Abstract. The spray atomization mechanisms under the conditions common for the Diesel engines are very complex and not completely understood. At the same time the detailed spray information is necessary to provide a better control of the combustion process. The principal difficulty of numerical spray simulation is the correct representation of the both characteristic zones of spray: dense near the nozzle and dilute downstream.

Combining the advantages of Eulerian and Lagrangian approaches, ELSA model is able to predict continuously the whole spray evolution. In the dense zone the spray and its gaseous environment are presented as an effective single-phase fluid with a highly variable density. To describe the dispersion of the liquid, the transport equations for the liquid mass fraction and for the liquid/gas interface density are solved. The transition to the Lagrangian calculation is applied when the spray is considered to be diluted enough. The initialization of the droplet characteristics (such as diameter or velocity) and also the position of the generated droplets are determined directly from the Eulerian description and not set a priori as in the classical Lagrangian approach.

This complete Eulerian-Lagrangian spray atomization model has been implemented into the computational fluid dynamics code STAR-CD. The model implementation is validated by comparing predicted liquid and vapour penetrations with experimental data reported in literature. Once validated, the ELSA model is coupled with an inside nozzle simulation to study the impact of internal nozzle flow (geometry, cavitation formation) on the spray and its characteristics.

1. Introduction

The main difficulty of numerical spray simulation is the correct representation of the both characteristic zones of spray: dense near the nozzle and dilute downstream. The Eulerian approach seems to be more appropriate to describe the dense zone because no droplet is formed and even a continuous medium of liquid can exist. So, the description of the spray inside this zone as a set of droplets is not the most suitable. On the other hand, the use of the classical Lagrangian approach inside the diluted zone could permit to benefit of the important background accumulated for this kind of spray representation. Combining the advantages of Eulerian and Lagrangian approaches, ELSA (Eulerian-Lagrangian Spray Atomization) model is able to predict continuously the whole spray evolution from the injector nozzle to the final dilute spray region. Moreover it is well known that the details of the internal nozzle flow induce considerably the spray formation and its characteristics. It is especially true when cavitation occurs inside the nozzle. The numerical simulation of this flow could provide the “realistic” conditions to initialize ELSA simulation and so, take into account the velocity and turbulence distribution over the nozzle exit section as well as their temporal evolution during injection.

The present paper contains the first validations of the ELSA model implemented into the commercial code STAR-CD. These validations are composed of two experimental data bases [5, 7] including the measurements of liquid and vapour penetrations obtained for non-vaporizing and vaporizing sprays under in-cylinder thermodynamic conditions around injection timing. The second phase of this work is the coupling of the inside nozzle flow with ELSA model. The fulfilment of this coupled simulation and the study of the internal flow influence on the spray formation is the principal aim of the present work and will be presented into the final paper.

2. Eulerian Lagrangian Spray Atomization model

ELSA model was proposed in 2001 by R. Borghi and A. Vallet [8] and since has been under development [1, 2, 3, 4 and 6]. This model is intended for application to turbulent spray with both high
Reynolds and high Weber numbers. The model version implemented into STAR CD code and used for all presented calculations is issued from the Ph.D thesis of P.A. Beau [1].

ELSA model combines the Eulerian approach in the near-nozzle region and Lagrangian approach in the region downstream of the nozzle. In dense region of the spray, liquid and its gaseous environment are represented as an effective single-phase fluid with a highly variable density. To describe the dispersion of the liquid, the transport equation of the liquid mass fraction is solved with a gradient law closure applied to model the turbulent liquid flux. A liquid/gas interface density is also transported in order to determine the mean size of the liquid fragments. The switch to the Lagrangian calculation is applied when the spray is considered to be diluted enough. The initialization of the droplet characteristics is determined directly from the Eulerian description and not set a priori as in the classical Lagrangian approach.

2.1 Liquid dispersion modeling

In dense region of the spray, the liquid and its gaseous environment is considered as an effective single phase of liquid and gas mixture. The mean properties of this effective fluid or mixture (like mean density \( \overline{\rho} \) or Favre averaged mean velocity \( \overline{U_i} \)) are defined with the following relationships:

\[
\frac{1}{\overline{\rho}} = \frac{\overline{\rho}_l}{\rho_l} + \frac{1 - \overline{\rho}_l}{\rho_g} \quad (1)
\]

\[
\overline{U_i} = \overline{\rho}_l U_{ij} + \left(1 - \overline{\rho}_l\right) U_{g,ij} \quad (2)
\]

\[
\overline{p} = \frac{(1 - \overline{\rho}_l) \rho_l R \overline{T_l}}{1 - \overline{\rho}_l \cdot \overline{\rho}_l} \quad (3)
\]

Here \( \overline{\rho}_l \) is liquid mass fraction and \( \rho_l \) and \( \rho_g \) stand respectively for the liquid and gas densities. In the equation of state (3), we take into account the volume occupied by liquid.

The classical transport equations are solved for these mean variables:

\[
\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho} \overline{U}_j}{\partial x_j} = 0 \quad (4)
\]

\[
\frac{\partial \overline{\rho} \overline{U}_i}{\partial t} + \frac{\partial \overline{\rho} \overline{U}_j \overline{U}_i}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} - \frac{\partial \rho u_j^* u_j^*}{\partial x_j} \quad (5)
\]

It should be noticed that the last equation does not contain any momentum exchange terms between liquid and gaseous phases. In order to model the liquid dispersion, this set of equations is completed by the transport equation for the liquid mass fraction:

\[
\frac{\partial \overline{\rho} \overline{\rho}_l}{\partial t} + \frac{\partial \overline{\rho} \overline{U}_j \overline{\rho}_l}{\partial x_j} = -\frac{\partial \rho u_j^* y^*}{\partial x_j} \quad (6)
\]

In the Eqs. (5) and (6), there are 2 turbulent fluxes to be closed. The turbulent stress tensor is modelled with a classical \( k - \varepsilon \) model closure. Concerning the liquid turbulent diffusion flux, the gradient law approximation is applied:

\[
\rho u_j^* y^* = -\overline{p} \frac{\nu_l}{Sc_l} \frac{\partial \overline{\rho}_l}{\partial x_j} \quad (7)
\]
2.2 Liquid/gas interface density

In order to characterize the size of the liquid fragments resulted from the jet atomization, the notion of liquid surface density is introduced. This variable is defined as the quantity of liquid/gas interface per unit of volume \( \Sigma \ (m^{-1}) \). Using this new variable, one can obtain the Sauter mean diameter of droplet: \( D_{32} = 6 \bar{\rho} \bar{Y}_l / \left( \rho \Sigma \right) \). A transport equation for liquid surface density is postulated by analogy with the flame surface density [8]:

\[
\frac{\partial \bar{\rho} \bar{\Omega}}{\partial t} + \frac{\partial \bar{\rho} \bar{U}_j}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \bar{\rho} v_x \frac{\partial \bar{\Omega}}{\partial x_j} \right) + \bar{\rho} \left( \dot{\bar{\Omega}}_{\text{init}} + \dot{\bar{\Omega}}_{\text{mean}} + \dot{\bar{\Omega}}_{\text{turb}} + \dot{\bar{\Omega}}_{\text{coll}} + \dot{\bar{\Omega}}_{\text{coal}} \right) \tag{8}
\]

Here, Beau [1] introduced the other notion of liquid/gas interface per unity of mass that is defined as \( \bar{\Omega} = \Sigma / \bar{\rho} \ (m^2/kg) \).

The production and destruction of liquid surface are accounted for with source terms detailed below. The first term source \( \dot{\bar{\Omega}}_{\text{init}} \) in Eq. (8) permits to initialize the calculations since all other terms source are proportional to \( \bar{\Omega} \):

\[
\dot{\bar{\Omega}}_{\text{init}} = \begin{cases} 
2 \frac{v_x}{Sc} \frac{6 \bar{\rho}}{\rho_s \rho_l L_i} \frac{\partial \bar{Y}_l}{\partial x_i} \frac{\partial \bar{Y}_l}{\partial x_i}, & \text{if } \bar{Y}_l(1 - \bar{Y}_l) \leq 0.001 \\
2 \frac{v_x}{Sc} \frac{\bar{\Omega}}{\bar{Y}_l(1 - \bar{Y}_l)} \frac{\partial \bar{Y}_l}{\partial x_i} \frac{\partial \bar{Y}_l}{\partial x_i}, & \text{otherwise}
\end{cases} \tag{9}
\]

The three next terms correspond to the production of liquid surface density due to the mean or turbulent stresses and due to the collisions:

\[
\dot{\bar{\Omega}}_{\text{mean}} = \frac{\bar{\rho} u_i u_i}{\bar{\rho} \bar{k}} \frac{\partial \bar{U}_i}{\partial x_j} \bar{\Omega}; \quad \dot{\bar{\Omega}}_{\text{turb}} = \frac{\bar{\Omega}}{\tau_i} \quad \text{and} \quad \dot{\bar{\Omega}}_{\text{coll}} = \frac{\bar{\Omega}}{\tau_{\text{coll}}} \tag{10}
\]

The last term in the right hand of Eq. (8) deals with destruction of surface density due to coalescence:

\[
\dot{\bar{\Omega}}_{\text{coal}} = -\frac{1}{\tau_{\text{coal}} \Omega_{\text{crit}}} \bar{\Omega}^2 \tag{11}
\]

More details about the model closure and parameters can be found in Ph.D. thesis of P.A. Beau [1].

2.3 Transition from Eulerian to Lagrangian formulation

As mentioned before, Eulerian part of the model is coupled with the classical Lagrangian formulation. So, there are 3 characteristic zones of spray: dense zone, transition zone and diluted one. The Eulerian formulation is applied into the whole numerical domain. Once the spray is considered to be diluted enough the Lagrangian droplets are generated. The criterion switch is based on the value of liquid volume fraction that is linked to the ratio of mean free path between two droplets and mean equivalent radius of the droplets in the cell. In this paper, the transition is done when the liquid volume fraction becomes lower than 0.01. The transition zone is composed of the computational cells that form the border with the dense zone (i.e. zone where the liquid volume fraction is greater than 0.01) and only one parcel is generated per transition cell and per time step.
The initialization of the characteristics (such as diameter or velocity) and location of the generated droplets are determined directly from the Eulerian description and not set a priori as in the classical Lagrangian approach. The mean number of droplets per generated parcel is obtained from the mass conservation.

3 Validation tests

The ELSA approach described above was implemented into STAR CD code. In order to validate its implementation, comparisons with two experimental series were realized. The first series was carried out by Naber and Siebers [5] in Sandia National Laboratory, the second one – by Verhoven et al. [7] in Institut Francais du Petrole. Naber and Siebers [5] investigated ambient gas density and fuel vaporization effects on diesel spray penetration over a wide range of gas density. Verhoven et al. [7] varied temperature and density of the ambient gas as well as the fuel injection pressure.

3.1 SANDIA results

The injector and fuel used by Naber and Siebers [1] are a high-pressure, common rail diesel fuel injector and a Phillips research grade diesel fuel. The fuel density is 705 kg.m\(^{-3}\) at the considered injection temperature of 440 K. The injector has a fast opening time, i.e. time required to reach the full injection rate, and a constant injection rate. Ambient gas density effects on sprays are examined by comparing injections over a wide range of ambient gas density (3 to 124 kg.m\(^{-3}\)). Fuel vaporization effects are examined by comparing injections into non-vaporizing (ambient temperature of 450 K) and vaporizing (ambient temperature of 1000 K) inert environments at the same density.

All the calculations are performed using a 2D axis-symmetric mesh composed of 10000 cells. The cell size of 10 to 20 microns across the nozzle diameter is needed to perform an accurate modelling of the near injector zone.

Figures 2 and 3 show the comparison of vapour and liquid penetrations predicted using the present ELSA model and experimental data of Naber and Siebers [5]. Figure 2 shows the liquid penetrations obtained under the non-vaporizing conditions (six ambient gas densities). It is observed that the liquid penetrations predicted by the ELSA model are in good agreement with the experimental ones. It can be concluded that ELSA model reproduces the main trend shown by the experimental penetration data, i.e. the decrease in penetration with an increase in ambient density under non-vaporizing conditions.

The effect of vaporizing on spray penetration is more controversial. Naber and Siebers [1] observed that vaporization reduces or slows penetration with an influence more important as density is weaker. The reduction was as much as 20% at the lowest densities. Figure 3 shows the liquid and

<table>
<thead>
<tr>
<th>Ambient gas density (kg.m(^{-3}))</th>
<th>Ambient gas temperature (K)</th>
<th>Fuel pressure (MPa)</th>
<th>Time to full injection rate (μs)</th>
<th>Bernoulli’s velocity (m.s(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.57</td>
<td>455</td>
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<td>70</td>
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<td>137</td>
<td>70</td>
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<td>452</td>
<td>140</td>
<td>70</td>
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<td>30.0</td>
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<td>3.3</td>
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<td>137</td>
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<td>618.9</td>
</tr>
</tbody>
</table>

All the calculations are performed using a 2D axis-symmetric mesh composed of 10000 cells. The cell size of 10 to 20 microns across the nozzle diameter is needed to perform an accurate modelling of the near injector zone.

Table 1. SANDIA experimental conditions
vapour numerical penetrations obtained for vaporizing injection conditions. During the earliest stage, both liquid and vapour penetration have the same rate until the liquid core had reached its ultimate length. After this time, the vapour continues to penetrate into the chamber at a similar rate to the liquid spray injected under non-vaporizing conditions into an equivalent ambient density. So, the vapour penetrations obtained with ELSA model are overestimated compared to experimental results (right part of Fig. 3).

![Fig. 2. Liquid penetration versus time for non-vaporizing sprays](image1)

![Fig. 3. Liquid (left) and vapor (right) penetrations versus time for vaporizing sprays](image2)

### 3.2 IFP results

All the measurements reported by Verhoven et al. [7] were made in a high pressure and temperature diesel simulation cell. The gases within the cell were heated and pressurized. The experiments were conducted in a mixture composed of 86.8% N₂, 1.7% CO₂ and 11.5% H₂O. The sprays were created with injector supplied by Ganser Hydromag (nozzle hole diameter \( d = 200 \mu m \)). Dodecane was used as single component fuel. Table 3 lists the variations into experimental conditions studied by Verhoven et al. [7].

<table>
<thead>
<tr>
<th>Case number</th>
<th>Ambient gas density (kg.m⁻³)</th>
<th>Ambient gas temperature (K)</th>
<th>Fuel pressure (MPa)</th>
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<tr>
<td>1</td>
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</tr>
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</tr>
</tbody>
</table>

Spray tip penetrations vs. time for both the liquid and vapor parts of the spray were measured. Their comparisons with the numerical penetrations are given in Fig. 4 for selected experimental conditions. All the numerical results predicted by ELSA model are in good agreement with the experiment and following Verhoven et al. [7], we can conclude that:
a) Liquid and gas penetrations are respectively weakly dependent on the injection pressure (Case 4) and on the gas temperature (Case 2);
b) Liquid penetrations decrease with increasing gas temperature (Case 2) and with increasing gas density (Case 5);
c) Vapour penetrations decrease with decreasing fuel injection pressure (Case 4) and with increasing gas density (Case 5).

4. ELSA model coupled with nozzle flow simulation

In every calculations presented previously, the injector’s outlet section has been considered as an inlet boundary for ELSA model with homogenous conditions on its surface. In this section, more realistic injection conditions with non-uniform distributions at the injector outlet have been tested. These distributions are determined through hydraulic calculations inside the injector’s nozzle. These calculations have been performed independently from ELSA calculations using STAR-CD with Rayleigh model activated in order to take into account the cavitation effect.

4.1 Boundary conditions – coupling with hydraulic calculation

Two Bosch injection nozzles with six holes are being considered:
(1) a cavitating nozzle (nozzle 195 Kf0) with cylinder-shaped and non hydro-eroded (sharp) holes and an outlet diameter $D_{inj} = 147 \mu m$;
(2) a non-cavitating nozzle (nozzle 194 Ks1.5) with cone-shaped (ratio of 1.5) and hydro-eroded (rounded-inlet) holes and an outlet diameter $D_{inj} = 138 \mu m$.

A series of results obtained from stationary calculations carried out at several needle lifts for each considered nozzle (provided by Renault) is available. The 2D fields of longitudinal velocity, kinetic turbulent energy, its dissipation rate and volume fraction of vapour at the injector’s outlet section can be determined through these results. The experimental injection rate is used to define the moment when each needle lift should take place. ELSA calculations are performed for a single hole of each nozzle in the conditions of experimental measurements of liquid penetrations: ambient gas pressure $p_{ch} = 10\ bar$, fuel injection pressure $p_{inj} = 800\ bar$, injection duration $T_{inj} = 500\ \mu s$ and liquid density $\rho_l = 750\ kg/m^3$.

4.2 Numerical characteristics of ELSA calculations

The structure of the 3D mesh used for ELSA calculations is represented in Fig. 6. One can find here several views of this mesh in the plane perpendicular to the injection’s direction: zones 1 and 2 are the usual zones of an O-mesh whereas zones 3 and 4 (the last one represents the nozzle outlet) are integrated in order to have a thinner mesh in the area close to the injector. In z direction, the mesh is non uniform with the stretch ratio of 1.02.
4.3 Comparisons

The following experimental results provided by Renault and CORIA are available for comparisons:
1) lengths of the liquid penetration,
2) droplets’ velocities.

The experimental penetrations are obtained in the same injection conditions as the ones applied in the ELSA calculations: $p_{inj} = 800$ bars, $p_{ch} = 10$ bars and $T_{inj} = 500$ $\mu$s. However, velocities measurements are only available for $T_{inj} = 1000$ $\mu$s and so, the comparison with ELSA will be more difficult.

Figure 7 shows the comparison of the liquid penetration for two nozzles. A delay between numerical and experimental penetrations is observed. Indeed, it can be seen that numerical spray penetration is composed of two distinct periods: an initial slow penetration period followed by a fast penetration period whereas experimental penetrations are more linear. After 0.25 ms of injection, numerical and experimental rates of penetration are almost the same. It can also be noticed that numerical penetrations are quite close for the two nozzles, cavitating or non-cavitating, which is also the case for measured penetrations.

![Figure 7. Liquid penetration evolution: cylindrical and conical nozzles](image)

On the following figure, a comparison of the two nozzles based on the velocity profiles obtained at 0.5ms is carried out. The numerical results confirm close behaviour of the two injectors already observed experimentally.
5. The spray structure

The spray structure obtained under non-vaporizing conditions is presented and discussed in this section. Figure 9 shows some snapshots of the spray solution obtained at different portion of the spray tip. Circles are used to represent the liquid in the discrete Lagrangian part while contours are used to represent the liquid in the continuous Eulerian part.
In figure 10 the structure of the spray is represented at 0.5 ms highlighting the different zone of the spray. The chosen time after injection is 0.5 millisecond. The spray structure shown in this figure indicates clearly the presence of a continuous liquid region at the nozzle exit and persist several nozzle diameter downstream the injection direction. It is also shown droplet with relatively small diameter around this continuous part. The development of the discrete part with large droplets diameter takes place near the half of the spray length as it is expected.

Conclusions

An Eulerian Lagrangian Spray Atomization model has been implemented into commercial code STAR-CD. The model validation was carried out by means of experimental data of vaporizing and non-vaporizing sprays under in-engine like conditions in a constant-volume bomb. It was found that ELSA calculations are able to capture the effects of gas density on liquid and vapour penetrations.

Then, ELSA simulations with inflow boundary conditions obtained from inside nozzle flow modelling were performed for two non-cavitating and cavitating nozzles. The comparison with the measurements was based on the data for liquid penetration and droplet velocity. For the considered injection conditions (ambient gas pressure and fuel injection pressure), a very close behaviour has been observed for the sprays formed by two different nozzles as expected by the measurements.

The spray structure indicates clearly the presence of a continuous liquid region at the nozzle exit and persist several nozzle diameter downstream the injection direction. It is also shown droplet with relatively small diameter around this continuous part. The development of the discrete part with large droplets diameter takes place near the half of the spray length as it is expected.
References


