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Additional Information

Numerical simulation of primary atomization in diesel spray at low injection pressure

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Abstract

Atomization involves complex physical processes and gas-liquid interaction. Primary atomization on diesel spray is not well understood due to the difficulties to perform experimental measurements in the near nozzle field. Hence computational fluid dynamics (CFD) has been used as a key element to understand and improve diesel spray.

A recent new code for incompressible multiphase flow with adaptive octree mesh refinement has been used to perform simulations of atomization at low injection pressure conditions. The multiphase flow strategy to manage different flows is the volume of fluid (VOF) method. The adaptive mesh allows to locally refine the mesh at each time step where a better resolution is needed to capture important gradients instead of using a static mesh with a fixed and high number of cells which, in turns, would lead to an unaffordable computational cost. Even with this approach, the cell number is very high to achieve a Direct Numerical Simulation (DNS) at reasonable computational cost. To reduce the computational cost, an idea has been explored, the possibility of setting a maximum number of cells of the domain. Following this idea, the code has been tested with different configurations to understand their effects on numerical stability, the change in different spray parameters and the benefits achieved in terms of execution time. The outcomes have been validated against a theoretical model.

Keywords: diesel spray, atomization, Gerris, DNS, VOF

1. Introduction

Atomization process in a spray has been an important issue for researchers during last decade, due to its presence in many industrial applications. In particular, this is extreamely important in

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Diesel Engines, where combustion efficiency and pollutant formation are a consequences of spray atomization and fuel-air mixing process [1, 2, 3, 4, 5].

As a result of these studies, several tools have been developed for modeling macroscopic spray behaviour [6, 7]. Nevertheless, there are still uncertainties related with internal nozzle flow and its link with spray formation and primary break-up [8, 9, 10].

Last decades have been characterized by a continuous increase in computational resources. For the study of diesel spray this increase allows to move forward to use more complex models for breakup, evaporation, coalescence, turbulence, etc.

In terms of turbulence modelling, the classes of models from lower to higher computational cost are: RANS (Reynolds averaged Navier-Stokes) [11, 12], LES (large eddy simulations) [13, 14] and DNS (direct numerical simulations) [15, 16, 17]. While RANS methods have been used along several decades, the use of LES models is more recent and even now the computational requirements for the use of DNS is still very high for study typical current conditions in diesel engines.

However, despite all the computational difficulties some researchers [16, 17, 18] have tried to use DNS approach for the study of Diesel sprays. Some basic procedures have been adopted by these researchers in order to be able to perform DNS simulations in sprays, such as, decreasing injection velocity and reducing the domain for studying only the first millimeters, and so, taking into account only primary atomization. It is also used an Adaptative Mesh Refinement (AMR) method to reduce the computational cos of simulations [17, 18]. Even with this simplifications, in the present paper, the numerical cost to simulate around 8 millimeters of the spray has been around 2 months running over 32 CPUs on a blade server Fujitsu BX920.

The aim of this paper is to study the potential of a new code [19, 20] to perform simulations of primary atomization in diesel sprays with DNS approach. For this purpose the same strategy used by other researchers described before [16, 17, 18] for reducing the computational time has been used: Low spray velocity, small domains (just to consider only the first atomization and breakup length) and the application of AMR algorithm.

The present paper has been split into 6 sections. In Section 2, a brief description of the numerical code will be performed. After that, in Section 3, a mesh sensitivity study performed over several parameters that define the mesh will be reported. In Section 4 the outcomes of the computational simulations will be validated against a theoretical model available in the literature (which in turns has been widely validated). After the validation, in Section 5, a study on the influence that the use of periodic perturbation in the injection velocity has on the results will be described. Finally, in Section 6 the main conclusions will be drawn.

2. Numerical Code

For this study, the numerical code Gerris developed by Stéphane Popinet [19, 20] has been used. This code solves Navier-Stokes equations with surface tension for incompressible flow (1)–(3)

$$\rho \left(\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot (2\mu \mathbf{D}) + \sigma k \delta_s \mathbf{n}, \tag{1}$$

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = \mathbf{0}, \tag{2}$$

$$\nabla \cdot \mathbf{u} = \mathbf{0}, \tag{3}$$

where $\rho = \rho(\mathbf{x}, t)$ is the fluid density, $\mathbf{u} = \left(u_x, u_y, u_z \right)$ is the fluid velocity, p is the pressure field, $\mu = \mu(\mathbf{x}, t)$ is the dynamic viscosity, $\mathbf{D}$ is the deformation tensor, σ is the surface tension

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coefficient, k and $\mathbf{n}$ are the curvature and the normal vector to the interface, respectively, and δ_s is the Dirac distribution which expresses that the surface tension term is active only in the interface.

In the simulations whose results are presented here, diesel fuel is injected into a gas environment, thus, density and viscosity depend of the concentration of diesel, c, in the following way

$$\rho(c) = c\rho_f + (1 - c)\rho_a, \tag{4}$$

$$\mu(c) = c\mu_f + (1 - c)\mu_a, \tag{5}$$

where ρ_f and ρ_a are the fuel and air density, respectively, and μ_f and μ_a represent the fuel and air dynamic viscosity.

The advection equation for density (2) can be replaced by an advection equation for the concentration (6):

$$\partial_t c + \nabla \cdot (c\mathbf{u}) = \mathbf{0}. \tag{6}$$

Concerning the numerical approach to solve (1)–(3), a brief but accurate summary of the numerical discretization and schemes is provided at following paragraph. The fully detailed numerical approach can be found in [19, 20], where numerical and discretization schemes are explained. A second-order scheme is used for time discretisation at any given time-step n:

$$\rho_{n+\frac{1}{2}}\left(\frac{\mathbf{u}_{n+1} - \mathbf{u}_n}{\Delta t} + \mathbf{u}_{n+\frac{1}{2}} \cdot \nabla \mathbf{u}_{n+\frac{1}{2}}\right) = -\nabla p_{n+\frac{1}{2}} + \nabla \cdot \left(\mu_{n+\frac{1}{2}}\left(\mathbf{D}_n + \mathbf{D}_{n+1}\right)\right) + (\sigma k \delta_s \mathbf{n})_{n+\frac{1}{2}}, \tag{7}$$

$$\frac{c_{n+\frac{1}{2}} - c_{n-\frac{1}{2}}}{\Delta t} + \nabla \cdot (c_n \mathbf{u}_n) = \mathbf{0}, \tag{8}$$

$$\nabla \cdot \mathbf{u}_n = \mathbf{0}. \tag{9}$$

The calculation of the velocity and the pressure field are decoupled through an intermediate velocity, $\mathbf{u}_\star$, using the Chorin's projection method [21]:

$$\mathbf{u}_{n+1} = \mathbf{u}_\star - \frac{\Delta t}{\rho_{n+\frac{1}{2}}}\nabla p_{n+\frac{1}{2}}, \tag{10}$$

and the system is simplified into the following expresion

$$\rho_{n+\frac{1}{2}}\left(\frac{\mathbf{u}_\star - \mathbf{u}_n}{\Delta t} + \mathbf{u}_{n+\frac{1}{2}} \cdot \nabla \mathbf{u}_{n+\frac{1}{2}}\right) = +\nabla \cdot \left(\mu_{n+\frac{1}{2}}\left(\mathbf{D}_n + \mathbf{D}_\star\right)\right) + (\sigma k \delta_s \mathbf{n})_{n+\frac{1}{2}}, \tag{11}$$

$$\frac{c_{n+\frac{1}{2}} - c_{n-\frac{1}{2}}}{\Delta t} + \nabla \cdot (c_n \mathbf{u}_n) = \mathbf{0}, \tag{12}$$

$$\nabla \cdot \mathbf{u}_\star = \nabla \cdot \left(\frac{\Delta t}{\rho_{n+\frac{1}{2}}}\nabla p_{n+\frac{1}{2}}\right). \tag{13}$$

The advective term in Equation (11), $\mathbf{u}_{n+\frac{1}{2}} \cdot \nabla \mathbf{u}_{n+\frac{1}{2}}$ is computed using the Bell-Colella-Glaz second-order unsplit upwind scheme [22, 19], which is numerically stable for CFL numbers smaller than one. The advection equation (12) for the volume concentration is solved using a piecewise-linear geometrical Volume-of-Fluid (VOF) scheme [20].

The surface-tension term in Equation (11), $(\sigma k \delta_s \mathbf{n})_{n+\frac{1}{2}}$, is computed as described by Stéphane Popinet [20] combining a continuum-surface-force (CSF) approach and a height-function curvature estimation. This approach solves the known parasitic currents problem that are found classically in CSF when a stationary droplet in theoretical equilibrium is considered.

An important feature of the code is the octree mesh for 3D (or quad mesh in 2D) that allows adaptive refinement in each time-step. Three different criteria for the refinements have been used: in terms of vorticity to a proper characterization of the turbulence, in terms of gradient of concentration to accurately capture the interface and in terms of radius of curvature to describe the break-up process.

This code has been validated against linear instability theory [15] considering two-phase parallel mixing layers comparing the predicted temporal growth of small disturbances induced in the flow, obtaining a good agreement between numerical and theoretical results. The errors of the position of the maximum height of the wave were always below 5%. The ability of the code to simulate primary applications in jets at low velocity (20 m/s) has been also tested in that paper, as well as for the case of a hollow-cone atomizer with same velocity but adding swirl movement. The results were compared with experimental images, obtaining similar flow patterns experimentally and computationally.

Using low jet velocity, the code has been also used to predict the behaviour of impinging jets in [23]. In this paper, the authors compared the liquid sheet morphology for two identical liquid jets impinging at a given instant. They obtained numerical convergence and good agreement with experimental results based on measurements of droplet size. Finally, in [17], the code is used to simulate a spray of a diesel injector. Results obtained from the code were compared in terms of droplet radius with experiments from Hiroyasu and Kadota [24].

3. Mesh Sensivity

Concerning to the mesh, 3 parameters have been studied: cell size, domain width and maximum number of cells.

3.1. Cell Size

As it is showed in Figure 1, a coarse mesh results in a lack of accuracy and unrealistic spray with big droplets and very low atomization. However, a finer mesh is able to accurately capture the physics of the spray at the expense of increasing the number of cells, and consequently the computational time.

In the computational study, several minimum cell sizes ranging from 24 μm to 1 μm (Table 1) were studied. Something to highlight is that when the minimum cell size is divided by 2 the number of cells increase roughly by a factor of 8 (in the case of a uniform mesh they increase exactly by a factor of 8).

minimum cell sizes (μm)	1, 1.5, 2, 3, 4, 6, 8, 9, 12, 16, 24

Table 1: Minimum cell size cases

A mesh independence study involving different minimum cell sizes was performed to establish the cell size requirements depending on the parameter of the spray to be analyzed. From this study two different requirements for the cell size have been achieved: for the study of an external property of the spray, such as the spray penetration, the convergence is achieved for a cell size of 9 μ, while for the study of an internal spray characteristic, such as the breakup length a minimum cell size of 2 μ is required. The study was performed by comparing the numerical results in terms of penetration or breakup length coming from different meshes (decreasing the
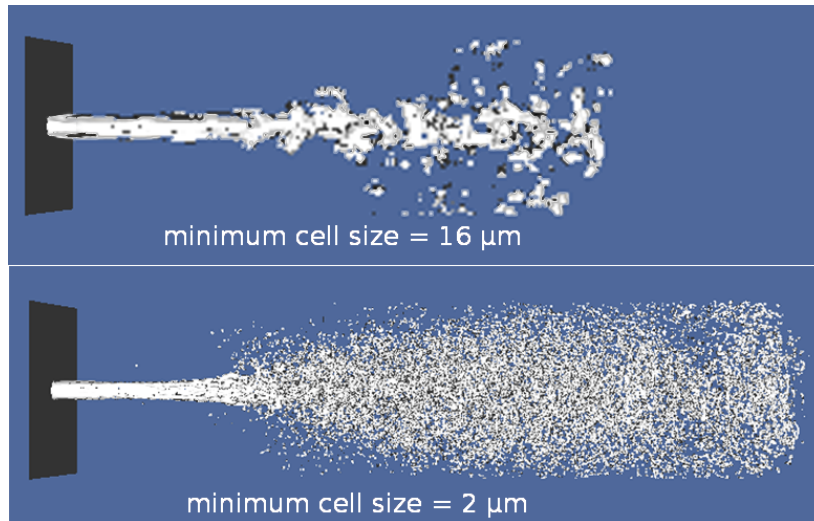
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Figure 1: Minimum cell size

minimum cell size) in order to detect the convergence of results, and therefore the cell size which guarantees best results with low computational cost.

3.2. Domain Width

In Figure 2 the domain of the simulation is shown. This domain is characterized by the width, L and the length, which is five times the width. In the Figure the diameter of the orifice where the fuel is injected is represented by D_0. Free stream boundaries have been set at the top and at the bottom of the domain. With the aim of reducing as much as possible the computational cost, small values of L/D_0 where initially tested, but important divergence problems arisen when the fuel droplets approached to the vicinity of the boundaries. In particular, the problem is produced when a vorticity field placed around the spray tip, where velocity dramatically increases, approaches to the free stream boundaries.

In order to optimize the domain, three different L/D_0 ratios have been tested (5, 10 and 20).

Results are plotted in Figure 3. In the upper part, the simulation time is displayed versus the number of iterations. In the bottom of the Figure, the time-step is plotted against the same parameter. As can be seen, for the smaller value ($L/D_0 = 5$), the time-step is dramatically reduced (from iteration 2000 on) and tends asymptotically to zero, resulting in the higher number of iterations required to make the simulation progress. Nevertheless, no significative differences were found in terms of time-step when comparing the cases of $L/D_0 = 10$ and $L/D_0 = 20$. In order to guarantee convergence and reduce the domain size as much as possible (less computational cost) a domain width orifice diameter ratio of 10 has been used.

3.3. Maximum Number of Cells

Due to the Adaptative Mesh Refinement (AMR) algorithm used, the number of cells drastically increases along the simulation when the number of droplets increases due to the atomization process. In order to avoid an increase without limit and a saturation of the computational
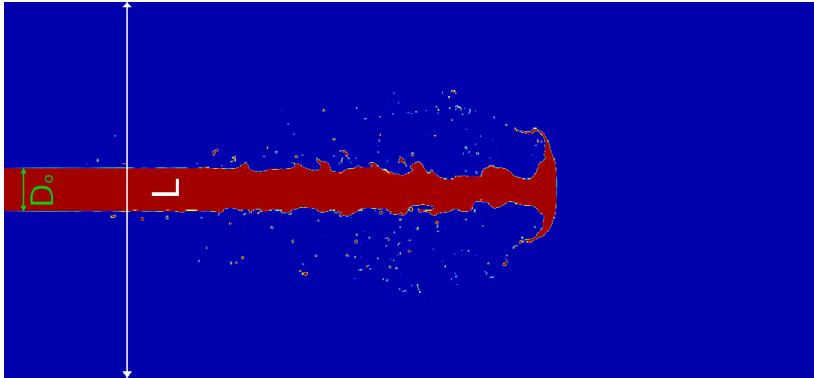
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Figure 2: Domain width
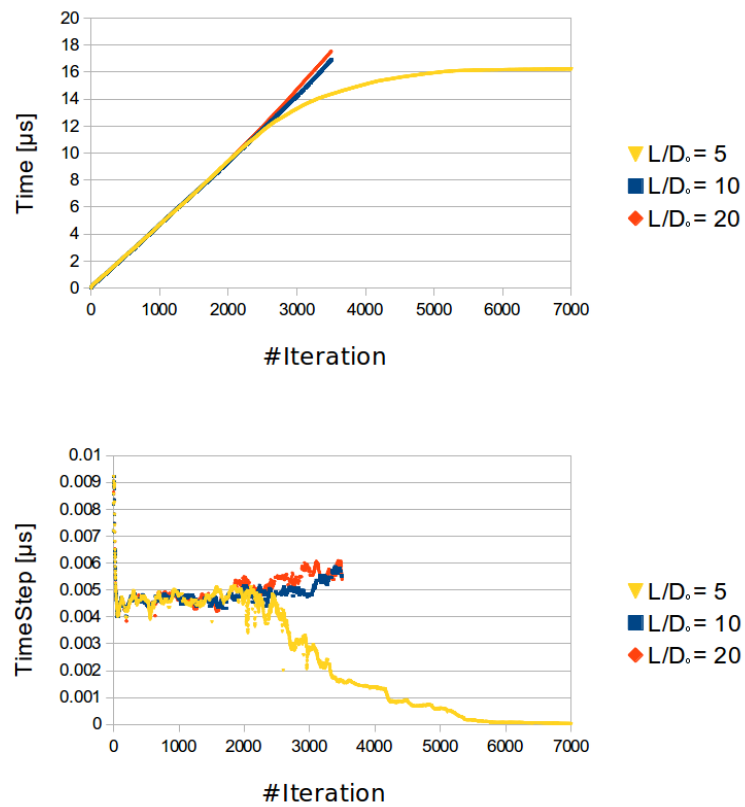

Figure 3: Domain width - orifice length ratios

resources (32 CPUs per simulation), the effect on the results of limiting the maximum number of cells has been studied. As showed in Table 2, six different limits have been tested.

Maximum number of cells [-]	Maximum number of cells per CPU (32 CPUs) [-]
800k	25k
1.6M	50k
3.2M	100k
6.4M	200k
12.8M	400k

Table 2: Maximum number of cells

During the simulation, when the maximum number of cells is reached, cells are created or removed according to AMR cost function criteria, suffering a redistribution but keeping the total number. In Figure 4, the axial velocity of the spray is depicted versus the axial position for all the tested maximum number of cells. The case of a simulation time of 10 μs is exhibited in the upper part and the case of 18 μs in the bottom part. It can be noted that for 10 μs (upper part), the spray tip penetration is around 2 *mm* and the maximum number of cells is not supposed to be reached in any case, and so, all the plotted cases behave exactly in the same way. Nevertheless, after 18 μs of simulation (bottom part), the spray tip penetration is around 3 *mm*, and due to the spray development and atomization, the use of a limitation of 25k would lead to stability and convergence problems.

In order to study the first 7-8 millimeters of the Diesel spray where primary atomization takes place [8], the results of this study has proved that it is required to use the extreme case of 12.8 M cells as a maximum value (that is the same 400k cells per CPU) because with this value convergence and stability problems are avoided even when the maximum number is reached.

4. Validation

The theoretical model from Desantes et al. [25] have been used for validation. It is a theoretical model for the non-perturbed zone length and the drop of velocity in the spray axis in the main region of the spray. As it is drawn in Figure 5, the non-perturbed zone is the axial distance from the orifice where there is only liquid in the axis (liquid core) and the axial velocity is equal to the injection velocity and so, it is not perturbed by the entrained air. The main region is the zone where the liquid core does not further exist because all the fluid has been atomized into small droplets and the axial velocity decreases with the axial position [6, 7, 8].

This model has been extensively validated against measurements of axial velocity in the spray axis obtained with a phase Doppler particle analyzer (PDPA) [7, 25] and also using X-ray projected mass distribution measurements [8, 26] that were converted into fuel mass concentration in the axis. The relationship between axial velocity and axial mass concentration through the Schmidt number [8, 26] allowed validating also this theoretical model with those complex measurements.

The model is based in momentum flux conservation and considers local density variations inside the spray and a generic Schmidt number. A complete model description and the assumptions under the model is derived are given in [26] where the following equation (14) that relates the velocity in the axis with the axial position is obtained:
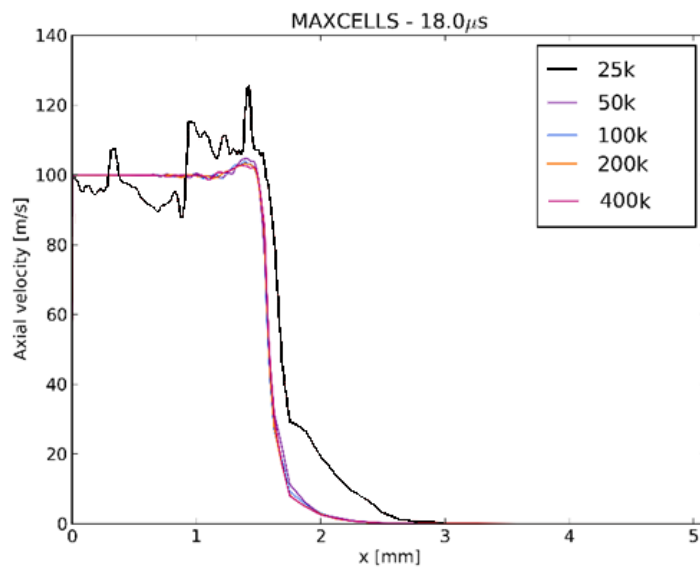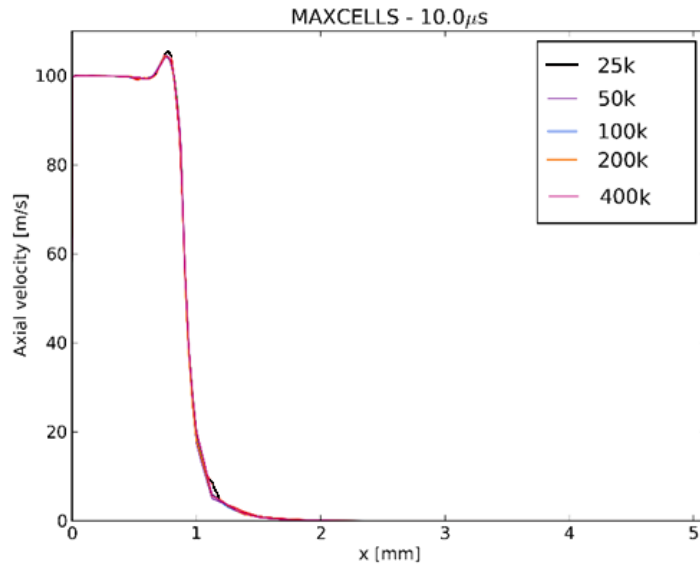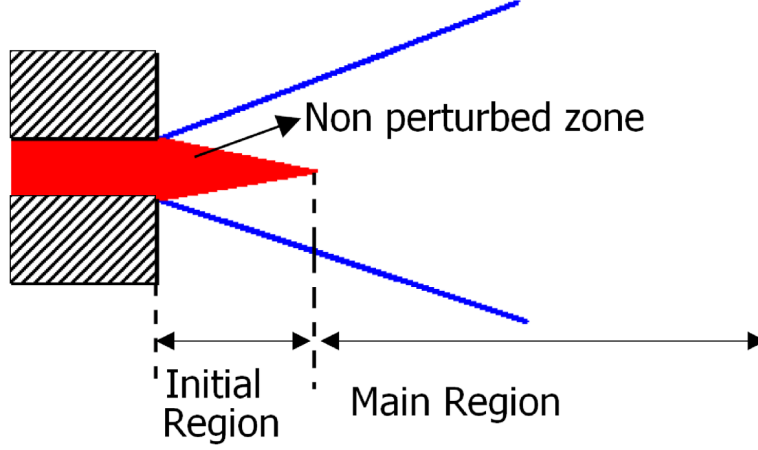
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Figure 4: Maximum number of cells - divergence

Figure 5: Spray zones

$$M_0 = \frac{\pi}{2\alpha}\rho_\alpha \tan\left(\frac{\theta_u}{2}\right) x^2 U_{axis}^2 \sum_{i=0}^{\infty} \frac{2}{2+i \cdot \text{Sc}} \left[\left(\frac{U_{axis}}{U_0}\right)\left(\frac{1+\text{Sc}}{2}\right)\frac{\rho_f - \rho_a}{\rho_f}\right]^i, \qquad (14)$$

where M_0 is the axial momentum flux, Sc is the Schmidt number, ρ_f is the density of the fuel, ρ_a is the density of the air, $U_{axis} = U_{axis}(x)$ is the velocity in the axis, α is the shape factor of the Gaussian profile representative of the radial component of the velocity inside the spray, and θ_u is the velocity spray cone angle.

A case with the physical characteristics of Table 3 has been set up and the outcomes have been compared in terms of velocity drop in the axis with the one expected by Equation (14). The comparison have been performed with 2 Schmidt numbers, Sc = 0.6, which was demonstrated in [26] to be inside a suitable Schmidt number range in diesel sprays [8, 26], and Sc = 1, which is normally used for spray modelers because it simplifies equation (14) [6]. A more scientific reason that justifies the use Sc = 1 is the fact that, although an optimal value of Sc = 0.6 could explain the axial velocity drop along the spray axis, the breakup length is better estimated with the 0D mathematical model when a value of Sc = 1 was used [26].

In Figure 6 the drop in the velocity along the axis of the spray is shown. Results coming from the theoretical model (with two values of Schmidt number) are compared to the results of the 3D simulation. For this last, the value of the spray angle was calculated by fitting the radial velocity profiles to Gaussian profiles following the same procedure described in [25]. From the results it can be observed a good agreement between the theoretical model and the simulation. It is worthy of mention that, as was the case in the comparison of the 0D model with experimental X-ray projected mass distribution measurements [8, 26], the results of the 3D simulation (in that case experimental values) are closer to the velocity decrease provided by the 0D model when a Schmidt number of 0.6 is used, and, what is more important, the simulation and the 0D model basically provide the same intact length with small deviation when the Schmidt number equals unity.

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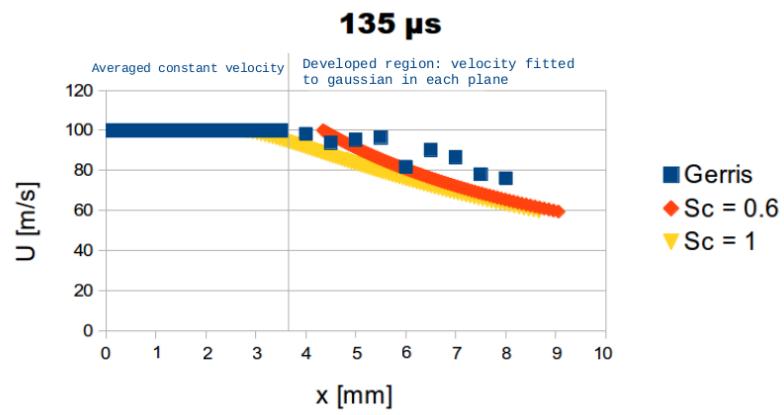| D_0	156 μm
ρ_f	843 kg/m^3
ρ_a	17 kg/m^3
μ_f	2.4e-3 Pa ·s
μ_a	2.872e-5 Pa ·s
U$_0$	100 m/s
σ	2.5e-2 N/m

Table 3: Physical characteristics for validation

Figure 6: Axial velocity drop

5. Influence of Periodic Velocity Perturbation

After the validation, the influence of a periodic perturbation in the injection velocity (inlet boundary condition) on the atomization process has been analysed. In order to achieve this objective, a small sinusoidal perturbation in the inlet velocity given by equation (15) has been considered for several frequencies, f:

$$U = U_0 \left(1 + 0.05 \sin \left(2\pi \cdot f \cdot t \right) \right). \tag{15}$$

This sinusoidal perturbation simulates the pressure oscillations that normally occur in actual injection systems mainly due to the dynamic behavior of the injector.

The exterior non-perturbed length parameter, L_{np}, has been chosen in order to study the influence of the perturbations on the spray morphology. As it is drawn at Figure 7, L_{np} is the length measured from the orifice where there is not perturbation in the spray surface, so, there is not atomization or it is negligible.
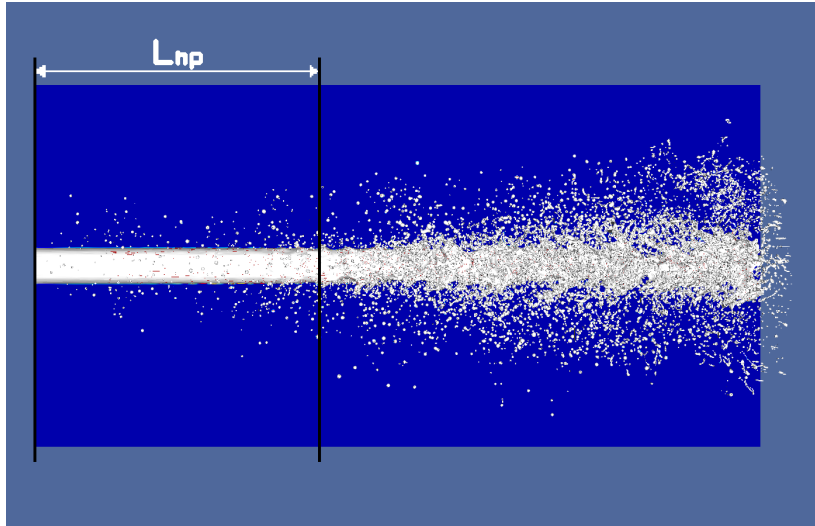

Figure 7: Exterior non-perturbed length

The physical characteristics of the fuel used to perform this study are showed at Table 4.

For this study, the frequency has been varied from 0.2 MHz to 2.2 MHz in steps of 0.2 MHz and also a lowest frequency of 0.1 MHz has been tested. Outcomes have been drawn at Figure 8. As can be observed the tendency of L_{np} over frequency has been captured in a good fit. Higher frequency implies lower L_{np} and L_{np} tends asymptotically to zero as the frequency grows. This result implies that pressure perturbation in the injection system that induce velocity fluctuations could improve the atomization of the spray (diminution of L_{np}).

6. Conclusions

In this section, the main conclusions of the work presented in this paper are drawn:

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D_0	100 μm
ρ_f	696 kg/m^3
ρ_a	25kg/m^3
μ_f	1.2e-3 Pa ·s
μ_a	1.0e-5 Pa ·s
U_0	100 m/s
σ	6.0e-2 N/m

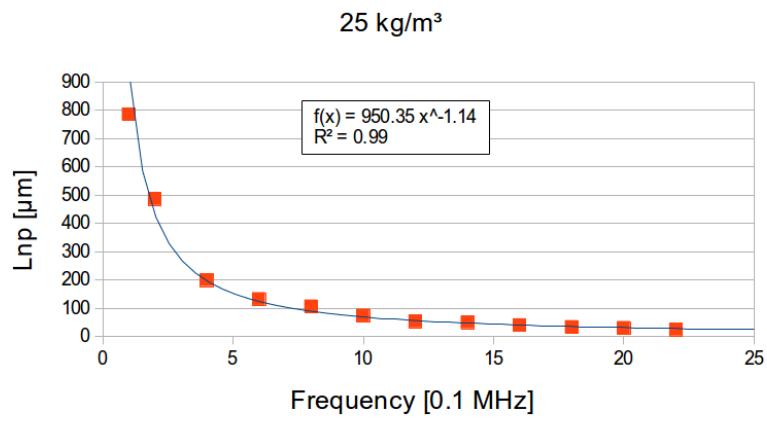Table 4: Physical characteristics for periodic perturbation study

Figure 8: Exterior non-perturbed length over frequency

In this paper, a new multiphasic code for incompressible flow has been studied for using in diesel spray simulations. The study has been performed using low injection velocity in order to reduce the computational cost. First of all, a mesh sensitivity study has been performed over the different possible parameters defining the mesh, namely, domain width, refinement levels and limiting the maximum number of cells in the domain. From this first study the following conclusions have been extracted:

- Two different refinement levels should be used depending on the objective:

    - For the study of external properties of the spray like the spray penetration, a cell size of 9 micrometers has been found to guarantee convergence and reliable results.

    - For the study of inner properties such as droplet characteristics or liquid core length, a cell size of 2 micrometers is required.

- In order to guarantee convergence and reduce the domain size as much as possible and so, reducing the computational cost, a domain width-orifice diameter ratio, L/D of 10 has been obtained as an optimal value to study the first millimeters of the spray (about 8 millimeters).

- In order to study the first millimeters of a diesel spray (8 millimeters), a maximum number of cells of 12.8M cells has been found to be enough to reduce convergence problems.

The code has been validated by comparing with a theoretical 0D model based on momentum flux conservation in the spray. This 0D model has been extensively validated previously with complex measurements using X-Rays. The validation has been made in terms of the velocity evolution in the spray axis and liquid core length. The results of the simulations showed an acceptable agreement of the model with the 0D model results in predicting the axial velocity and the liquid core length.

Finally, the influence of periodic perturbation of the injection velocity on the spray atomization has been studied. This perturbation simulates the pressure oscillations that normally occur in the injection process of Diesel injection systems, which in turns, lead to injection velocity oscillations. A sinusoidal function with amplitude variation of 5% and different frequencies has been tested. The level of atomization has been characterized using the external non-perturbed length (L_{np}) which is the length of the spray closer to the orifice where there is no perturbation in the surface, and so, atomization does not take place.

From this final study, the following conclusions have been drawn:

- The non-perturbed length clearly depends on the frequency: the higher the frequency of the perturbation, the lower the non-perturbed length. An exponential function has been found to fit the results with high level of reliability ($R^2 = 0.99$).

- From this finding, it can be conclude that oscillations in the injection velocity enhance the atomization process.

Acknowledgements

Nomenclature

c: concentration
D: deformation tensor
D_0: orifice diameter
f: frequency
k: curvature
L: domain width
M: momentum flux
n: normal vector
p: pressure
Sc: Schmidt number
u: velocity
Greek symbols:
α shape factor
δ_s Dirac distribution
θ_u velocity spray angle
μ dynamic viscosity
ρ density
σ surface tension coefficient
Subscripts:
f: fuel
a: air

Conflict of Interest Statement

The authors declare that there is no conflict of interests regarding the publication of this article.

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