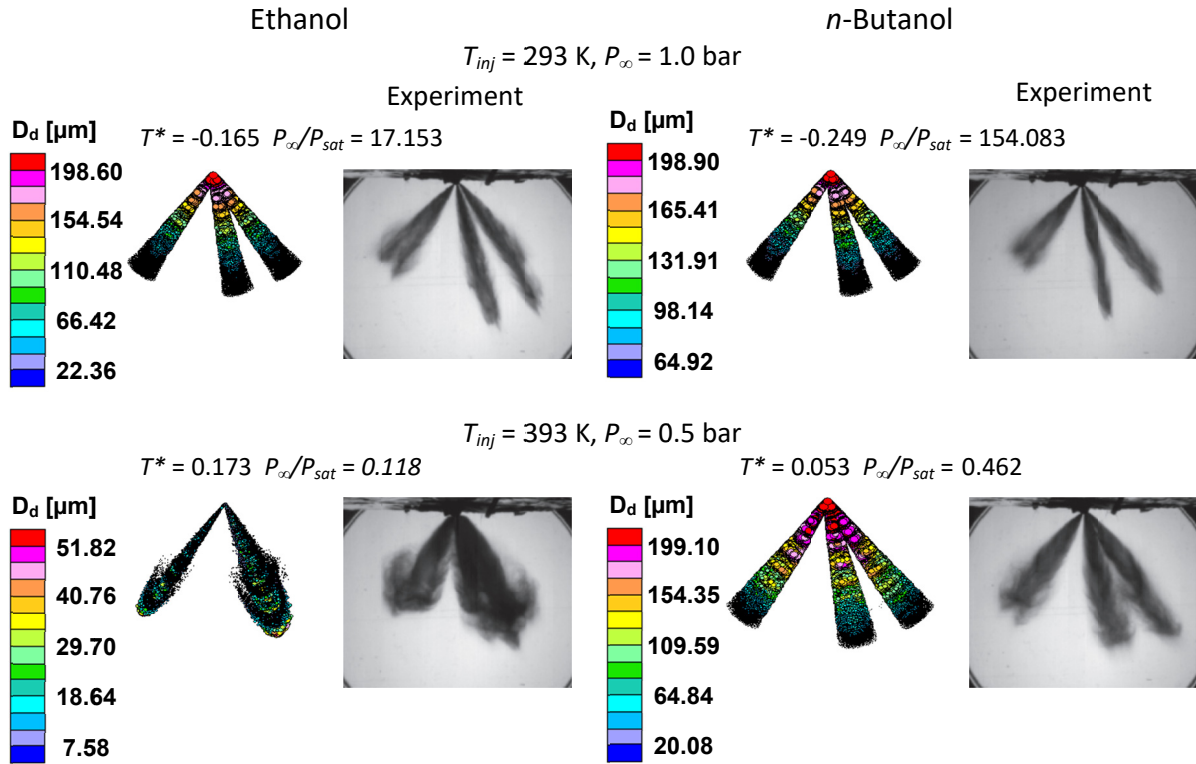
**Figure 7.** Normalised droplet diameter reduction factor for all fuels at pressures of  $P_{\infty} = 1.0, 0.5$  and  $0.3$  bar.



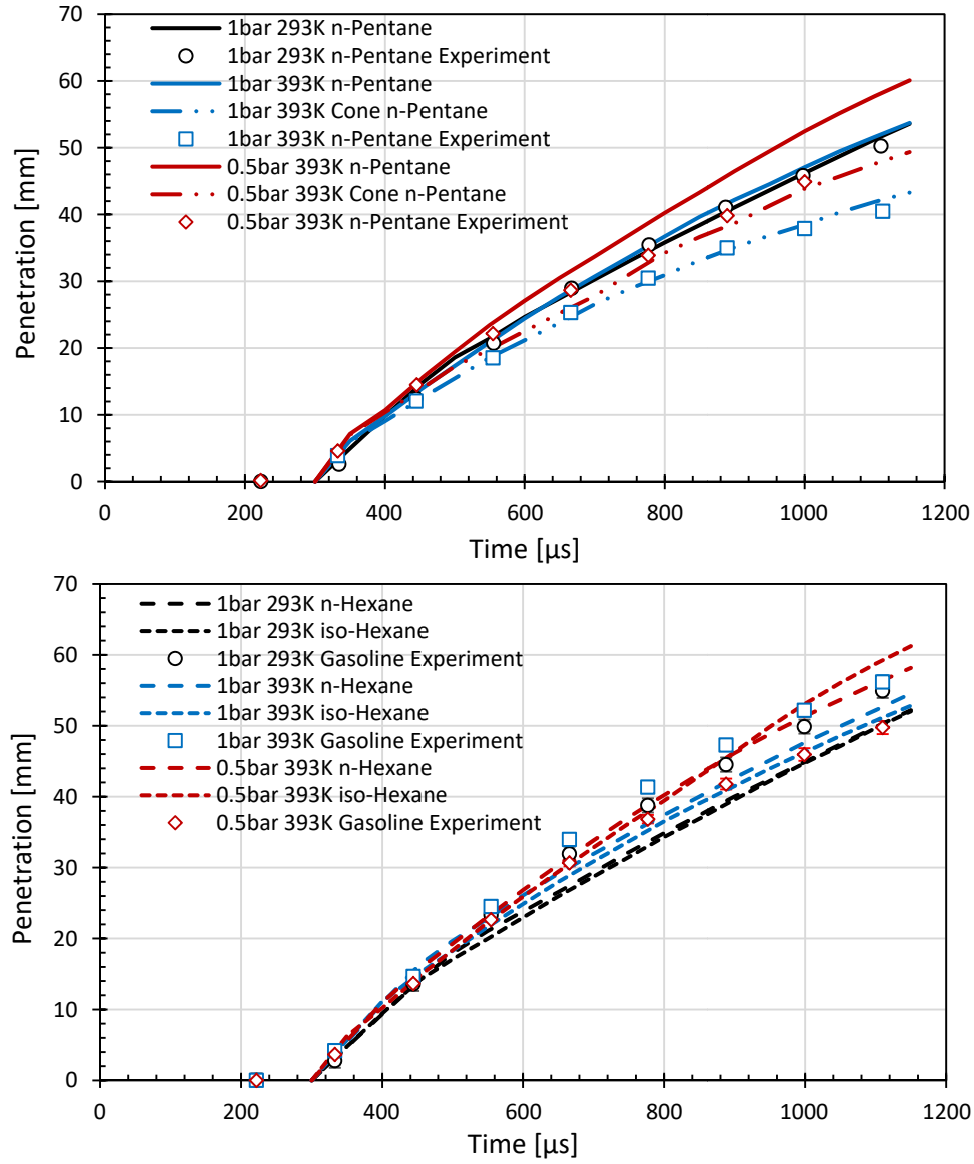
**Figure 8.** 6-hole asymmetric injector spray formation at 777  $\mu\text{s}$  ASOI (including injection delay), *n*-Pentane, *n*-Hexane and *iso*-Hexane. Experiments can be found in [40], Gasoline and *n*-Pentane.



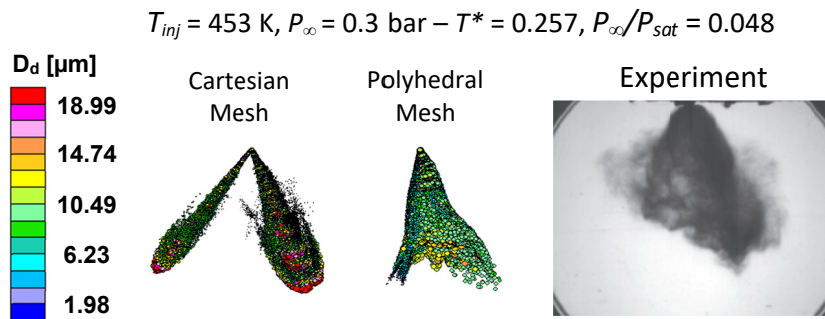
**Figure 9.** 6-hole asymmetric injector spray formation at 777 μs ASOI (including injection delay), *n*-Pentane front view (see Table 1). Experiments can be found in [40], Gasoline.



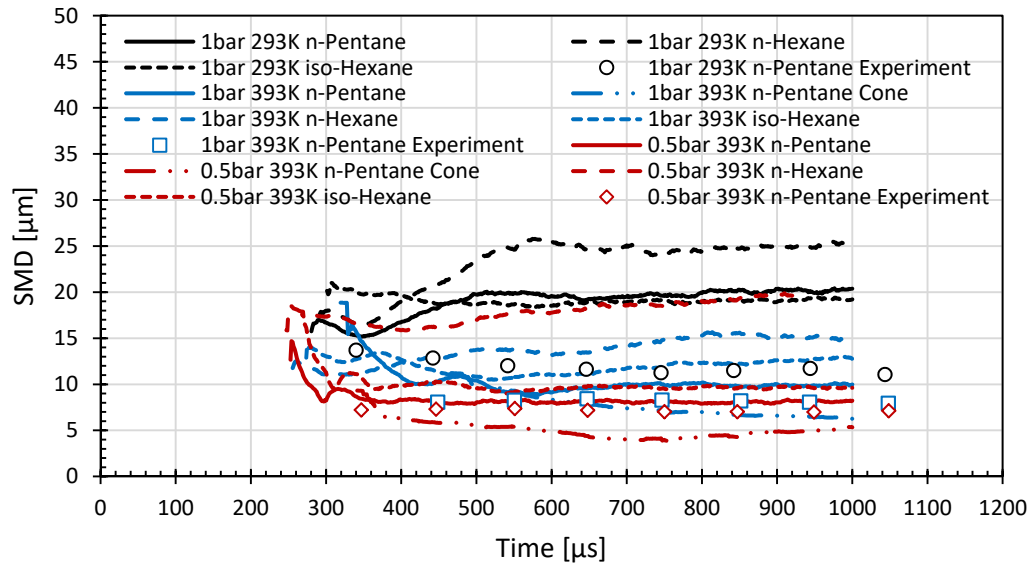
**Figure 10.** 6-hole asymmetric injector spray formation at 777 μs ASOI (including injection delay), Ethanol, *n*-Butanol. Experiments can be found in [40], Ethanol, *n*-Butanol.



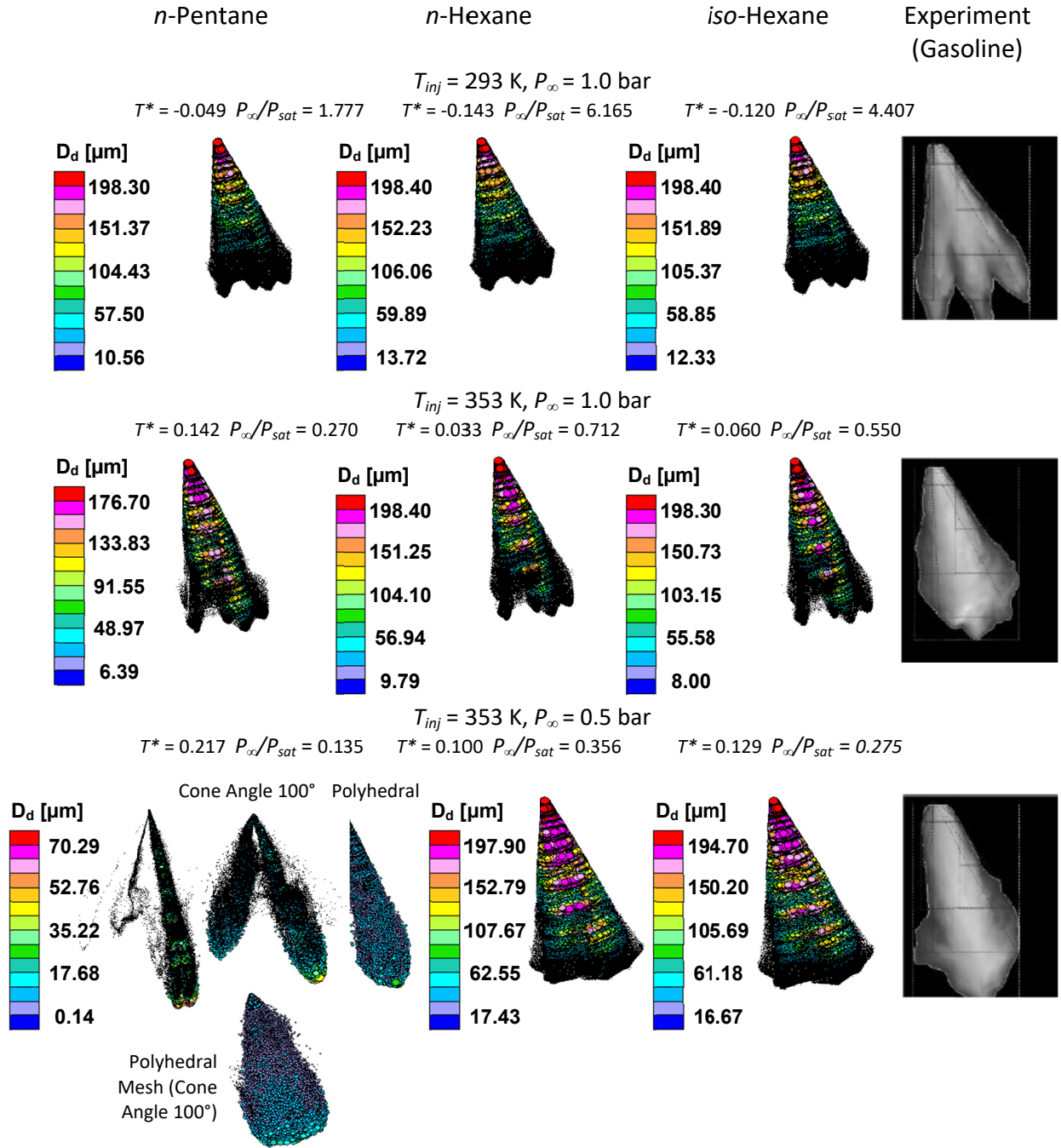
**Figure 11.** Liquid spray penetration using the 6-hole asymmetric injector, *n*-Pentane, *n*-Hexane and *iso*-Hexane. Experiments can be found in [40].



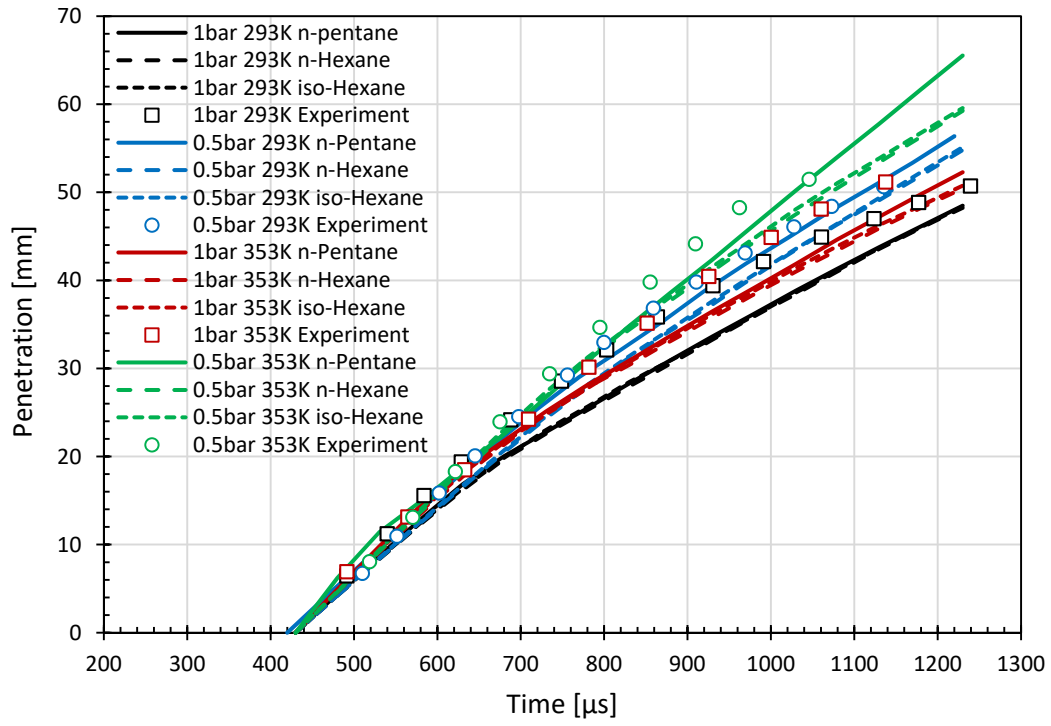
**Figure 12.** Spray formation of 6-hole asymmetric injector at  $T_{inj} = 453 \text{ K}$ ,  $P_{\infty} = 0.3 \text{ bar}$ , *n*-Butanol. Experiments can be found in [40], *n*-Butanol.



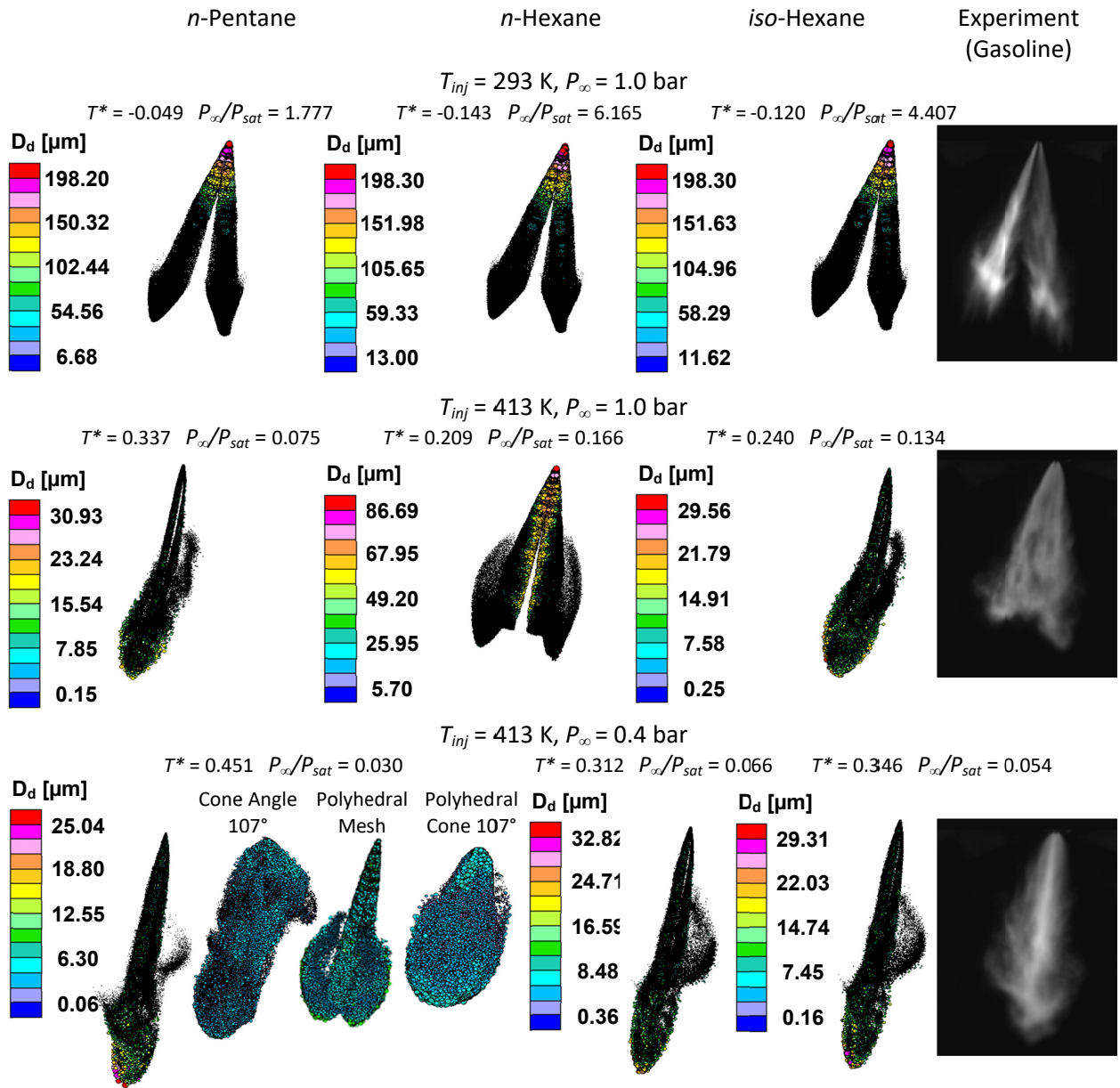
**Figure 13.** Time-varying SMD of 6-hole asymmetric injector at 25 mm downstream of the nozzle exit, *n*-Pentane, *n*-Hexane, *iso*-Hexane. Experiments can be found in [40], *n*-Pentane.



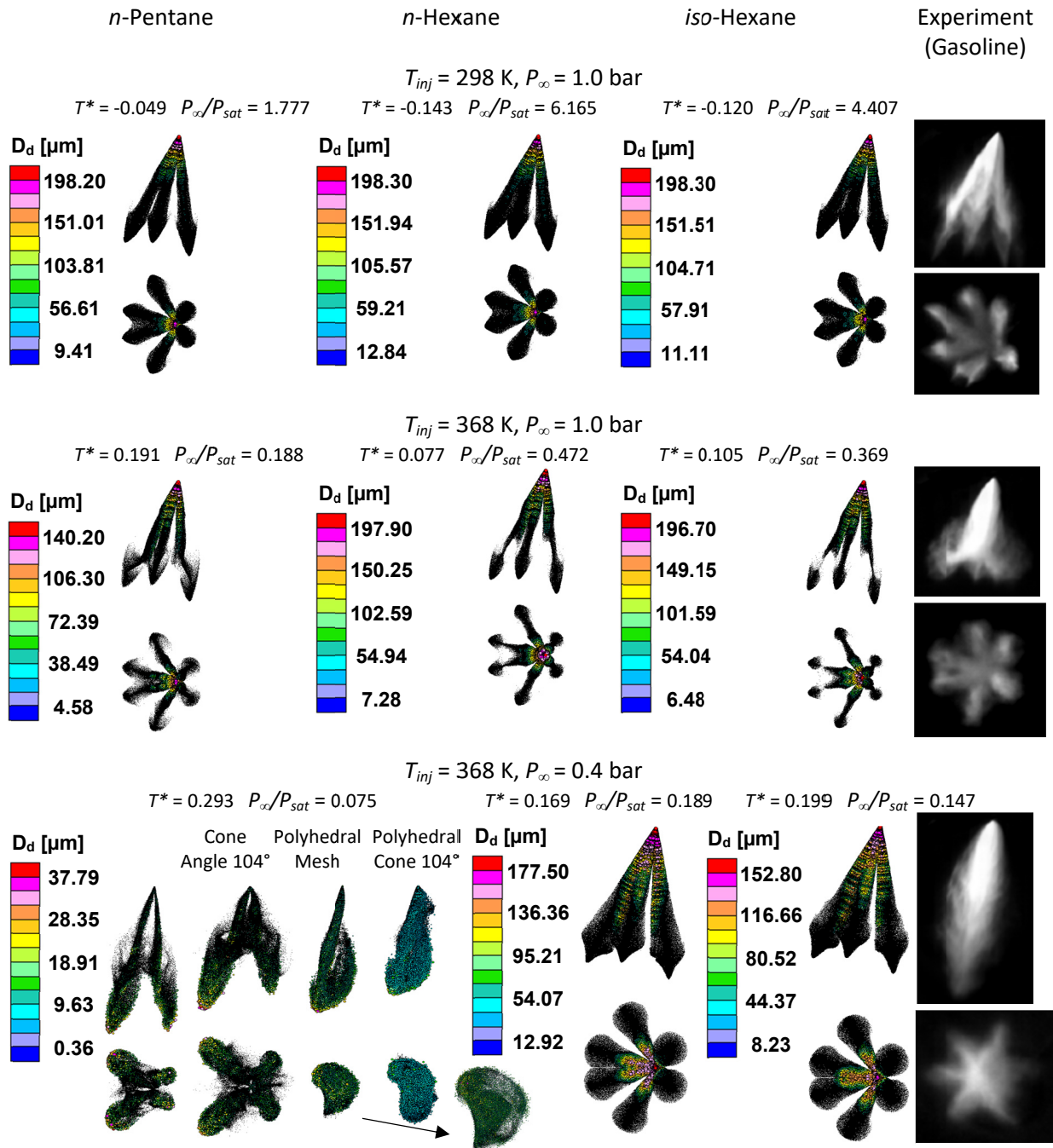
**Figure 14.** 7-hole asymmetric injector spray formation at 888  $\mu\text{s}$  ASOI, *n*-Pentane, *n*-Hexane, *iso*-Hexane. Experiments can be found in [39], Gasoline.



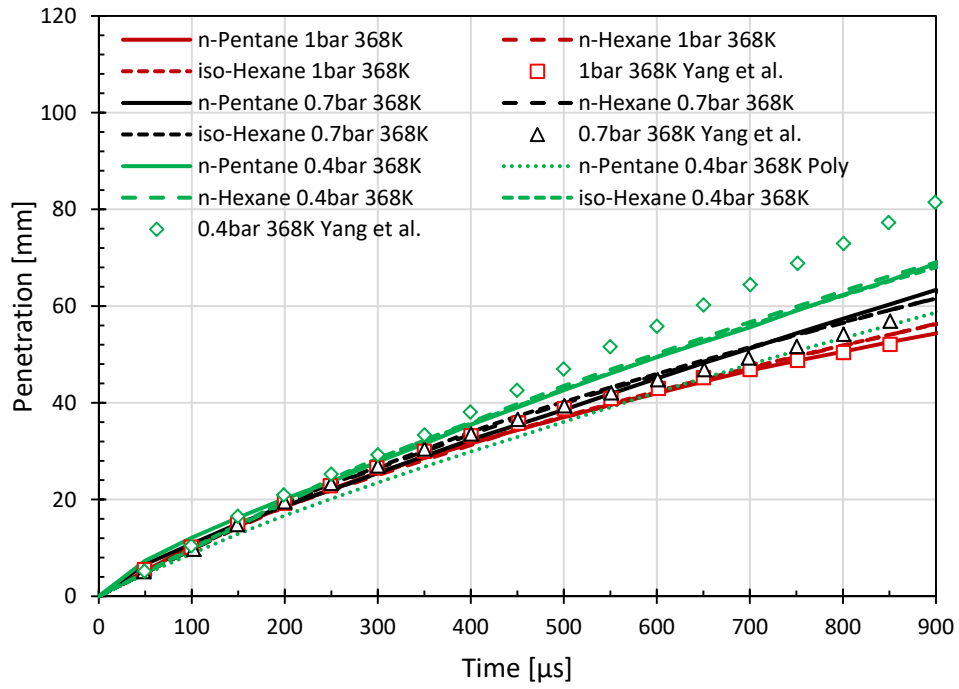
**Figure 15.** Liquid spray penetration predictions of *n*-Pentane, *n*-Hexane and *iso*-Hexane. Experiments can be found in [39], Gasoline.



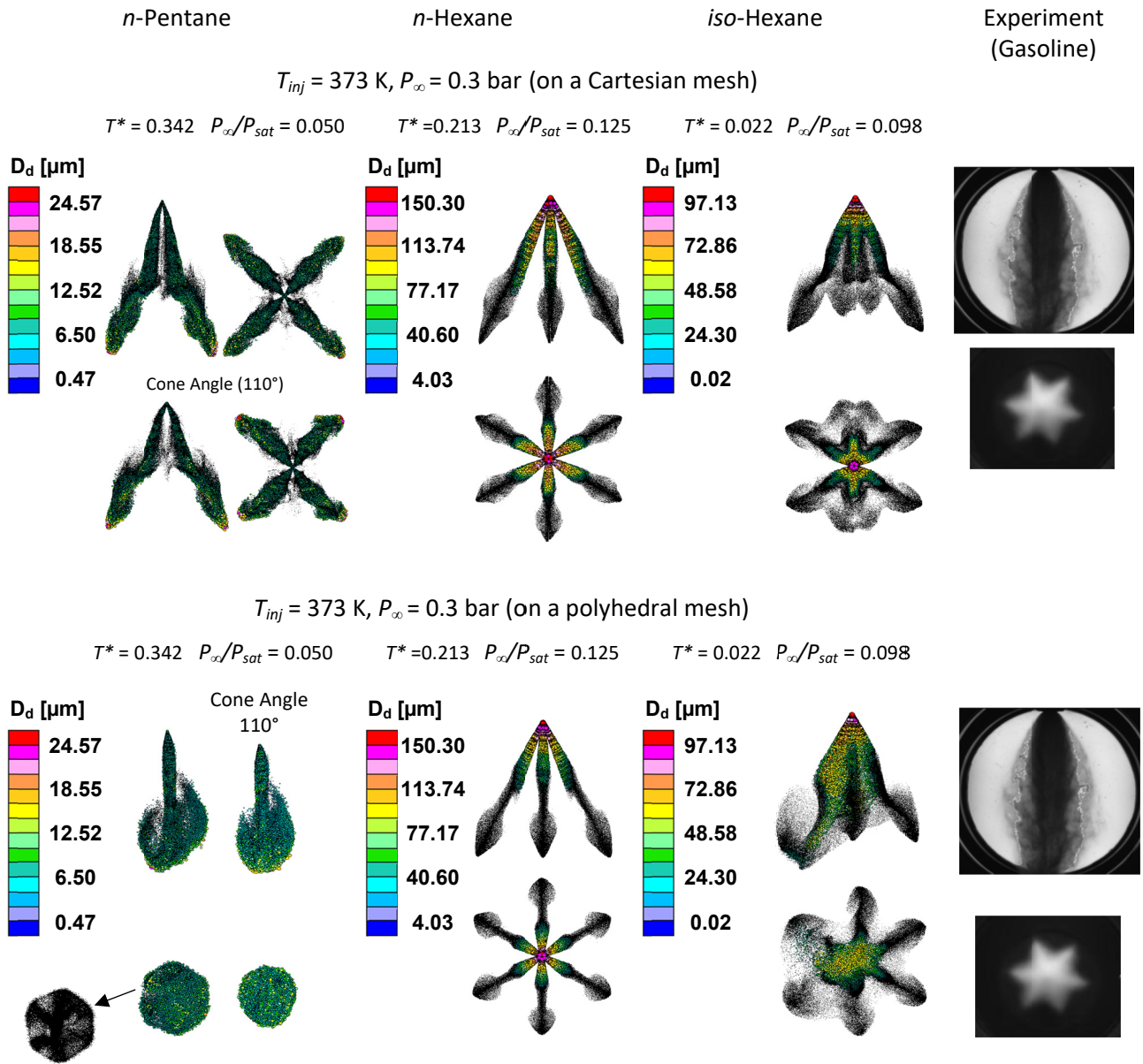
**Figure 16.** 2-hole asymmetric injector sprays at 800  $\mu\text{s}$  ASOI, *n*-Pentane, *n*-Hexane and *iso*-Hexane. Experiments can be found in [38], Gasoline.



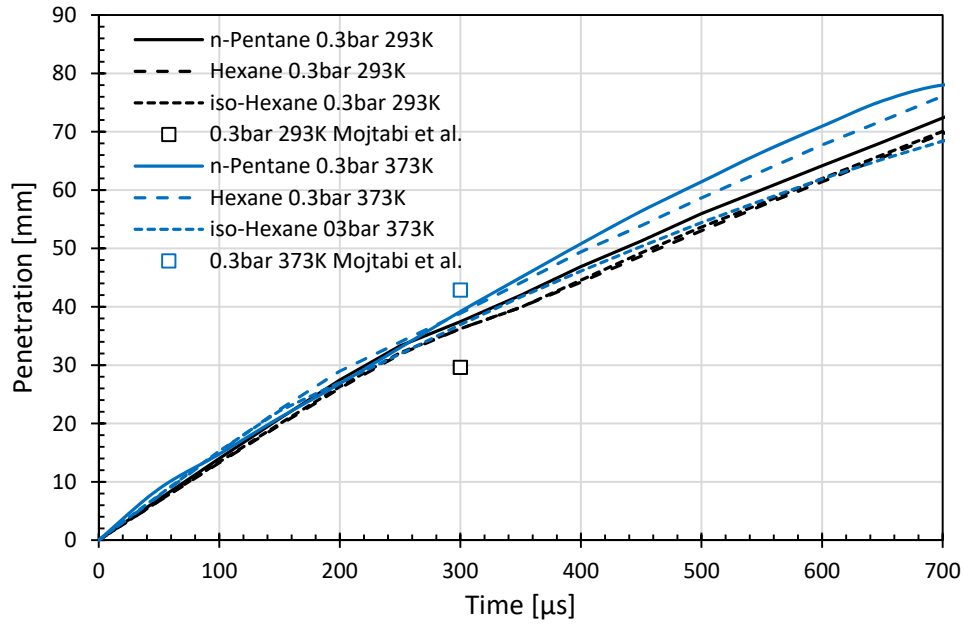
**Figure 17.** 6-hole asymmetric injector sprays at 800  $\mu\text{s}$  ASOI, *n*-Pentane, *n*-Hexane and *iso*-Hexane. Experiments can be found in [38], Gasoline.



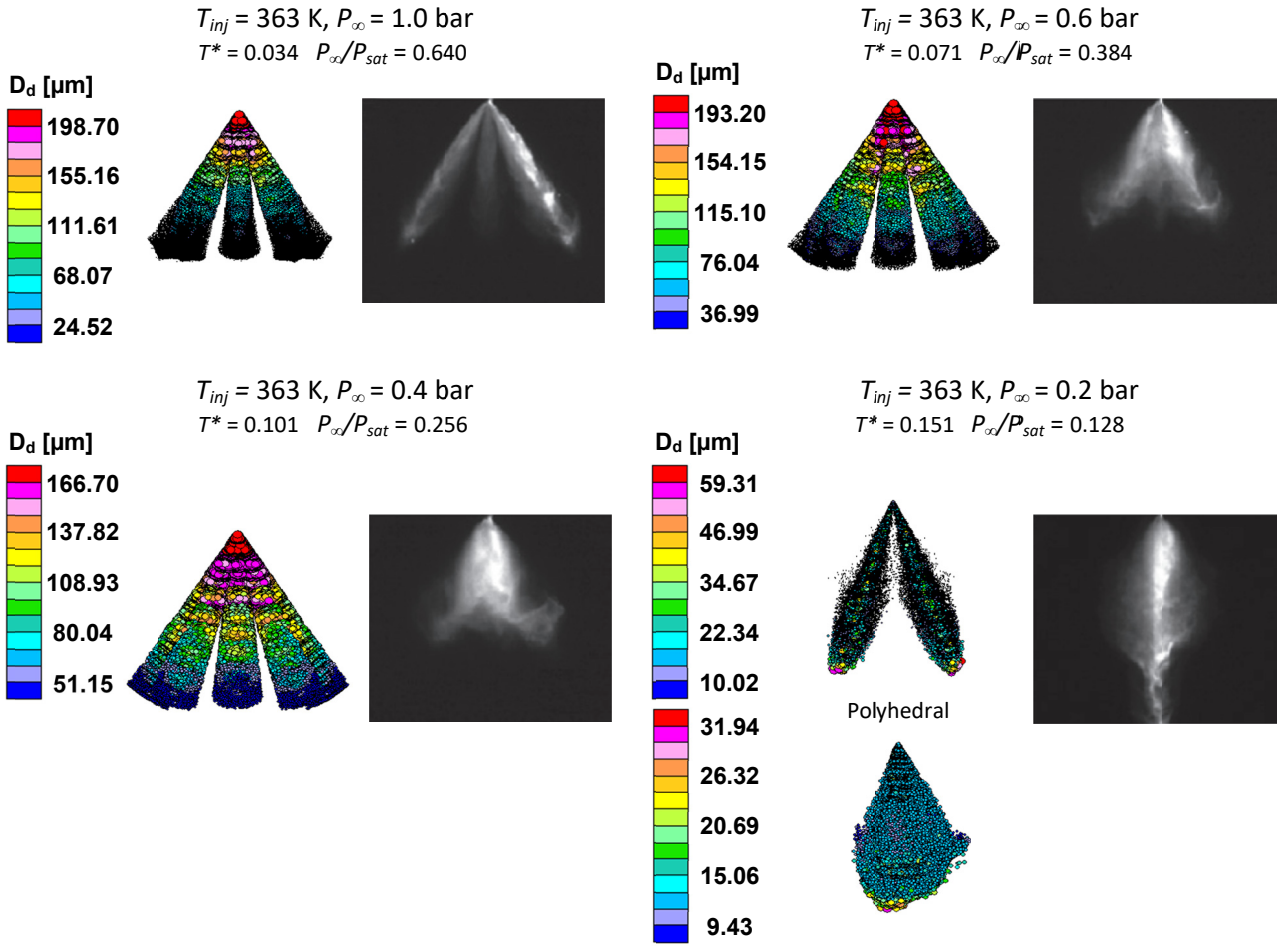
**Figure 18.** Liquid spray penetration predictions of a 6-hole asymmetric injector, *n*-Pentane, *n*-Hexane and *iso*-Hexane. Experiments can be found in [38], Gasoline.



**Figure 19.** Spray formation using a Cartesian mesh (top) and a polyhedral mesh (bottom). *n*-Pentane, *n*-Hexane and *iso*-Hexane compared to experiments from [37], Gasoline.

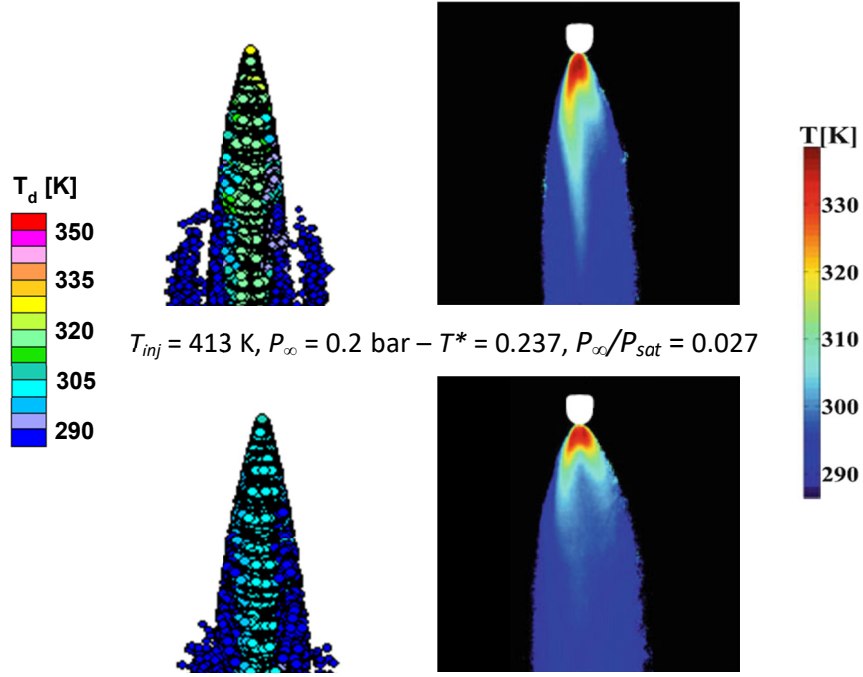


**Figure 20.** Liquid penetration of a 6-hole symmetric injector at  $P_{\infty} = 0.3$  bar and  $T_{inj} = 293\text{--}373$  K. Experiment can be found in[37].

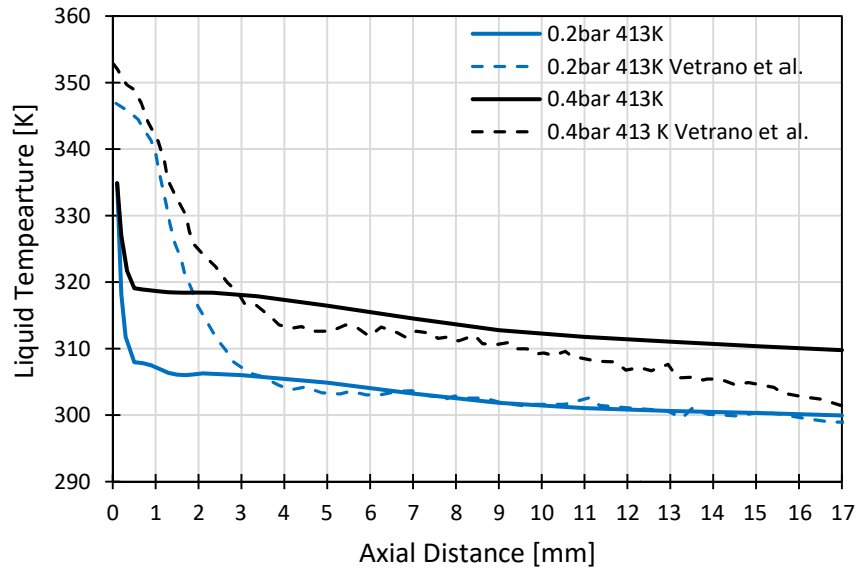


**Figure 21.** Sprays with reducing  $P_\infty$  at 600  $\mu$ s ASOI, Ethanol. Experiments can be found in [4]. Polyhedral mesh case included for extreme flash-boiling case ( $P_\infty = 0.2$  bar).

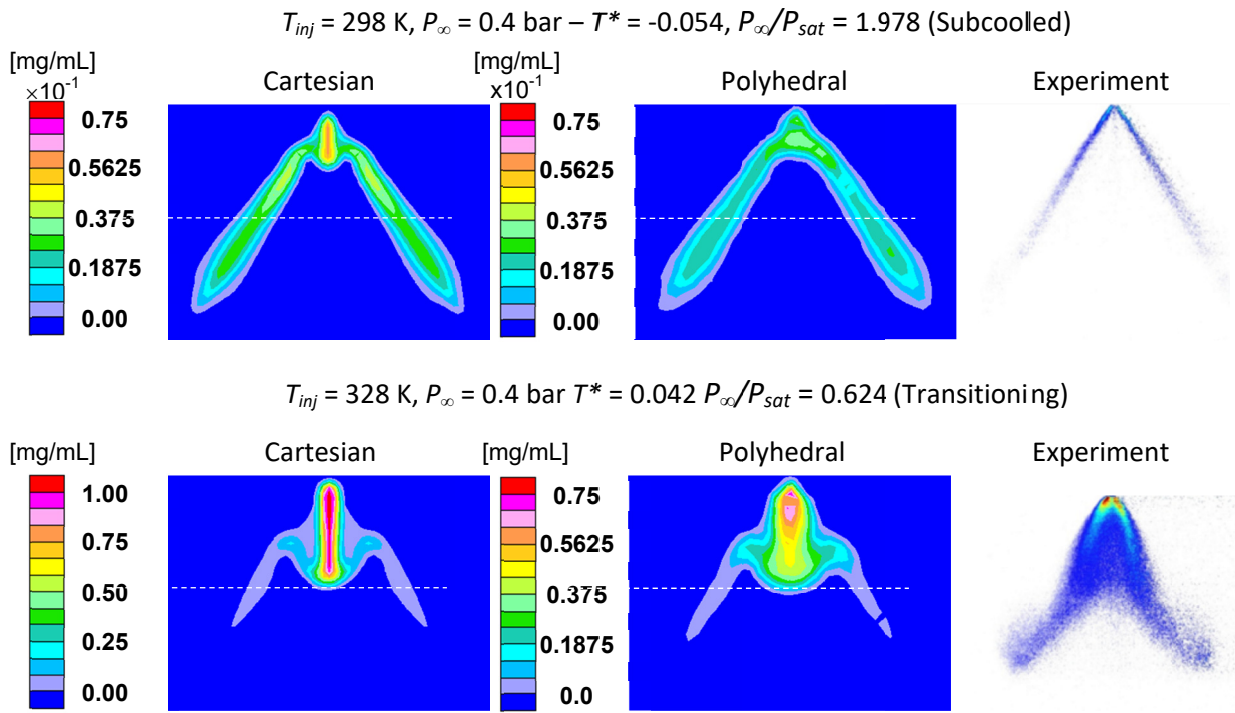
$$T_{inj} = 413 \text{ K}, P_{\infty} = 0.4 \text{ bar} - T^* = 0.202, P_{\infty}/P_{sat} = 0.053$$



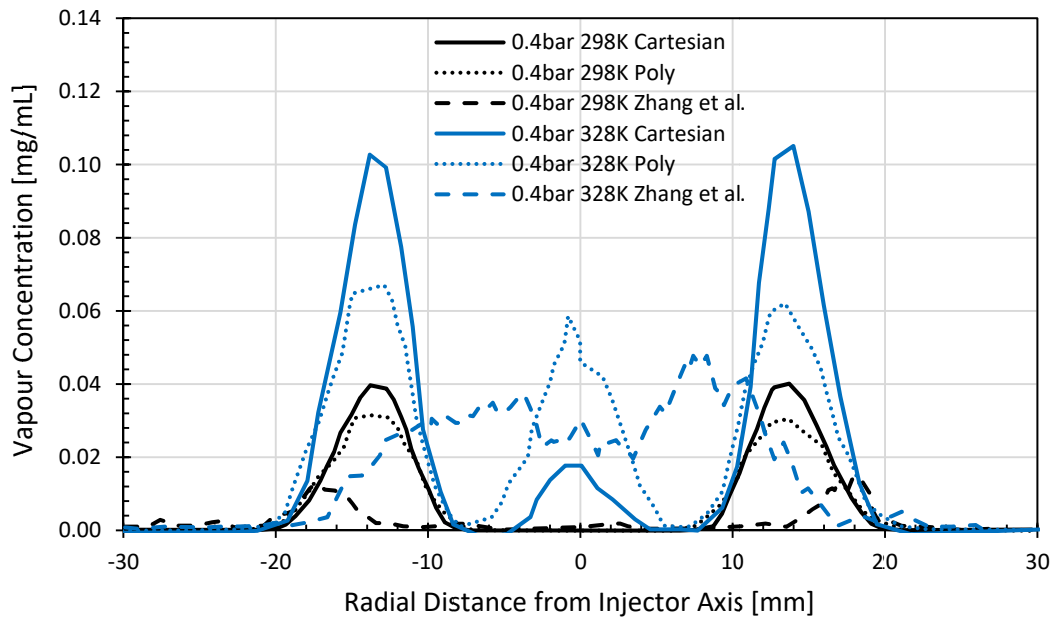
**Figure 22.** Droplet temperature of single-hole spray on a 2 mm plane cutting through the central axis of the injector compared to PLIF experiment of [55], Ethanol.



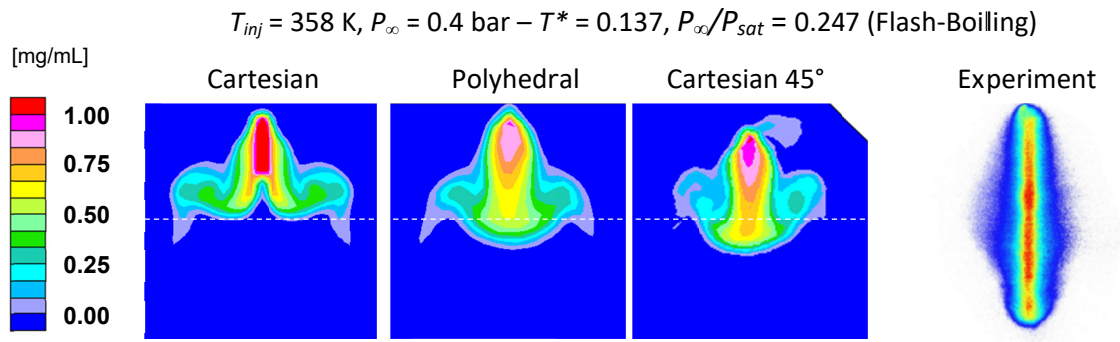
**Figure 23.** Average liquid/droplet temperatures taken at 2 mm intervals on the central axis of the plume compared to PLIF experiment of [55], Ethanol.



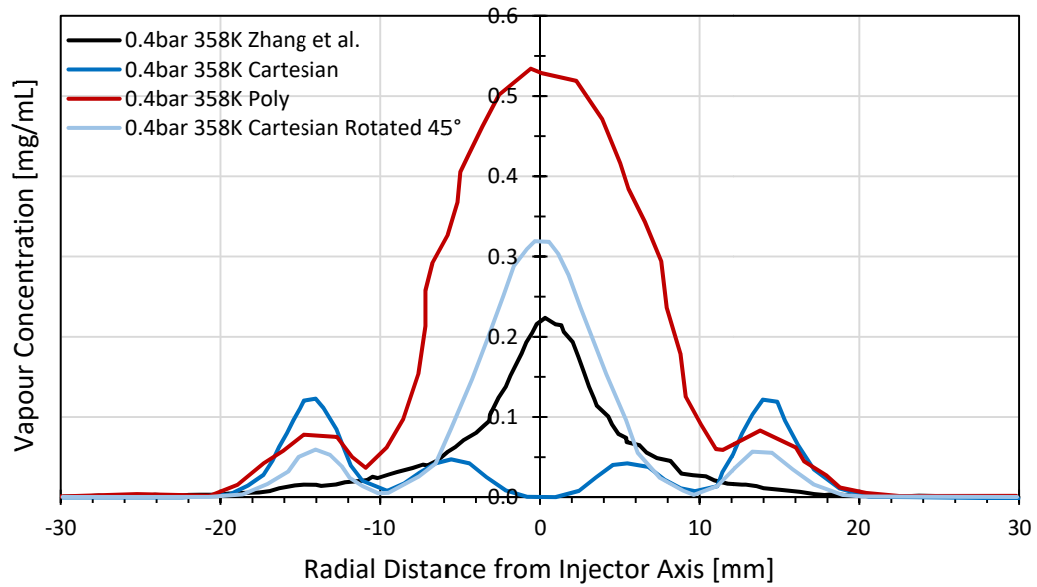
**Figure 24.** Vapour concentration of *n*-Hexane plotted on a plane cutting through the central axis of the injector. Compared to LIEF experiments of [56].



**Figure 25.** Vapour concentration of *n*-Hexane at 20 mm downstream of the nozzle exit at varying radial distances from the injector axis. Compared to LIEF experiments of [56].



**Figure 26.** Vapour concentration of *n*-Hexane plotted on a plane cutting through the central axis of the injector. Compared to LIEF experiments of [56].



**Figure 27.** Vapour concentration of *n*-Hexane at  $T_{inj}=358 \text{ K}$ , 20 mm downstream of the nozzle exit at varying radial distances from the injector axis. Compared to LIEF experiments of [56].