Full internship report

Modelling of evaporating droplets in a monodisperse spray and vortex ring-like structure in internal combustion engines

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**Notations**

CFD – Computational Fluid Dynamics;

c\textsubscript{p} – heat capacity of a particle material;

C – distance parameter : \( C = \frac{DBD}{d} \);

d – droplet diameter;

DBD – distance between droplets;

k – gas thermal conductivity;

m – mass;

Re – Reynolds number, \( Re = \frac{\rho Ud}{\mu} \);

SHRL – Sir Harry Ricardo Laboratory;

T – gas temperature;

TBD – time between droplets’ injection;

u – velocity component along x-axis;

U – droplet velocity scale;

UoB – University of Brighton;

UDF – user-defined function written in C, ANSYS Fluent.

Greek letters:

\( \rho \) – density;

\( \mu \) – dynamic viscosity;

Subscripts:

\( i \) – index for number of droplets, time steps, or components;

\( g \) – gas (air) parameter;

\( p \) – particle parameter.
I. **Introduction**

This report covers two subjects studied during the three month placement in the University of Brighton, School of Computing, Engineering and Mathematics, Centre for Automotive Engineering, Sir Harry Ricardo Laboratories (SHRL), modelling research group, from the 13\textsuperscript{th} of January to the 4\textsuperscript{th} of April 2014.

The first part of the report is focused on droplet evaporation process and interaction between droplets in a fuel spray. When a fuel spray is injected into an engine cylinder a large quantity of droplets is formed, often travelling in groups, hence the droplet-to-droplet interactions take place. A better knowledge of the phenomenon will allow us to significantly improve and control fuel evaporation in engines, thus improving the engine efficiency. Whilst droplets are moving in clusters under realistic engine spray conditions, our study will focus on a simplified case of droplets moving in a straight line at a certain distance between the droplets, in a mono-disperse spray. This will allow us to compare our results with available experimental data for droplet tracking and evaporation.

This study is conducted in the frameworks of two research projects at the SHRL, UoB:

- ‘Energy Efficiency and Environment: a Cross-Channel Cluster (E3C3)’ [12]

Current study directly feeds into the projects, and the results of the research are expected to be implemented into the above mentioned projects directly after the placement.

In the process of the research, it has been revealed that the standard ANSYS Fluent post-processing output options do not allow us to track individual particle data. Communication with ANSYS Support and development of a corresponding UDF module took few weeks. During this period another project was considered.

The second topic focuses on vortex ring behaviour. This structure can be formed when air and/or fuel spray is injected into a cylinder. The vortex ring formation and evolution are investigated. Vortex ring size, its travel distance and other flow parameter dependence on different input parameters are considered. The vortex ring behaviour is studied in the frameworks of projects at the SHRL:

- ‘Development of the full Lagrangian approach for the analysis of vortex ring-like structures in disperse media: application to gasoline engines’ [14]
- ‘Combustion Engine for Range-Extended Electric Vehicle (CEREEV)’ [15].
Each section begins with introduction, then the underlying theory and methodology are described in detail. The research is based on CFD (ANSYS Fluent and ANSYS CFX). The validation and development ANSYS Fluent via new UDFs has been performed. The results of numerical modelling are discussed; recommendations for future research are made.

Acknowledgements

The author is grateful to the INTERREG IVa (Project E3C3, Reference 4274) for financial support. Research teams on the EU INTERREG E3C3 and EU INTERREG CEREEV projects are warmly thanked for their contribution, especially Dr. Steven Begg for the lab tour and useful discussions, Dr. Vyacheslav Stetsyuk for a very interesting lecture on Laser Induced Fluorescence applied to automotive research. The supervisory team are thanked for their support and guidance.
II. Investigation of evaporating droplet dynamics

1. Introduction and motivation

Dynamics of a droplet is influenced by its surround area. An isolated droplet in a large volume of gas, with nothing near to it, might have a behaviour that drastically differs from that of a droplet injected close to a wall or in a series of droplets. In other words, presence of a wall boundary and neighbouring droplets may have a real impact on the heat and mass exchange, and dynamics of droplet. Evaporation of a fuel droplet into air is different from its evaporation into a mixture composed of air and fuel vapour.

The purpose of current study is investigation of interactions between evaporating droplets of fuel, determination of the influence of the distance between the droplets on their velocity and evaporation rate.

There are research papers where this topic was studied (e.g. [1] and [2]), but the current understanding of droplet-to-droplet interaction is far from being sufficient. Usually simple configurations are used to study these kinds of physical phenomena properties.

The number of droplets directly influences the heat and mass transfer. The more droplets are injected, the more vapour emerges, and consequently gas properties change. The velocity of a closely injected droplet is also influenced by the wake of a previous one.

Droplet size, velocity, temperature and distance between them can be independently set at the injection. Ambient conditions can be monitored as well [3]. Then, this kind of droplet flow is an interesting tool to work on droplet-to-droplet interactions.

Fundamentally, this project is a small part of a full multi-components droplets study [11, 12]. The aim is to create the more realistic model validated by a comparison with known experimental data [4]. The current study is also based on [4], the flow parameters are set close to that in the paper [4].

Objectives

Consider dynamics of one to ten droplets, injected one after another with same velocity, mass, temperature and pressure. Our main goal is to reveal the effect of a large number of droplets on their behaviour.

The section includes the description of the methods and validation of the simulations, two cases – the case of a single droplet and the case of a series of droplets, conclusion.
2. Methodology and results

The droplet dynamics is investigated using ANSYS Fluent CFD code. The study begins with the validation of modelling to ensure that our results are reliable. The first problem considered is motion of a droplet of water; the flow is simulated numerically and results are compared to the known analytical solutions – droplet velocity and temperature relaxation processes.

The convergence of the numerical method is validated as well by reducing the value of computational time step. It was assured that the time step is fine enough.

Full description of ANSYS Fluent case for each simulation is presented in the corresponding section. To perform the study three UDFs (User-Defined Functions) were added to ANSYS Fluent CFD code in order to generate the required output parameters, which cannot be provided by standard ANSYS Fluent output options. The UDFs make it possible to monitor each particles mass, position, velocity, temperature and diameter. These UDFs were developed in the SHRL modelling research group (Dr Rybdylova, private communication).

Validation of CFD results

a) Droplet velocity and temperature relaxation

The motion of a single droplet of water is considered; the results of numerical simulation are compared to the known analytical solutions.

The momentum balance equation of a particle, moving in one direction (along x-axis) at low Reynolds number, without evaporation, takes form [3]:

\[ m_p \frac{du_p}{dt} = 3\pi \mu (u - u_p) \]  

(1)

The Reynolds number is small:

\[ Re = \frac{\rho u_d \mu}{\nu} < 0.5 \]  

(2)
Here, \( \mu \) – air viscosity; \( \rho \) – air density, \( U \) – droplet velocity scale (initial droplet velocity, if air is quiescent), \( d \) – droplet diameter, \( u_p \) – current droplet velocity, \( u \) – velocity of air, \( m_p \) – mass of a particle.

In the simplified case, air is still \( (u = 0) \), using (1) then:

\[
\frac{du_p}{dt} = -\beta u_p
\]  

\[
\beta = \frac{3\pi d\mu}{m_p}
\]  

Then the solution of (3) is:

\[
u_p = u_{p0}e^{-\beta t}
\]  

Where \( u_{p0} \) – initial droplet velocity.

The same kind of solution can be obtained for temperature relaxation process. The energy balance equation for a non-evaporating droplet, assuming that there is no temperature gradient in it is:

\[
c_p m_p \frac{dT_p}{dt} = 2\pi dk (T - T_p)
\]  

Here \( c_p \) – heat capacity of a particle material, \( T_p \) – particle temperature, \( T \) – gas (air) temperature, \( k \) – gas thermal conductivity.

Here the same method, as the one that was used for equation (3), is used. Introduce a parameter:

\[
\gamma = \frac{2\pi dk}{c_p m_p}
\]  

Then for constant air temperature and non-evaporating conditions, the solution of (6) is:

\[
T_p = T + (T_{p0} - T)e^{-\gamma t}
\]  

Where \( T_{p0} \) is the initial particle temperature

For the first case (velocity relaxation), a motion of a droplet of water is simulated using ANSYS Fluent. The choice of water is explained by the water properties – water is
harder to evaporate in comparison to acetone and ethanol (fuel liquid). Moreover, droplet and gas temperatures are set to be equal (300K).

In settings of discrete phase model, “virtual masses force”, “pressure gradient force” and “multicomponent acting on droplets” were deactivated as these processes are not taken into account in eq. (1).

This validation can only be performed for flows with Re < 0.5. Knowing all the parameters, it’s simple to find a velocity value corresponding to Reynolds number value under the limit. In Table 1 the results based on the definition of the Reynolds number (equation (2)) are presented:

<table>
<thead>
<tr>
<th>Re</th>
<th>0 &lt; Re &lt; 0.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>ρ (kg m⁻³)</td>
<td>1.1766</td>
</tr>
<tr>
<td>d (m)</td>
<td>1.338 • 10⁻⁴</td>
</tr>
<tr>
<td>μ (Pa·s)</td>
<td>1.79 • 10⁻⁵ [16]</td>
</tr>
<tr>
<td>U (m/s)</td>
<td>0 &lt; U &lt; 6.2997 • 10⁻²</td>
</tr>
</tbody>
</table>

Table 1. Velocity value interval satisfying the Stokes flow criteria

The velocity values obtained using ANSYS Fluent for the case of U = 0.6 m/s are presented in Fig 1. They are compared with the analytical solution. As it can be clearly seen the results are in good agreement. The maximum difference between the results is 0.4093%. The difference may be attributed to ANSYS Fluent dynamic drag model.
Δₘₐₓ = 0.4093\%

For temperature relaxation simulation, a static droplet is considered, and water is used as a droplet material. The values of gas and droplet temperatures are considered in this study to be very close, in order to make other thermal effects negligibly small in numerical simulations. For this case, droplet is injected at 290K into air at 300K.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_p ) (J/kg.K)</td>
<td>4182 [ANSYS]</td>
</tr>
<tr>
<td>( d ) (m)</td>
<td>( 1.338 \times 10^{-4} )</td>
</tr>
<tr>
<td>( k ) (W/m.K)</td>
<td>( 2.42 \times 10^{-2} ) [ANSYS]</td>
</tr>
<tr>
<td>( T ) (K)</td>
<td>300</td>
</tr>
<tr>
<td>( T_{p0} ) (K)</td>
<td>290</td>
</tr>
<tr>
<td>( \gamma )</td>
<td>3.885821</td>
</tr>
</tbody>
</table>

Table 2. Summary of the parameters for temperature analytical comparison

The velocity values obtained using the analytical solution and ANSYS Fluent are presented in Fig 2. As it can be clearly seen the results are practically the same.
\[ \Delta_{\text{max}} = 0\% \]

b) Convergence of CFD code

Most of the results presented in this section of the report (III. “Investigation of evaporating droplet dynamics”) correspond to the simulations with a time step equal to \(10^{-5}\) s. This value of the time step was validated as well. In order to check the convergence, the time step was refined, the results of calculations compared. The chosen criteria is:

\[
\frac{|\text{case}_1 - \text{case}_2|}{\frac{\text{case}_1 + \text{case}_2}{2}} \leq 1\%
\]  

Here, \(\text{case}_i\) stands for: data from series “i” corresponding to the same time instance \(t_n\) (velocity, temperature, etc.)

The test case chosen for this validation is as follows: two droplets are injected into a rectangular domain. The temperature of the droplets is 300K, temperature of air is 500K (see section III.4 “Series of droplets” for more details). Then the calculations with different time steps were performed, the output data collected using the UDFs (see III. 2. Methodology and
results). The results were processed: velocity components, droplets masses, temperatures and diameters were plotted and compared.

The residuals of these parameters are presented in Table 3. From this table it can be concluded that the choice of the time step size is reasonably good; no further refinement is needed.

<table>
<thead>
<tr>
<th>Droplet 1</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Ux</td>
<td>Mass</td>
<td>Temperature</td>
<td>Diameter</td>
</tr>
<tr>
<td>MAX</td>
<td>0.0418%</td>
<td>0.0050%</td>
<td>0.0086%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Droplet 2</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Ux</td>
<td>Mass</td>
<td>Temperature</td>
<td>Diameter</td>
</tr>
<tr>
<td>MAX</td>
<td>0.0720%</td>
<td>0.0086%</td>
<td>0.0148%</td>
</tr>
</tbody>
</table>

Table 3 – Convergence residuals of the simulations with the two time steps: $10^{-5}$s, $5\times10^{-6}$s
3. Single droplet evaporation

Problem formulation

First, the case of a single droplet motion is considered. The purpose of this study is to calculate droplet velocity and evaporation rate. The droplet consists of two components – 75% acetone and 25% ethanol, the initial droplet velocity is 12.75 m/s (Re = 101.2).

The simulation domain and the ambient conditions are the same for the both studies (single and a series of droplets). The injection takes place in a box representing a cylinder filled with air (P = 1 atm) (see Figure 3). A droplet of a $1.338 \times 10^{-4}$ m diameter and $9.65737 \times 10^{-10}$ kg is injected at $t = 0$ s (see Table 4 for the summary of inputs).

![Fig 3 A schematic diagram of ANSYS Fluent computational domain and case setup.](image)
Droplet temperature (°C / K) 32.5 / 305.66
Gas temperature (°C / K) 226.85 / 500
Droplet diameter (µm) 133.8
Mass droplet (kg) 9,6574.10^{-10}
Mass flow (Kg/s) 9,6574.10^{-5}
Time step (s) 1.10^{-5}
Number of time steps 1000

Table 4. Physical parameters for the single droplet evaporation case

Numerical parameters:
- Maximum number of iterations: 1000
- Time step: 1.10-5 s
- Total calculation time: 10ms

**Calculation of droplet mass:**

Mass of a droplet can be calculated using the formula:

\[
m_d = \rho_{\text{liquid}} \times \frac{4}{3} \cdot \pi \cdot r^3
\]

Where: \( \rho_{\text{liquid}} = \sum_{i=1}^{n} \vartheta_i \cdot \rho_{\text{liquid}(i)} \) — density of a mixture;
\( \vartheta_i \) — volume fraction of the i-th components (dimensionless parameter);
\( \rho_{\text{liquid}(i)} \) — density of the i-th component (kg·m\(^{-3}\)) and
\( r = \frac{d_{\text{droplet}}}{2} = \frac{d}{2} \) — radius of a droplet.

In the general case the density of a mixture is defined by the formula:

\[
\rho_{\text{liq,mix}} = \rho_{\text{liq,acetone}} \times \frac{V_{\text{acetone}}}{V_{\text{liq,mixture}}} + \rho_{\text{liq,ethanol}} \times \frac{V_{\text{ethanol}}}{V_{\text{liq,mixture}}}
\]

Corresponding densities were calculated using the Elbro’s Volume calculation method [6]:
\[ V = \sum n_i \times \Delta v_i \]

\[ \Delta v_i = A_i + B_i T + C_i T^2 \]

The values for the coefficients A, B and C for the working temperature \( T = 300K \) are provided in the Ebro’s table (see table 5 for the extract)

<table>
<thead>
<tr>
<th>Group</th>
<th>( A \text{ [cm}^3\text{/mol]} )</th>
<th>( 10^3 B \text{ [cm}^3\text{/mol K]} )</th>
<th>( 10^5 B \text{ [cm}^3\text{/mol K}^2\text{]} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( CH_3 )</td>
<td>18.96</td>
<td>45.58</td>
<td>0</td>
</tr>
<tr>
<td>( CH_2OH )</td>
<td>39.460</td>
<td>-110.60</td>
<td>23.31</td>
</tr>
<tr>
<td>( CH_2CO )</td>
<td>42.180</td>
<td>-67.17</td>
<td>22.58</td>
</tr>
</tbody>
</table>

Table 5. Elbro’s table [6]

Example of calculation for ethanol:

\[ \Delta v_{C_2H_6O} = \Delta v_{CH_3} + \Delta v_{CH_2OH} \]

\[ \Delta v_{C_2H_6O} = \left( A_{CH_3} + B_{CH_3} T + C_{CH_3} T^2 \right) + \left( A_{CH_2OH} + B_{CH_2OH} T + C_{CH_2OH} T^2 \right) \]

\[ V_{C_2H_6O} = (18.96 + 4.56 \times 10^{-2} \times 298.15 + 0 \times 298.15^2) + (39.46 - 1.11 \times 10^{-1} \times 298.15 + 2.33 \times 10^{-4} \times 298.15^2) \approx 59.8 \text{cm}^3\cdot\text{mol}^{-1} \]

Ethanol → \rho_{C_2H_6O} = \frac{V_{C_2H_6O}}{m_{C_2H_6O}} = \frac{59.8}{46} \approx 770 \text{kg} \cdot \text{m}^{-3}

The density of acetone is calculated using the same algorithm:

Acetone → \rho_{C_3H_6O} = \frac{V_{C_3H_6O}}{m_{C_3H_6O}} = \frac{748}{58} \approx 776 \text{kg} \cdot \text{m}^{-3}

Finally we obtain:

\[ m_d = 9.65737 \times 10^{-10} \text{ kg} \]

During the CFD calculation, the volume fractions change due to evaporation, thus resulting in changing \( \rho_{\text{liquid}} \) as well. However, in our case, the two species, ethanol and acetone, are considered (“n” is equal to 2), and the densities of the both components are almost equal (about 770 kg·m\(^{-3}\)). Hence density variations are negligibly small.
4. Results

Firstly, the check of mass conservation was performed. To do this validation, the droplet mass is monitored, along with evaporated acetone and ethanol vapour mass. In this case, the droplet mass is very small. Basically, the absolute values are close to the accuracy of ANSYS Fluent calculations. It shall be kept in mind that ANSYS Fluent stops further droplet evaporation when the droplet size reaches a minimum limit.

The evaporated acetone and ethanol gas mass in air obtained at the end of the calculation are added to droplet mass obtained at the same step; then this number was compared with injected droplet mass. In Figs 4 and 5 you can see acetone and ethanol gas mass evolutions in the cylinder, and droplet mass evolution together with its trend line till the droplet is fully evaporated. Since a droplet is 75% acetone and 25% ethanol, the mass of acetone in the air is higher.

![Fig. 4. Acetone and ethanol vapour mass time evolution](image)
Acetone gas mass | $4.9887 \cdot 10^{-11}$ kg
---|---
Ethanol gas mass | $1.6629 \cdot 10^{-11}$ kg
Droplet residual mass | $9.9922 \cdot 10^{-10}$ kg
Sum | $9.6574 \cdot 10^{-10}$ kg

*Table 6 – summary for a full evaporation*

The method of calculation is the same as the one used to validate the size of the time step (Eq 8). Here it was used to define the difference of mass between injected mass and fully evaporated mass.

$$\left| \frac{m_1 - m_2}{m_1 + m_2 / 2} \right| \leq 1\%$$

It is obtained as the result: residual is equal to: $1.5 \cdot 10^{-4}\%$
Some other results of the simulation are presented in Fig 6 & Fig 7 showing variation of the droplet velocity and diameter.

**Fig 6. Droplet’s velocity evolution with time (x-component of the velocity)**

**Figure 7 – Droplet’s diameter evolution along time**
5. A series of droplets

Problem formulation

The setup for this study is similar to that as for the single droplet; the difference is that now droplets form a series as shown in Fig 3. The purpose is to inject fuel droplets (75% acetone 25% ethanol), and investigate droplet dynamics (velocity, heat and mass transfer), varying the number of droplets injected. The droplets form a chain (series) of initially identical droplets moving in x-direction with a certain distance between the droplets.

- Define droplet-to-droplet parameters

To investigate the interaction between droplets the following parameters were introduced: droplet diameter (d), distance between droplets (DBD), and the distance parameter (C, nondimensional).

\[ C = \frac{DBD}{d} \]

Or

\[ DBD = C \times d \]

The time between droplets (TBD) is related to the droplet velocity (U)

\[ TBD = \frac{DBD}{U} \]

In the current study, the droplet parameters are presented in table 7:

| Distance between droplets | 1.164\cdot10^{-3} | m |
| Time between droplets     | 9.12988\cdot10^{-3} | s |

Table 7. Droplet-to-droplet parameters

The motion of 1 to 10 droplets is investigated; see Table 8 for the injection times.

<table>
<thead>
<tr>
<th></th>
<th>fluent starts injection at (sec)</th>
<th>fluent stops injection at (sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st drop is at</td>
<td>0</td>
<td>1.00E-05</td>
</tr>
<tr>
<td>2nd drop is at</td>
<td>9.1299E-05</td>
<td>1.0130E-04</td>
</tr>
<tr>
<td>3rd drop is at</td>
<td>1.8260E-04</td>
<td>1.9260E-04</td>
</tr>
<tr>
<td>4th drop is at</td>
<td>2.7390E-04</td>
<td>2.8390E-04</td>
</tr>
<tr>
<td>5th drop is at</td>
<td>3.6520E-04</td>
<td>3.7520E-04</td>
</tr>
<tr>
<td>6th drop is at</td>
<td>4.5649E-04</td>
<td>4.6649E-04</td>
</tr>
</tbody>
</table>
6. Results

A series of simulations were conducted: ten cases with various numbers of droplets. The droplets are moving in the $x$-direction and they form a monodisperse spray (the initial diameters of droplets and velocities are identical). This arrangement will be referred to as *droplets moving in series*.

Case 1 corresponds to a single droplet motion. Case 2 corresponds to two droplets, Case 3 to three droplets and so on.

This arrangement made it possible to compare droplet behaviour under various conditions: different number of droplets in the series, different droplet position in the series. Figures 8 to 12 show droplet velocity, mass, temperature, diameter, and evaporation rate for the case with ten droplets. Droplet velocity and mass are also supplied with a polynomial trend of the 2\textsuperscript{nd} order with the value of $R^2$.

Having obtained trends for a droplet mass using standard MS Excel ‘Trendline’ option, the evaporation rate is calculated as a derivative of the mass. The droplet velocities decrease and temperature increase due to the relaxation process. Diameters and masses decrease as droplets evaporate. Evaporation rate increases, the absolute value of evaporation rate decreases, which corresponds to the fact that the evaporation slows down as the droplet reduces in size. The same behaviour takes place in other cases (series of 1 to 9 droplets) as well.

<table>
<thead>
<tr>
<th>Droplet</th>
<th>Injection Time</th>
<th>Mass 1</th>
<th>Mass 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>7th</td>
<td>5.4779E-04</td>
<td>5.5779E-04</td>
<td></td>
</tr>
<tr>
<td>8th</td>
<td>6.3909E-04</td>
<td>6.4909E-04</td>
<td></td>
</tr>
<tr>
<td>9th</td>
<td>7.3039E-04</td>
<td>7.4039E-04</td>
<td></td>
</tr>
<tr>
<td>10th</td>
<td>8.2169E-04</td>
<td>8.3169E-04</td>
<td></td>
</tr>
</tbody>
</table>

Table 8. Droplets injection timetable
Figure 8. Velocity for each of the ten droplets (with trend line equations)

Figure 9. Mass for each of the ten droplets (with trend line equations)
Figure 10. Temperature graph for each of the ten droplets

Figure 11. Diameter evolution with time for each of the ten droplets
The results were processed and compared in two ways:

- for the individual members of a series;
- for the droplets in the same positions in different series.

All the expressions for trends of droplet velocity, mass, and evaporation rate evolutions are listed in Tables 13 to 15 (please see Appendix B).

As these two types of analysis show, the behaviour of all droplets is almost the same. This can be clearly seen by the residual values.

Residuals have been calculated to estimate the difference (i) in a single case – difference in motion of droplets in a single series; and (ii) difference of a droplet motion on a certain position in different conditions (depending on the length of a series of particles). First, velocity and mass of the first and the last droplet in the ten droplets case are compared using the formula (8). The results are (see Table 9):

<table>
<thead>
<tr>
<th>Ux</th>
<th>mass</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.5015\cdot 10^{-2} %</td>
<td>1.1353 \cdot 10^{-2} %</td>
</tr>
</tbody>
</table>

Table 9. Velocity and mass residuals between the 1st and the 10th droplets of the ten droplets case
The same kinds of residuals have been calculated for the fifth droplet in the fifth and tenth cases (5 and 10 particles in series) (see Table 10 below).

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Ux</strong></td>
<td><strong>mass</strong></td>
</tr>
<tr>
<td>7.9462%</td>
<td>9.4492\times10^{-2}%</td>
</tr>
</tbody>
</table>

Table 10. Velocity and mass residuals between the 5th droplet of the five droplets case and the 5th droplet of the ten droplets case

In both cases the absolute values of residuals are negligibly small. Hence, ANSYS Fluent models do not take into account the presence of other particles, as it has been seen for the simulations of 1 to 10 droplets for the calculation time of 10 ms (10^{-2}s).

7. Conclusion

The motion of evaporating droplets is modelled numerically using ANSYS Fluent with UDFs that allow tracking the motion of the droplets.

First the validation of the calculations was performed: velocity relaxation and temperature relaxation processes were simulated, numerical data compared with analytical solution, results are in good quantitative agreement (max residual is 0.4093\%). The value of the simulation time step and convergence of the numerical method were proved by reducing the time step.

Then series of 1 to 10 droplets were considered. The velocity and temperature of droplet relaxes to the surrounding gas velocity and temperature. As the droplet moves in the hot air, it evaporates; the absolute value of evaporation rate decreases with time.

The behaviour of droplets in different cases was compared. First, the data from a single case was analysed. Even for the case of 10 droplets, the difference between the first and the last droplet velocity and mass is negligibly small (the corresponding residuals are 9.5015\times10^{-2} % and 1.1353\times10^{-2} %). Then parameters of a droplet injected on the same position were compared. In this case, again, the difference is negligibly small.

In the case considered, ANSYS Fluent models were verified against simple single droplet cases. But ANSYS Fluent models do not take into account group effect, observed in experiments.
III. Vortex ring flow modelling

1. Introduction and motivation

Vortex rings are a particularly fascinating fluid mechanical phenomenon. From initial stage of jets to volcanic eruptions or the propulsive motion of some aquatic creatures, as well as the discharge of blood from the left atrium to the left ventricular cavity in the human heart [13], vortex rings can be identified as the main flow feature.

Vortex rings are of fundamental importance in fluid mechanics. In particular, this is indicated by the fact that a visualized cross-section of a vortex ring is put on the cover of Batchelor’s textbook [7]. The phenomenon of vortex formation is used for producing thrust and lift by insects, fishes, and animals. They’re also capable to transport neutrally buoyant materials [8]. Recently they have found their further applications for creating virtual reality in the field of entertainment. There is an attempt to use an air cannon, as a means of olfactory display, to deliver flavour encapsulated in a vortex ring to a targeted person. In a theatre, virtual reality contents are created solely by image and sound. Reality is enhanced if we appeal to tactile display. A mini-theatre is proposed in which air cannons are integrated to produce vortex rings delivering, in synchronization with the image and the sound, so that the audience experiences direct impact and flavour [2].

Vortex rings appear when an area is speeded up (corresponding to the middle of the first circle taking place at the beginning) in one direction. Due to viscosity the accelerated fluid particles make the fluid around them to spin in a tangent displacement to the initial direction. With this particles moving, the ring grows up, moving in the same direction as well. Then, the fluid rotating on toroid surface unequally loses speed and the structure dissipates, keeping expanding and moving forward (see figure 13).

This project is also linked to CEREEV project (Combustion Engine for Range-Extended Electric Vehicle) [14], and the project on the Lagrangian approach to describe two-phase flows in vortex-ring-like flows [15]. In fact, CEREEV forms an international research group working on a new kind of efficient engine. Vortex ring and vortex-ring-like structures appear during injections in a combustion camera [9]. A good description of this process is required to improve efficiency, reduce fuel consumption, which is the topic of ‘Development of the full Lagrangian approach for the analysis of vortex ring-like structures in disperse media: application to gasoline engines’ project as well. In the frameworks of CEREEV project it was also requested to enhance the combustion by injecting air into the camera. In the current study the flow is modelled using the geometry of a test rig prepared for the CEREEV project (See experimental rig pictures in Appendix C)
Objectives

In the current study, injection of air in a cylinder is investigated using CFD (ANSYS CFX). The simulation case is prepared: first the geometry model is designed (based on CEREEV experimental rig); then the computational domain is discretised; the physical properties and conditions are specified; the simulations are launched; and then the results are processed. The objective of this study is to quantify the influence of inlet pressure and of the injection’s duration on Vortex behaviour. The evolution of the radius and the travel distance and propagation velocity of a vortex ring are investigated (see following Figure 14).
2. Problem formulation and setup

In the current study, injection of air into a cylinder filled with quiescent air is investigated using CFD (ANSYS). See IV.2.b. and IV.2.b. for more details on initial conditions and flow conditions (e.g. injection duration and injection pressure). The computational domain is a rectangular box (see Fig. 15). The injector is placed in the centre of the top cylinder face, and it protrudes by 4 millimetres inside. The injector is a cylinder with a diameter of 200μm.

In our case, cylinder and injector are fully filled with air. The air in cylinder is quiescent at 1 atm, the same fluid (air) is injected with higher pressure. No-slip conditions are specified on the walls.

Figure 15 – Initial setup

Figure 15 – zoom on injection point
- **Design the geometry**

  For our study, ANSYS CFD (Design Modeller) is used to create a new geometry (See Figure 16) for our calculations.

  ![Figure 16- Box geometry (Design Modeler)](image)

- **Meshing**

  Then, the computational domain is discretised to calculate the parameters required at each point. See Figures 17-21 for the global meshing, followed by some more precise views (cut view and zoom on injecting point).

  The base meshing chose is a coarse one, automatically generated, the minimum for orthogonal quality is 0.2274 (ANSYS recommends this value to be not less than 0.05) with a total of 31 841 nodes for 156 426 elements.
<table>
<thead>
<tr>
<th>Topic</th>
<th>Placement report – Interactions between droplets / Vortex rings</th>
</tr>
</thead>
</table>

**Figure 17.** Box’s global meshing (ANSYS Meshing tool)

**Figure 18&19.** Box cut meshing (Vertical plan with zoom on injection point)
Figure 20&21. Box’s cut meshing (Vertical elements cut with zoom on injection point)
• **Boundary and initial conditions**

At this stage, boundary and initial conditions are specified using ANSYS CFX-Pre (see IV.2.b).

Boundary conditions:

- Inlet boundary conditions for air injection. Air is injected by the injector nozzle.
- Outlet condition at the bottom (piston)
- No-slip conditions on the walls

Solution initialization: The cylinder is filled with quiescent air at one atm.

![Figure 22. Box simulation parameters definition (ANSYS CFX-Pre)](image-url)
Flow conditions

The Table 12 references boundary and initial parameters for case considered. See Fig. 23 for injection conditions.

![Diagram of injection window](image)

**Figure 23. Injection window**

### Input parameters

<table>
<thead>
<tr>
<th><strong>BC : inlet</strong></th>
<th>test 1</th>
<th>test 2</th>
<th>test 3</th>
</tr>
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<td>1.5</td>
<td>2</td>
</tr>
<tr>
<td>Temperature (°C)</td>
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<td></td>
<td></td>
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<tr>
<td>Density (kg/m³)</td>
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<table>
<thead>
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<th><strong>IC in cylinder</strong></th>
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<th></th>
</tr>
</thead>
<tbody>
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<td></td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>20</td>
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<tr>
<td>Density (kg/m³)</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Injection duration (ms)</strong></th>
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</tr>
</thead>
</table>

The Table 12 presents how inlet pressure study is investigated. In different simulation the inlet pressure value is changed; and its influence on vortex ring behaviour is studied. However once this mode is done, a user is able to change any parameter to quantify its influence on vortex ring formation.

This study being at its really first step (no geometry created yet), the first goal targeted to this project is to be able to visualise correctly vortex rings appearance when post-processing will be applied on the case file. Therefore the geometry must be correctly created, boundary conditions have to be precisely set and relevant post-processing process chosen to provide the best views.
3. Results

Review of the preliminary results obtained

The air injection through a nozzle of 200 µm in diameter turned out to be a complicated problem to solve numerically. A series of issues appeared, due to the lack of time only few of them were resolved. First of all, the full mimicking of the experimental conditions was not achieved (e.g. the bottom side is open; the injection duration is much less than supposed to be).

Here some results of numerical simulations using ANSYS CFX are presented. In fig. 25 to 29 you can see the air velocity projected on a symmetry plane. At the beginning, injection forms a strong jet and a vortex ring close to the top. As the jet propagates down, the vortex ring moves in the same direction and expands. After the injection is over, the jet intensity reduces dramatically, and the vortex ring disappears.

![Figure 24. Velocity vectors at t=2\cdot10^{-5}s for 2bar injection pressure at inlet](image)
Figure 25. Velocity vectors at $t=6 \times 10^{-5}$ s for 2bar injection pressure at inlet

Figure 26. Velocity vectors at $t=1 \times 10^{-4}$ s for 2bar injection pressure
Figure 27. Velocity vectors at $t=2 \cdot 10^{-4}$s for 2bar injection pressure at inlet

Figure 28. Velocity vectors at $t = 3 \cdot 10^{-4}$s for 2bar injection pressure at inlet
In Fig. 30 – 34 pressure distribution in cross-section by the symmetry plane is presented. The pattern is rather complex.

The quality of the results is not satisfying and could be considered as preliminary. Improvement of the mesh quality is essential for further investigation. The step distribution of inlet pressure is also a subject of consideration. A smoother and more realistic distribution should be applied. Finally, the geometry of the nozzle affects the flow.

![Figure 29&30 – Pressure distribution at t=2·10^{-5} s & 6·10^{-5} s for 2bar injected](image1)

![Figure 31&32 – Pressure distribution at t=1·10^{-4} s & t=2·10^{-4} s for 2bar injected](image2)
4. Conclusions for air spray study

During the study the number of problems modelling the air injection into a cylinder has arisen. Due to the limited time devoted to the project only few of them were resolved. Still a case file allowing preliminary simulations was obtained, though not all the experimental conditions were met.

The air injection into a cylinder filled with quiescent air through a cylindrical nozzle of 200 µm in diameter was modelled and the results were processed using ANSYS DesignModeler, ANSYS Meshing, ANSYS CFX-Pre, ANSYS CFX and ANSYS CFX-Post. The vortex ring formation, propagation and dissipation were observed.

Improvement of the mesh quality, substitution with a smoother and more realistic distribution of the inlet pressure (instead of step function) should be applied to achieve more accurate results. More details on the geometry of the nozzle are needed in order to obtain more realistic data.
IV. Conclusions

During the placement in the University of Brighton, School of Computing, Engineering and Mathematics, Centre for Automotive Engineering, Sir Harry Ricardo Laboratories (SHRL), modelling research group, from the 13\textsuperscript{th} of January to the 4\textsuperscript{th} of April 2014, two projects were investigated. The first project was focused on the modelling of the droplet evaporation process and droplet-to-droplet interactions, while the second one was focused on the modelling of the vortex ring flow. The research was based on using CFD tools – ANSYS Fluent and ANSYS CFX. To perform the study, a series of tutorials on numerical modelling using ANSYS 14.5 tools (Workbench, DesignModeler, Ansys Meshing, CFX-Pre, CFX, CFX-Post, Fluent) was undertaken. Also during the placement I had lectures from Dr. Oyuna Rybdylova, Dr Vyacheslav Stetsyuk, attended two seminars and had a laboratories tour following by a meeting with Dr. Steven Begg).

The project is focused on droplet evaporation process and interactions between droplets moving in clusters, the modelling was based on ANSYS Fluent simulation. The work was conducted in the frameworks of ‘Investigation of heating and evaporation of multi-component droplets’ and ‘Energy Efficiency and Environment: a Cross-Channel Cluster (E3C3)’ projects at the SHRL. In this project a relevant case file was modified to simulate a series of injections, and the UDFs were added in order to be able to process the particle data.

Project began with validating the calculations; analytical solutions for velocity and temperature relaxation were compared with numerical data. Good agreements have been obtained (max residual 0.4093\%). Therefore, series of droplets (from one to ten droplets) were considered. Each case was run with Fluent to obtain droplets parameter evolutions with time.

Each case and each droplet data were processed; trends calculated. Two types of analysis were performed. The first comparison was focused on the difference in motion of droplets in a single series. Results for the first and the tenth droplets of the ten droplets case were discussed in detail. The agreement between the results was very good (velocity residual was equal to 9.5015·10\textsuperscript{-2} % and mass residual was equal to 1.1353·10\textsuperscript{-2} %). Then comparison was operated for droplets on a certain position in different conditions (depending on the length of a series of particles). The residuals for the two fifth droplets of the five and the ten droplets cases were presented. Here again the difference was negligibly small.

To conclude, in this considered case, ANSYS Fluent calculations were checked using simple cases of droplets moving in tandem. The fact is that group effects observed in experiments seem not to be taken into account by ANSYS Fluent models.
The second project is focused on vortex ring flows, the investigation is based on ANSYS CFX. The vortex ring behaviour is studied in the frameworks of ‘Development of the full Lagrangian approach for the analysis of vortex ring-like structures in disperse media: application to gasoline engines’ and ‘Combustion Engine for Range-Extended Electric Vehicle (CEREEV)’ projects at the SHRL. Here the modelling included designing the geometry, meshing, setting up the simulation and post-processing.

A number of problems appeared along the modelling of the air injection. Due to a short time allocated to this project, only the first problems were solved. Some preliminary studies were performed by modifying some parameters which allowed us to run some calculations, but not fully following the experimental conditions (provided by CEREEV).

ANSYS DesignModeler, ANSYS Meshing, ANSYS CFX-Pre, ANSYS CFX and ANSYS CFX-Post were the tools used to observe flow parameters, vortex ring formation, vortex ring propagation or dissipation which was the goal of this project.

Further studies were mentioned to improve this model. First, improvements of the mesh quality and of the injection window had to be investigated to increase calculation accuracy. Also, an improvement of injection nozzle geometry has to be performed to provide more realistic data.

The results of the activity on both projects are demanded; summaries will be included into E3C3 and CEREEV projects. The results on air injection and vortex formation were presented on a CEREEV meeting (please see the Appendix).
References


[16] – ANSYS database (ANSYS Fluent 14.5)
V. Appendix

(A) Participation in research activity of the SHRL:

- Research seminar: Monday 27th of January, 16h-17h, Watts Building Room 504
  Spreading and splashing behaviour of an complex impact droplet
  Prof. Alidad Amirfazli
  Department of Mechanical Engineering
  York University, Toronto

- Research seminar: Wednesday 26th of March, 16h-17h, Watts Building Room 504
  Floasys: a platform for CFD Workflow Management
  Mr. Donato Pirozzi
  ISISLab, Dipartimento di Indormatica, University of Salerno

  General discussion on Mr. Donato Pirozzi’s work and context of CEREEV/collaboration possibilities.

- CEREEV meeting:

  Presentation of air injection simulation results by Adrien Oger

  Thursday 27th of March, 14:00-17:00,
  SHRL Laboratories
### Trends of a Particle Velocity, Mass and Evaporation Rate

#### Velocity

<table>
<thead>
<tr>
<th>Droplet 1</th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
<th>Case 4</th>
<th>Case 5</th>
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</thead>
<tbody>
<tr>
<td>y = 3.4838E+04x² - 9.8292E+02x + 1.2703E+01</td>
<td>y = 3.4833E+04x² - 9.8298E+02x + 1.2703E+01</td>
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<table>
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<th>Case 7</th>
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<th>Case 10</th>
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**Table 13. Velocity equations worksheet from 1 to 10 droplets cases**
## Mass

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<tr>
<th>Droplet 1</th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
<th>Case 4</th>
<th>Case 5</th>
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**Table 14.** Mass equations worksheet from 1 to 10 droplets cases
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<th>Droplet 2</th>
<th>Droplet 3</th>
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<td>Droplet 8</td>
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</tr>
</tbody>
</table>

Table 15. Evaporation rate equations worksheet from 1 to 10 droplets cases.
(C) CEREEV experimental rig

Experimental rig; calibration and tuning of the measuring equipment.