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ILASS–Europe 2017
28th Conference on Liquid Atomization and Spray Systems

The Universitat Politècnica de València (UPV), Spain, is honored to host the 28th edition of the European Conference on Liquid Atomization and Spray Systems from the 5th to the 8th September 2017, organized by CMT-Motores Tèrmicos and ILASS Europe.

Our University is located on the east coast of Spain in the beautiful city of Valencia with very good connections to the rest of Spain. It hosts about 36000 students, who attend the courses given by it’s over 2800 academic staff. It has reached international renown, attracting every year over 2000 Erasmus students, which ranks UPV as the 6th hosting institution in Europe.

Now, let me briefly present the main organizer of this conference, CMT Motores Térmicos. It is an internationally well-known research institute of the Universitat Politècnica de València dedicated to research on thermo-and fluid dynamics processes in direct injection engines. Its staff comprises over 120 people, with 41 faculty members and about 60 research assistants (mainly Ph.D students). Our institute has a total annual budget of 16 M€ coming from projects with private companies and public administrations. Two visits to our CMT laboratories have been scheduled during the ILASS conference, and participants will be welcome to discover our state of the art facilities, which comprise 16 engine test cells and another 20 specific test installations. Among these, 8 test benches dedicated to sprays, including a high pressure and high temperature vessel, a rapid compression machine, a transparent engine and several hydraulic test benches to measure injection rate and spray momentum.

With three keynote lectures and a total of 135 oral presentations distributed in 28 sessions, the ILASS 2017 Conference program reflects the success of this edition, in line with previous ones. There are three main topics: Automotive Sprays, Atomizers, and Atomization & Droplets, with about 30 papers each. The rest of the papers are grouped in four smaller topics: internal nozzle flow, combustion, experimental techniques, and atmospheric & medical sprays. A closer look at the program reveals the extensive participation of both industry and academia, with the common objective of sharing the latest scientific advances to help improve knowledge about the atomization processes for different applications.

Last but not least, I would like to convey our warmest welcome to all the guests attending the conference, wishing them a fruitful conference and enjoyable stay in Valencia.

Prof. Raul Payri
ILASS 2017 Conference Chairman
CONFERENCE CHAIRMAN

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A study of the controlling parameters of fuel air mixture formation for ECN Spray A

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Abstract

Designing future ultra-high efficiency, ultra-low emission engines requires an in depth understanding of the multi-scale, multi-phase phenomena taking place in the combustion chamber. The performance of the fuel delivery system is key in the air fuel mixture formation and hence the combustion characteristics, however in most spray modelling approaches is not considered directly. Thus, it is important to understand how the selection of models mimic injection process affect predictions. In this paper we present an Eulerian-Lagrangian framework based on OpenFOAM libraries to model spray injection dynamics. The framework accounts for primary droplet formation (based on a parcel method with predefined initial droplet size distribution), secondary droplet breakup, evaporation and heat transfer. In order to account for the interaction of droplets with turbulence, simulations were performed within the LES context with two different turbulence models. A systematic variation of the key injection parameters (parcel number, parcel size distribution) of the parcel method as well as the grid size was considered. Varying the parcel number affects the initial droplet size distribution which in turn, depending on the selection of the turbulence and the evaporation sub-models, affects: spray dispersion; spray penetration; and subsequent droplet size distribution. Results were validated against the baseline experimental data for evaporating ECN Spray A with n-dodecane chosen as a surrogate for Diesel fuel.

Keywords

ECN Spray A, Eulerian-Lagrangian, LES, OpenFOAM

Introduction

In both Diesel and spark ignition engines fuel is injected into the combustion chamber at elevated pressures. Nowadays realistic injection pressures for common-rail Diesel reach up to 3500 bars. The reason behind the need for such extreme pressures is to promote primary and secondary atomisation until a combustible mixture is formed. The higher the injection pressure the higher the shear between the static air within the combustion cylinder and the liquid. At extreme ambient pressures and temperatures the fuel can even exhibit supercritical behaviour that causes a reduction in its surface tension. Combustion occurs in a lifted, turbulent diffusion flame mode. Numerous studies indicate that the combustion and emissions in such engines are strongly influenced by the lifted flame characteristics, which are in turn determined by fuel and air mixing in the upstream region of the lifted flame, and consequently by the liquid breakup and spray development processes [1, 19, 14, 5, 6]. These processes clearly play a critical role in determining the engine combustion and emission characteristics.

From a numerical standpoint simulating spray combustion in modern engines involves a number of challenges mostly associated with the multiphase, multi-scale nature of the phenomenon. Scales vary from the molecular level (reactions) to microns (droplets) to mm (turbulence) and to meters (combustor dimensions). Thus, ‘all component—all scale’ analysis with direct numerical simulations (DNS) is prohibitive with the current computational capabilities for real size combustors. Only a very limited number of studies have been performed in engines with DNS [18]. Reynolds Averaged Navier Stokes (RANS) [17] and more recently Large Eddy Simulation (LES) based approaches are typically employed for engine simulations [7, 3, 22, 12]. RANS, which is the industrial standard approach is based on ensemble averaged governing equations. Although numerically efficient and relatively accurate in predicting the qualitative behaviour of the sprays, RANS cannot predict the local unsteadiness in the mixing flow field. This is a considerable drawback considering that ultra-high injection pressures promote supersonic behaviour of the jet and locally the creation of shock waves that further promote unsteadiness [15]. Moreover, RANS does not allow the study of cycle-to-cycle variation phenomena relevant to the spray evolution that currently is a subject that attracts considerable interest, and is also linked to spray spatial and temporal variations. The LES approach, which is based on spatially filtered governing equations, can capture the large scale flow structures based on the filter size. However, the unresolved small-scale structures are still modelled, which makes LES dependent on the sub grid scale models used and the grid resolution. Since LES can capture local unsteadiness and is computationally more attractive than a DNS based approach, it has received significant attention in the past decade, especially for simulation of internal combustion engines.

An additional difficulty in the modelling of turbulent combustion in realistic engine geometries is that in the effort to reduce computational cost and grid complexity, in many of the existent approaches the injector is not simulated directly and the effects of the in-nozzle flow and primary atomisation are modelled indirectly. The existent models based on the so-called parcel method have considerable weaknesses, the most important of which is the fact that...
the injected (initial) droplet size distribution needs to be selected a-priory. If experimental data are not available then fine tuning is required, making the final results dependent on the degree of tuning. Moreover, these models are mostly tailored to intermediate injection pressures of equipment of the past as well as to the RANS context. Extending these models to the LES context, understanding the resulting challenges and suggesting modifications is an area of active research. The sensitivity of the predictions to the injection model also undermines efforts for better evaporation and combustion models since in sprays all the phenomena present are interlinked and the injection part is a key controlling parameter of the initial mixture formation. For instance, even if the evaporation model predicts accurately the droplet size reduction because of heat transfer, if the parcels initially injected represent droplets with sizes considerably smaller than the real ones, simulations of liquid penetration will fail because the droplets will evaporate considerably quicker.

In recent years, various studies were performed in both experimental [9, 14] and numerical front [21, 20, 22, 23] in an effort to better understand spray dynamics at ultra-high pressures. Within the experimental results several institutions have provided high-fidelity measurements of macroscopic spray parameters such as spray penetration, liquid length and vapor penetration as well combustion related parameters such as ignition delay, lift-off length, and soot emissions for a range of fuels, ambient and injection conditions. Such datasets can be accessed through the Engine Combustion Network [11].

Experimental data
In the current work we use experimental data from Sandia National Laboratories at operating conditions known as ECN 'Spray A' (see Table 1). A constant-volume, quiescent, pre-burn-type combustion vessel is used to generate high-temperature and high-pressure gases. A premixed combustible mixture is spark-ignited. The combustion products are cooled until they reach the desired pressure and temperature. Then the diesel fuel injector is triggered and fuel injection occurs. The conditions for n-dodecane used as a surrogate of diesel fuel. In Fig 1 the experimental pictures of Spray A at three different time instances obtained with different techniques is presented. In pictures from both techniques the light blue line indicates the liquid penetration vs time [11]. The time instances were selected to correspond to the time instances that numerical results will be presented in the following sections.

![Figure 1. Experimental images of Spray A at three different time instances obtained with different techniques. In pictures from both techniques the light blue line indicates the liquid penetration vs time [11].](image)

Numerical setup
The numerical simulation of the two-phase flows is performed in the framework of an Eulerian-Lagrangian approach within an Open Source code (OpenFOAM) [8]. The governing equations were solved on two different grid sizes. For

<table>
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<th>Table 1. Summary of experimental conditions [11].</th>
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<tr>
<td>Experimental conditions</td>
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<tr>
<td>--------------------------</td>
</tr>
<tr>
<td>Ambient temperature (K)</td>
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<tr>
<td>Ambient density (kg/m^3)</td>
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<tr>
<td>Composition</td>
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<tr>
<td>Injection pressure (bar)</td>
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<tr>
<td>Fuel temperature (K)</td>
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<tr>
<td>Nozzle diameter (µm)</td>
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<tr>
<td>Duration of injection (ms)</td>
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<tr>
<td>Total mass injected (mg)</td>
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<td>Fuel density (kg/m(^3))</td>
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the rest of the paper we use the notation “Grid 1” for the coarser grid with average cell size of 0.5 mm and “Grid 2” for a finer grid with average cell size of 0.3 mm. The time step is calculated based on the Courant number criterion: 
\[ C_{O_{\text{max}}} = \frac{n\Delta t}{\Delta x} \]
where \( \Delta x \) is the grid size while \( \Delta t \) is the time step. For the calculations presented in the results section the \( C_{O_{\text{max}}} = 0.1 \).

**Turbulence model**

LES is based on the idea of computing the large, energy-containing eddy structures (filtered quantities) which are resolved on the computational grid, whereas the smaller, more isotropic, sub-grid structures (SGS) are modelled. The filter width is taken as the cube root of the local grid cell volume. The effect of the small scales is obtained through the sub-grid scale stress term \( \tau_{ij}^{\text{SGS}} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j \) that must be modelled. There are two popular types of turbulence models: a) algebraic eddy viscosity models in which the stress tensor \( \tau_{ij}^{\text{SGS}} \) is related to the resolved strain rate tensor \( \bar{S}_{ij} \) by means of a scalar eddy viscosity given by an algebraic equation; b) one-equation eddy viscosity models. Both model groups are based on the Boussinesq hypothesis associating \( \tau_{ij}^{\text{SGS}} \) with a SGS turbulent viscosity \( \mu_T \). However their main difference is that one-equation SGS models overcome the deficiency of local balance assumption between the SGS energy production and dissipation adopted in algebraic models. Such a phenomenon may occur in high Reynolds number flows and/or in the cases of coarse grid resolutions. In this paper we assess two models (one of each group): The Wall-Adapting Local Eddy-viscosity model (WALE) [13] which is an algebraic eddy viscosity models and the Kinetic Energy Model (KEM) [24] that belongs to the category of one-equation eddy viscosity models. The main difference between the proposed WALE model in comparison to other models of this group, is that the SGS viscosity is dynamically computed with the square of the velocity gradient tensor rather than the resolved strain rate tensor used in Smagorinsky-type models that have been tested in previous work [21] for Spray A. This velocity tensor can not only account for the effects of both strain and rotation rate of the smallest resolved turbulence fluctuations, but also recover the proper near-wall scaling for the eddy viscosity without requiring dynamic procedure. Moreover, the WALE model is invariant to any coordinate translation or rotation and no test-filtering operation is needed, it is therefore considered well suitable for LES in complex geometries [13] as the ones in IC engines.

**Injection model**

As mentioned in the introduction one of the greatest challenges associated with the Eulerian-Lagrangian approach is modelling the near-nozzle flow. In this region a liquid core forms from the liquid fuel being injected through the injector. Ligaments are separated from this liquid core and form droplets that evaporate and mix with the ambient gas. When a combined Eulerian-Lagrangian framework is used then the fuel spray is treated as a dispersed liquid phase, which moves and interacts with the surrounding continuous gas phase. The spray is represented by an ensemble of discrete “parcels”. Each parcel contains a number of droplets with the same size, velocity and temperature. Droplets in a parcel are considered as spherical, which is a rather strong assumption especially for regions close to the nozzle where ligaments instead of droplets are expected to be formed. The droplet parcels are tracked in a Lagrangian fashion as they move through the gas phase, exchanging mass, momentum and energy. The effect of the droplet parcels on the continuous phase due to drag, heat and mass transfer is implemented via source terms in the gas phase conservation equations.

Figure 2 shows a schematic of the injection process modelled in our current calculations. The injection model is a solid-cone injection model. The user supplies a drop diameter probability density function (PDF) with parameters. In our work we have examined two different models a) a Rosin-Rammler (RR) [2] with spreading parameter \( n = 3 \) and mean diameter \( \bar{d} = 50 \mu m \). The RR distribution function is based on the assumption that an exponential relationship exists between the droplet diameter, \( d \), and the mass fraction \( Y_d \) of droplets with diameter greater than \( d \): 
\[
Y_d = e^{(\bar{d}/d)}
\]
b) A fixed value distribution with mean droplet size \( \bar{d} = 90 \mu m \). In this method all droplets injected have the same size and their size only changes as they move through the domain because of evaporation and secondary break up. One point that should be made is that for sprays with low initial velocity, the droplets can retain their sizes for quite a long period after the primary breakup. It is, therefore, essential to provide a correct droplet size distribution for fuel sprays of low injection velocity, such as the pressure-swirl type of gasoline injector. For diesel sprays of high initial velocity, the droplet size distribution is not expected to be as important to the final droplet distribution if an appropriate model for the secondary breakup is applied. The higher the initial velocity of the jet, the sooner the secondary breakup occurs and the lower the dependence of the final droplet sizes on the droplet size distribution of the primary breakup.

The velocity of the injected parcel is calculated as 
\[
\dot{m}_d = \frac{m}{C_d p A}
\]
where \( A \) is the area of the injection (defined by the diameter of the nozzle), \( C_d \) is the discharge coefficient (=0.9) and \( \dot{m} \) is the mass flow rate. Within this model the velocity vector direction is defined by a random angle size within a limit (in our case 10°) which is a user-defined constant and does not depend on the droplet size which might lead to inaccuracies. It should be underlined that the mass (or volume) given initially to each parcel depends on the mass flow rate profile of the injector while the mean droplet size characterising the parcel depends on the initial distribution. This means that the number of droplets in each parcel is a statistical number which can vary from a fraction of a droplet to thousands of droplets depending also on the number of parcels used. The higher the number of parcels used the lower the number of droplets each
It becomes evident that one of the most important parameters in this injection model is the number of parcels injected per second (PPS). The higher the PPS the more accurate is the representation of the initial pre-selected distribution. For the case of a fixed droplet size this is not particularly important since even a small size of parcels is enough for the statistical representation of the injection process while for the case of the RR the number of parcels is more important to faithfully reproduce the droplet size distribution.

Parcel Tracking

In Lagrangian spray simulations, the particles representing the liquid are moving in a fixed Eulerian framework as described above. Tracking them and defining the cells they go through are clearly important issues. In OpenFOAM the approach used is the face-to-face tracking. The process can be described in four steps [10]: 1) Initially the parcel is moved until it reaches a cell boundary or the entire time step if it remains in the same cell; 2) Then a check is performed to evaluate if the parcel changes cell; 3) The time it took to move out of the first cell is calculated, and the parcel properties are updated; 4) Following the momentum change to the cell that the parcel has been in are added. If the parcel still has time left to move we go back the the first step of the algorithm. Parcels tracked by face-to-face tracking cannot ‘skip’ cells, which improves the predictions of transfer of mass, momentum and energy.

Secondary breakup

The breakup model used is the Kelvin-Helmholtz-Rayleigh-Taylor (KHRT) model [16]. This model, along with the TAB model, is one of the most widely used in Lagrangian spray simulations today. The KHRT model was chosen here since previous studies (within the RANS context) have indicated its superior performance under Diesel conditions [4]. It should be mentioned that it is also possible to use the TAB model, but often in conjunction with some form of primary atomisation model. The TAB model tends to break up the droplets very rapidly. The KHRT model includes two modes of breakup: KH breakup, accounting for unstable waves growing on the liquid jet due to differences in velocity between the gas and liquid; and RT breakup, accounting for waves growing on the droplets’ surface due to acceleration normal to the droplet-gas interface. The relative performance of the two models within the LES context needs to be also examined in a future study.

Summary of Test Cases

In Table 2 a summary of all the cases considered in this paper is provided.

Results and discussion

Figure 3 shows predicted and measured liquid spray penetration at different times after start of injection (ASOI) under non-reacting conditions for n-dodecane at an ambient temperature of 900 K. Liquid penetration is defined as the axial location encompassing 97% of the injected mass at that instant in time. The first observation is that for Cases 1-3 that the RR is used as initial distribution the results show great sensitivity to the particle number. Case 3 (with the lower number of particles and thus the less accurate representation of the RR) shows closer agreement with the experiments. This can be considered an indication that the RR with the selected parameters might not be
the optimum distribution for this spray condition. Moving to a finer grid it can be seen that rather surprisingly for both Cases 4 and 5, irrespectively of the number of parcels used a considerably higher liquid penetration is predicted in comparison to the coarser mesh. Also the predictions are less dependent on the PPS number. Differences can only be noticed when a considerably low number of PPS is used as in Case 6. Using though 50,000 PPS is not a reasonable number to represent any spray statistics and thus it is not considered in the liquid penetration predictions. An additional interesting point is that the turbulence model appears to play a considerable role. Case 1 and 3 are run with the same number of parcels as Case 7 and 8 as well as the same grid however the liquid penetration predicted is different. For Case 7 and 8 regardless of the number of parcels the predictions agree with the experiments while for Case 1 and 3 the predictions depend on the number of parcels. An additional case (Case 9) is run with the KEM model and with 20 million PPS. It can be seen that for this case since the initial distribution is different (a fixed mean diameter value for all the injected droplets is chosen) the predictions are slightly different than Cases 7 and 8 although still in reasonably good agreement with the experiments. Finally it should be mentioned that looking at pictures in Fig 1 for all cases the spray disperses less than in experiments and potentially an even higher grid resolution with modifications to the particle model is required.

Figure 3. Measured [11] and predicted liquid penetration vs. time for the cases of Table 2

In order to get a better understanding of the conditions leading to these differences we include in our analysis Figs 4-6 that demonstrate the C_{12}H_{26} (vapour) contour at two different time instances. We can see that in Fig 4 for the cases that use a rather large number of parcels (20,000,000 and 2,000,000) the results are similar. The length of the spray is similar while we can see that the vapour (indicated by the bright red areas of high C_{12}H_{26}) starts being formed even very close to the injection point. The behaviour is different in Fig 5 in which a higher grid resolution is used. The vapour diffuses less while it penetrates more. However the areas of high vapour concentration are at the tip of the spray and not close to the injection point. This behaviour is not compatible to what has been reported in the literature when different codes are used (see for example [21]). It should be underlined that the different grid sizes, apart from the direct effect they have on the turbulence resolution, also affect the parcel injection method because for the current calculations the time step is adjusted based on the Courant number. The average time step for Grid 1 $\Delta t = 2.5 \times 10^{-7}$ s while for Grid 2 $\Delta t = 1.3 \times 10^{-7}$ s. The difference in the time step means that even for the cases that the same number of parcels per second is injected (for example Case 1 and 4) in reality a different number of parcels is injected per time step leading to a different representation of the initial droplet distribution PDF.

<table>
<thead>
<tr>
<th>Test Case</th>
<th>PPS</th>
<th>Grid Size (mm)</th>
<th>Turbulence Model</th>
<th>Initial Distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>20,000,000</td>
<td>0.5</td>
<td>Wale</td>
<td>RR</td>
</tr>
<tr>
<td>Case 2</td>
<td>2,000,000</td>
<td>0.5</td>
<td>Wale</td>
<td>RR</td>
</tr>
<tr>
<td>Case 3</td>
<td>200,000</td>
<td>0.5</td>
<td>Wale</td>
<td>RR</td>
</tr>
<tr>
<td>Case 4</td>
<td>20,000,000</td>
<td>0.3</td>
<td>Wale</td>
<td>RR</td>
</tr>
<tr>
<td>Case 5</td>
<td>2,000,000</td>
<td>0.3</td>
<td>Wale</td>
<td>RR</td>
</tr>
<tr>
<td>Case 6</td>
<td>50,000</td>
<td>0.3</td>
<td>Wale</td>
<td>RR</td>
</tr>
<tr>
<td>Case 7</td>
<td>2,000,000</td>
<td>0.5</td>
<td>KEM</td>
<td>RR</td>
</tr>
<tr>
<td>Case 8</td>
<td>200,000</td>
<td>0.5</td>
<td>KEM</td>
<td>RR</td>
</tr>
<tr>
<td>Case 9</td>
<td>20,000,000</td>
<td>0.5</td>
<td>KEM</td>
<td>Fixed Value</td>
</tr>
<tr>
<td>Case 10</td>
<td>20,000,000</td>
<td>0.5</td>
<td>KEM</td>
<td>RR</td>
</tr>
</tbody>
</table>

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Moreover, the size of the time step is linked to the time that the particles interact with the underlying gas properties as explained in the Section “Parcel Tracking”. For Grid 1 the average local Courant number is 0.0005 while for Grid 2 is 0.0009. The difference in the local Courant number results because of the turbulence resolution locally which leads to a different local velocity. This implies that in reality for Grid 2 the particles remain less time in the cell, and thus they have less time to interact with the underlying Eulerian velocity field and exchange momentum which might explain why for the Grid 2 the spray penetrates much more than the other cases. Looking at Fig 6 we can see that when KEM turbulence model is used less sensitivity to the other parameters is noticed (PPS and initial distribution). The vapour penetration for all cases is similar however the distribution of the vapour is different. High vapour concentration (bright red areas) is seen through the spray for Case 7 while some isolated dense regions are noticed for Case 8. For Case 9 the behaviour is closer to Case 7 although a more uniform dispersion is noticed which might be attributed to the fact that less randomness is introduced in the inlet since all droplets have the same diameter.

Figure 4. $C_{12}H_{26}$ contour plots for two different time instances using Grid 1 and WALE turbulence model.

Figure 5. $C_{12}H_{26}$ contour plots for two different time instances using Grid 2 and WALE turbulence model.

Figure 7 shows the scatter plot of droplet diameter versus velocity magnitude ( coloured by temperature) for the total number of the droplets in the domain at $t = 3$ ms for three different simulation cases. In all cases the PPS is 20 million. We will use this figure in order to get a better insight into the links between the predictions of the droplet size, the droplet velocity and the droplet temperature. For all cases the droplet size is mostly clustered in the range of 1-4 µm and only few parcels have diameters above 10 µm. Also we can see that in all cases droplets with smaller diameters have lower velocities while the droplets with larger diameters have higher velocities in some cases reaching up to 500 m/s. For Cases 1 and 4 the behaviour is similar although we can see that droplets with similar diameter for Case 1 have considerable lower velocity. For Case 4 there is a greater variation of the droplet velocity even for droplets with similar sizes. Droplets with small diameter 2-4 µm have velocities ranging 200 m/s-300 m/s and the temperature depends on the velocity. Droplets with higher velocities have also lower temperature since they have less time to interact with the underlying flow field. For case 9 the behaviour is different and we can see a more linear relation between droplet size and velocity. Also we can see that for droplets in the range of 2-4 µm the temperatures are higher (above 550K) Figure 8 shows the number of droplets vs droplet sizes for the axila locations. Top raw is at $x = 0.003$ m (close to the injector) and bottom raw at $x = 0.09$ m (close to the tip of the spray). In all cases the PPS is 20 million
Figure 6. C_{12}H_{26} contour plots for two different time instances using Grid 1 and KEM turbulence model.

Figure 7. Scatter plot of droplet diameter versus velocity magnitude (coloured by temperature) for the total number of the droplets in the domain at t=3ms for three different cases. In all cases the PPS is 20 million.

and the samples were taken for t = 0.6 ms. It can be seen that close to the injector the droplet distribution as expected is different depending the selection of the initial distribution. When the RR distribution is used regardless of the turbulence selection model (for Case 1 Wale and for Case 10 KEM) the droplet distribution is similar. Much narrower distribution around droplet sizes of 3 µm is noticed when a fixed value distribution is used (Case 9). Also it can be noticed that in both case the initial droplet size reduces rapidly. For example for Case 9 all droplets are injected with an average diameter of 90 µm and after 3 mm their size has already reduced to 3 µm. Further downstream as expected the effect of the initial distribution reduces and all three cases predict an average droplet size of 2 µm. Moving from 3 mm to 9 mm the droplet radius reduction rate is smaller.

Conclusions
In this work we present an LES Eulerian-Lagrangian framework within OpenFOAM for the modelling of high pressure injection dynamics of ECN Spray A conditions. The framework accounts for primary droplet formation (based on a parcel method), secondary droplet breakup, evaporation and heat transfer. The sensitivity of the framework to different parameters that affect the predictions of the local mixture formation during breakup and evaporation is considered. Initially a systematic variation of the key injection parameters (parcel number, parcel size distribution) of the parcel method as well as the grid size is presented. Varying the parcel number affects the accuracy of the representation of the initial droplet size distributions, which in turn, depending on the selection of the initial droplet PDF, turbulence model and the evaporation model, affects a) spray dispersion b) spray penetration and c) downstream droplet size distribution. Moreover, two different turbulence models are considered. The selection of the turbulence model appears to be of high importance. For the cases considered the KEM model results are less sensitive to the other parameters (PPS, initial droplet PDF). Finally a rather unexpected discrepancy between the predictions of the coarse and the fine grid is noticed which is attributed to the algorithm for the parcel method and the adjustable time step used for the calculations. More detailed examination of the droplet diameter statistics including analysis of their radial distribution will be the subject of future work.

Acknowledgements
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Figure 8. Number of droplets vs droplet sizes for two axial locations. Top raw is at $x = 0.003 \text{ m}$ (near-nozzle region) and bottom raw at $x = 0.09 \text{ m}$ (close to the tip of the spray). In all cases the PPS is 20 million and the samples were taken for $t = 0.6 \text{ ms}$.

References

Evidence of vortex driven primary breakup in high pressure fuel injection
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Abstract
This paper is to present a detailed case study on how the nozzle flow dynamics influences the primary breakup in the spray formation process of diesel injection. The investigation was based on a 3-hole real-application nozzle with highly tapered injection holes using a URANS-LES (Large Eddy Simulation) hybrid approach in combination with the coupled Volume of Fluid (VOF) and Level Set method. High resolution LES was applied to simultaneously resolve the multi-scale nozzle flow dynamics downstream of the needle seat and the primary breakup process in the near-nozzle spray. Phase Contrast X-ray imaging (PCX) was applied to characterize the liquid-gas interfaces in the near-nozzle spray for validation purposes. The results provide detailed information on how the vortex shedding and vortex interactions in the injection hole drives the jet deformation, ligament and droplet formation in the primary breakup process.

Keywords
Primary breakup, Fuel injection, Vortex dynamics, LES, Phase Contrast X-ray imaging

Introduction
Clean internal combustion engine technology improvement requires the capability to control and optimise the fuel-gas mixing, ignition, and combustion process. However, how to transfer the individual engine requirements on the spray to a specific nozzle design still remains a challenging engineering task. One blocking point is the lack of detailed understanding on the fundamental physics of the primary breakup process. This process involves highly complex multi-phase and multi-scale fluid dynamics phenomena, including turbulence, cavitation and their interaction. A significant number of investigations have been dedicated to the cavitation phenomenon over the last 30 years. As for turbulence, the scales and dynamics of the vortex structures in the nozzle flow need to be understood. Two experimental investigations have reported vortex phenomena in injection nozzles. One is the cavitation visualisation of (1) in a real-size VCO nozzle. The vapour distribution in the injection holes indicated the occurrence of strong swirling vortex structures and vortex shedding. Though the investigation was focused on the in-nozzle flow, the authors proposed that the vortex shedding can impact the jet breakup downstream of the injection hole exit. Another is the string cavitation characterization in a scale-up nozzle (2), which demonstrated that string cavitation is caused by large-scale vortex strings in the sac and injection holes and has a correlation with the fluctuation of the spray dispersion angle. Nevertheless, the vortex structures are expected to be much more complex and have richer scales in real applications due to much higher velocity gradients. It is almost impossible to make detailed experimental characterization of field turbulence and vortex dynamics inside a real-size nozzle due to the small dimensions and high speed of the problem. CFD simulation is advantageous over measurement techniques to gain insight into the nozzle flow dynamics and vortex structures and their impact on the spray as shown in (3), (4). In order to resolve the involved multi scale and dynamic phenomena, Scale-Resolved Simulation approaches (SRS), such as LES, are needed.

For the primary breakup diagnostic, several effective visualization techniques have been developed in the current century. It is worth mentioning the high resolution PCX imaging developed at Argonne National Lab (5), and the recent application of Transmitted Light Microscopy to the near-nozzle spray visualization (6). Both tools are useful for the characterization of the liquid-gas interface in the primary breakup process having different strengths. From the simulation point of view, interface tracking techniques like the Level-set method have been successfully applied to resolve the liquid-gas interface in the ligament and droplet formation process (7) (8). In order to obtain
detailed information on how the fluid dynamic instabilities in the nozzle flow trigger ligament and droplet formation and how the nozzle geometry influences those processes and consequently the spray structure, techniques allowing for simultaneous diagnostic of the nozzle flow and the near-nozzle spray are needed. Considering the limitation of measurement techniques for the characterization of field turbulence in a real-size fuel injection nozzle, Scale-Resolved Simulation is a more feasible tool for this purpose. The main issue for simulation is how to deal with the cavitation phenomenon using an interface tracking technique, which naturally requires applying Direct Numerical Simulation (DNS) and is still beyond the capability of most available CFD codes and computational power. An alternative is to treat cavitation by using the Volume of Fluid (VOF) approach, which is a naturally conservative method tracking the volume fraction of a particular phase in each cell rather than the interface itself, being effective for the in-nozzle flow analysis but at the expense of having an excessive numerical diffusion for the jet breakup prediction. This approach might be useful for predicting the liquid jet fragmentation and fuel distribution in the breakup process, but might not be able to provide details for the droplet formation process.

Considering the strength and limitations of both measurement and simulation techniques, the authors have adopted a correlation based approach for years to work out understanding on how nozzle design and operating conditions influence on the spray behaviour. This approach involved the application of simulation for the nozzle flow and measurement techniques for the near-nozzle spray characterization and identifying links between both (4), (9), (10), (11). These successful studies have given the authors confidence in the simulation tools (ANSYS CFX and Fluent) for the nozzle flow diagnostic. In this work we present a detailed case study on the primary breakup of Diesel fuel jet injected from a so-called High Performance atomization (HP) hole nozzle (12). The HP hole uses very high hole taper (K-factor = (Dout-Din)/10 [µm] = 5, see Figure 1) to increase the hydraulic efficiency and the spray momentum rate. The target is to make a direct investigation on how the nozzle flow dynamic impacts the primary breakup and to reveal the flow dynamic processes in detail. Since the high hole taper prevents the occurrence of cavitation, the coupled VOF-Level Set LES method (13) can be applied simultaneously to resolve the nozzle flow and the liquid jet primary breakup. In order to ensure the numerical quality, the influence of grid resolution on the simulation results has been carefully analysed. Phase Contrast X-ray imaging (PCX) was applied to visualize the liquid-gas interface structures for the near-nozzle spray to support the simulation analysis. The experimental investigation was carried out for injection pressures from 400bar to 2000bar using a spray chamber at atmospheric pressure. The simulation case study was carried out for the injection pressure of 800bar.

Simulation setup
The simulation was performed with the software ANSYS Fluent 16.2 adopting a hybrid URANS-LES approach and using a 120-degree sector nozzle model. The computational domain was divided into two subdomains as shown in Figure 2. The sub-domain upstream of the seat sealing was solved with URANS using a tetrahedral mesh and the sub-domain downstream of the seat sealing, including the near-nozzle spray region, with LES using high-quality hexahedral cells. A careful best practice study was carried out to ensure the quality of the simulation results. It was verified that the location of the URANS-LES interface is far enough from the region of interest to avoid causing a distortion of the results. At the URANS-LES interface, only the pressure and velocity fields were interpolated without introducing any artificial disturbance to the LES flow. Regarding the numerical setup, a VOF - Level Set method (13) was applied to simultaneously resolve the nozzle flow and jet breakup. A standard k-ω SST turbulence model was used in the URANS domain and the Wall-Adapting Local Eddy (WALE) sub-grid scale (SGS) viscosity model (14) in the LES domain owing to its ability to correctly predict the near-wall eddy viscosity.

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A fully implicit, 2nd-order time-accurate scheme was used together with a 2nd-order scheme for spatial discretization. In order to ensure sufficient numerical resolution, the following criteria were used: local SGS eddy viscosity ratio below 1, local CFL number below 2, and $y^+<1.0$.

Two different meshes were utilized in the discharge volume in order to assess the effects of mesh resolution. A coarser mesh (mesh 1) was defined with ~15 million cells and an average cell size of ~5.7μm, and a finer mesh (mesh 2) with ~31 million cells and an average cell size of ~3μm for the domain outside of the nozzle. The time-step for mesh 1 was $\Delta t = 5\times10^{-3}$ s and for mesh 2 was $\Delta t = 2.5\times10^{-3}$ s to ensure numerical stability. Each simulation was first run with URANS for 100μs and then switched to LES for 50μs for initialization purpose to ensure proper development of LES flow. After initialization, the simulation ran further for 100 μs to provide sufficient data for statistical sampling and analysis.

![Figure 2: Computational domain decomposition and Hybrid LES mesh for the nozzle tip.](image)

**Experimental setup**

The PCX imaging was performed at the XOR 7ID beamline in the Advanced Photon Source (APS) to visualize the near-nozzle spray. The third generation synchrotron x-ray beam can produce ultra-short x-ray pulses and weak interaction with the object materials. With these features and the high transmittance of the x-ray in dense materials, it becomes possible to capture the instantaneous liquid-gas interface structures in the near-nozzle spray. After passing thought the spray, the x-ray beam forms a phase-contrasted image on a scintillator crystal CCD camera. The field of view of the camera was 1.734mm x 1.310mm with a pixel resolution of 0.66 µm/pixel when a 20 times objective lens was used. The imaging frequency is 50kHz, or 20µs per image. A detailed description of the experimental setup can be found in (9).

**Results and discussion**

**Liquid-gas interface structures: mesh resolution effect**

Similar liquid core interface structures and jet breakup patterns were predicted on both meshes, but the higher resolution of mesh 2 captured much more small droplets. Ideally, a proper post-processing tool for scale separation and calculation should be developed and used to assess the minimum droplet size which can be captured by each mesh. As this tool was not available a concept of interface diffusion thickness is used instead. This value is calculated using the Level Set function ($\phi$) and liquid volume fraction, and is introduced to help estimate the mesh resolution effect on the diffusion of the liquid-gas interface structures. The interface diffusion is a result of mesh resolution and diffusion caused by numerical schemes. Therefore, this method is also useful for a coarse estimation of the smallest droplet resolution as will be explained. The process of the interface smearing due to numerical diffusion is schematically plotted in Figure 3 a) for a single droplet. The Level set function is exactly zero at the interface and has a value equal to the distance to the interface (with a positive or negative sign...
according to the convention for each phase) for any other points (13). Initially, the droplet is bounded by a sharp interface \( \phi = 0 \) where the liquid volume fraction jumps from \( \alpha_L = 0 \) outside the droplet to \( \alpha_L = 1 \) inside the droplet. After a number of time steps the interface smears, leading to a smooth volume fraction variation across the interface. In this new state, the region where \( \alpha_L = 1 \) is restricted to some cells in the center of the droplet, bounded by a surface where \( \phi = 0 \). Taking \( \alpha_L = 0.01 \) as the threshold of the interface diffusion, the thickness of the diffused interface \( d_{1\%} \) can be estimated using the distance between the volume fraction iso-surface, \( \alpha_L = 0.01 \) and the iso-surface \( \phi = 0 \). Under a symmetric interface diffusion assumption the diameter \( d \) of a spherical droplet is \( 2r \leq d \leq 2r + 2d_{1\%} \), where \( r \) is the distance from the droplet core center to the undiffused droplet core interface \( \phi = 0 \). The smallest spherical droplets near the intact liquid core (\( \alpha_L = 1 \)) are only distributed over one or a few cells, leading to \( r \sim 0 \). In such cases, \( d \sim 2d_{1\%} \) is a reasonable estimate of the actual characteristic droplet size.

An instantaneous near-nozzle spray visualisation is presented in Figure 3 b) for both meshes using the instantaneous liquid volume fraction iso-surfaces 0.01 colored by \( d_{1\%} \). The colour scale threshold chosen here is aimed at separating the smallest droplets \( d_{1\%} < 10 \mu m \) from the larger droplets and the liquid core interface. It is observed that Mesh 1 only captured a few droplets with \( d_{1\%} < 10 \mu m \) very close to the liquid core during initiation of breakup. Further downstream, only larger droplets and ligaments are resolved with increasing diffusion due to mesh coarsening. In contrast, mesh 2 is fine enough to capture droplets smaller than \( 10 \mu m \) over the entire primary breakup region modelled. In addition, it is noted that the diffusion thickness is low for the liquid core obtained based on both meshes. Therefore, it is safe to say that the mesh resolution is unlikely to influence the numerical observations of the liquid jet deformation and ligament formation phenomena in the primary breakup process.

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Liquid-gas interface structures: LES solution vs. PCX spray images

Comparison for the liquid-gas interface structures between LES solution and PCX spray images should be based on a statistical approach. This is hindered by the differences in the physical time durations and the time resolution between simulation and measurement. Spray imaging was performed for an injection duration of 1ms at full needle lift and at a time interval of 20\( \mu s \) per image (50 images in total). The physical time in simulation was 100\( \mu s \) for both meshes. Flow visualisation images were stored every \( 5\times10^{-8} \) s. Obviously, the time resolution and the image number in the measurements were not sufficient in the sense of a rigorous statistical analysis of the near-nozzle spray structures, while the physical time duration in the simulation is too short as it is limited by the available computational resources. Under these limitations, effort was made to identify similarities between the instantaneous spray morphologies captured by PCX imaging and by the simulations.

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The LES results for mesh 1 and mesh 2 are treated as independent time series, considering the fact that the initialization has an influence on the flow development. The mesh 1 solution of the near nozzle spray was found to have a close correlation with 7 out of the 50 PCX spray images recorded over the open needle operation time interval. Sample results are presented in Figure 4, where the LES near-nozzle sprays are represented by using the iso-surface of 0.1 liquid volume fraction. The predicted undisturbed liquid core before the initiation of jet breakup is obviously longer than the measurement, but the simulation is able to capture some features observed in the PCX spray images. For example, a linear streak crossing the liquid core very close to the nozzle exit can be recognized from both the predicted and measured spray (Figure 4, left). In particular, a close similarity between both is observed at the lower side of the spray, where the wavy structures begin to break up into smaller structures and droplets. Figure 4 right shows another example. The wavy structures with higher local breakup intensity on the upper side of the spray as recorded by the PCX imaging are also captured in the simulation. In addition, a “horizontal boundary” between the continuous un-atomized liquid core (lower part of the spray) and the upper spray regions with small structures can be well noted both from the PCX spray image and the LES solution.

**Figure 4:** Instantaneous LES liquid volume fraction iso-surfaces (value=0.1) on mesh 1 (top) vs. PCX images (bottom)

The LES solution on mesh 2 was found to produce similar spray features with 8 out of the 50 PCX images. Figure 5 shows for the correlations between some example mesh 2 results and PCX spray images. The LES spray in the left image shows a braid-like (helical) structure appearing on the upper side of the very initial jet, which can also be noticed from the PCX spray image. This type of structures are caused by vortex shedding and rotating string vortices occurring in the nozzle flow and will be discussed in detail in the next section. In addition, similar vertical streaks are observed both in simulation and measurement. The LES spray on the right shows a close similarity in terms of breakup patterns and spray shape to the corresponding mesh 1 result shown on the right of Figure 4. As with the mesh 1 result, the wavy structures on the upper side of the spray correlate well with the PCX image.

**Figure 5:** Instantaneous LES liquid volume fraction iso-surfaces (value=0.1) for mesh 2 (top), PCX images (bottom).
These results show a clear impact of the mesh resolution on the small structures and droplets in the near-nozzle spray. However, both meshes have captured some breakup patterns and morphological features of the spray, which can be recognized in PCX spray images, are therefore valid. Since the mesh 2 results were only very recently obtained in this work, the understanding on the physics of the primary breakup process reported below is mainly derived from the mesh 1 solution.

**Vortex driven primary breakup process**

Figure 6 illustrates the correlation between the predicted vortex structures and near-nozzle spray structures obtained on mesh 1 together with a similar PCX spray image. Two type of vortices can be observed in the nozzle flow. Small-scale vortices and vortex shedding occur at the upper lip of injection hole inlet as the flow turns into the hole. At the same time, large-scale string vortices are generated in the bulk flow of weak shear due to flow recirculation in the sac and flow acceleration into the hole. The results indicate that the upper-lip vortex shedding and the interaction between the string vortices and the shed vortices in the nozzle are the triggering mechanism of ligament formation in the primary breakup region. A vortex shedding event produces low momentum vortices and a pulsation in the local flow. The shed vortices interact with the string vortices in the injection hole. As they exit the injection hole they transfer their local instability and their pulsating momentum into the liquid jet, causing its deformation and the development of ligaments.

![Figure 6](image)

**Figure 6:** Correlation between vortex shedding in the nozzle and jet breakup: vortex structure \((Q=1e13 \text{ [s}^{-2}\text{]})\), predicted spray morphology (liquid volume fraction 90%), and PCX image (bottom).

This vortex-driven ligament formation and breakup process is illustrated in Figure 7 using a time sequence of instantaneous results for the vortex flow and near-nozzle spray. At a certain time instant \(t_0\), the string vortices move upwards and interact with the shed vortices close to the hole exit, creating a local flow instability and upward momentum. This pulsating momentum is transported into the near-nozzle flow after a shed vortex leaves the injection hole exit. At \(t_0 + 0.45 \mu s\) the upward moving shed vortex triggers the wavy surface vortex enhanced by the interaction with the surrounding gas. This vortex causes deformation of the liquid jet on the upper side, leading to wavy liquid-gas interface structures. At \(t_0 + 2 \mu s\) the surface vortex gets further developed due to air-liquid interaction and the liquid surface deformation continues to grow causing the roll-up of the liquid-gas interface and ligament formation. At \(t_0 + 5 \mu s\) the surface vortices lose their momentum, get separated from the high speed bulk flow and decompose into smaller vortices causing atomization of ligaments and formation of droplets. A detailed video showing this process is available in (15).
In addition, large scale vortex strings are high energy containing structures. Their morphology, location and motion direction have an important impact on the primary breakup behaviour as is shown in Figure 8 using selected instantaneous results. In case (a), the string vortices move upwards. This triggers liquid core deformation and ligament formation further downstream on the upper side of the jet. The string vortices are pushed downwards by the strong shed vortices at the hole exit in case (b), leading to liquid-core deformation on the lower side. In case (c), the string vortices show an unstable “S”-shape motion, causing an earlier jet breakup both on the upper and lower sides. In contrast, relatively undisturbed flow with all large vortices well aligned with the injection hole axis is predicted close to the injection hole exit in (d). Under this situation, weak perturbations on the liquid jet and thus weak jet breakup is observed.
Conclusions
A detailed case study was carried out on the primary breakup process in high pressure fuel injection based on a production diesel nozzle design. A coupled VOF-Level Set LES simulation methodology was applied to simultaneously resolve the multi-scale flow dynamics in the nozzle and the jet primary breakup process after the hole exit. Phase Contrast X-ray imaging was applied to characterize the liquid-gas interface in the near-nozzle spray. The simulation successfully reproduced many structures of the spray captured by the PCX imaging. It was observed from the simulations that, as the flow is deflected into the nozzle hole, it triggers vortex shedding events, producing high speed, energetic vortex structures and local flow instabilities. These structures continue to develop into the liquid jet and initiate the deformation and ligament formation processes within the primary spray breakup. Additionally, vortex ejection from the nozzle causes small surface vortices at the liquid-gas interface that interact with the surrounding gas and ultimately lead to droplet formation. These results provide evidence for a vortex driven atomization mechanism. With this understanding, fuel injector nozzle designs can be optimized by control and optimization of the vortices.

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References
9. Correlating the Nozzle Flow to Spray and Primary Breakup using Visualization and Multi-phase Simulation. Lai M-C; Wang F; Xie X; Shi J; Dober G; Guerrassi N; Meslem Y. Rouen : s.n., 2014. SIA.
CFD simulations of the diesel jet primary atomization from a multihole injector

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Abstract
High pressure multi-hole diesel injectors are currently used in direct-injection common-rail diesel engines for the improvement of fuel injection and air/fuel mixing, and the overall engine performance. The resulting spray injection characteristics are dictated by the injector geometry and the injection conditions, as well as the ambient conditions into which the liquid is injected. The main objective of the present study was to design a high pressure multi-hole diesel injector and model the two-phase flow using the volume of fluid (VOF) method, in order to predict the initial liquid jet characteristics for various injection conditions. A computer aided design (CAD) software was employed for the design of the three-dimensional geometry of the assembly of the injector and the constant volume chamber into which the liquid jet emerges. A typical six-hole diesel injector geometry was modelled and the holes were symmetrically located around the periphery of the injector tip. The injector nozzle diameter and length were 0.2 mm and 1 mm, respectively, resulting in a ratio of nozzle orifice length over nozzle diameter L/D = 5. The commercial computational fluid dynamics (CFD) code STAR-CD was used for the generation of the computational mesh and for transient simulations with an Eulerian approach incorporating the VOF model for the two-phase flow and the Rayleigh model for the cavitation phenomenon. Three test cases for increasing injection pressure of diesel injection from the high pressure multi-hole diesel injector into high pressure and high temperature chamber conditions were investigated. From the injector simulations of the test cases, the nozzle exit velocity components were determined, along with the emerging liquid jet breakup length at the nozzle exit. Furthermore, the spray angle was estimated by the average radial displacement of the liquid jet and air mixture at the vicinity of the nozzle exit. The breakup length of the liquid jet and the spray cone angle which were determined from the simulations, were compared with the breakup length and cone angle estimated by empirical equations. From the simulations, it was found that cavitation takes place at the nozzle inlet for all the cases, and affects the fuel and air interaction at the upper area of the spray jet. Furthermore, the spray jet breakup length increases with elapsed time, and when the injection pressure increases both the breakup length and the spray cone angle increase.

Keywords
Diesel injector, VOF, atomization.

Introduction
The main objective of the present work was to characterize the flow phenomena at the exit of the nozzle of a multihole Diesel injector. It was of main interest to examine the behaviour of the emerging two-phase flow spray jet with emphasis in the primary spray jet atomization. The objectives included, first the setup of the CFD model for a typical three-dimensional valve-covered orifice (VCO) sac-less six-hole diesel injector for carrying out the analysis of the initial spray characteristics, namely the liquid breakup length and the spray angle at the nozzle exit. The second objective was the calculation of the primary atomization characteristics with empirical equations and to compare the empirical data with the simulations. The injector which was used had sharp nozzle entry, a nozzle diameter equal to 0.2 mm and a ratio of nozzle orifice length over nozzle diameter L/D = 5.

Previous experimental [1, 10, 14, 15] and computational [1, 6, 9, 11, 13] studies investigated the internal and external flow of diesel injectors. In some experiments, large scale transparent injectors were used [8], [12], and it was found that cavitation phenomena are present. Experimental studies [10, 14] revealed that the emerging liquid jet is affected by both cavitation and the interaction with the surrounding gas flow. Various methodologies were adopted for injector flow simulations, including the VOF method [8] and the large eddy simulation (LES) framework [5]. The simulations from previous studies revealed that strong vortex structures were generated around the liquid jet penetrating in the gas phase and these were the results of velocity relaxation inside the liquid [8]. However, as it was reported in [8], the problem of jet disintegration is complex and not well understood.

The effect of injection pressure on the initial spray atomization characteristics predicted from simulations and comparisons with pertinent data estimated from empirical models, have not been found by the author of the
present work in published work. Thus, it is required to quantify the effects of the injection pressure on the injected spray jet, as well as compare the primary spray atomization characteristics from simulations with data from empirical equations. In the present work, the adopted CFD methodology is described first. Then, the results for three test cases at low, medium and high injection pressure of the diesel injector into high pressure and high temperature chamber conditions are presented. Finally, conclusions and recommendations are provided.

Methodology

The CFD methodology along with the simulations setup are described first, followed by the illustration of the empirical equations which were used for the calculation of the liquid jet breakup length and the spray jet angle. For the CFD simulations, the CFD code STAR-CD [3] was used. The Eulerian modelling methodology employing the VOF method was utilized, which included the mass, momentum and energy conservation equations for the two phases. The interface-capturing method in the VOF method was employed, by computing the convective terms in the volume fraction equations using the High-Resolution Interface-Capturing (HRIC) model [3]. For the two-phase flow modelling, the pressure in the two phases was assumed to be the same. A constant value of surface tension was used, with which the normal force due to the surface tension is treated using the continuum surface force (CSF) model [3], while the tangential force is not accounted. The CSF model provides a source term in the momentum conservation equation. The turbulence was modelled with the k-ε high Reynolds number RNG model [17], and the boundary layer was handled with the standard wall functions. The MARS [3] differencing scheme was used for the discretization of the conservation equations. Transient simulations were carried out, and the SIMPLE algorithm [3] was employed for the numerical solution of the problem.

A VCO sac-less six-hole diesel injector and a constant volume chamber were assembled for the computational mesh generation. The injector design was based on typical injector geometries found from literature ([10, 11, 14, 15]). The three-dimensional injector which was designed with a CAD software [4] is shown in Figure 1. The injector design was for a six-hole diesel injector whose nose holes were symmetrically located around the periphery of the injector tip as shown in Figure 1. The nozzle entry was designed with sharp edge at the body of the injector. The injector nozzle diameter and length were 0.2 mm and 1 mm, respectively, resulting in a ratio of nozzle orifice length over nozzle diameter L/D = 5. The designed constant volume chamber had length 5 mm which corresponds to 25 D distance downstream the nozzle, and a square cross-sectional area with side width 1 mm. The constant volume chamber was assembled at the tip of the nozzle exit, and the centreline of the nozzle and the symmetry axis of the chamber coincided. The computational mesh was generated with the automatic mesh generation tool of STAR-CD [3], where prism type cells computational were used. The resulting mesh was composed of around 850000 cells and it is presented in Figure 2. The cell size ranged from 5 to 10 μm within the injector and the cell size varied between 10 to 20 μm in the constant volume chamber. Figure 2 includes the boundary conditions which were imposed for the simulation setup. Inlet boundary condition was defined at the entry of the injector on the top, shown in dark yellow color in Figure 2. Symmetry plane boundary conditions were imposed on the symmetry sides of the one-sixth segment of the injector, which are presented in violet color in Figure 2. No-slip wall boundary condition was imposed on the four sides of the chamber, which is indicated with orange color in Figure 2. Wall boundary condition was set at the remaining surfaces, including the injector shell, the nozzle and the back plane of the chamber where the nozzle tip was assembled. Pressure boundary condition

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was defined at the chamber front plane. At the pressure boundary, the pressure and temperature were set equal to 42 bar and 1000 K, respectively, which resemble diesel engine conditions during compression stroke.

Figure 2. Computational mesh and boundary conditions.

At the inlet boundary, the volume fraction of the fuel was set equal to 1 and uniform inlet velocities for the three test cases were defined. The code uses the inlet velocity and calculates the injection pressure at the inlet. For the simulations, n-heptane and air were utilized. The properties of n-heptane liquid, n-heptane vapour and air from the database of STAR-CD [3] were employed, and are contained in Table 1.

Table 1. Physical properties of the fuel and air.

<table>
<thead>
<tr>
<th>Property</th>
<th>Liquid</th>
<th>Vapour</th>
<th>Air</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (Kg/m³)</td>
<td>678.3</td>
<td>2.48639</td>
<td>1.18415</td>
</tr>
<tr>
<td>Molecular viscosity (Kg/ms)</td>
<td>3.92073 10⁻⁴</td>
<td>1.01377 10⁻⁵</td>
<td>1.855 10⁻⁵</td>
</tr>
<tr>
<td>Surface tension coefficient (N/m)</td>
<td>0.0727</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

For the initial conditions of the transient simulations, stagnant air was set in the computational domain. The simulations for the three test cases were performed for an injection duration of 1 ms. The computational time step size was constant and equal to 0.5 µs. The numerical processing of the simulations was performed on a sequential computer. The simulation results are presented and discussed in the next section.

In the present work, in the absence of experimental data for validation of the simulations, empirical equations were used in order to obtain data for comparison with the simulations. Empirical equations provide the primary atomization characteristics and are usually employed within the atomization modelling setup in diesel engine CFD simulations. From a literature survey, the empirical equations for the calculation of the breakup length and spray angle were adopted from [15] and [2], respectively. The liquid jet breakup length was estimated by the following empirical equation (from [15]),

\[ L = 0.39 \left( \frac{2 \Delta p}{\rho_l} \right)^{1/2} t \]  

where \( \Delta p \) is the pressure drop along the nozzle, \( \rho_l \) is the liquid density and \( t \) is the elapsed time after the start of injection. The cone angle for diesel jet spray in the atomisation region was calculated from the empirical equation of Arai [2] by,

\[ \theta = 0.017 \left( \frac{D^2 \rho_a \Delta p}{\mu_a^2} \right)^{0.25} \]  

where \( D \) is the nozzle diameter, \( \rho_a \) is the density of air in the chamber and \( \mu_a \) is the molecular viscosity of air.

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Results

In the present section, the results and discussion from the simulations for the three test cases are presented. For the test cases, the injection pressure was calculated by the code at the inlet boundary. The velocity at the inlet boundary, the resulting injection pressure and the mass flow rate of fuel are included in Table 2. The three cases denoted, low, medium and high injection pressure correspond to modern common rail system injection pressure. As it can be seen in Table 2, the injection pressure was 1124, 1669 and 2245 bar.

<table>
<thead>
<tr>
<th>Test case</th>
<th>Description</th>
<th>Inlet velocity (m/s)</th>
<th>$P_{\text{inj}}$ (bar)</th>
<th>Fuel mass flow rate (Kg/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Low injection pressure</td>
<td>20</td>
<td>1124</td>
<td>0.0422</td>
</tr>
<tr>
<td>2</td>
<td>Medium injection pressure</td>
<td>24</td>
<td>1669</td>
<td>0.0507</td>
</tr>
<tr>
<td>3</td>
<td>High injection pressure</td>
<td>28</td>
<td>2245</td>
<td>0.0592</td>
</tr>
</tbody>
</table>

First, the evolution of the VOF field from the simulations at the vertical symmetry section plane of the nozzle and the chamber are presented in Figure 3, 4 and 5. Then, comparisons of the VOF field and the velocity field between the three cases at 0.25 ms after start of injection (ASOI) are presented. Finally, the breakup length and spray jet cone angle from the simulations are compared with the empirical data.

For the low injection pressure, Case 1, the evolution of the liquid fuel injection and the propagation of the emerging fuel jet are presented with the VOF flow field in Figure 3. From the simulations of Case 1, it was found that the fuel starts to emerge from the nozzle exit at 0.2 ms after the start of the simulation. As it can be seen in Figure 3, there is cavitation area which is created at the upper edge of the nozzle inlet. The axial penetration of the spray jet increases with elapsed time, and at 0.3 ms the spray reaches the chamber front plane. Also, the spanwise spreading of the two-phase spray jet increases with time. A spray jet with VOF higher than 0.5, indicated with green colour, is present at the nozzle exit, which increases with time. For this case the spray jet slightly bends at an angle of around 10°, which is the effect of the induced gas recirculation at the upper area of the spray jet.

The emerging spray jet, for the medium injection pressure case is presented in Figure 4, at time 0.2, 0.25 and 0.35 ASOI. The simulations of the medium pressure case revealed that by increasing the injection pressure for 1124 to 1669, then the required time for the fuel to emerge from the nozzle exit is 0.18 ms. The cavitation area is present at all times after start of injection and the spray jet recirculates at the upper area of the emerging jet at a...
downstream distance of seven nozzle diameters. The spray jet core with VOF higher than 0.5, is almost symmetrical and has a length of around five nozzle diameters.

The results for Case 3 are included in Figure 5, at 0.15, 0.2 and 0.25 ms ASOI. For the high injection pressure case, the time needed by the fuel to exit the nozzle was 0.14 ms, and this is lower than the time needed for the low and medium injection pressure cases. Figure 4 shows that the vortex structure at the upper area of the spray becomes stronger and that a small amount of fuel accumulates near the wall at the vicinity of the nozzle. Also, it can be observed that the fuel air mixture travels downstream and accumulates towards the front plane of the chamber at 0.25 ms. The VOF and velocity fields for the three are further discussed and compared below.
Figure 6. Comparison of the VOF field of Case 1, 2 and 3 at 0.25 ms ASOI. It can be observed that the spray jet for the low injection pressure case is narrower that the spray of the higher injection pressure cases. This observation reveals that the spray cone angle increases when the injection pressure increases. Regarding the spray jet, it can be seen that the penetration of the spray core with VOF greater than 0.5 increases when the injection pressure increases. However, for the high injection pressure cases there is a core at the vicinity of the nozzle and an accumulated spray jet towards the front plane of the chamber.

Figure 7. Comparison of the velocity field of Case 1, 2 and 3 at 0.25 ms ASOI. As it can be observed in Figure 7, for all the cases there is a recirculation at the nozzle entry which is the cavitation zone, and the flow has higher velocities at the lower area of the nozzle. By increasing the injection
pressure, then the nozzle velocity increases. The increase of the injection velocity induces a recirculation zone at the upper area of the spray. The recirculation zone becomes stronger with increasing injection velocity and this can be also seen in Figure 6, where the spray recirculation zone occurs for the medium and high injection pressure cases. For the low injection pressure case, the injection velocity is not sufficiently high and the recirculation in upper area affects the spray which slightly bends as observed in Figure 6 and 7.

The estimated breakup length from the simulations is compared against the calculated breakup length from the empirical equation in Figure 4. The time of the start of injection for Case 1, 2, and 3 was adjusted with the values of 0.2, 0.18 and 0.14 ms. This was done for the purpose of comparison, and it is considered as the delay time for the emergence of the liquid jet from the nozzle exit. Figure 8 compares the breakup length data estimated from the simulation against the calculated empirical data for each case. From the simulations, the breakup length was estimated at the distance from nozzle where the VOF value was equal and greater than 0.3. For both the simulation and the experimental data, the breakup length increases with time, as it can be observed in Figure 8. Here, it is noted that the empirical expression does not account for the phenomena of evaporation, while the present simulation was carried out in a chamber with high pressure and temperature conditions and the evaporation was simulated. Thus during the early injection period, for each case, there is slight under prediction of the breakup length and this considered as a very good agreement. However, in Figure 8 it can be seen that for later times the breakup length is substantially underpredicted by the simulation, and this can be explained by the evaporation phenomena which are not considered in the empirical equation.

**Figure 8.** Comparison of the breakup length between simulation and empirical data with elapsed time after the start of injection into the chamber.

**Figure 9.** Comparison of the spray jet angle between simulation and empirical data for increasing injection pressure at 0.25 ms ASOI.
The spray jet angle from the simulations was estimated at 0.25 ms ASOI for the three test cases. Tangents from the nozzle exit upper and lower edges were drawn to the outer edge of the jet spray at five diameters distance from the nozzle exit, and the average angle for each case was found. The spray cone angle from the simulations for each test case is compared against the empirical data in Figure 9. As it can be seen in Figure 9, there is very good agreement on cone angle for the low injection pressure case, while for the medium and high injection pressure the cone angle is slightly overpredicted. It can be observed that the cone angle increases linearly when the injection pressure increases. The differences between the predictions and the empirical data can be explained by the spanwise spreading of the spray jet in the simulation and the interaction with the surrounding gas. However, in order to be able to draw firm conclusions about the overprediction of the cone angle at higher injection pressures, it will be required to carry out further simulation investigation and compare with experimental data. Furthermore, it will be required to assess available empirical data and the conditions under which the empirical expressions can be applied, since in the present work high injection pressures and evaporating conditions were simulated. In the following section, the main conclusions from the present work are described and recommendations for future work are provided.

Conclusions and recommendations
From the three test cases of increasing injection pressure into high pressure and temperature chamber conditions, it was found that cavitation takes place and affects the fuel and air interaction at the upper area of the spray jet. The predicted jet breakup length increases with elapsed time. When the injection pressure increases, then both the breakup length and the downstream penetration of the spray jet increase. The spray cone angle estimated at the vicinity of nozzle exit increases with increasing injection pressure. When the injection pressure doubled, then the cone angle increased by around 50%. Comparisons with empirical data revealed that there is very good agreement on the breakup length size during the early stages of injection, for all the test cases. However, when time elapses from the start of injection then the predicted breakup length is underpredicted because of the evaporation phenomena, which are not accounted in the empirical expression.

In future work a bigger constant volume chamber should be used in order to examine the downstream behaviour of the atomized jet and the resulting downstream spray cone angle. It is recommended to use the predicted values of breakup length and spray cone angle from the present simulations in combination with the Eulerian-Lagrangian framework for simulation of direct injection diesel engine sprays, which should be validated against experimental data in order to reach robust conclusions.

Acknowledgements
The provision of computer facilities by Frederick University is acknowledged.

References

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Large eddy simulations of atomisation and sprays: application to a high pressure multihole injector

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Abstract
A weak coupling strategy is proposed to simulate the pressurised spray without any empirical readjustment. Volume Of Fluid is used to simulate the nozzle internal flow with cavitation and its primary atomization into ligaments. Lagrangian simulations are then used to get the spray evolution, even temporal. Large Eddy Simulations are used for these two simulations types. The coupling between both is realized by a recording and an analysis of the ligaments with local break up modelling into drops. Two test cases are presented, the second one deals with full, complex geometry, 6-holes Gasoline Direct Injection nozzle. Such approach shows a huge potential for prediction of the final spray from the nozzle geometry.

Keywords
Large Eddy Simulation, spray, multihole, atomization, Volume Of fluid

Introduction
The present work is driven within the industrial automotive contextual aim of reducing the carbon particles emission of car engines. It has been shown that these emissions can be linked to the liquid wall films generated by the penetration of gasoline sprays (i.e. drop jets generated by pressurized atomizer, without assistance of a coflow) impacting on the engine walls. Therefore a better understanding of these sprays physics through simulations is needed. To do so, we developed an Euler-Lagrange solver, implemented in the OpenFOAM platform which allows us to model the non-evaporating gasoline sprays from high-pressure injectors: Large Eddy Simulation (LES) is used for the carrier phase whereas Lagrangian simulation is used for the dispersed phase. A 2-way coupling between the 2 phases and several subgrid submodels have been investigated [1]. The Lagrangian simulation uses the treated results of a Large Eddy-Volume Of Fluid simulation of the cavitating and atomizing flow within and at the close exit of the nozzle. This strategy is efficient because at least one order of magnitude separates the characteristic times of each type of flow but request an effort in the coupling which is specifically described in the present paper.

Simulation Approach
Second order numerical schemes are used for spatial and temporal discretisations. The numerical developments are based on OpenFoam® platform. For the Volume Of Fluid (VOF) approach, first-order reconstruction of the interface is used together with the sharpening process of Weller, see for instance [2]. The subgrid models used in this work are the one-equation eddy for the LES-VOF and the dynamic Smagorinski for the lagrangian-LES. The choice of the first one is due to the presence of walls and flow detachment inside the nozzle, and the choice of the second one is due to the capture of transitional turbulent jet flow that requires a minimum of numerical dissipation. For more details on the lagrangian simulations, the readers are referred to Helie et al. [1]. To carry out the lagrangian computation of the drops, a special attention is required for the spray inlet condition. This is done through an original weak coupling with LES-VOF simulation of the flow in the internal part and close-vicinity of the nozzle (see for instance [3]). The liquid instantaneous presence and the associated velocity field are stored to be reused identically as input of the spray. The primary atomization process is then analysed and a modelling approach is proposed in 2 steps: Firstly, a rupture into ligaments, almost bidimensional, and a second step where these ligaments propagate further and atomise into rounded ligaments and then into drop populations. Figure 1 left indicates the sketch of this process for one single ligament, the flow being a set of numerous different ligaments. This paradigm of considering a set of different ligaments that will be individually modeled is, to our knowledge, new. The first step is captured with a limited computational effort in the LES-VOF simulation, whereas the second step will be approached using well-established sheet atomization models from the literature. The first
step from the LES-VOF results gives the ligament structures at each instant, and the atomization model returns the final drop size population.

Figure 1: Left, schematic of the atomisation model for one specific sheet; Right: effect of the sheet stretching

It has to be noted that, at least in this particular case of these nozzles, the result of the primary rupture is to break the circular liquid jet into bidimensional sheets, mostly due to 1) the presence of vapor locations in between the liquid sheets 2) the hydrodynamic in the nozzle that generates an expanding flow at the exit. Therefore the analysis is done on each individual, 2D sheet. Evidence of such sheets will be shown later Figure 1 and 4. Obviously this is a strong modeling assumption, and a limit of the present approach that should be completed for a more universal model and different nozzle types. The break-up of bidimensional sheets to ligaments is based on the instability theory of thin sheet. The growing rate and therefore the final size with $\Lambda = \frac{2\pi}{K_s}$ are chosen according to Senecal et al. [4].

$$\omega = -2v_1k^2 + \left(4v_1^2k^4 + \left(\frac{P_0}{P_g}\right)U^2k^2 - \frac{\sigma k}{\rho_l}\right)$$  \hspace{1cm} (1)

and

$$D_{ligaments} = \sqrt{\frac{16\Lambda}{\omega}}$$  \hspace{1cm} (2)

The primary ligaments are then submitted to instabilities, and they are subsequently atomized in drops, using simple model [5]:

$$K_{ligaments} = \frac{1}{D_{ligaments}} \left(0.5 + \frac{3\mu}{2\sqrt{\rho_l \sigma D_{ligaments}}}\right)^{-1/2}$$  \hspace{1cm} (3)

allowing to derive :

$$D_{drops} = \left(\frac{2\pi D_{ligaments}}{K_{ligaments}}\right)^{1/3}$$  \hspace{1cm} (4)

The initial model of Senecal [4] was initially developed for thin sheets as resulting from swirl atomizer. The validity hypotheses are to have a small ratio of density between gas and liquid, which is the case in gasoline engines where the spray is injected in limited counterpressure and to have a Weber number $We > 27/16$ which is the case in current high pressure injection. In our cases, $h > 2\mu m$ and $U_{rel} > 125 m/s$, then $We > 1.79 > 27/16$. The break-up length $L = U_{rel} \cdot \tau$ with the break-up time $\tau = 12/\omega(\Lambda)$ results typically in our cases $L~\Omega$(mm) ; $\tau ~\Omega$(5-10us) which looks reasonable based on the data available from the literature.

A specificity of our case is the stretching due to the nozzle exit angle $\varphi$ (Figure 1 right). Due to the internal flow, as characterised for instance by the hole exit angle, the liquid films are extended radially. Each sheet can be stretched...
during the break-up time and so by conservation of the mass, its thickness will then diminish. This effect is quantified using the estimation of the flow stretching along the centre of the ligaments and then reintroduced as a correction parameter in the model. An interesting property of the Senecal model equation (1-2) is that instabilities are independent from the sheet thickness. More details of the practical numerical implementation can be found in ref [1]. The typical steps are illustrated Figure 2. The cross stream slice is extracted at one instant at 500um from the hole from the LES-VOF, where the ligaments are separated. Ligaments thickness is extracted using a distance function from centre to boundary (this last one being associated to an arbitrary iso-level of VOF). Then the coefficients due to the stretching but also due to the breakup into drops, equation (4), are computed (bottom left). This local computation is an improvement of the procedure used in ref [1], where the coefficients were estimated only in an average way. All together, it is easy to return the drop population locally (bottom right), the one that will be reinjected stochastically in the lagrangian simulations. Lagrangian computations cannot be described here into detail but are identical to ref [1]. The mesh is identical when comparing different geometries.

Figure 2: Ligaments analysis principle on an instantaneous slice. (a) Initial alpha field; (b) distance function at the center of the ligaments; (c) coefficient between ligament and drop size (d) final deduced drop size on this field. The slice is taken perpendicularly to the main direction of the hole. One ligament identification, as modelled fig 1, is indicated on (a), white arrow.

Testcases
The fuel atomizer used here as reference are a special Continental GDI prototype, 3-hole injector (first test, each hole has a different diameter), and 6-hole injector (second test, each hole is inclined differently). The first testcase (Table 1) has holes that are 7% convergent, their length is 345micron, the needle lift is 75um. The second testcase (Table 2) has a needle lift of 100um, with different geometries, extracted from the remeasured ones. The hexahedral mesh is around 15 Mo cells for each case. Each hole is followed by a conical external domain that is meshed up to a length of 5 diameters (Figure 3). The simulations are two-phase (not 3-phase, which is a limitation of the present approach). Experimental (fixed) mass flow rate is imposed at the inlet, pressure at the exit.

Table 1. First testcase, periodic 3-hole injectors

<table>
<thead>
<tr>
<th>Hole #</th>
<th>b angle [*]</th>
<th>L/D</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>30</td>
<td>1.7</td>
</tr>
<tr>
<td>2</td>
<td>30</td>
<td>2.0</td>
</tr>
</tbody>
</table>

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Table 2. Second testcase, 6-hole injector

<table>
<thead>
<tr>
<th>Hole #</th>
<th>b angle [°]</th>
<th>L/D</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>20</td>
<td>1.68</td>
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<td>2</td>
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<tr>
<td>5</td>
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<td>1.76</td>
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<tr>
<td>6</td>
<td>20</td>
<td>1.68</td>
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</tbody>
</table>

Results and discussion, first testcase

The atomization process that has been mentioned above is clearly illustrated Figure 4 for the first testcase. Slices perpendicular to the hole direction are showed in the second part of the hole and in the first part of the atomisation process. The flow development in the hole and at the exit clearly exhibits the breakup into ligaments mostly due to 1) a huge presence of cavitation 2) the ligaments are separated thanks to the radial velocity at the hole exit (as visualised experimentally with the close spray angle at hole exit for instance). A limited hole-to-hole interaction inside the sac volume has been found, due to the high distance between the holes, as only 3-hole are implemented in this prototype test injector. Whatever the hole, shear cavitation is developing largely and reaches the hole exit, even if a small convergence of the hole geometry is present. For holes with the higher diameters, vortex cavitation also develops. Hydraulic flip appears while D is increased. Increasing the hole diameter the primary atomization length is increasing.

Figure 4 : Instantaneous snapshot of the Volume of Fluid (liquid: red color), 200bar fuel pressure. Left: large hole diameter; center: medium hole diameter; right: small hole diameter. The slices are placed at the hole middle, hole exit, one and two diameters distance after the hole exit (hole length is 345micron)
In the first application case, each hole has a different diameter. This characteristic is visible in the development of the plumes, computed separately here, Figure 5. The spray from the first hole is much larger than the one from the last, small, hole. The Q-criterion as an indicator of the centers of the vortices classically defined by:

\[ Q = \frac{1}{2} (\tilde{S}_{ij} \tilde{S}_{ij} - \tilde{D}_{ij} \tilde{D}_{ij}) \]

where \( \tilde{S}_{ij} \) is the strain-rate tensor and \( \tilde{D}_{ij} \) is the rotation-rate tensor defined as:

\[ \tilde{D}_{ij} = \frac{\partial \tilde{u}_i}{\partial x_j} - \frac{\partial \tilde{u}_j}{\partial x_i} \]

displays, in both cases, roll-up structures close to the injection location which then evolve in helicoidal structures [1]. In the spray from the small hole, this transition to turbulence is longer: indeed, the spray is denser and its exchange with the entrained gas is expected to be reduced.

As expected, the studied spray is not sensitive to the smallest scales (\( \ell_p/\ell_q > 1 \) and \( D_p/\ell_q > 1 \)). On the other hand, it is sensitive to the sub-grid scale eddies (\( \ell_p/\ell_{edg} < 1 \)), so a basic sub-grid dispersion model have been introduced in order to take into account this interaction [1]. However, in this dispersion model the main driving factor remains the relative velocity between drops and eddies (\( \tau_{rel}/\tau_{edg} \ll 1 \)). Fortunately, as the turbulent fluctuations are mostly resolved, \( u'/\sqrt{\ell_{edg}} \approx 0.95 \), the influence of the turbulent dispersion model should remain limited.

To simulate the transient, the single additional input data that is needed is the mass flow rate as a function of time. The specific features at needle opening are initially neglected, using only full lift results, as will be discussed later. Temporal penetration curve in the direction of the spray are compared Figure 6. The global behaviour is satisfactory, slightly lower than the experimental one for the small hole case. Initially, a large difference was found for the medium-diameter hole. Its reason is now explained. Regarding the transient phenomena, in ref [6] the spray exhibited a flapping behaviour at the needle opening, impacting the spray penetration and which had been reproduced successfully in the simulations. In the present testcase, the transient influence of the needle opening is also highlighted. Indeed, with (only) the medium hole of this prototype injector a spurious behaviour was found experimentally: an important increase of the spray angle at the beginning of the injection: the exit angle is increasing.
from 25° to 45° during the period 0.1ms-0.4ms. When applying this angle increase in our simulation a satisfactory penetration is recovered back, which was not the case without taking this angle increase into account as the slope change was not captured (figure 6). This result confirms that the transient opening phase has to be measured into detail to be re-introduced empirically as in the present work. Otherwise moving mesh has to be used to simulate the opening needle phase as in ref [3].

**Results and discussion, second testcase**

Orientation angle B also clearly influences the cavitation behaviour, as seen Figure 8. Flow detachment is increasing with higher angles, and therefore the shear cavitation (right part of the nozzle slice) is progressively visible. For a small angle, a flow reattachment is visible on both sides, without hydraulic flip, and with a strong presence of cavitation vortex. For an intermediate to large angle, strong shear and vortex cavitation developments generate tridimensional effects and, in average, display a typical “smiley” shape.

In addition, the flow is strongly asymmetric and unsteady due to the hole-to-hole interaction in the nozzle flow development. The arrows refer to the vicinity of the next holes. The top arrow is in the direction of 20deg-hole; and bottom toward the 40deg-hole. This is a particular effect of this mirror geometry. It is of great interest to look into the vicinity of the holes (along the circumferential direction), see table 2 & fig 3 for the geometry. The 20deg-hole is in between 30deg-hole and 40deg-hole. The other holes have one neighbour with the same hole direction, reinforcing the stability of the flow. Only the intermediate hole direction has neighbour with different hole orientation.

![Figure 7: Time-average of volume of fluid. Red: liquid; blue: vapour. Flow is coming from the right side (needle seat). Top: Slice at the hole exit, perpendicular to the hole direction axis. Bottom: Cut-plan. Left: beta angle 20°; center: beta angle 30°; right: beta angle 40°. Arrow: see text](image)

The large beta angle shows a stable but reduced cavitating double contrarotating vortices. Stable attached shear cavitation is also present. It leads to a typical “smiley shape” that has been already described with a different injector design but still with a large beta angle of 40deg in ref [1]. Also coherent with this former paper, a side jet appears, due to the reorientation of a liquid sheet in between the two vortices. It can lead to small droplets with high velocity and angle on the side, as has been experimentally confirmed in the former work. Lastly, the higher angles (30deg-40deg) angles exhibit a hydraulic flip. As only two phases (vapour/liquid) are considered here, and not three phases (vapour/air/liquid), we can identify in this simplification a clear limit of the numerical model representation that will be overcome in the future works. It should be also noticed that the geometry has been generated from a complete 6-holes 3D design, and not from a mirror projected 3 hole case. Therefore, small geometrical differences are intended to be introduced from both sides. However this effect can be lower than in reality, for instance in case of some needle non-axisymetric positioning. This effect can also be damped by the limited resolution mesh. Indeed the flow is found quite stable in
time concerning its pattern, and even comparing the 2 sides. Considering one representative instantaneous flow event, the full picture is provided Figure 8. Differences are obviously observed, but the number and the area of the cavitating structures are almost identical when comparing both sides, even for 20deg-hole. The captured effect on the average mass flow rate is here not found as the main reason (average mass flow rate differs only by 3%, and instantaneous mass flow rate by less than 10%), but the average flow direction seems to break the symmetry for this 20deg-hole, as already discussed.

![Figure 8: Instantaneous snapshot of volume of fluid. Red: liquid; blue: vapour. Cut-plan at the hole exit, projected on a plane perpendicular to the injector central axis.](image)

The spray simulation is now realised with all the plumes injected together. As expected, some jet to jet interaction is observed, especially for the small drops that are entrapped in between the holes. Some turbulent eddies can also connect between the narrowest jets. The general comparison returns a very correct behaviour on Figure 9. The injector is inclined to get the central hole in the vertical direction at the center of the image. The estimation of the external angle depends on the thresholding level that is used, but the tendency is well recovered despite this simple offset.

![Figure 9: Instantaneous snapshots of the developed spray. Left: central hole is beta angle 20°; centre: central hole is beta angle 30°; right: central hole is beta angle 40°](image)

The experimental penetration is also correctly recovered in Figure 9 and Figure 10, even if the case to case difference is really small, below the RMS shot to shot variation. Interestingly, a manual recording of the typical size of the visible large scale structures of drop segregation returns also a good agreement which explains quantitatively the visible agreement between the images, with fish-bones and drop segregation structures.
Conclusions
Multijets spray structures, penetrations, and interactions are simulated with large Eddy Simulations. Differences between largely separated holes and narrow holes are depicted, with variations of hole diameters and orientation angles. Comparisons with local quantities will complete this work in the future.

Acknowledgements
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Nomenclature

- $D$: Hole diameter [m]
- $\rho_l$: Liquid volumetric mass density [kg/m$^3$]
- $\nu_l$: Liquid viscosity [kg/s.m]
- $\rho_g$: Gas volumetric mass density [kg/m$^3$]
- $\sigma$: Surface tension [N/m]
- $h$: Liquid sheet width [m]
- $\tau_p$: Drop relaxation time [s]
- $D_{ligaments}$: Drop diameter [m]
- $D_{drops}$: Drop diameter [m]
- $w$: Growing rate
- $k$: Wave number [m$^{-1}$]
- $\Lambda$: Maximum unstable wavelength [m]
- $K$: Wave number corresponding to the maximum growth rate
- $U_{rel}$: Relative velocity between the gas and the liquid [m/s]
- $\tau$: Break-up time [s]
- $L$: Break-up length [m]
- $u'$: Fluctuating velocity [m/s]
- $\tau_{sgs}$: Sub-grid time scale [s]
- $\tau_{rel}$: Time for a droplet to traverse an eddy in sub-grid scale [s]
- $\eta$: Kolmogorov time-scale [s]
- $\eta$: Kolmogorov length scale [m]
- $k_{sgs}$: Turbulent kinetic energy [m$^2$/s$^2$]

References

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Influence of liquid properties on ultrasonic atomization
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Abstract
Ultrasonic atomization is very convenient because it can generate droplets with diameters of a few microns and with very narrow size distribution. Besides, opposite to twin fluid nozzles, in ultrasonic atomization, droplet generation and transport are decoupled processes. Droplets are ejected from the liquid surface with very low velocities, so driving them is relatively simple. Although this atomization method is now common in some specific applications, for example in household humidifiers, there are still some details about the physics of this process that are not completely understood. Up to date, most of the published results have been limited to experiments with water. However, it has been demonstrated that atomization rates quickly decrease as liquid viscosity increases. This work analyzes the characteristics of ultrasonic atomization of some alternative fluids to determine if there is any influence of other physical properties such as surface tension or vapor pressure. Experiments are performed using a commercial piezoceramic disk with a resonance frequency of 1.65 MHz. The disk is excited with a sinusoidal signal with voltage amplitudes that go up to 60 V. Sprays are visually characterized analyzing instantaneous images and high speed video sequences. Besides atomization rates are calculated by measuring the weight loss in a fixed time.

Keywords
Ultrasonic atomization, ultrasound, piezoceramic.

Introduction
Ultrasonic atomization has some unique characteristics that are ideal for many specific applications. Typical examples are most commercial household air humidifiers, or some inhalers for drug delivery to the lungs. In these devices, atomization is achieved by vibration of an ultrasonic transducer submerged in a liquid volume. As a result, droplets can be generated from the liquid surface with diameters of a few microns, with very narrow size distribution, and with low velocity. Opposite to pressure and twin fluid nozzles, in which small droplet diameters are associated to high liquid and gas velocities, in ultrasonic atomization, droplet generation and transport are decoupled processes. Droplets are ejected from the liquid surface with very low velocity, so driving them is relatively simple.

The possibility to generate a cloud of droplets by means of ultrasonic waves was first reported by Wood and Loomis in 1927 [1]. Since then, many theoretical and experimental works have been published to explain the physics controlling this phenomenon. Two main mechanisms are considered to be responsible for the spray formation: cavitation inside the liquid mass and instabilities of standing waves on its free surface. Droplet detachment from wave crests can clearly be observed for low excitation frequencies but cannot be distinguished for frequencies in the MHz range. The importance of cavitation might be dependent on the forcing frequency or the ultrasonic power, but these extremes have not been demonstrated in a definite way. As confirmed by numerous experiments, it is now generally accepted that, in ultrasonic atomization, spray mean droplet diameter is essentially determined only by the oscillation frequency. The oscillation amplitude controls the spray flow rate but does not have a major influence on drop diameter [2]. When using ultrasonic transducers this amplitude is proportional to the driving signal voltage.

A major part of the published results are limited to water atomization. The influence of fluid physical properties has been studied in a relative low number of papers [3]. Most of them are based on experimental considerations [4,5], although some theoretical analysis can also be found [6]. Furthermore, in some of these works, the ultrasonic frequency is low [7]. Liquid viscosity does not substantially alter the droplet size distribution, but has a dramatic effect on atomization rate [8]. With the specific conditions in the present experiments, efficiency drops dramatically for kinematic viscosity values over 3x10⁻⁶ m²/s. This is a severe limitation that can preclude the use of this atomization method in many processes of industrial interest, for example in surface coating, or to introduce the droplets in a chemical reactor. However mists of viscous liquids can be obtained diluting them first in volatile solvents and atomizing the low viscosity mixture [9]. Once the solvent has evaporated, the result is a mist of a liquid that otherwise could not have been directly nebulized. To facilitate this possibility and advance in the
understanding of the dependence on different physical properties, this work analyzes the characteristics of ultrasonic atomization of some organic compounds. In particular, several alkanes and alcohols are considered. Results are compared to those obtained atomizing water in the same conditions. Measured parameters include atomization rate and droplet size distribution. Visual aspect of the sprays is also examined, recording instant images and high speed sequences.

Material and methods
In the experiments here described, atomization was performed using commercially available inexpensive ultrasonic transducers as the one shown in Fig. 2. They consist of lead zirconate titanate PZT-4 piezoceramic disks with a diameter of 20 mm, a thickness of 1.3 mm and a measured resonance frequency of 1.65 MHz.

The disks were excited with a sinusoidal wave coincident with the resonance frequency and variable amplitude. It has to be noted that disks of this type only oscillate with significant amplitude when the excitation wave coincides with the main resonance peak which is quite narrow. The resonant frequency depends on the ceramic type and the disk geometry, and this is the only frequency for which atomization occurs efficiently. A scheme of the oscillator circuit used to force the disks is presented in Fig. 2. It is very important to be sure that the disks operate submerged into the fluid volume, because in this way, the liquid also acts as a cooling medium preventing the disk from overheating. Otherwise, the Curie temperature, defined as the point where the material undergoes a transition from ferromagnetic to paramagnetic, might be reached. In this case, the magnetic moments would become randomly oriented, and the ceramic element would depolarize losing its electrostrictive properties. As the disk heating increases with the applied voltage, the maximum delivered value was limited to 80 V to avoid damaging the ceramic. Values over 100 V would also risk the integrity of the power transistor in the electronic oscillator circuit (marked as T in Fig. 2).

The disks were attached to the bottom plate of two different open vessels. The first one has a section of 18 cm x 18 cm and a height of 24 cm. It was used for the atomization rate measurements. A relatively large section was chosen to avoid a noticeable liquid heating from the piezoceramic transducer. The second one is even larger, with dimensions of 36 cm x 36 cm x 24 cm. This one was used for the image recording, to minimize possible interferences from the walls.

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To determine the atomization rates, the decrease in the liquid mass inside the vessel during a minimum time interval of 5 minutes was monitored by weighting it with a Kern FCB scales, capable of measuring a maximum mass of 8 kg with a precision of 0.1 g. For all the measurements the initial liquid level was identical and equal to 3 cm. Care was taken to evacuate the liquid droplets out of the atomizer to prevent condensation, suctioning them with an extraction fan. This extraction, however, was limited to the small droplets that form the spray mist and not to other larger drops. This group includes, for example, splashing caused by falling of the liquid cone tip onto the pool surface. This is mainly because these drops are not useful for most applications requiring small droplets where ultrasonic atomization could be a first choice. Besides, they can be filtered out in a relatively simple manner. This study will, thus, focus on the micron-sized droplets resulting from the ultrasonic atomization.

Droplet size distributions were measured with a Malvern Mastersizer S laser diffractometer equipped with a 300 mm focal length lens. According to the manufacturer specifications, this lens is suitable to cover a droplet diameter range from 0.5 µm to 900 µm. The maximum obscuration in the Malvern measurements was lower than 25%, with a minimum of 3.6%. The room was darkened to maximize the contrast for low obscuration values. To calculate the droplet size distribution, the polydisperse model of the Malvern software was selected. The small droplets were driven to the laser beam dragging them with an air flow. To visualize the atomization process, instantaneous images were acquired with a Hamamatsu 1,024 x 1,344 pixels 12-bit C4742-95-12 ORCA-ER CCD camera with a Sigma 70 – 200 mm zoom lens. Exposure time was set to 10 ms, and the covered field of view was 90 mm x 118 mm (87.8 µm/pixel). Image sequences were also acquired with a high speed CMOS RedLake Motion Pro HS4 camera, capable of recording 5,000 frames per second (fps) at a maximum image size of 512 x 512 pixels. Two different types of sequences were registered. The first one corresponds to a field of view of 130 mm x 130 mm, recording speed of 5000 fps and exposure time varying between 50 µs and 150 µs. The second configuration corresponds to close ups with a field of view reduced to 4.2 mm x 4.2 mm, recording speed of 3000 fps and exposure time of 330 µs. To achieve this magnification (8.2 µm/pixel), a Nikon PB6 bellows focusing attachment was placed between the camera and the lens, together with a set of three Kenko extension rings. Two 500 W halogen lamps were used as illumination source.

Experiments were performed atomizing several organic compounds as well as pure water. Table 1 summarizes the values of several physical properties that can be influential in the atomization process. Liquid selection includes three alkanes and three alcohols. Density and surface tension values are quite similar for all of them, in all cases lower than those for water. Viscosity and vapor pressure cover a wider range, increasing for increasing number of C atoms.

<table>
<thead>
<tr>
<th></th>
<th>Density ρ (kg/m³) 20°C</th>
<th>Viscosity μ (m²/s) 20°C</th>
<th>Surface tension σ (N/m) 20°C</th>
<th>Vapor pressure (Pa) 25°C</th>
<th>Compressibility modulus K (Pa)</th>
<th>Boiling Temperature (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>998.2</td>
<td>1x10⁻⁶</td>
<td>0.0728</td>
<td>3.167x10⁶</td>
<td>22.0x10⁶</td>
<td>100</td>
</tr>
<tr>
<td>Hexane</td>
<td>654.8</td>
<td>0.294x10⁻⁴</td>
<td>0.01843</td>
<td>20.4x10³</td>
<td>7.9x10³</td>
<td>69</td>
</tr>
<tr>
<td>Heptane</td>
<td>683.8</td>
<td>0.408x10⁻⁵</td>
<td>0.0197</td>
<td>6.06x10³</td>
<td>9.4x10⁸</td>
<td>98</td>
</tr>
<tr>
<td>Decane</td>
<td>730.0</td>
<td>0.92x10⁻⁶</td>
<td>0.02337</td>
<td>1.85x10³</td>
<td>11.0x10⁶</td>
<td>174</td>
</tr>
<tr>
<td>Methanol</td>
<td>781.8</td>
<td>0.745x10⁻⁵</td>
<td>0.02261</td>
<td>16.96x10³</td>
<td>8.23x10⁸</td>
<td>65</td>
</tr>
<tr>
<td>Ethanol</td>
<td>789.0</td>
<td>1.36x10⁻⁶</td>
<td>0.0228</td>
<td>7.924x10³</td>
<td>8.94x10⁸</td>
<td>78</td>
</tr>
<tr>
<td>2-Propanol</td>
<td>786.3</td>
<td>3.05x10⁻⁶</td>
<td>0.022</td>
<td>6.02x10³</td>
<td>7.5x10⁸</td>
<td>82</td>
</tr>
</tbody>
</table>

Results and discussion

Before presenting and discussing the results obtained from the different measurements, it can be interesting to describe the ultrasonic atomization process. It takes place according to the following scheme. The piezoceramic disk submerged below the fluid surface starts vibrating when excited with a 1.65 MHz sinusoidal wave. For low voltages the only noticeable effect is the appearance of some waves on the liquid surface over the disk. As the voltage is increased, this part of the surface assumes a conical shape most likely induced by an acoustic streaming phenomenon [10]. A further increase causes the elongation of the cone that forms a stem with a neck zone. Eventually, the tip of the cone detaches, and falls on the liquid pool forming big droplets due to splashing. When voltage surpasses a determinate value that depends on the liquid to be atomized and its viscosity, superimposed both to the whole mass displacement that produces the conical shape and the interfacial waves, a fine mist of small micron-sized droplets is generated, particularly in the middle part of the cone region. Together with it, some medium sized droplets are also ejected from the cone surface. The amount of this last type of droplets and their detachment velocity clearly increase with increasing forcing voltage. All these steps are

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illustrated in the series of images in Fig. 3, where water has been used as the atomized fluid. Voltages are 20 V, 30 V, 45 V and 55 V. It has to be remarked that although the response of the CCD camera is linear, to better discern low intensity details, the images are not displayed with a linear look-up table, but with a gamma \( \gamma = 2 \) grey scale according to the expression

\[
I_{\text{corr}} = I_{\text{max}} \left( \frac{I}{I_{\text{max}}} \right)^{1/\gamma}
\]

where \( I_{\text{corr}} \) are the intensity corrected values, and \( I_{\text{max}} \) is the maximum intensity.

**Figure 3.** Evolution of the ultrasonic atomization process for increasing voltages. From left to right: 20 V, 30 V, 45 V and 55 V. Atomized liquid is water.

**Atomization rate measurements**

A compilation of the results of the atomization rate measurements is presented in Fig. 4. From it, a first conclusion is noticeable. Water exhibits a trend that differs from the rest of liquids. While water atomization rate keeps increasing with voltage, all the other curves present a maximum for an intermediate voltage value, which varies between 35 V and 40 V. Although maximum voltage in this plot is limited to 60 V, values up to 80 V where tested without finding a maximum in the water graph. It is possible that still higher voltages could be required to reach it, but they would be out of the limits set for these experiments, as explained in Section 2. Setting aside water as a special case, the relative atomization rate values for the alkanes and alcohols have an inverse correlation with the kinematic viscosity, as shown in Fig. 5. Here, the maximum atomization rate for each liquid has been plotted as a function of the respective viscosity value. Again, this is in good agreement with the results in [8].

**Figure 4.** Atomization rate as a function of the forcing voltage for the different working liquids.
In order to perform ultrasonic atomization, the frequency and voltage are clearly visible, for decane, ethanol and water, this production is still in its initial stages. In the case of 2-propanol these droplets are almost not generated at all. Visual estimation of atomization intensity is in perfect agreement with the atomization rate values plotted in Fig. 4. From analysis of images obtained at different voltages, it can be concluded that production of the micron-sized droplets seems to be independent of the formation of the cone-shaped liquid fountain. Fountain height increases with voltage, but mist formation is inhibited for high viscosity values. It is interesting to note that according to the experiments in [8] working with mixtures of glycerol and water, ultrasonic atomization is difficult for kinematic viscosities over 3x10-6 m²/s. Viscosity of 2-propanol, for which fog production is very low, is slightly above this limit.

**Figure 5.** Maximum atomization rate for each one of the liquids as a function of the corresponding kinematic viscosity.

**Image analysis**

In order to confirm the results in Fig. 4, an analysis of instantaneous images of the atomization process has been performed. Figure 6 shows the situation for the different liquids at a common voltage of 30 V. As in Fig. 3, images are displayed with a γ = 2 look-up table. While for hexane, heptane and methanol the mist of small droplets is clearly visible, for decane, ethanol and water, this production is still in its initial stages. In the case of 2-propanol these droplets are almost not generated at all. Visual estimation of atomization intensity is in perfect agreement with the atomization rate values plotted in Fig. 4. From analysis of images obtained at different voltages, it can be concluded that production of the micron-sized droplets seems to be independent of the formation of the cone-shaped liquid fountain. Fountain height increases with voltage, but mist formation is inhibited for high viscosity values. It is interesting to note that according to the experiments in [8] working with mixtures of glycerol and water, ultrasonic atomization is difficult for kinematic viscosities over 3x10-6 m²/s. Viscosity of 2-propanol, for which fog production is very low, is slightly above this limit.

**Figure 6.** Ultrasonic atomization of different liquids for a common forcing voltage of 30 V
From the physical properties listed in Table 1, it is to be observed that the main difference between water and the rest of the liquids can be found in the values for surface tension and compressibility modulus, which are the highest. This could be a reason for its distinct behavior, but further research is required. Arguments are still required to explain the presence of the atomization rate maximum for some of the tested liquids. Figure 7 shows some images of heptane atomization for driving voltages of 25 V, 30 V and 55 V. Although for all the recorded images atomization seems to be more violent for higher forcing, what appears to increase in a higher degree is the formation of medium-sized droplets, in detriment of the production of the smallest ones. As in the present experiments the atomization rate measurements are limited to this last group of droplets, this might explain the maximum in the curves in Fig. 4.

![Figure 7. Ultrasonic atomization of heptane for forcing voltage values of 25 V, 30 V and 55 V.](image)

The process of droplet ejection from the cone surface is shown in Fig. 8. It corresponds to methanol atomization for a forcing voltage of 25 V. Time interval between frames is 333 μs. Relatively large droplets can be seen escaping from the liquid surface. The smallest droplets cannot be discerned individually, and they appear as a fine mist. As a first estimate, this indicates that their size has to be lower than 8 μm. The droplet size distribution measurements should confirm this extreme.

![Figure 8. Close up view of ultrasonic atomization of methanol for a forcing voltage of 25 V. Time interval between frames is 333 μs.](image)

**Droplet size distribution measurements**

Similarly to what happened for the atomization rate measurements, the specific experimental set up arranged to determine droplet size distribution only considers the small drops that form the mist. As they are dragged out of the recipient by a slow air flow, large droplets are effectively filtered out by effect of gravity. It is again to be reminded that large droplets are not considered of interest because they can be produced in an efficient way by a variety of atomization methods. It is the generation of micron-sized droplets what is difficult to achieve with other procedures alternative to ultrasonic atomization.

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Measurements for water were already obtained in previous works [2,8]. Some of them have been retaken to ensure repeatability. Main results are compiled in Fig. 9. As expected, it is confirmed that for the liquids in these experiments and for the droplets in the micron range, variation in their physical properties has a weak influence on the size distribution function. For most of the liquids, the shape of the distribution function is nearly identical, with two distinct peaks at 3.3 μm and 6.2 μm. Size distributions for hexane, ethanol and propanol show a slightly different shape. It may be due to the fact that accuracy of these measurements is somewhat lower. The measurements for hexane are inaccurate because they were affected by laser beam steering due to the high concentration of vapors. Non-zero results were obtained flowing the dragging air inside the liquid container with the ultrasonic transducer disconnected. However, we were unable to separate the vapor from the droplets to be measured. Ethanol and 2-Propanol measurements are also inaccurate because droplet concentration was very low and laser obscuration was below the recommended level. Measurements for the rest of the liquids seem to confirm the hypothesis postulated in many previous papers that relates droplet size only to ultrasonic frequency.

Conclusions
An experimental study has been conducted to analyze the characteristics of ultrasonic atomization when working with different organic compounds. Three alkanes (hexane, heptane and decane) and three alcohols (methanol, ethanol and 2-propanol) have been considered. Density and surface tension values are quite similar for all of them, in all cases lower than those for water. Viscosity and vapor pressure cover a wider range, increasing for increasing number of C atoms. Tests operating with water have also been performed for comparison purposes. A commercial piezoceramic disk with a resonance frequency of 1.65 MHz, has been used in the experiments. It has been forced with a sinusoidal wave coincident with the resonance frequency and variable amplitude. The maximum applied voltage has been limited to 80 V. In all cases, atomization rates have been measured. Sprays have been characterized analyzing instantaneous images and high speed video sequences, and measuring droplet size distribution functions. It has been observed that in the process of atomization a fine mist of small micron-sized droplets is generated, together with some medium sized droplets that are also ejected from the liquid surface. The amount of this last type of droplets and their detachment velocity clearly increase with increasing forcing voltage. In this study, attention has been only focused on the small drops that form the mist. The large droplets have not been considered of interest because they can be produced in an efficient way by a variety of atomization methods and can be easily filtered out. It is the generation of micron-sized droplets what is difficult to achieve with other procedures alternative to ultrasonic atomization. A somehow unexpected observation is that, contrary to the case of operation with water in which atomization rate always increases with voltage, alkane and alcohol atomization presents a maximum for a certain value, decreasing when voltage is further increased. The presence of this maximum can be attributed to an increase with voltage in the formation of medium-sized droplets, in detriment of the production of the smallest ones. Results also confirm that viscosity strongly conditions the atomization efficiency. On the other hand it has been verified that for a fixed ultrasonic frequency, size of the fog droplets seems to be independent of the liquid nature.
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References
Effect of excitation on gas centered swirl coaxial injectors

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Abstract
Studies on combustion instability in liquid rocket engines are important in improving combustion efficiency and preventing combustion chamber losses. To prevent combustion instability, methods such as baffles and cavities are used. The injector is located in the middle of the perturbation-propagation process in the rocket engine, so it is important to study the suppression of combustion instability using the design of the injector. Much research has been focused on the study of liquid excitation in a single injector; however, the actual injector used in a liquid rocket engine is a coaxial injector. In this study, the dynamic characteristics of a gas-centred swirl coaxial injector were investigated by varying the gap thickness and momentum-flux ratio. Spray photographs were captured by synchronizing a stroboscope and digital camera, and a high-speed camera and Xenon lamp were also used. To measure the liquid film, a measurement system was implemented using the electrical conductance method. For excitation of the gas, an acoustic speaker was used to impart a frequency to the gas. The gas velocity and effect of excitation were measured by hot-wire anemometry. A mechanical pulsator was used for liquid flow excitation. Liquid fluctuation was measured by a dynamic pressure sensor. In both gas and liquid excitation cases, the gain increased as the gap thickness decreased and the momentum-flux ratio increased. From these results, it can be concluded that gap thickness and momentum-flux ratio are major factors in suppressing combustion instability.

Keywords
Gas-centred Swirl Coaxial Injector, Excitation, Gain

Introduction
Research on combustion efficiency and combustion instability is important in the development of a liquid rocket engine. Combustion instability occurs in the combustion chamber when the combustion and the flow of the propellant supply system are combined. This not only reduces combustion efficiency, but also leads to combustion chamber losses in extreme cases. Disturbances that can occur in propellant supply systems ranges from a few Hz to a few thousand Hz, depending on the causes [1].

One of the causes of combustion instability is perturbations in the flow rate of the propellant to the combustion chamber, which can be caused by various factors. This disturbance of the flow travels through the feed line, the injector, and the combustion chamber, affecting the stability of the combustion. The pressure perturbation resulting from combustion instability can also affect the propellant flow in the feed system. Therefore, the design of an injector located in the middle of this process is of considerable importance. If the injector can serve as a shock absorber to reduce the disturbance from the supply line by optimized design, it would be able to prevent instability of the spray, which could cause combustion instability.

Research into the suppression of combustion instability through injector geometry has been going on since the 1990s. In 1996, Bazarov et al. found that the injector dynamics affected the instability of the liquid rocket engine [2]. In 2007, Soller et al. investigated the combustion instability of an oxidant-feed system and combustion chamber in various gas centred swirl coaxial injectors. They confirmed that the perturbation of the oxidant supply system affects the perturbation of the combustion chamber [3]. Heister et al. proposed several models of self-resonance phenomena of a close-type single swirl injector and analysed it numerically [4]. Fu et al. confirmed the dynamic characteristics of an open-type single swirl injector by changing the injector geometry using a mechanical pulsator.

The previous research only focused on the response characteristics to liquid disturbance in a single swirl injector. The phenomenon of propellant disturbance in a gas-liquid injector used in a liquid rocket engine has not been extensively studied. In this study, the dynamic characteristics of the spray from disturbances of the gas and the liquid were investigated by varying the gap thickness of the gas centred swirl coaxial injector, used mainly in the Russian multi-stage combustion cycle liquid rocket engine, such as the RD-170.
Material and methods
The experimental setup is shown in Fig. 1. In this experiment, air and water were used as the experimental fluids to represent oxidant and fuel, respectively. The apparatus comprises a function generator, a data acquisition system (DAQ), an injector, and a high-speed camera. The function generator supplied a constant frequency, and the voltage for the liquid film thickness was measured by the electrodes in the orifice. The method of measuring the liquid film thickness with electrodes, using the electrical conductivity of water, was proposed by Suyari and Lefebvre [5]. Two thin electrodes were placed at the end of the orifice to obtain the voltage generated by the liquid film thickness. The manifold pressure of the injector was measured by a static- and a dynamic-pressure sensor, and was recorded by the DAQ system. The spray image of the injector was obtained using a high-speed camera and a DSLR camera.

For the gas excitation, a speaker, amplified by an amplifier, was installed in the middle of the gas supply line to generate the perturbation of the gas flow. The influence of the gas velocity perturbation was measured by using hot-wire anemometry. For the liquid excitation, a mechanical pulsator was installed in the middle of the liquid supply line to generate perturbations in the pressure of the supplied liquid. The pulsator was designed to change the area of the flow path by rotating a plate at a predetermined speed, up to 1000 Hz.

The geometry of the gas-centred swirl injector used in the experiment is shown in Fig. 2. The gas orifice is located in the middle of the injector, surrounded by the liquid orifice. The gas is jetted and the liquid is swirled through the tangential inlet and injected. The diameter of the injector orifice was 8 mm (2Rn) and the gas orifice diameter (Dg) was 6 mm. The tangential inlet diameter (Rinlet) was 0.9 mm for the gas flow perturbation case, and 1.5 mm for the liquid flow perturbation case. The gap thickness (hgap) was set at 0.3 mm, 0.5 mm, and 0.7 mm.

In this experiment, the speaker frequency was varied from 200–1100 Hz at 100 Hz intervals to simulate disturbances in the oxidant excess gas. The liquid fuel disturbances were simulated by varying the pulsator frequency from 200–1000 Hz in 50 Hz increments. Experiments were carried out by setting the gap thickness, which influences the gas-liquid mixing and the gas-liquid momentum-flux ratio as the main parameter in the gas-liquid injector. The momentum flux ratio is defined by Eq. 1, and the experimental conditions are shown in Table 1.

\[ MR = \frac{\rho_g U_g^2}{\rho_l U_{ai}} \] (1)
Results and discussion

The thickness of the liquid film at the end of the injector orifice is an important factor influencing the spray angle, breakup length, and droplet size [6]. Therefore, understanding the change in liquid film thickness at the end of the orifice in response to the generated flow disturbances is important in terms of spray- and combustion-instability predictions. In this experiment, the response characteristics of the liquid film thickness to the perturbation during gas excitation and liquid excitation is expressed by the injector transfer function as shown in Eqs 2–4.

\[
ITF_{\text{gas}} = \frac{\text{output}}{\text{input}} = \frac{v'/r}{w'/0}
\]  
(2)

\[
ITF_{\text{liquid}} = \frac{\text{output}}{\text{input}} = \frac{v'/\rho}{p'/\rho}
\]  
(3)

\[
\text{gain} = |\text{ITF}|
\]  
(4)

In a gas centred swirl coaxial injector, the gap thickness is a geometric factor that determines the liquid film thickness in a liquid flow. Fig. 3 shows the results of the injector dynamic characteristics for varying gap thickness when the gas is excited while the gas and liquid are sprayed at the same time. As the gap thickness decreased, the gain increased. A decrease in the gap thickness means an increase in the lip thickness because the diameter of the gas and liquid orifices is kept constant. Larger lip thickness produces greater flow eddy [7]. Therefore, when the gap is thinner, i.e., when the lip is thicker, a large vortex forms, and the magnitude of the perturbation becomes larger.
Figure 3. Dynamic characteristics for varying gap thickness with gas flow perturbations

Figure 4 shows the response characteristics of the spray when only the gas is excited, the liquid flow rate is fixed, and the gas-liquid momentum-flux ratio is changed. The increase in the gas-liquid momentum-flux ratio means that the momentum of the gas relative to that of the liquid increases, resulting in a larger momentum transfer for the same mixing-zone length. Therefore, more gas velocity perturbations are transmitted to the liquid, which increases the liquid film tremor at the end of the orifice. However, it can be seen that the increase of the gain due to the increase of the momentum-flux ratio changes with frequency. The effect of the spray pattern on frequency is shown in Fig. 5. When the magnitude of the gain is larger, the liquid film thickness reduces because the effect of the excitation acted on strongly liquid flow. Thus, it can be seen that the spray breaks up quicker and has a qualitatively wider angle due to its earlier breakup.

Figure 4. Dynamic characteristics for varying momentum-flux ratios with gas flow perturbations
Liquid Excitation

Figure 6 shows the dynamic characteristics of the injector for the three gap thicknesses with liquid excitation, while the liquid flow rate is fixed without injecting gas. Gain changes and a phenomenon in which the gain decreased at a specific frequency (sharp drop) can be observed. When the gap thickness was 0.3 mm, the gain was more than twice that of the other cases, which is thought to be due to the liquid film thickness. As shown in Table 2, when the gap thickness was 0.3 mm, the liquid film thickness was approximately half that of the other two gaps. Such a thin liquid film is susceptible to tremors, so that the change in thickness was doubled due to the influence of the excitation. As the gap thickness increased, the frequency at which the gain decreased also decreased. This is because the gap thickness acts as a low pass filter; the fluid passing through the tangential inlet meets the gap, which is a suddenly enlarged space, and only the low-frequency fluid passes through.

![Figure 5. Spray pattern with gas excitation for h_{gap} = 0.5 mm and MR = 2; (a) f = 0 Hz, (b) f = 600 Hz, and (c) f = 1000 Hz](image)

Table 2. Film thickness and film thickness fluctuation for varying gap thicknesses.

<table>
<thead>
<tr>
<th>Gap thickness [mm]</th>
<th>Film thickness @ 300 Hz [μm]</th>
<th>Film thickness fluctuation @ 300 Hz [μm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.3</td>
<td>480.70</td>
<td>55.84</td>
</tr>
<tr>
<td>0.5</td>
<td>714.82</td>
<td>26.97</td>
</tr>
<tr>
<td>0.7</td>
<td>887.77</td>
<td>29.21</td>
</tr>
</tbody>
</table>

Figure 7 shows the results of the dynamic characteristics with different gas-liquid momentum-flux ratios when the gas and the liquid were injected simultaneously, with only the liquid having flow perturbations. An increase in the
gas-liquid momentum-flux ratio leads to the formation of a thin liquid film thickness that is susceptible to perturbations, thereby increasing the gain. It was also considered that the gas momentum added to the liquid tremor, and increased the gain. Figure 8 shows the spray pattern at three different frequencies. It can be seen that the spray has a clear single layer of the liquid mass concentrated at every excitation period in the case where the gain was larger, similarly to the case of gas flow perturbations.

Figure 7. Dynamic characteristics for varying momentum-flux ratios with liquid flow perturbations

Figure 8. Spray pattern with liquid excitation for \( \text{h}_{\text{gap}} = 0.5 \text{ mm} \) and \( \text{MR} = 2 \); (a) \( \text{f} = 0 \text{ Hz} \), (b) \( \text{f} = 400 \text{ Hz} \), and (c) \( \text{f} = 900 \text{ Hz} \)

Conclusions
To investigate the dynamic characteristics of a gas-centred swirl coaxial injector, which is used mainly in a multi-stage combustion cycle engine, a speaker and a mechanical pulsator were used to generate gas- and liquid-flow perturbations. The effect of the geometry on the dynamic characteristics was investigated by varying the gap thickness, and the dynamic characteristics of the injector were determined by varying the momentum flux ratio. In the case of gas excitation, the gain increased as the gap thickness decreased. It is considered that as the gap thickness decreased and the lip became thicker, a larger vortex formed, resulting in a larger gain. As the momentum flux ratio increased, the gain increased. This is because more of the gas momentum was transferred to the liquid, as the momentum of the gas relative to that of the liquid increased.

In the case of liquid excitation, the gain increased as the gap thickness decreased. Because of the spatial limitations of the smaller gap thickness, a thin liquid film was formed and was susceptible to tremors, which are caused by the influence of the excitation. As the momentum flux ratio increased, the gain increased. This is thought to be due to the momentum of the gas being transmitted to the liquid.
From these results, it can be concluded that the gap thickness is considered to be the main geometric factor for suppressing combustion instability, and that the momentum-flux ratio was also a factor for suppressing combustion instability.

Acknowledgements
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Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
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<tbody>
<tr>
<td>ITF</td>
<td>injector transfer function</td>
</tr>
<tr>
<td>t'</td>
<td>film thickness fluctuation [μm]</td>
</tr>
<tr>
<td>T</td>
<td>average of film thickness [μm]</td>
</tr>
<tr>
<td>p'</td>
<td>manifold pressure fluctuation [bar]</td>
</tr>
<tr>
<td>P</td>
<td>average of manifold fluctuation [bar]</td>
</tr>
<tr>
<td>MR</td>
<td>momentum flux ratio</td>
</tr>
<tr>
<td>ρ_g</td>
<td>density of gas</td>
</tr>
<tr>
<td>ρ_l</td>
<td>density of liquid</td>
</tr>
<tr>
<td>u'</td>
<td>gas velocity fluctuation [m/s]</td>
</tr>
<tr>
<td>U</td>
<td>average of gas velocity [m/s]</td>
</tr>
<tr>
<td>U_g</td>
<td>velocity of gas</td>
</tr>
<tr>
<td>U_ail</td>
<td>axial velocity of liquid</td>
</tr>
<tr>
<td>D_g</td>
<td>diameter of the gas orifice</td>
</tr>
<tr>
<td>R_m</td>
<td>distance from the centre of the injector orifice to the centre of the tangential inlet</td>
</tr>
<tr>
<td>R_o</td>
<td>radius of the injector orifice</td>
</tr>
<tr>
<td>R_inlet</td>
<td>radius of the tangential inlet</td>
</tr>
</tbody>
</table>

References

Effect of liquid viscosity on the aerodynamic breakup of non-spherical droplets

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*Corresponding author: k.bergeles12@imperial.ac.uk

Abstract
This paper studies the effect of liquid viscosity on the atomisation regimes of initially spherical and non-spherical droplets and also kinematic characteristics of non-spherical droplets. The droplets consisted of water-glycerol solutions with viscosities ranging from 6.3 to 697 mPa.s, and the initial aspect ratio was 1<AR<2. The range of We number was from 10 to 200 and of the Oh number from 0.01 to approximately 4. The experimental findings showed that the equivalent Weeq and Oheq numbers, proposed in previous work [1] for water droplets, are also applicable to spherical and non-spherical droplets in the range of Oh numbers of this study in order to classify the breakup regimes on the existing morphological charts. The kinematic characteristics of the centre of mass for droplets with AR=1.2 are evaluated and the role of viscosity examined in the no breakup and bag-stamen regimes.

Keywords
non-spherical, droplet, breakup, aerodynamic

Introduction
Understanding the physics and nature of liquid droplet-air interaction, investigating the droplet internal and external flow and capturing droplet deformation and breakup is of importance in various scientific fields and technological applications [2]. In some technological applications, such as automotive sprays, the need is to avoid the generation of the largest droplets. Although their number density is low, these sizes carry a disproportionate fraction of the injected fuel, which evaporates slowly, and follow ‘ballistic’ trajectories resulting in locally overly rich mixtures, associated with undesirable emission characteristics.

The literature on experimental droplet atomisation assumes an initial spherical droplet. In other words, most research classifies and investigates the breakup modes under morphological regimes treating the droplet as a sphere. However, in regions of intense atomisation, as found in the interior of the crankcase, the technological motivator of the present work, droplets are known to have an initial non-spherical shape before the interaction with the flow inside the crankcase.

According to Hinze [3] droplet deformation occurs as the value of We becomes greater than one (We > 1). The external aerodynamic force acting on the droplet’s surface, which scales as ρu² becomes larger than the counteracting force owing to the surface tension σ/d₀ of the liquid. The deformation evolves to breakup at the critical value of Weeq≈12 number. In cases where We ≈ Weeq number simple breakup mechanism occurs, while for increasing We number, the disintegration of the droplet becomes a more chaotic atomisation process.

Pilch and Erdman [4] performed experiments to quantify characteristic variables of the breakup process, classifying the breakup modes. For increasing We number the atomisation regimes found were the vibrational, bag, bag-stamen, sheet stripping and catastrophic breakup as shown in Figure 1. The normalised displacement xₙₙ (Eq. (1)), velocity uₙₙ (Eq. (2)) and acceleration αₙₙ (Eq. (3)) of the centre of mass of the droplet were also presented. The study modelled the droplet as a rigid sphere, neglecting mass loss during the atomisation, as also the droplet breakup relative to the flow assuming an average, constant drag coefficient C₉ through the breakup process.

\[ xₙₙ = \frac{x_d}{d₀} = \frac{3}{8} C_d (t^{*})^2 \] 

\[ uₙₙ = \frac{u_d}{u_g \cdot \epsilon^{0.5}} = \frac{3}{4} C_d t^{*} \] 

\[ \alphaₙₙ = \frac{\alpha_d \cdot d₀}{u_g^{2} \cdot \epsilon} = \frac{3}{4} C_d \] 

where xₙₙ, uₙₙ, αₙₙ are the dimensioned displacement, velocity and acceleration of the centre of mass of the droplet.

The timescale t* of the atomisation phenomenon (Eq. (4)) equals to:

\[ t^{*} = \frac{t \cdot u_g \epsilon^{1/2}}{d₀} \] 

where ϵ is the density ratio ρ₀/ρₙ, t is the dimensioned time and C₉ is the droplet drag coefficient which remains constant during the atomisation and equal to C₉ = 2.5 and C₉ = 1.7 for compressible and incompressible flows respectively.

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We < 12
Atomisation regime
12 < We < 50
Bag breakup
50 < We < 100
Bag-stamen breakup
100 < We < 250
Sheet stripping
We > 250
Catastrophic breakup

**Figure 1.** Morphological classification of breakup modes based on $We$ number as derived by Pilch and Erdman [4]

In addition Pilch and Erdman [4] proposed a third degree polynomial to express the droplet displacement $x_d^*$ (Eq. (5)), velocity $u_d^*$ (Eq. (6)) and acceleration $a_d^*$ (Eq. (7)) using the empirical constant $B$ to provide a correct initial behaviour.

\[
x_d^* = \frac{x_d}{d_0} = \frac{3}{8} C_d (t^*)^2 + B (t^*)^3
\]

\[
u_d^* = \frac{u_d}{u_g \epsilon} = \frac{3}{4} C_d t^* + 3B (t^*)^2
\]

\[
a_d^* = \frac{\alpha_d d_0}{u_g^2 \epsilon} = \frac{3}{4} C_d + 6B t^*
\]

with $C_d = 1$, $B = 0.116$ for compressible flow and $C_d = 0.5$, $B = 0.0758$ for incompressible flow. The correlation assumes a constant drag coefficient $C_d$ of a rigid constant-mass sphere. The change of the frontal area of the droplet due to deformation is not taken into account. Moreover, the equations are valid for the period of time until the velocity of the droplet is 60% of the velocity of the flow.

The transition between two breakup regimes has been found to be a function of the $We$ and $Oh$ number and independent of the density ratio or the $Re$ number. These transitional $We$ numbers have been quantified by Brodkey [5] in Eq. (8) and Gelfand [6] in Eq. (9).

\[
We_{crit} = We_{crit,0} \left(1 + 1.077 Oh^{1.6}\right)
\]

\[
We_{crit} = We_{crit,0} \left(1 + 1.5 Oh^{0.74}\right)
\]

where $We_{crit}$ is the transitional $We$ number for increased $Oh$ number and $We_{crit,0}$ is the transitional $We$ number for $Oh \rightarrow 0$ respectively.

However a gap exists in the literature of the droplet atomisation as all the previous analytical work and interpretation of experimental data assumed initial spherical droplets.

**Experimental arrangement and measurement technique**

The experimental arrangement is shown in Figure 2. The main components are a Tec5 ultrasonic levitator which is used to levitate individual droplets and control their sphericity, a Photron CMOS high-speed camera for the imaging of the breakup and a nozzle controlled by a high-speed solenoid valve which produces the cross-flow that atomises the droplet.

**Droplet levitation:** An ultrasonic wave is emitted from the transducer of the levitator, which is reflected back to its source by a reflector, creating a vertical standing wave. A single droplet with diameter of the order of one millimetre is
The acoustic pressure induced on the upper and lower pole of the droplet plays a minor role during the deformation and atomisation process. For a millimetre droplet, the lift force generated by the acoustic pressure balances the gravitational force and caused a total pressure within the droplet to increase by approximately 10 Pa. The acoustic pressure is the cause of transformation of the spherical droplet shape into an oblate spheroidal shape, due to surface tension, approximately 70 Pa for the maximum AR. The minimum dynamic pressure of the flow is 500 Pa, therefore the contribution of the maximum acoustic pressure to the droplet atomisation is an order of magnitude lower compared to the minimum dynamic pressure of the flow. As a result, the role of the acoustic pressure on the atomisation is expected to be negligible.

**Gas flow:** The droplets were impulsively accelerated by a sudden gust of air, which was released from a pressure chamber by a fast solenoid valve. The cross-flow consisted of filtered air at room temperature 20°C. The air jet flow was ejected through a nozzle with 10mm diameter. The velocity at the exit of the nozzle was measured using a Dantec hotwire device to examine the uniformity and repeatability of the velocity profile. The velocity profile of the flow as a function of time is close to a step function with accelerations ranging from 1928 up to 13·10^3 m/s^2 over the range of experiments. The coefficient of variance of the acceleration is lower than 8% for all operating conditions. The maximum and mean velocity value of the flow were measured at four distinct points at a radius of 2mm and at the centre of the nozzle. The measurements, show an almost uniform velocity profile with a standard deviation well below 3%, thus the droplet atomisation occurs under a uniform velocity profile. However, for low air velocities, discrepancies in the flow are larger, but still within an acceptable range with maximum standard deviation of around 4.3%.

**High-speed imaging:** The shadowgraphic technique is employed for the visualisation of the droplet breakup. A Photron high-speed CMOS camera records the droplet breakup at a frame rate of 20 kHz. The spatial resolution of the images is 512 x 256 pixels with 5/s exposure time. A commercial Nikon lens (f-number f/2.8) with appropriate extension tubes and a teleconverter (TELEPLUS MC7 AF 2.0X DGX) are used leading to an image magnification of 12.3 μm/pixel. The imaged area of the camera is 6.2 mm x 3.1 mm in the xy plane as shown in Figure 2. Due to the high acquisition rate, the droplet breakup was temporally resolved. The camera was placed perpendicular to the flow direction and it was focused on the symmetry plane of the droplet. The synchronisation of the solenoid valve with the high-speed camera was achieved using a SRS 535 digital delay generator. Finally, a back illumination lamp of 1000 W was used and uniform illumination was accomplished with ground glass diffusers. The processing of the images was performed in Matlab environment using an in-house code and in ImageJ [7], an image manipulation software.

For the present study three glycerol-water solutions were produced and the viscosity measured using a viscometer. The physical properties were derived for 20°C ambient temperature and the characterisation error is within 2%. Table 1 summarises the physical properties of the glycerol-water solutions.

---

**Table 1. Physical properties of glycerol-water solutions at 20°C ambient temperature**

<table>
<thead>
<tr>
<th>Name (% glycerol)</th>
<th>Dynamic viscosity [μL/m]</th>
<th>Kinematic viscosity [ν] [mm²/s]</th>
<th>Density [ρ] [kg/m³]</th>
<th>Surface tension [σ] [mN/m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mix-1 (50%)</td>
<td>6.386</td>
<td>5.674</td>
<td>1125.5</td>
<td>68.5</td>
</tr>
<tr>
<td>Mix-2 (80%)</td>
<td>58.96</td>
<td>48.839</td>
<td>1207.3</td>
<td>65.5</td>
</tr>
<tr>
<td>Mix-3 (97%)</td>
<td>697</td>
<td>557.15</td>
<td>1251.0</td>
<td>63.0</td>
</tr>
</tbody>
</table>

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Morphological classification of droplet breakup

The breakup modes appearing for increasing $We$ numbers are the no, bag, bag-stamen and sheet stripping breakup modes. These regimes change for increasing $Oh$ numbers and it must be pointed out that the transition between breakup regimes is not a step function but it occurs gradually. Therefore the characterisation of a breakup could be difficult and rather arbitrary, especially between bag-stamen and sheet stripping breakup regimes and also for viscous liquids.

The most commonly used theoretical curves describing this transition of the breakup modes are produced by Brodkey [5] (Eq. (8)) and Gelfand [6] (Eq. (9)). According to these relations, a steep change in the transitional $We$ numbers appears for higher $Oh$ number ($Oh > 0.1$). From this $Oh$ number and onward the liquid viscous forces become dominant and an exponential change occurs to the transitional $We$ numbers.

The morphological classification in the $Oh - We$ number plane of the present experimental data is shown in Figure 3. The derivation of the dimensionless numbers was done with the equivalent droplet diameter $d_e$. Overlapping regions appeared, especially in the bag and bag-stamen breakup regimes for Mix-1 (50% glycerol) and Mix-2 (80% glycerol) solutions.

The theoretical curve of Brodkey [5] and Gelfand [6] are also presented in Figure 3. The regime boundaries are approximately flat for $Oh < 0.1$; Gelfand’s relation [6] produces higher transitional $We$ numbers for lower $Oh$ numbers than Brodkey’s [5], however the latter one predicts a steeper change in the transitional $We$ numbers. The theoretical curves of Brodkey [5] and Gelfand [6] predicting the breakup regime boundaries should be taken as a general rule.

For $Oh > 0.05$ the discrepancies of the two theoretical curves become significant, showing that the transition criteria of breakup regimes for increasing $Oh$ are not well defined even for initially spherical droplets. The experimental data does not agree with the predicted transitional $We$ numbers because the initial sphericity of the droplet has not taken into consideration by the theoretical curves.

Figure 4 is the representation of the breakup modes in $We_{eq} - Oh_{eq}$ plane. The derivation of the dimensionless numbers was done with the equivalent droplet diameter $d_{eq}$ (Eq. (11)). The equivalent $We_{eq}$ [1] (Eq. (10)) number for deformed droplet is:

$$We_{eq} = \frac{\rho \alpha^2 d_{eq}^2}{\sigma}$$  \hspace{1cm} (10)

where $d_{eq}$ is the equivalent diameter and defined in Eq. (11)

$$d_{eq} = \frac{d_x^2}{d_y}$$  \hspace{1cm} (11)

where $d_x$, $d_y$ are the stream-wise and cross-stream diameter of the droplet respectively. In the case of the spherical droplet, the equivalent diameter is equal to the diameter of the droplet $d_0$, based on its volume. In the same way the equivalent $Oh_{eq}$ [1] is formulated (Eq. (12))

$$Oh_{eq} = \frac{\mu}{\sqrt{\rho \sigma d_{eq}}}$$  \hspace{1cm} (12)

Figure 3 and Figure 4 map the breakup mode of both initially spherical and non-spherical droplets; however the initial sphericity of the droplets is not illustrated in the figures for clarity purposes. The introduction of $d_{eq}$ to the $Oh$ number gives $Oh_{eq} < Oh$; in other words the equivalent diameter $d_{eq}$ "reduces" the effect of liquid viscosity (and as a consequence of the overall $Oh$ number) to the transition of breakup modes. For the same $We$ number, higher initial $d_{eq}$ leads to lower $Oh_{eq}$ compared to a spherical droplet ($d_0$, $Oh$) resulting to a "higher" breakup regime. The combined effect of the equivalent $Oh_{eq}$ and $We_{eq}$ is to translate the experimental data upwards and to the left; meaning that if one is held constant the introduction of $d_{eq}$ leads to "higher" breakup regimes.

For the two least viscous solutions (50% and 80% glycerol) the overlapping of the experimental data appears decreased compared to the $We$-$Oh$ plane representation. Additionally, both sets of experimental data are in better agreement with the two theoretical curves (Figure 8 and Figure 9).

The equivalent dimensionless groups ($We_{eq}$ and $Oh_{eq}$) incorporate the initial non-sphericity of the droplets which lead to a better mapping of the experimental data than the conventional $We$ and $Oh$ numbers. For droplets with $Oh > 1$ (97% glycerol) the regions where breakup modes overlap remains. As the viscosity effects become dominant, the role of $Oh$ number becomes important.

Effect of liquid viscosity to the kinematic characteristics of droplets

The displacement $x^*_t$, velocity $u^*_t$ and acceleration $a^*_t$ of the centre of droplet’s viewable area are presented as a function of dimensionless time $t^*$ for water and three glycerol-water solutions (50%, 80% and 97% glycerol). The results of the study are split in two sections, for low and high $We$ numbers, or in other words for no and bag-stamen breakup regimes. The aspect ratio $AR$ chosen for this study is $AR = 1.2$. It could be achieved with all liquid with satisfactory repeatability leading to minimisation of the errors regarding the droplet’s volume and initial $AR$; both of the errors are below 5%. For the normalisation of the results the diameter $d_0$ is used. This is done in order to maintain the physical meaning of the kinematic characteristics. For example, an initially spherical droplet translates faster than an initially non-spherical. When $d_{eq}$ is employed for the normalisation of the velocity this would not be the case for the non-dimensional velocity $u^*_t$. However, in the present paper, since the is constant ($AR = 1.2$), diameter $d_{eq}$ could be used as well as it is the same for all breakup cases presented.
Figure 3. Morphological classification of breakup modes of spherical and non-spherical droplets consist of water and Mix-1, 2 and 3 (50%, 80% and 97% glycerol) in \( W_e - Oh \) plane derived with \( d_0 \)

Figure 4. Morphological classification of breakup modes of spherical and non-spherical droplets consist of water and Mix-1, 2 and 3 (50%, 80% and 97% glycerol) in \( W_{eq} - Oh_{eq} \) plane derived with \( d_{eq} \)

Low \( W_e \) number - No breakup regime

The \( W_e \) number ranges from 10 to 13 with the \( Oh \) number being \( 3.4 \times 10^{-3} \), 0.02, 0.19 and 2.2 for increasing liquid viscosities. The diameter \( d_0 \) based on the droplet volume is \( d_0 = 1.25 \pm 0.05 \) mm and the AR = \( 1.20 \pm 0.02 \). The variation in the values for \( W_e \) number occurs due to the difference in the physical properties of the liquids, namely the density and the surface tension.

Figure 5a presents a comparison of the non-dimensional displacement \( x_\ast \) of the centre of viewable area of the droplet with dimensionless time \( t_\ast \) for the four liquids (water and 50%, 80% and 97% glycerol) with the 3rd degree fitting curve of Pilch and Erdman [4] which is independent of viscosity. The fitting curve generally under-predicts the displacement of the droplet and this is mainly due to the increased frontal area of the droplets compared to the spherical droplet assumed by the 3rd degree fitting curve.

Figure 5b shows the non-dimensional velocity \( u_\ast \) of the centre of viewable area of the droplet. For glycerol-water solutions, after they achieve their maximum deformation \( d_{\ast \max} \) which occurs at \( t_{\ast \max} = 1.18 \), 2.55 and 2.6 for 50%, 80% and 97% glycerol solutions respectively, they continue to translate with constant frontal area approximately equal to their maximum deformation.

Regarding the water droplet, its velocity \( u_\ast \) oscillates due to the changes of the frontal area of the droplet. At \( t_{\ast \max} = 1.07 \) the water droplet achieves its maximum deformation \( d_{\ast \max} = 1.42 \), however at \( t_{\ast \max} = 2.6 \) it becomes nearly spherical again. The reason why the oscillatory behaviour did not appear to that extent for the glycerol-water solutions is because the increased viscosity dampens the droplet oscillations. This oscillatory behaviour is not predicted by the 3rd degree fitting curve.

The velocities of the droplet as they exit the imaged area are \( u_\ast = 2.6, 2.8, 3.3 \) and 3.0 for increasing liquid viscosity and are directly related to the droplet frontal area.

The extent of the droplet’s oscillatory behaviour decreases with the increase of the liquid viscosity as also does its effect on the translation behaviour of the droplet. Figure 5c shows the temporal evolution of the normalised acceleration of the droplet \( \alpha_\ast \). The data for the acceleration were derived by fitting a 5th degree polynomial to the displacement data of the four liquids and taking the second derivative of the polynomial. A 5th degree polynomial was used so that its second derivation was a third degree, which is able to predict the oscillation; the correlation coefficient is more than 0.95 regarding the displacement data. The bars in Figure 5c indicate the difference of the fitting curve value from the corresponding value of the experimental data for the acceleration \( \alpha_\ast \).
Comparison of the temporal evolution of the (a) displacement $x^*_d$, (b) velocity $u^*_d$ and (c) acceleration $\alpha^*_d$ of oblate droplets ($AR=1.2$) under the no breakup regime for water, 50\%, 80\% and 97\% glycerol solutions with the 3$^{rd}$ degree fitting curve.

Figure 5.
Figure 6. Comparison of the temporal evolution of the (a) displacement $x^*_d$, (b) velocity $u^*_d$ and (c) acceleration $\alpha^*_d$ of the centre of mass of oblate droplets ($AR=1.2$) under the bag-stamen breakup regime for water, 50%, 80% and 97% glycerol solutions with the 3$^{rd}$ degree fitting curve [4].

High $We$ number - Bag-stamen breakup regime

Figure 6 presents the measured displacement $x^*_d$, and the deduced velocity $u^*_d$ and acceleration $\alpha^*_d$ of the droplet centre of mass with time for various liquid viscosities. The gray area of the figures correspond to the breakup initiation time $t^*_\text{init}$ of the most viscous case and is equal to $t^*_\text{init}=1.02$; the corresponding breakup initiation time for the least viscous droplet is $t^*_\text{init}=0.97$.

At short times the effect of increasing viscosity on both displacement and velocity is minor, despite the order of magnitude in the viscosity differences. Detailed differences can be seen in the acceleration values (Figure 6c). The acceleration of the water droplet at time $t^*=0$ is smaller than the acceleration for the more viscous droplet due to the higher initial deformation. In later times, due to its higher frontal area the acceleration increases and consequently its velocity increases and its displacement overtake the other droplets. It is of interest to notice that the three more viscous cases have almost the same velocity and displacement and trajectory differentiation starts much later in time, in fact approximately around the breakup initiation time.

Conclusions

The role of the initial sphericity of the droplet on the breakup process was experimentally investigated, over a range of $We$ from 10 to 200 and of the $Oh$ number from 0.01 to approximately 4. It was observed that the breakup modes of initially spherical droplets were in good agreement with the literature but equivalent $We_{eq}$ and $Oh_{eq}$ numbers were required to extend the existing morphological classification charts for initially non-spherical as well as spherical...
droplets. For the higher $Oh$ numbers ($Oh>1$) not a discernible distinction between breakup modes was possible. The kinematic characteristics of droplets of $AR=1.2$ showed that the liquid viscosity has an important role through the dampening of the internal flow field and two viscosity droplets are accelerated at higher rates due to faster deformation which results in greater frontal area.

Acknowledgments
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Nomenclature

\begin{align*}
t & \text{ time [s]} \\
*t & \text{ dimensionless time [-]} \\
AR & \text{ aspect ratio [-]} \\
We & \text{ Weber number [-]} \\
We_{eq} & \text{ equivalent Weber number [-]} \\
Oh & \text{ Ohnesorge number [-]} \\
Oh_{eq} & \text{ equivalent Ohnesorge number [-]} \\
\rho_{g,l} & \text{ gas, liquid density [kg/m}^3\text{]} \\
u_g & \text{ gas velocity [m/s]} \\
d_0 & \text{ volume based droplet diameter [m]} \\
d_{eq} & \text{ equivalent droplet diameter [m]} \\
\mu_{g,l} & \text{ gas liquid dynamic viscosity [Pas]} \\
\sigma & \text{ surface tension [N/m]} \\
\epsilon & \text{ density ratio [-]} \\
C_d & \text{ drag coefficient [-]} \\
x_d & \text{ dimensionless droplet displacement [-]} \\
u_d & \text{ dimensionless droplet velocity [-]} \\
\alpha_d & \text{ dimensionless droplet acceleration [-]}
\end{align*}

References

Numerical Investigation of Droplet Impact on Smooth Surfaces with Different Wettability Characteristics: Implementation of a dynamic contact angle treatment in OpenFOAM

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Abstract
The “Direct Numerical Simulations” (DNS) of droplet impact processes is of great interest and importance for a variety of industrial applications, where laboratory experiments might be difficult, costly and time-consuming. Furthermore, in most cases after validated against experimental data, they can be utilised to further explain the experimental measurements or to extend the experimental runs by performing “virtual” numerical experiments. In such “DNS” calculations of the dynamic topology of the interface between the liquid and gas phase, the selected dynamic contact angle treatment is a key parameter for the accurate prediction of the droplet dynamics. In the present paper, droplet impact phenomena on smooth, dry surfaces are simulated using three different contact angle treatments. For this purpose, an enhanced VOF-based model, that accounts for spurious currents reduction, which has been previously implemented in OpenFOAM CFD Toolbox, is utilised and further enhanced. Apart from the already implemented constant and dynamic contact angle treatments in OpenFOAM, the dynamic contact angle model of Kistler, that considers the maximum advancing and minimum receding contact angles, is implemented in the code. The enhanced VOF model predictions are initially compared with literature available experimental data of droplets impacting on smooth surfaces with various wettability characteristics. The constant contact angle treatment of OpenFOAM as well as the Kistler’s implementation show good qualitative and quantitative agreement with experimental results up to the point of maximum spreading, when the spreading is inertia dominated. However, only Kistler’s model succeeds to accurately predict both the advancing and the recoiling phase of the droplet impact, for a variety of surface wettability characteristics. The dynamic contact angle treatment fails to predict almost all stages of the droplet impact. The optimum version of the model is then applied for 2 additional series of parametric numerical simulations that identify and quantify the effects of surface tension and viscosity, in the droplet impact dynamics.

Keywords
Droplet impact, dynamic contact angle treatment, VOF, OpenFOAM

Introduction
In the last 20 years, many investigations of droplet impact have taken place experimentally as well as numerically. Wettability constitutes an important controlling parameter in the dynamics of droplet impact, as it can completely alter the impact characteristics and output [1]. The “Direct Numerical Simulations” (DNS) of droplet impact processes is of great interest and importance for a variety of industrial applications, where laboratory experiments might be difficult, costly and time-consuming. Furthermore, in most cases after validated against experimental data, they can be utilised to further explain the experimental measurements or to extend the experimental runs by performing “virtual” numerical experiments. In such “DNS” calculations of the dynamic topology of the interface between the liquid and gas phase, the selected Dynamic Contact Angle (DCA) treatment is a key parameter for the accurate prediction of the droplet dynamics, since it underpins the wettability characteristics of the simulated phenomenon. The droplet impact of water on a flat, solid surface has been studied by Pasandideh-Fard et al. [2]. A numerical solution of the Navier-Stokes equations, using a modified SOLA-VOF method was utilised to model the interface deformation. Yokoi et al. [3] investigated liquid droplet impact behaviour onto a dry and flat surface numerically and compared their results with experimental data, indicating the significant role of the DCA modelling in reproducing the droplet impact behaviour. Their numerical method consists of a Coupled Level Set and VOF framework (CLSVOF), a volume/surface integrated average based multi-moment method, and a continuum surface force model. The experimental work of Antonini et al. [4] is focused in the understanding of the effect of surface wettability on impact characteristics of water drops, onto solid dry surfaces. Their results indicated the role of advancing contact angle and contact angle hysteresis as fundamental wetting parameters. They also found that, generally, if Reynolds (Re) and Weber numbers (We) are high enough, the spreading drop can be
The document discusses drop impact phenomena on smooth, dry surfaces and presents a numerical model for simulating these phenomena. The model utilizes and compares three different numerical treatments for the contact angle at the solid-liquid-gas triple contact line against existing literature. Experimental data from previous studies is used to validate the model. The optimal version of the proposed numerical framework is then applied for two additional series of parametric numerical simulations (virtual experiments) that isolate, identify, and quantify the effects of surface tension and viscosity, in the droplet impact dynamics. The effect of the varied parameters on the droplet spreading factors with time is identified and quantified, and comparisons with the theoretical correlation by Roisman for the maximum droplet spreading factor are also conducted. The proposed correlation is given by Equation 1.

\[ \beta_{\text{max}} = 0.87 Re^{1/5} - 0.4 Re^{2/5} We^{-1/2} \]  

(1)

### Numerical Method

With the VOF approach, the transport equation for the volume fraction, \( \alpha \), of the secondary (dispersed) phase is solved simultaneously with a single set of continuity and Navier–Stokes equations for the whole flow field. The corresponding volume fraction of the primary phase is simply calculated as \( 1 - \alpha \). The main underlying assumptions are that the two fluids are Newtonian, incompressible, and immiscible. The governing equations can be written as:

\[ \nabla \cdot \vec{U} = 0 \]  

(2)

\[ \frac{\partial p_b \vec{U}}{\partial t} + \nabla \cdot \left( p_b \vec{U} \vec{U} \right) = -\nabla p + \nabla \cdot \left( \rho_b \left( \nabla \vec{U} + \nabla \vec{U}^T \right) + \rho_b f + F_D \right) \]  

(3)

\[ \frac{\partial \alpha}{\partial t} + \nabla \cdot \left( \alpha \vec{U} \right) - \nabla \cdot \left( \alpha (1 - \alpha) \vec{U}_p \right) = 0 \]  

(4)

where the bulk fluid properties are calculated as weighted averages of the individual phase properties as follows,
In the VOF method, $\alpha$ is advected by the velocity field. For the case of incompressible flow, this is equivalent to volume fraction conservation, which makes the method mass conservative. Interface sharpening is very important in simulating two-phase flows of two immiscible fluids. In OpenFOAM the sharpening of the interface is achieved artificially by introducing an extra compression term in the advection equation of $\alpha$ (last term in the left-hand side of Eq. 4). $U_r$ is the artificial compression velocity which is calculated from the following relationship,

$$U_r = n_f \min \left[ c_r \left| \frac{\delta \alpha}{\delta t} \right| \right] \max \left( \frac{\delta t}{\tau_r} \right)$$  \hspace{1cm} (7)

Finally, the surface tension force is modelled as a volumetric force using the Continuum Surface Force (CSF) method by Brackbill et al. [10], applying the following equations:

$$F_s = \gamma \kappa (\nabla \alpha) \hspace{1cm} (8)$$

$$\kappa = \nabla \cdot \left( \frac{\nabla \alpha}{|\nabla \alpha|} \right) \hspace{1cm} (9)$$

where $\gamma$ is the surface tension coefficient and $\kappa$ is the curvature of the interface. As mentioned in the introduction section of the present paper the utilized numerical framework constitutes an enhanced version of the original VOF-based solver of OpenFOAM [8], that suppresses numerical artefacts of the original model, known as “spurious currents”. The proposed enhancement involves the calculation of the interface curvature $\kappa$ using the smoothed volume fraction values $\bar{\alpha}$, which are obtained from the initially calculated $\alpha$ field, smoothing it over a finite region near the interface. All other equations are using the initially calculated (non-smoothed) volume fraction values of $\alpha$. Further details on the proposed numerical modelling framework can be found in [8].

In OpenFOAM, there are two ways to predict the evolution of the contact angle between the liquid-gas interface and the solid wall boundary. The simplest approach is to assign a constant value equal to the equilibrium contact angle, and therefore neglecting the contact angle hysteresis. This is usually known as static or constant contact angle treatment. A more complicated approach involves the application of a contact angle that varies with respect to the instantaneous flow quantities. Such treatments are known as dynamic contact angle treatments (DCA). The original distribution of OpenFOAM includes both a CCA treatment as well as a DCA treatment.

For the purposes of the present investigation, after the satisfactory predictions in a similar investigation by Criscione et al. [11], the adopted, enhanced, VOF-based solver from the work of Georgoulas et al. [8], is further improved by implementing an additional DCA treatment in the solver. The proposed treatment, is known as Kistler’s model [12], and it calculates the DCA, $\theta_d$, using the Hoffman function, $f_{\text{Hoff}}$, as follows:

$$\theta_d = f_{\text{Hoff}} \left[ C_a + f_{\text{Hoff}}^{-1} (\theta_r) \right] \hspace{1cm} (10)$$

where $\theta_r$ is the equilibrium contact angle. The capillary number, $C_a$, is calculated as $C_a = \frac{U \alpha}{\gamma}$ and $U_{CL}$ is the spreading velocity of the contact line. $f_{\text{Hoff}}^{-1}$ is the inverse function of “Hoffman’s” empirical function which is given in the following form [11].

$$f_{\text{Hoff}} = \cos \left[ 1 - 2 \tanh \left( 5.16 \left( \frac{x}{1.31 \times 10^{-6}} \right)^{0.706} \right) \right] \hspace{1cm} (11)$$

Validation of Numerical Method

All simulations presented in the present paper constitute 2D axisymmetric runs. The computational domain is a 5° wedge, with 5 mm width and 8 mm height. The computational mesh consists of 1.6 million hexahedral cells (1000x1600x1). The dimensions of the computational domain and the total number of computational cells, were
selected after an initial sensitivity analysis and a mesh independency study, respectively. The computational
domain, mesh and boundary conditions are illustrated in Figure 1. To validate the adopted, enhanced, VOF-based
solver for droplet impact cases and compare the numerical predictions with the previously mentioned, contact
angle treatments, four different, literature available, experiments on droplet impact are numerically reproduced. In
the first case, all three contact angle models are tested, while in the rest three cases only Kistler’s dynamic
contact angle is used, to reproduce the proposed experimental runs. The initial conditions and the wetting
characteristics of the proposed experimental runs are summarized in Table 1.

As it can be seen for the axisymmetric simulations of the present paper, a structured computational mesh,
consisting of hexahedral and prismatic elements was used, with grid clustering towards the bottom left corner of
the computational domain (centre of droplet impact). At the solid walls, a no-slip velocity boundary condition was
used with a fixed flux pressure boundary condition for the pressure values and a contact angle condition,
according to the selected in each case treatment, for the volume fraction values. These contact angle boundary
conditions are used to correct the surface normal vector, and therefore adjust the curvature of the interface near
the wall, in relation to the prescribed wettability characteristics. At the outlet, a fixed valued (atmospheric)
pressure boundary condition and a zero-gradient boundary condition for the volume fraction were used, while for
the velocity values a special (combined) type of boundary condition was used that applies a zero-gradient when
the fluid mixture exits the computational domain and a fixed value condition to the tangential velocity component,
in cases that fluid enters the domain. Further details regarding the utilised boundary conditions can be found in
OpenFOAM Documentation [13].

<table>
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<th>D₀ [m]</th>
<th>U₀ [m/s]</th>
<th>We</th>
<th>Re</th>
<th>θₑ [°]</th>
<th>θₐ [°]</th>
<th>θᵣ [°]</th>
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<td>132</td>
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<tr>
<td>IV</td>
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<td>0.44</td>
<td>5.3</td>
<td>880</td>
<td>158</td>
<td>165</td>
<td>142</td>
</tr>
</tbody>
</table>

As it can be observed from Table 1, the selected validation cases constitute experiments with various impact as
well as wettability characteristics. Experiments I and II constitute droplet impacts in hydrophilic surfaces, while in
experiments III and IV hydrophobic and super-hydrophobic surfaces are used for the impacts, respectively.
As mention previously, in the case of Experiment I all three different contact angle treatments are used to
numerically reproduce the considered droplet impact. A macroscopic comparison of the numerical predictions for
the droplet evolution with the corresponding experimental snapshots at the same time instances, for each
treatment, is illustrated in Figure 2. For a more quantitative comparison, the contact diameter of the droplet with
the solid surface with respect to time is plotted for each of the three numerical simulations as well as for the
experimental measurements, in the diagram of Figure 3.
Figure 2. Droplet evolution with time - Comparison of numerical predictions for all three contact angle treatments (present investigation) with corresponding experimental snapshots from [2]. The velocity magnitude field in a central vertical section of the droplet, is also shown in the numerical snapshots.

Figure 3. Contact diameter with time - Comparison of numerical predictions (present investigation) for all three contact angle treatments with corresponding experimental data from [2].

After examining Figures 2 and 3, it is obvious that both the CCA and DCA treatments implemented in the original distribution of OpenFOAM fail to predict the experimental data, while Kistler’s DCA treatment follows the experimental points well, both before and after the maximum spreading. However, in order to further check the validity of the Kistler's DCA treatment for cases with varying wettability characteristics, three additional, literature available experimental runs that are reported in [3] and [7], are numerically reproduced. In more detail, another hydrophilic (Experiment II), a hydrophobic (Experiment III) and a super-hydrophobic case (Experiment IV) are selected for this purpose. A macroscopic comparison of the numerical predictions for the droplet evolution with the corresponding experimental snapshots, is illustrated in Figure 4. For a more quantitative comparison, the contact diameter of the droplet with the solid surface with respect to time, is plotted for each case in the diagrams of Figure 5.

Figure 4. Droplet evolution with time - Comparison of numerical predictions (present investigation) using Kistler's dynamic contact angle treatment with corresponding experimental snapshots reported in [3] (top) and [7] (middle) and (bottom). The velocity magnitude field in a central vertical section of the droplet, is also shown in the numerical snapshots.
As it can be observed, Kistler’s DCA treatment successfully predicts the spatial and temporal evolution of the droplet in all stages of the considered impacts. Therefore, it can be concluded that the utilised enhanced VOF framework in conjunction with the implemented DCA treatment of Kistler, can safely be applied for the investigation of droplet impacts through “virtual” numerical experiments, as it successfully predicts the droplet impact stages in hydrophilic, hydrophobic and super-hydrophobic cases.

Parametric Analysis – Effect of fluid viscosity and surface tension

In the present section of the paper, the optimum version of the VOF-based numerical framework that is presented and validated against experimental data in the previous sections, is further applied for the conduction of two additional series of parametric numerical simulations. The proposed numerical experiments mainly aim to identify and quantify the effects of viscosity and surface tension on the spatial and temporal evolution of the droplets after their impact on a hydrophilic surface. Furthermore, the validity of a widely used theoretical correlation by Roisman [9] (Equation 1) for the case of “virtual” fluids is assessed. For this purpose, the validation case reproducing Experiment II is selected as the base case for the proposed parametric numerical investigations. In the first parametric investigation 5 additional simulations are conducted “virtually” varying only the liquid viscosity, by factors of 0.5, 1.5, 2.0, 3.0 and 3.5, while keeping all the other properties and impact characteristics constant and equal to the base case. In the second parametric investigation, again 5 additional simulations are conducted virtually varying only the surface tension coefficient, by factors of 0.5, 1.5, 2.0, 3.0 and 3.5, while keeping all the other properties and impact characteristics constant and equal to the base case. The evolution of the spreading factor $\beta$ with dimensionless time $t^*$ for each case is plotted. The spreading factor is calculated as the contact diameter over the initial droplet diameter $r_l$ while the dimensionless time $t^*$ is calculated as $t \frac{D_l}{D_0}$. The effects of the variation of viscosity and surface tension on the spreading factor $\beta$ with respect to dimensionless time $t^*$ are given in Figures 6(a) and 6(b). In each case the corresponding maximum spreading factor from Equation 1 (Roisman correlation [9]) is plotted for comparison purposes.
Figure 6. (a) Spreading factor vs dimensionless time – effect of viscosity variation (b) spreading factor vs dimensionless time – effect of surface tension variation. Dotted lines correspond to the maximum spreading factor as predicted using the theoretical correlation of Roisman [9] (Equation 1).

As it can be observed from Figure 6 (a), as viscosity increases both the spreading as well as the recoiling stages of the droplet are dumped. It is characteristic however that the proposed effect, is more intense around the maximum spreading stage of the droplet, while it appears to be negligible during the initial spreading and the later recoiling stages. It can also be seen that the theoretical correlation of Roisman, in each case slightly over-predicts the resulting maximum spreading factors from the numerical simulations, by 2% up to 4%. Examining Figure 2 (b), it can be observed that as surface tension increases, the maximum spreading is significantly reduced and the recoiling stage is strengthened. The proposed effect is quite evident from the first stages of the spreading and it progressively increases towards the last stages of the recoiling phase. It is characteristic that a variation of the surface tension coefficient by a factor of just 0.5 can significantly alter the post-impact dynamics of the droplet. As for the comparison with the theoretical correlation of Roisman an increasing deviation from the numerically predicted maximum spreading factor is observed with the corresponding increase of the surface tension. The deviation between the theoretical and numerical maximum spreading factors in this case varies from 0.85% up to 55%.

The results from the present parametric investigation illustrate that the correlation proposed by Roisman [9] can be safely used for the prediction of the maximum spreading of viscous fluids with viscosities up to 3.5 times higher than water, but it significantly fails to predict the maximum spreading for fluids with surface tension more than two times the surface tension of water, such as metal fluids.

Conclusions

In the present paper, Kistler’s DCA model has been implemented in a previously improved version of the VOF-based solver of OpenFOAM. The performance of the proposed contact angle treatment is compared with the existing contact angle treatments of OpenFOAM’s original distribution, through comparison with literature reported experimental measurements on water droplets impacting on hydrophilic surfaces. To further test the revealed accuracy of the proposed DCA implementation, three additional experimental runs are numerically reproduced; a second hydrophilic case as well as a hydrophobic and a super-hydrophobic case. In all cases, Kistler’s model implementation in the utilised, enhanced VOF-based solver, successfully predicts the spreading, recoiling and rebounding stages of the droplet impact. Further application of the numerical model for the conduction of two additional series of parametric numerical experiments identifies and quantifies the effects of viscosity and surface tension variation in the post-impact stages of the droplet evolution. Comparison of the numerical predictions with a widely accepted theoretical correlation [9], indicate that the proposed correlation can be safely applied to predict the maximum spreading of fluids with higher viscosity than water but not for fluids with more than two times the surface tension of water. Finally, from the overall presentation and analysis of the results it is obvious that the proposed enhanced VOF framework can be safely used to further examine the effects of a variety of important controlling parameters to the post-impact characteristics of droplets impinging on solid surfaces with various wetting characteristics, ranging from hydrophilic to super-hydrophobic cases.

Nomenclature

$\beta_{\text{max}}$ maximum spreading factor [-] (contact droplet diameter / initial droplet diameter)
$Re$ Reynolds Number [-]
$We$ Weber Number [-]
$U$ velocity vector [ms$^{-1}$]
$\rho_f$ volumetric representation of the gravitational force [kg/m$^3$s$^{-2}$]
$p$ pressure [Pa]
$\rho_b$ bulk density [kg m$^{-3}$]
$\mu_b$ bulk viscosity [kg m$^{-1}$ s$^{-1}$]
$\alpha$ volume fraction [-]
$\rho$ density of phase 1 [kg m$^{-3}$]
$\beta$ density of phase 2 [kg m$^{-3}$]
$\mu$ viscosity of phase 1 [kg m$^{-1}$ s$^{-1}$]
$\mu_\phi$ viscosity of phase 2 [kg m$^{-1}$ s$^{-1}$]
$\gamma$ surface tension [Nm$^{-1}$]
$\kappa$ curvature of the interface [m$^{-1}$]
$F_r$ volumetric representation of the surface tension force [kg m$^{-2}$ s$^{-2}$]
$U_g$ artificial compression velocity [m s$^{-1}$]
$n_k$ cell surface normal vector
$\varphi$ mass flux [kg s$^{-1}$ m$^{-2}$]
$s_f$ surface area of the cell [m$^2$]
$C_r$ interface compression coefficient [-]
$a$ smoothed volume fraction [-]
$\theta_e$ equilibrium contact angle [$^\circ$]
$\theta_a$ advancing contact angle [$^\circ$]
$\theta_r$ receding contact angle [$^\circ$]
$\theta_d$ dynamic contact angle [$^\circ$]
$f_{Hoff}$ Hoffman function [-]
$C_o$ capillary number [-]
$D_0$ initial droplet diameter [m]
$U_0$ impact velocity [m s$^{-1}$]

**Subscripts**

$b$ bulk
$p$ cell
$f$ face

**References**


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A model for mono- and multi-component droplet heating and evaporation and its implementation into ANSYS Fluent

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Abstract
A model for heating and evaporation of mono- and multi-component droplets, based on analytical solutions to the heat transfer and species diffusion equations in the liquid phase, is summarised. The implementation of the model into ANSYS Fluent via User-Defined Functions (UDF) is described. The model is applied to the analysis of pure acetone, ethanol, and mixtures of acetone/ethanol droplet heating/cooling and evaporation. The predictions of the customised version of ANSYS Fluent with the newly implemented UDF model are verified against the results predicted by the previously developed in house, one-dimensional code.

Keywords: Droplets, multi-component fuel, heating, species diffusion, evaporation.

Introduction
The problem of modelling droplet heating and evaporation is a longstanding one and has been widely discussed in the literature [1-3]. Modelling of these processes is an integral part of the analysis of many engineering processes, including those which take place during spray combustion in Diesel engines [4]. The models incorporated in Computational Fluid Dynamics (CFD) codes used for the analysis of these processes, are based on a number of assumptions, the applicability of which to practical engineering problems is not at first evident [2-4]. One of these assumptions is that there is no temperature gradient and/or recirculation inside droplets, which could be justified in the case when liquid thermal conductivity is infinitely large. Liquid thermal conductivity is indeed much larger than that of gas in most cases, and this has been generally considered as a justification of the abovementioned assumption [4]. This approach, however, overlooks the fact that heating and evaporation of droplets in most engineering applications is not a steady state, but transient process, for which heat transfer is characterised by thermal diffusivity rather than thermal conductivity. The thermal diffusivity of liquid, in contrast to thermal conductivity, is much lower than that of gas in most cases. This allows us to question the widely used assumption that temperature gradients inside droplets can be ignored when modelling droplet heating and evaporation. The need to take into account temperature gradient inside droplets was highlighted in many experiments including those discussed in [5] (see also [2]).

The authors of [6] were perhaps the first to describe the preliminary results of implementation of a model for droplet heating and evaporation, taking into account the effects temperature gradient and recirculation inside droplets, into the commercial CFD software ANSYS Fluent. This problem was investigated later in more details in [7]. In the latter paper, the results of the implementation of the model of mono-component droplet heating and evaporation in ANSYS Fluent, using User-Defined Functions (UDF), was described. The predictions of the customised version of ANSYS Fluent were verified against experimental measurements performed at the Combustion Research Facility, Sandia National Laboratories, Livermore, California and results predicted by in-house research code for an n-dodecane droplet heated and evaporated in hot air. The main limitation of the model described in [7] was that it is applicable only to mono-component droplets, while most droplets used in engineering, including automotive applications, are multi-component. For the case of multi-component droplets, the process of species diffusion inside droplets needs to be taken into account alongside the heat transfer process [2]. The characteristic times of species diffusion are generally much longer than temperature relaxation times. Thus, taking into account species diffusion inside droplets is expected to be even more important than taking into account temperature gradients.

The main focus of our paper is on the generalisation of the results reported in [7], to the case of multi-component droplets, using the results of preliminary analysis presented in [6]. In contrast to mono-component droplets, the
modelling of multi-component droplets needs to take into account both heat and species transfer processes inside droplets. The model to be used in our analysis is based on analytical solutions to the heat transfer and species diffusion equations in the liquid phase and is described in detail in [2]. The effect of recirculation in the liquid phase is taken into account based on the Effective Thermal Conductivity (ETC)/ Effective Diffusivity (ED) model [2]. The Abramzon and Sirignano approach [8] is used for modelling the gas phase.

The main ideas of the model used in our analysis are summarised in the following section, based on [2]. Then the details of the implementation of the model into ANSYS Fluent are described. The predictions of the version of ANSYS Fluent, with the new model implemented into it, will be compared with the predictions of the previously developed one-dimensional code for the case of heating/cooling and evaporation of acetone/ethanol droplets. The choice of these droplets was based on the fact that the predictions of the one-dimensional code for them were validated against experimental data [9]. Then the main results of the paper are summarised.

Basic equations and approximations

The heat transfer inside the droplets is described by the one-dimensional heat transfer equation, assuming that all processes are spherically symmetric. The analytical solution to this equation is presented as [2]:

\[
T(r, t) = \frac{1}{r} \sum_{n=1}^{\infty} \left( I_n - \frac{R_d \sin \lambda_n}{\lambda_n^2} \zeta(0) \right) \exp\left( -\frac{\kappa \lambda_n^2 t}{b_n} \right) - \frac{R_d \sin \lambda_n}{b_n \lambda_n^2} \int_0^t \frac{d\zeta(t)}{dt} \exp\left( -\frac{\kappa \lambda_n^2 (t - \tau)}{b_n} \right) d\tau \sin \left[ \lambda_n \frac{r}{R_d} \right] + T_{\text{eff}}(t),
\]

where \( r \) is the distance from the droplet centre, \( R_d \) is the droplet radius, \( \lambda_n \) are positive solutions to the eigenvalue equation (numeration starts from the first positive root, the roots are in ascending order):

\[
\lambda \cos \lambda + h_0 \sin \lambda = 0,
\]

\[
b_n = \frac{1}{2} \left( 1 + \frac{h_0}{h_0^2 + \lambda_n^2} \right), I_n = \int_0^{R_d} \frac{r}{R_d} T(r, 0) \sin \left[ \lambda_n \frac{r}{R_d} \right] dr, h_0 = \frac{h R_d}{k_{\text{eff}}} - 1, h = \frac{k_g N_u k_g}{2 k_{\text{eff}}},
\]

\( T(r, 0) \) is initial temperature distribution inside the droplet,

\[
\kappa = \frac{k_{\text{eff}}}{c_l \rho_l R_d^2}, \zeta(t) = \frac{h T_{\text{eff}}(t) R_d}{k_{\text{eff}}}, T_{\text{eff}} = T_g + \frac{\dot{m}_d L}{2 \pi R_d N_u k_g},
\]

\( c_l \) and \( \rho_l \) are liquid specific heat capacity and density, respectively, \( L \) is specific heat of evaporation, \( h \) and \( N_u \) are convection heat transfer coefficient and Nusselt number for the gas phase, respectively, \( T_g \) is the ambient gas temperature, \( k_g \) is gas thermal conductivity, \( \dot{m}_d \) is droplet evaporation rate, \( k_{\text{eff}} \) is the effective conductivity of the liquid phase:

\[
k_{\text{eff}} = \left( 1.86 + 0.86 \tanh \left( 2.225 \log \left( \frac{\text{Pe}_l}{30} \right) \right) \right) k_l.
\]

\( k_l \) is the liquid thermal conductivity, \( \text{Pe}_l = \text{Re} \text{Pr} \) is the liquid Peclet number.

The introduction of \( k_{\text{eff}} \) was made within the so called the Effective Thermal Conductivity (ETC) model developed to take into account the effects of droplet velocity on the average value of its surface temperature. Obviously, this model cannot adequately describe the distribution of temperature inside droplets due to recirculation triggered by their relative velocities. Assuming that the time dependence of \( \zeta \) is weak (this is particularly good approximation when Equation (1) is applied to a short time step (see below)), the terms proportional to the time derivative of \( \zeta \) can be considered small. This allows us to simplify Equation (1) to:

\[
T(r, t) = \frac{1}{r} \sum_{n=1}^{\infty} \left( I_n - \frac{R_d \sin \lambda_n}{\lambda_n^2} \zeta(0) \right) \exp\left( -\frac{\kappa \lambda_n^2 t}{b_n} \right) \sin \left( \lambda_n \frac{r}{R_d} \right) + T_{\text{eff}}(t).
\]

The droplet evaporation rate \( \dot{m}_d \) is estimated as:

\[
\dot{m}_d = -2 \pi R_d \rho_g \ln(1 + B_M) \text{Sh}^*,
\]
where $D$ is the binary diffusion coefficient in the gas phase,

$$Sh^* = 2 + \left(1 + \text{Re}_d \text{Sc}^{1/3} \max(1, \text{Re}_d^{0.077})\right)^{-1}, F(B_M) = \left(1 + B_M\right)^{0.7} \ln \frac{1 + B_M}{B_M},$$

$B_d$ is the Spalding mass transfer number, $\text{Sc}$ is the Schmidt number. $h$ and $Nu$ are linked by the equation:

$$h = \frac{k_g \text{Nu}}{2R_d},$$

$$\text{Nu} = \frac{\ln(1 + B_T)}{B_T} \nu^* \nu^* = 2 + \left(1 + \text{Re}_d \text{Pr}^{1/3} \max(1, \text{Re}_d^{0.077})\right)^{-1}, F(B_T) = \left(1 + B_T\right)^{0.7} \ln \frac{1 + B_T}{B_M},$$

$Nu$ is the Nusselt number, $B_T$ is the Spalding heat transfer number and $\text{Pr}$ is the Prandtl number for the gas phase.

In the limit of infinitely large liquid thermal conductivity, Equation (1) can be simplified to (see [2] for the details):

$$c_p m_d \frac{dT}{dt} = Nu \frac{k_g}{2R_d} A_d (T_g - T_s) + L m_d,$$

(6)

Where $m_d$, $A_d$ and $T_s$ are the droplet mass, surface area and surface temperature, respectively. The derivation of Equation (1) was based on the assumption that $h$ and $T_g$ are constant during the process of droplet heating and evaporation which is not satisfied in most engineering applications (e.g. the reduction of $R_d$ during the evaporation process would lead to an increase in $h$). That means that neither Equation (1) nor Equation (4) can be used directly during the whole period of droplet heating and evaporation. Both these equations, however, can be used during short time steps $\Delta t$ when the assumption of constant $h$ and $T_g$ is valid. In this case, the solution to these equations at the end of the time step can be used as the initial condition for following time step with updated values of all other parameters, if necessary. As in [7] our analysis is based on Equation (4).

As in the case of heat transfer equation inside droplets, we assume that species diffusion inside them is described by the one-dimensional species diffusion equation and all processes are spherically symmetric. The analytical solution to this equation for the mass fractions $Y_i$ is presented as [2]:

$$Y_i(r, t) = \epsilon_i + \frac{1}{r} \exp \left[\sum_{n=1}^{\infty} \frac{1}{b_{Yn}} \exp \left[\frac{-D_{eff} \lambda_n^2}{R_d} \frac{1}{t} \left(I_{0n} + \epsilon_i \frac{1}{\lambda_n} \left(1 + h_{Y0} \right) \sinh \left(\lambda_0 \frac{r}{R_d}\right) \right] \sinh \left(\lambda_n \frac{r}{R_d}\right) \right] \right],$$

(7)

where $\lambda_0$ and $\lambda_n$ are solutions to the eigenvalue equations:

$$\lambda_0 \cosh \lambda_0 + h_{Y0} \sinh \lambda_0 = 0, \lambda_n \cos \lambda_n + h_{Yn} \sin \lambda_n = 0, \ (n = 1, 2, ...).$$

(8)

$\lambda_n \ (n \geq 1)$ are in ascending order,$\epsilon_i = \frac{Y_{vis,i}}{\sum_i Y_{vis,i}}, Y_{vis}$ is vapoour mass fraction at the surface of the droplet,

$$b_{Y0} = -\frac{R_d}{2} \left(1 + \frac{h_{Y0}}{h_{Tg} - \lambda_0^2}\right), b_{Yn} = \frac{R_d}{2} \left(1 + \frac{h_{Y0}}{h_{Tg} + \lambda_n^2}\right), h_{0Y} = -\left(1 + \frac{\alpha R_d}{D_t}\right),$$

$$I_{00} = \int_0^{R_d} \frac{Y_i(r, 0) \sinh \lambda_0 \frac{r}{R_d} dr, I_{in} = \int_0^{R_d} \frac{r}{R_d} Y_i(r, 0) \sin \left[\lambda_n \frac{r}{R_d}\right] dr, n \geq 1,}$$

$Y_i(r, 0)$ is the initial $i$th species mass fraction distribution inside the droplet. $D_{eff}$ is the effective species diffusivity in the liquid phase assumed to be the same for all species and defined as [2]

$$D_{eff} = \left(1.86 + 0.86 \tanh \left(2.22 \log \left(\frac{Pe_t}{30}\right)\right)\right) D_l,$$

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$D_l$ is the liquid diffusivity, $Pe_l = Re_l Sc_l$ is the liquid Peclet number referring to species diffusion. The introduction of $D_{lw}$ was made within the so-called Effective Diffusivity (ED) model developed to take into account the effects of droplet velocity on the average values of its surface mass fractions in the liquid phase. This model cannot adequately describe the distribution of species inside droplets due to recirculation triggered by their relative velocities. Vapour molar fractions of species at the surface of the droplets and the corresponding molar fractions in the liquid phase are linked by Rault law [2].

**Implementation of the model into ANSYS Fluent**

Equation (7) was implemented into the customised version of ANSYS Fluent alongside with the previously implemented Equation (4). The right-hand sides of these equations were calculated via the User Defined Functions (UDF); thermodynamic and transport parameters were calculated based on the average temperature inside the droplets, using Simpson's method [10]. The droplet volume was discretised into $N_v = 500$ concentric layers to calculate the series in Equations (4) and (7). The integrals ($I_n$ and $I_o$) and average temperatures inside droplets were also calculated using the Simpson's method with 501 points for 500 layers. At each time step temperatures and species distributions were calculated from Equations (4) and (7). Time-steps for calculations were taken equal to $\delta t = 10^{-6}$ seconds. The roots of the eigenvalue Equations (2) and (8) were found using the bisection method with accuracy of $10^{-6}$.

**Results and discussion**

The newly developed customised version of ANSYS Fluent was applied to the analysis of cooling and evaporation of droplets of ethanol, acetone and mixture of ethanol and acetone, as described in the experiments the results of which are presented in [9]. The transport and thermodynamic properties of acetone and ethanol were taken from [9]. The initial droplet temperatures were in the range 293-296 K, while the temperatures of ambient air were in the range 305-312 K at atmospheric pressure. Gas parameters in the vicinity of the droplet surface were calculated based on reference temperature $T_{ref} = (2T_s + T_g) / 3$. 200 eigenvalues were used to calculate temperature distribution and 10 eigenvalues were used to calculate species mass fraction distribution. Gas and liquid properties are taken from [5,11].

The results predicted by ANSYS Fluent were verified against the results predicted by the one-dimensional in-house code. The predictions of the latter code, in their turn, were verified against the predictions of the code based on the numerical solutions of the heat transfer and species diffusion equations [9]. This allows us to use the abovementioned code (IHC) as the reference code to verify the results for heating and evaporation of droplets of various compositions predicted by the new customised version of ANSYS Fluent.

The results of the comparison between ANSYS Fluent and in-house code for the temperatures at the centre and surface of the droplet and droplet average temperature are shown in Figs. 1-5 for various droplet and gas parameters and various compositions of droplets: pure acetone (Fig. 1), pure ethanol (Fig. 2), 75% ethanol and 25% acetone (Fig. 3), 50% ethanol and 50% acetone (Fig. 4), 25% ethanol and 75% acetone (Fig. 5). Input parameters used in calculations are summarised in Table 1. As can be seen from these figures, in all cases the agreements between Fluent and IHC results are reasonably good. The percentage errors for the abovementioned three temperatures after 7 ms is between 1.0-4.0% for acetone, 6.0-6.1% for ethanol, between 2.0-3.5% for the mixture with 25% of ethanol, between 0.5-1.8% for the mixture with 50% of ethanol and between 0.3-1.8% for the mixture with 75% of ethanol. Note that the results shown in Figs. 1 and 2 were obtained without using the new features of the ANSYS Fluent code developed in our work (they could be obtained based on the version of the code developed in [7]). In all cases shown in Figs. 1-5 the changes in droplet radii were small and the corresponding curves are not shown.

**Table 1** Droplet and gas temperatures, droplet diameters and approximations of droplet velocities, inferred from [11] and used in calculations.

<table>
<thead>
<tr>
<th>Composition</th>
<th>Droplet temperature (K)</th>
<th>Droplet diameter (µm)</th>
<th>Gas temperature (K)</th>
<th>Droplet velocity approximations in m/s (t is in ms)</th>
</tr>
</thead>
<tbody>
<tr>
<td>acetone</td>
<td>308.25</td>
<td>143.4</td>
<td>294.65</td>
<td>12.81 – 0.316t</td>
</tr>
<tr>
<td>ethanol</td>
<td>311.15</td>
<td>140.8</td>
<td>295.15</td>
<td>12.30 – 0.344t</td>
</tr>
<tr>
<td>+25% ethanol</td>
<td>305.65</td>
<td>133.8</td>
<td>294.25</td>
<td>12.75 – 0.370t</td>
</tr>
<tr>
<td>+50% ethanol</td>
<td>310.65</td>
<td>142.7</td>
<td>293.95</td>
<td>12.71 – 0.488t</td>
</tr>
<tr>
<td>+75% ethanol</td>
<td>311.75</td>
<td>137.1</td>
<td>294.75</td>
<td>12.28 – 0.306t</td>
</tr>
</tbody>
</table>
As can be seen in Figs. 1-5 the difference between the temperatures at the centre and surface of the droplets and droplet average temperatures is approximately 2-9 K, which cannot be ignored in most engineering applications. This difference was ignored in the conventional version of ANSYS Fluent (e.g. [4]), which cannot be justified in the general case. The agreement between ANSYS Fluent and IHC results gives us confidence in applying the new customised version of ANSYS Fluent to more complex problems that those presented in Figures. 1-5.

**Figure 1.** Time evolution of an acetone droplet surface, average and centre temperatures ($T_s$, $T_{av}$ and $T_c$) (see Table 1). ANSYS Fluent results (dotted curves) and compared with results of the previously developed In house code (IHC) (dashed and solid curves).

**Figure 2.** Time evolution of ethanol droplet surface, average and centre temperatures ($T_s$, $T_{av}$ and $T_c$) (see Table 1). ANSYS Fluent results (dotted curves) and compared with results of the previously developed In house code (IHC) (dashed and solid curves).
Figure 3. Time evolution of 75% ethanol and 25% acetone droplet surface, average and centre temperatures ($T_s$, $T_{av}$ and $T_c$) (see Table 1). ANSYS Fluent results (dotted curves) and compared with results of the previously developed In house code (IHC) (dashed and solid curves).

Figure 4. Time evolution of 50% ethanol 50% acetone droplet surface, average and centre temperatures ($T_s$, $T_{av}$ and $T_c$) (see Table 1). ANSYS Fluent results (dotted curves) and compared with results of the previously developed In house code (IHC) (dashed and solid curves).
Conclusions

A model for heating and evaporation of mono- and multi-component droplets, based on analytical solutions to the heat transfer and species diffusion equations in the liquid phase, is summarised. The implementation of the model into ANSYS Fluent via User-Defined Functions (UDF) is described. The model is applied to the analysis of pure acetone, ethanol, and mixtures of acetone/ethanol droplets heating/cooling and evaporation. The predictions of the customised version of ANSYS Fluent with the new model implemented into it are verified against the results predicted by previously developed one-dimensional in-house code based on the analytical solutions to the heat transfer and mass diffusion equations. The latter code in its turn was verified against the predictions of the in-house code developed at the University of Nancy (France) and validated against experimental data obtained at the same university.

The agreement between the predictions of these codes is shown to be reasonably good for mono-component (pure acetone and ethanol) and multi-component droplets comprising acetone with 25, 50 and 75-percentage mass fractions of ethanol, with input parameters used for previous validation of the in-house code. This gives us confidence in using the new customised version of ANSYS Fluent for the analysis of more complex engineering processes.

Acknowledgements

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### Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Bu; Br$</td>
<td>Spalding mass and heat transfer numbers</td>
</tr>
<tr>
<td>$b_n$</td>
<td>Parameter introduced in (1)</td>
</tr>
<tr>
<td>$b_{Yn}$</td>
<td>Parameter introduced in (7)</td>
</tr>
<tr>
<td>$c_p$</td>
<td>Specific heat capacity at constant pressure</td>
</tr>
<tr>
<td>$D$</td>
<td>Binary diffusivity coefficient of vapour in air</td>
</tr>
<tr>
<td>$F$</td>
<td>Function introduced in $Sh^<em>$ and $Nu^</em>$</td>
</tr>
<tr>
<td>$h$</td>
<td>Convection heat transfer coefficient</td>
</tr>
<tr>
<td>$h_0$</td>
<td>Parameter introduced in (2)</td>
</tr>
<tr>
<td>$h_{Y0}$</td>
<td>Parameter introduced in (8)</td>
</tr>
<tr>
<td>$I_n$</td>
<td>Integrals, used in Solutions (1) and (4)</td>
</tr>
<tr>
<td>$I_{in}$</td>
<td>Integrals, used in Solution (7)</td>
</tr>
<tr>
<td>$j$</td>
<td>Parameter, defined in (3)</td>
</tr>
<tr>
<td>$k$</td>
<td>Thermal conductivity</td>
</tr>
<tr>
<td>$L$</td>
<td>Latent heat of evaporation</td>
</tr>
<tr>
<td>$m$</td>
<td>Mass</td>
</tr>
<tr>
<td>$ṁ_d$</td>
<td>Evaporation rate</td>
</tr>
<tr>
<td>$M$</td>
<td>Molar mass</td>
</tr>
<tr>
<td>$N_L$</td>
<td>Number of layers inside a droplet</td>
</tr>
<tr>
<td>$Nu$</td>
<td>Nusselt number</td>
</tr>
<tr>
<td>$Pe$</td>
<td>Peclet number</td>
</tr>
<tr>
<td>$P$</td>
<td>Pressure</td>
</tr>
<tr>
<td>$Pr$</td>
<td>Prandtl number</td>
</tr>
<tr>
<td>$q$</td>
<td>Heat flux</td>
</tr>
<tr>
<td>$r$</td>
<td>Distance from the centre of the droplet</td>
</tr>
<tr>
<td>$R_d$</td>
<td>Radius of a droplet</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Greek symbols</th>
<th>Definition</th>
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</thead>
<tbody>
<tr>
<td>$ε$</td>
<td>Vapour species mass fractions</td>
</tr>
<tr>
<td>$κ$</td>
<td>Parameter introduced in (1)</td>
</tr>
<tr>
<td>$λ_n$</td>
<td>Eigenvalues</td>
</tr>
<tr>
<td>$μ$</td>
<td>Dynamic viscosity</td>
</tr>
<tr>
<td>$ρ$</td>
<td>Density</td>
</tr>
<tr>
<td>$φ$</td>
<td>Parameter defined by Equation (4)</td>
</tr>
<tr>
<td>$Χ$</td>
<td>Correction function defined by Equation (1c)</td>
</tr>
<tr>
<td>$ζ$</td>
<td>parameter defined by (1c)</td>
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<table>
<thead>
<tr>
<th>Subscripts</th>
<th>Definition</th>
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<tbody>
<tr>
<td>$d$</td>
<td>Droplet</td>
</tr>
<tr>
<td>$eff$</td>
<td>Effective</td>
</tr>
<tr>
<td>$g$</td>
<td>Gas</td>
</tr>
<tr>
<td>$int$</td>
<td>Internal</td>
</tr>
<tr>
<td>$l$</td>
<td>Liquid</td>
</tr>
</tbody>
</table>

### References


Modelling of spheroidal drop evaporation with non-uniform temperature conditions

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Abstract
The heating and evaporation of single component spherical and spheroidal drops in gaseous quiescent environment are predicted, accounting for the effect of a non-uniform distribution of the temperature at the drop surface. The analytical solution of the species conservation equations in the proper coordinate system (spherical/spheroidal) is implemented to numerically solve the energy equation in a rectangular domain. The effect of temperature non-uniformity on the local Nusselt number and global heat and evaporation rates is calculated for different species, drop deformation and gaseous temperature.

Keywords
Drop evaporation, spheroidal coordinates, non-uniform Dirichlet Boundary conditions.

Introduction
Most of the models predicting the drop heating and evaporation to be implemented in CFD codes for dispersed phase applications rely on the assumption that drops are spherical, thus allowing a simpler solution in spherical coordinates of the energy and species conservation equations. However, experimental investigation on liquid drops in multi-particle systems has revealed that they are subject to significant shape deformations while interacting with the carrier phase [1-3], due to the interaction of surface tension and fluid-dynamic stresses on the drop surface [3]. Numerical investigations on oscillating drops [4,5] have shown that the vapour and heat fluxes on the drop surface are not uniform and they were empirically correlated to the local mean curvature of the surface [1,6]. Analytical modelling of the heating and evaporation of spheroidal drops have shown that the local vapour and heat flux scale with the fourth root of the Gaussian curvature [7, 8] and later the same result was extended to a wider class of drop shapes [9].

When dynamical simulation of droplet heating and evaporation is necessary, uniform drop temperature is often assumed, on the basis of a commonly accepted belief that the internal recirculation would maintain uniform conditions. However a more accurate simulation can be obtained by using the concept of effective conductivity, firstly introduced by [10], to account for the effect of recirculation (see also [11] and [12]) and, although this cannot properly describe the temperature field inside the droplet, it can give a better estimation of the droplet surface temperature [13].

Recent modelling of heating and evaporation of spheroidal droplets [14] revealed that the uneven distribution of fluxes on the drop surface causes a corresponding uneven distribution of temperature on the drop surface, during most of the drop lifetime. This non-uniform temperature distribution affects the heat and vapour flow fields in a non negligible way.

The motivation of the work reported here is to investigate, through a combined analytical-numerical solution of the species and energy conservation equations, the effect of non-uniform Dirichlet boundary conditions at the drop surface (for spheroidal liquid drops) on the local heat and mass transfer coefficients.

Mathematical modelling
The evaporation of a single-component drop under quasi-steady conditions in a quiescent atmosphere, where the Stefan flow characterises the flow field, is described by the species conservation equations coupled with the energy conservation equation:

\[ \nabla \cdot n_j^{(r)} = 0 \quad p = 0.1 \]  

(1)

where:

\[ n_j^{(r)} = \rho U_j \chi_j^{(r)} - \rho D_{ij} \nabla \chi_j^{(r)} \quad p = 0.1 \]  

(2)
are the mass fluxes, \( p=1 \) stands for the evaporating component and \( p =0 \) for the gas. After summation, equations (1) yield the mass conservation equation:

\[
\nabla_j \rho U_j = 0
\]

These three equations are then not independent and one of the species conservation can be disregarded. Moreover, assuming that the diffusion of component \( p =0 \) into the drop can be neglected, the mass flux of the component \( p =0 \) is nil at drop surface and then is nil everywhere. This last observation, after introducing the new variable: \( G = \ln(1 - \chi^{(1)}) \), and assuming constant properties, allows to write the conservation equations under the form:

\[
\nabla^2 G = 0
\]

(see also [9] for further details). The evaporation model is coupled with the energy equation, which has the form:

\[
Le^{-1} \nabla_j G \nabla^2 T - \nabla^2 T = 0
\]

where \( Le = \frac{k}{\rho D_v c_p} \) (see again [9] for further details).

### Spherical and spheroidal drops

Equation (4) and (5) can be used to model heating and evaporation of drops of any shape, since the drop shape enters the problem through the boundary conditions. The case of spherical and spheroidal drops can be more easily treated solving the problem in proper coordinate systems. Using the spherical coordinates:

\[
x = R_0 \frac{1 - \eta^2}{\zeta} \cos \varphi; \quad y = R_0 \frac{1 - \eta^2}{\zeta} \sin \varphi; \quad z = R_0 \frac{\eta}{\zeta}
\]

where:

\[
\zeta = \frac{R_0}{r}; \quad \eta = \cos \theta
\]

the drop surface of a spherical drop is defined by the equation \( \zeta = \zeta_0 \) and similarly in spheroidal prolate and oblate coordinates:

\[
x = a \sqrt{\zeta^2 - 1} \sqrt{1 - \eta^2} \cos \varphi; \quad y = a \sqrt{\zeta^2 - 1} \sqrt{1 - \eta^2} \sin \varphi; \quad z = a \zeta \eta \quad \text{(prolate)}
\]

\[
x = a \sqrt{\zeta^2 + 1} \sqrt{1 - \eta^2} \cos \varphi; \quad y = a \sqrt{\zeta^2 + 1} \sqrt{1 - \eta^2} \sin \varphi; \quad z = a \zeta \eta \quad \text{(oblate)}
\]

the drop surface (a prolate or oblate spheroid, see figure 1) is again defined by the equation \( \zeta = \zeta_{0\beta} \) but it must be noticed that now the coordinates \( \zeta \) and \( \eta \) have different definitions.

![Drop shapes and definition of semi-axes \( a_z \) and \( a_r \).](image)

For spheroidal drops, an equivalent radius \( R_0 \) can be defined as the radius of a spherical drop having the same volume, and the constant \( a \) in equations (8) can be related to this radius by:

\[
a = R_0 \left| \frac{1 - \varepsilon^2}{\varepsilon^{1/3}} \right|^{1/2}
\]

where the eccentricity parameter \( \varepsilon \) is defined as the ratio between the axial and radial drop semi-axes (see again figure 1).

An analytical solution of equation (3) has the following form, for the prolate, oblate and spherical drops:
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Figure 2(a) shows qualitatively a sample of the vapour field around a prolate water drop with the eccentricity parameter $\varepsilon$ equal to 2.5; the surrounding gas temperature at free stream condition is fixed equal to 700K, the vapour mass fraction at infinity is taken equal to zero and the average surface temperature of the drop is equal to 340K, while seven different surface temperature profiles are imposed, defined by the maximum temperature difference at the drop surface as follows:

$$\Delta T = T_s(\zeta_0, \eta = 1) - T_s(\zeta_0, \eta = 0)$$ \hfill (15)\hfill

Figure 2. G-field and vapour flux around (a) prolate ($\varepsilon=2.5$) and (b) spherical water drops, for different surface temperature profiles; $T_\infty=700K$, $G_\infty=0$, $T_s=340K$.

The flow field is substantially affected by the non-uniform temperature boundary conditions at the drop surface, since vapour recirculation can be observed when the local surface temperature drops below the dew point value of the surrounding gas. The effect is mainly related to the temperature distribution and it is not peculiar of deformed drops, figure 2(b) shows the vapour distribution and flux around a spherical drop having a non-uniform surface temperature, and similar paths can be observed.

The calculated vapour distribution (equation 10a) is then used to numerically solve equation (5) and the local surface heat flux can be calculated. Figure 3(a) shows the heat fluxes, non-dimensionalised by the factor

$$\frac{2R}{(T_s - T_\infty)k}$$

for the case of a prolate drop ($\varepsilon=2.5$) while figure 3(b) shows the local Nusselt number, defined as:

$$Nu(\eta) = \frac{\Phi(\eta)2R}{[T_s(\eta) - T_\infty]k}$$ \hfill (16)\hfill

along the surface. The case $\Delta T =0$ is the one with uniform surface temperature and for this case the function $Nu(\eta)$ can be found analytically (see [14]), showing that the surface curvature itself influences this parameter. The results for $\Delta T \neq 0$ show that the surface heat flux is strongly influenced by the non-uniform temperature distribution (see figure 3a). The local Nusselt number is also influenced by the non-uniform temperature distribution, but to a lesser extent, specially close to the “pole” ($\eta=1$) where the effect of the different temperature distribution is lower (figure 3b).
These effects are clearly not peculiar of one particular species but their magnitude depends on the thermophysical characteristics of the species. Calculations were performed selecting five different species, whose properties are reported in Table 1. These species represent some of the most common working fluid used for spray modelling in industrial applications.

<table>
<thead>
<tr>
<th>Species</th>
<th>Mm (kg/kmol)</th>
<th>$T_{b,n}$ (K)</th>
<th>$L(T_{b,n})$ (kJ/kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>water H$_2$O</td>
<td>18.02</td>
<td>373.15</td>
<td>2257.4</td>
</tr>
<tr>
<td>ethanol C$_2$H$_6$O</td>
<td>46.07</td>
<td>351.39</td>
<td>850.53</td>
</tr>
<tr>
<td>acetone C$_3$H$_6$O</td>
<td>58.08</td>
<td>329.22</td>
<td>501.85</td>
</tr>
<tr>
<td>n-octane C$<em>8$H$</em>{18}$</td>
<td>114.23</td>
<td>398.80</td>
<td>301.10</td>
</tr>
<tr>
<td>n-dodecane C$<em>{12}$H$</em>{26}$</td>
<td>179.34</td>
<td>489.50</td>
<td>256.70</td>
</tr>
</tbody>
</table>

Table 1. Molar mass, normal boiling temperature and latent heat of evaporation for the selected liquid species.

The profiles of the local Nusselt number ($Nu$) and the percentage deviation $\Delta\%$ from the values obtained with a surface temperature uniformly equal to the mean temperature are presented in Fig. 4 for each fluid. These results were obtained maintaining constant the drop deformation ($\varepsilon=2.5$) and the gas temperature ($T_{\infty}=500$K) and setting the drop mean surface temperature equal to the corresponding quasi-steady (sometimes called plateau or asymptotic [16]) temperature. The deviations from the uniform temperature case are relatively small for water and n-dodecane while they are more relevant for acetone and n-octane. The different behaviour is due to a combination of the effects of boiling temperature and latent heat of vaporisation. These peculiarities should be considered when approximating the heat transfer coefficient from the analytic relation that can be deduced from the uniform surface temperature analysis [9, 14].

The drop deformation has an effect on the deviation of the local Nusselt number from the values for the uniform temperature case, as reported in figure 5. The increase of the deformation decreases the deviation, which should be expected since the effect of curvature becomes dominant over the effect of temperature non-uniformity when $\varepsilon$ increases.

Also the increase of the gas temperature has a similar effect (see figure 6), since in this case the relative non-uniformity of the temperature difference between drop and gas decreases, leaving again the curvature as the dominant parameter.

Finally the evaporation rates and the sensible heat rate, calculated integrating the species and heat fluxes over the drop surfaces, are reported in figure 7 as a function of the temperature non-uniformity for the case of n-dodecane. The temperature non-uniformity has a non neglectful effect on the evaporation rate, which mainly increases when the temperature becomes non-uniform, reaching relative variation of about 30% for the case $\Delta T=40^\circ$C, with a peculiar behaviour for small temperature non-uniformity, which may cause a small decrease of the evaporation rate (around 1%) when $\Delta T=+10^\circ$C. The heat rate instead increases for positive values of $\Delta T$ and decreases for negative values, but the maximum differences are lower than 8%.
Figure 4. Local Nusselt number ($\text{Nu}$) and percentage deviation ($\Delta\%$) from the uniform surface temperature case for five species: water, acetone, ethanol, n-octane, n-dodecane, for different $\Delta T$ ($\varepsilon=2.5$, $T_\infty=500K$, $T_s=225K$).
Figure 5. Local Nusselt number ($\textit{Nu}$) and percentage deviation ($\Delta \%$) (figures (a) and (b) respectively) for different values of $\varepsilon$ (n-dodecane, $T_\infty = 700\, \text{K}$, $T_s = 380\, \text{K}$, $\Delta T = 20\, \text{K}$, $P = 10^5\, \text{Pa}$).

Figure 6. Local Nusselt number ($\textit{Nu}$) and percentage deviation ($\Delta \%$) (figures (a) and (b) respectively) for different $T_\infty$ (n-dodecane, $\varepsilon = 2.5$, $T_s = 380\, \text{K}$, $\Delta T = 20\, \text{K}$, $P = 10^5\, \text{Pa}$).

Figure 7. Evaporation rate and heat rate for a n-dodecane prolate drop ($\varepsilon = 2.5$) as a function of the temperature profile; the values are non-dimensionalised by the respective values for the uniform surface temperature case.

Conclusions
The effect of temperature non-uniformity on the heating and evaporation of spherical and spheroidal drops in a still gaseous environment are investigated analytically and numerically. The species conservation equations are analytically solved in proper coordinate systems (spherical or spheroidal) and the energy equation is numerically solved in the same coordinate system.
A detailed analysis is reported for the case of a prolate evaporating drop, accounting for different species (water, acetone, n-octane, ethanol, n-dodecane), different gas temperature, drop deformation and temperature non-uniformity.

The effects on the local mass flux can become quite important, with local re-circulations when the temperature differences between the drop pole and equator become relative large (20 to 40°C).

The local Nusselt number is found to depend on local curvature and temperature, although for not too large values of the maximum surface temperature variation (less than 20°C) the effect of curvature prevails and the analytical values obtained for the uniform temperature case are still usable with acceptable errors.

The local heat transfer coefficient is less affected by the non-uniformity of surface temperature when the deformation is large and when the gas temperature increases.

The total evaporation rate is affected by the temperature distribution and can increase up to 30% when drop non-uniformity is increased up to 40°C, still maintaining the same average surface temperature. The heat rate is less affected showing deviation less than 8% for temperature difference between drop pole and equator as large as 40°C.

References

Nomenclature
Roman symbols
- \( a \) length scale in spheroidal coordinate [m]
- \( b, c, d \) constants, eqs. (10) [-]
- \( c_{p,v} \) vapour heat capacity [J/kgK]
- \( D_{10} \) mass diffusivity \([m^2/s]\)
- \( G \) non-dimensional function [-]
- \( k \) thermal conductivity \([W/mK]\)
- \( L_e \) Lewis number [-]
- \( m_{ev} \) evaporation rate \([kg/s]\)
- \( M_m \) molar mass \([kg/kmol]\)
- \( n_s \) mass flux \([kg/sm^2]\)

Greek symbols
- \( \varepsilon \) drop eccentricity parameter [-]
- \( \chi \) mass fraction [-]
- \( \gamma, \eta, \zeta \) spheroidal coordinate system [-]

Subscripts
- \( k, p \) index [-]
- \( ref \) reference case [-]
- \( v \) vapour [-]
- \( \infty \) at infinite [-]
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