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ESTIMATION OF A SUITABLE RANGE FOR THE SCHMIDT NUMBER IN DIESEL SPRAYS AT HIGH INJECTION PRESSURE THROUGH A THEORETICAL DERIVATION.

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ABSTRACT

The aim of this paper is to estimate a suitable range for the Schmidt number value in non-evaporative diesel sprays. For this purpose, mass distribution data obtained from Xray absorption experiments existing in literature and a theoretical derivation for spray microscopic characteristics have been combined. Firstly, a procedure based on Gaussian concentration profiles has been proposed in order to interpret X-ray absorption results and relate them to physical parameters as local concentration or spray density. After this, information about FWHM (Full Width at Half Maximum) values has allowed to estimate spray angle in the tested conditions by the definition of Gaussian profiles for the mass radial distribution inside the spray. Following, a theoretical model dependent on momentum flux and Schmidt number has been used to simulate local mass concentration evolution along the spray axis and compare it with the values obtained from the experiments. The combination of the experimental and the theoretical data has allowed to estimate a suitable range for the Schmidt number value in such conditions as those existing in Diesel sprays.

Keywords: Diesel sprays, near field, Schmidt number, concentration, modeling, X-rays.

List of symbols

Α	Outlet orifice section ([m ²])
C(x,r)	Local spray mass concentration ([-])
$C_{axis}(x)$	Concentration at a determined axial position of the spray ([-])
D	Mass diffusivity ($[m^2/s]$)
D_i	Orifice diameter at the inlet section ([m])
D_o	Orifice diameter at the outlet section ([m])
f	Generic radial function for spray velocity distribution ([-])
i	Counter in the Taylor series ([-])
Ι	X-ray beam intensity after passing through the spray ([photons/s])
I_0	X-ray beam incident intensity ([photons/s])
j	Counter in the calculation of Mean Squared Deviation from FWHM data ([-])
k-factor	Degree of conicity of the orifice, defined as $k - factor = \frac{D_i[\mu m] - D_o[\mu m]}{10[\mu m]}$
M'	Projected mass obtained from x-ray measurements ([kg/m ²])
\dot{M}	Momentum flux ([N])
Мо	Momentum flux at the nozzle orifice outlet ([N])
MSD_{θ_m}	Mean Squared Deviation in the calculation of spray angle from FWHM
	measurements ([kg/m ²])
$m_a(x,r)$	Air mass ([kg])
$m_f(x,r)$	Fuel mass ([kg])
\dot{m}_{f}	Fuel mass flow rate ([kg/s])
Ν	Number of terms in the Taylor series ([-])
n_x	Number of measuring points in the axial direction ([-])

Pback	Backpressure ([Pa])
P _{in}	Injection pressure ([Pa])
r	Radial coordinate ([m])
<i>r</i> ₁	Radial position of the x-ray beam at the central plane of the spray ([m])
R(x)	Radius of the spray obtained from velocity profile ([m])
$R_m(x)$	Radius of the spray obtained from concentration profile ([m])
Sc	Schmidt Number ([-])
$U_{axis}(x)$	Velocity at the spray's axis in the axial position x ([m/s])
U_o	Orifice outlet velocity ([m/s])
U(x, r)	Local spray velocity in the axial position x and the radial position r ([m/s])
$V_a(x, r)$	Local volume occupied by air ([m ³])
$V_f(x, r)$	Local volume occupied by fuel ([m ³])
x	Axial coordinate ([m])
Z.	Axial perpendicular coordinate used in the experimental x-ray measurements
	([m])

Greek symbols:

Coefficient of the Gaussian radial profile for the axial velocity ([-])
Deviation in the prediction of M' from the spray width measurements at a
determined axial position ([kg/m ²])
Equivalent diameter ([m])
Outlet diameter of the nozzle's orifice ([m])
Fuel extinction coefficient ([m ² /kg])
Local spray density defined as $\rho = \frac{m_a(x, r) + m_f(x, r)}{V_a(x, r) + V_f(x, r)}$ ([kg/m ³])

$\rho_L(x, r)$	Local fuel density defined as $\rho_L(x, r) = \frac{m_f(x, r)}{V_a(x, r) + V_f(x, r)}$ ([kg/m ³])
$ ho_a$	Ambient density ([kg/m ³])
$ ho_{f}$	Fuel density ([kg/m ³])
ν	Kinematic viscosity ([m ² /s])
π	Pi number ([-])
θ_m	Spray cone angle obtained from mass distribution ([°])
$ heta_{\!u}$	Spray cone angle obtained from velocity distribution ([°])

1. Introduction

High pressure sprays have been widely used in many different applications (combustion processes, internal combustion engines, etc.). Despite having been studied over decades, this kind of sprays involves many complex physical phenomena, such as atomization, coalescence, mass and momentum transfer and evaporation, and there are important questions related with these processes that still remains unclear [1]- [3]. One of the important aspects that have to be taken into account in the design process of pressure atomizers and injectors is the distribution of mass and velocity over the entire spray. This is especially relevant in applications such as diesel spray combustion, since the flame location and characteristics are a result of the air-fuel mixing process. In this sense, both spray macroscopic characteristics, as spray tip penetration or cone angle [4]-[8], and microscopic features like droplet size, velocity or local concentration [9]-[13] have been measured with the help of different experimental techniques. Additionally, several theoretical models have been developed to understand and predict spray behavior [14]-[18]. As a result of most of these studies it can be seen that momentum flux at the nozzle exit can be considered as one of the most important

parameters for the characterization of sprays [15],[17],[19]-[22]. For this reason, several experimental techniques have been developed for measuring momentum flux [23],[24]. Some studies have revealed that Schmidt number has a significant influence on spray characteristics, especially in the near-nozzle field (axial positions lower than 50 D_o), where primary and secondary atomization take place [17]. Nevertheless, most of the experimental data available in the literature is restricted to positions far from the nozzle exit, where the spray concentration values are small enough to use optical techniques as PLIF (Planar Laser Induced Fluorescence) [25][26] or PDPA (Phase Doppler Particle Analyzer) [9],[10],[11], [16], [17]. In fact, typical ranges of study for these techniques are 20-50 millimeters, which implies axial positions higher than 200D_o. For this reason, there are still few contributions that give accurate estimations for Schmidt number in diesel sprays. Only Prasad and Kar [27] gave a range of value of 0.7-0.8 using an injection pressure of 10-20 MPa and nozzle diameters between 0.4 and 0.57 mm. Nevertheless, injection parameters were quite far from current diesel injection conditions, both in terms of injection pressures and nozzle diameters. In the last years, several researchers have made an effort to characterize Diesel spray behavior in the near-nozzle field [28]-[30]. In this sense, Argonne National Laboratories have developed a technique for quantifying projected density distribution inside the spray based on X-ray absorption. The advantage of using X-rays is that while other radiations in the electromagnetic spectra (as for example visible light) are rapidly attenuated by fuel particles, intensity loss for the X-rays is much lower, so that it can be used even in the densest zones of the spray [31]-[34].

In this paper, a combination of a theoretical spray model and X-ray measurements performed at Argonne National Laboratories is used to estimate Schmidt number of a diesel spray for two different nozzles. In the literature, X-ray absorption results express

mass distribution inside the spray by an integrated parameter along the line-of-sight (projected mass density). Thus, the first step for this analysis consists in converting these results to local microscopic parameters such as local density or mass concentration. Afterwards, results about spray width based on Full Width Half Maximum parameter (FWHM) are used for quantifying spray cone angle. For this purpose, Gaussian radial mass concentration functions are used and fitted to the experimental values of FWHM. After this, axial evolution of X-ray absorption measurements is compared with the results obtained by a theoretical model which depends on Schmidt number. Thus, an estimated range for this parameter can be obtained.

Considering the procedure previously described, two important findings will be obtained. On the one hand, a methodology will be described in order to convert X-ray experimental data to local concentration values, which is a more usual parameter to describe spray behavior. On the other hand, the analysis of data available will lead to obtain a suitable range for Schmidt number under realistic Diesel spray conditions, which is an important parameter to describe spray dynamics, especially for modeling purposes. Furthermore, the ability of this model to predict spray characteristics in the near-nozzle field will be analyzed, showing the potential of a simplified model to study the evolution of local velocity and concentration near the nozzle exit. As far as the structure of the paper is concerned, the article is divided in 5 sections. Firstly, in section 2, the model is presented, together with the radial profiles used for the variables studied along the paper (local velocity and local mass concentration). In section 3, a description of the X-ray absorption technique is made, as well as the experimental conditions and processing tools are summarized. Analysis of radial distribution results for the two nozzles is performed in section 4, leading to obtaining the spray cone angle value for the

tested conditions. After this, a comparison of the axial evolution of X-ray measurements and the predictions obtained by the theoretical model is made for different Schmidt numbers. Finally, in section 5, the most important conclusions of the work are drawn.

2. Spray model

2.1. Background

Diesel sprays have been traditionally divided in two different regions depending on its internal characteristics (Figure 1). In the first region (or intact core length) the fuel on the spray axis has not been perturbed by entrained air, and therefore

local fuel mass concentration, defined as $C_{axis}(x) = \frac{m_f(x)}{m_a(x) + m_f(x)}$, can be

considered as unity, and the local velocity value at the spray axis is still the same as the exit velocity.

The extension and behavior of this region is a consequence of primary atomization process, which depends on several physical phenomena such as flow turbulence or cavitation [1],[35],[36]. Nevertheless, the length of this region is usually in the range of $10D_o$ for typical injection conditions.

In the main or fully developed region, any section of the spray includes a significant amount of entrained air [36]. According to previous studies, the behavior in this region can be properly characterized in terms of momentum flux at the nozzle exit

[9],[20],[22], being the momentum flux at the nozzle exit equal to $M_o = m_f U_o$, with

 m_f , the fuel mass flow rate, and U_o the orifice outlet velocity.

Adler and Lyn [1] were one of the first authors to propose a study of sprays using a continuous model of gas jet, stating that this was justified due to the similarity between

gas jets and sprays from the point of view of basic mechanism. Since then, many other researchers have followed this path, as for example Rife and Heywood [6] who developed a model to predict spray behavior based on gas jet equation, or Prasad and Kar [27], who performed an investigation in order to analyze the processes of diffusion of mass and velocity obtaining quantitative data for treating the diesel spray as a turbulent jet. These and many other investigations imply that many results from the literature concerning gas jets will be directly applicable to sprays.

Nevertheless, it must be considered that, for a given nozzle geometry, the jet has a constant cone angle [37] which depends neither on injection pressure nor on ambient density, while the diesel spray has a cone angle that depends on the operating conditions [5], [35],[36], or indirectly on the presence or not of cavitation [19],[30],[38].

Additionally, it has been seen that spray aperture has different behavior in the two zones previously described (see Figure 1), probably due to the fact that atomization has not been completed [3][28]. Anyway, as a simplification, many studies consider a constant spray cone angle equal to the one corresponding to the main region of the jet or spray [1][14][27][39].

One of the important implications of the analogy between a gaseous jet and a spray is self-similarity. Rajaratnam [42] among others [3][27][37] [40] [41][44], found that, for any section in the fully develop region of the spray, if the velocity at any radial position is divided by the velocity at the axis and plotted versus the normalized radius (r/R), where r is the radial coordinate and R the spray radius at which velocity profile reaches 1% of its axial value, it has a unique evolution.

This result can be expressed as:

$$U(x,r) = U(x,0)f(r/R(x))$$
⁽¹⁾

where f is a radial profile for the velocity U. The same result is obtained if fuel concentration is considered:

$$C(x,r) = C(x,0) \left[f(r / R(x)) \right]^{Sc}$$
⁽²⁾

where *Sc* is the effective Schmidt number, which represents the ratio of effective momentum diffusivity to effective mass diffusivity and represents the relative rate of momentum and mass transfer, including both molecular and turbulent contributions. It is defined as:

$$Sc = \frac{v}{D}$$
(3)

with v the kinematic viscosity, and D the mass diffusivity.

Self-similarity hypothesis has shown to be adequate in many studies, and different radial profiles have been proposed in the literature[40]-[44]. The main consequence of this hypothesis is that the problem of calculating velocity or concentration distribution along the spray can be simplified to the calculation of the values of these parameters at the axis, as characteristics at any other position can be derived from the results at the axis as long as the function *f* in Equations (1) and (2) is known.

2.2. Theoretical derivation

The theoretical model considered in the current work is obtained under the hypothesis that momentum flux in the axial direction is conservative along the spray axis and, consequently, equal to momentum flux at the nozzle exit for any axial position. This fact has been confirmed by momentum flux measurements [45] and can be expressed as:

$$\dot{M}_{o} = \dot{M}(x) \tag{4}$$

where M_o and M(x) are the momentum flux through a spray cross section at the orifice outlet and at a distance *x*, respectively. If it can be assumed that the radial profile

of the velocity at the nozzle exit is flat, momentum flux can be defined as $M_o = m_f U_o$, as was introduced in section 2.1. Influences of a non-flat profile have been studied by Post *et al.*[46]. They show that, if two sprays have different radial profile shapes but the mass and axial momentum fluxes have the same value, the influence of the profile shape is confined to the initial region. In the main jet region, the distribution of axial velocity is identical at any axial position. Nevertheless, even when trying to analyze spray behavior in the near-nozzle field, it is usually difficult to obtain precise information about the actual shape of the velocity profile at the nozzle exit. Anyway, it is important to consider that when high injection pressure are used, as it is the case of the current analysis, considerably turbulent velocity profile is expected, which would not be too far from the flat profile assumption.

In order to develop expression (4), momentum must be integrated over the whole section, assuming cylindrical symmetry of the spray or jet:

$$\dot{M}_{o} = \dot{M}(x) = \int_{0}^{\infty} 2\pi\rho(x,r)rU^{2}(x,r)dr$$
(5)

where the x-coordinate coincides with the spray axis, and the r-coordinate is the radial position (perpendicular to the spray axis). In this expression, U(x,r) is the local spray velocity and $\rho(x,r)$ is the local density in the gas jet or diesel spray defined as:

$$\rho(x,r) = \frac{m_a(x,r) + m_f(x,r)}{V_a(x,r) + V_f(x,r)}$$
(6)

being $m_f(x,r)$ and $V_f(x,r)$ the local mass and volume of fuel, and $m_a(x,r)$ and $V_a(x,r)$ the local mass and volume of air.

The density at an internal point of the spray, taking into account the local concentration, can be written in terms of spray local concentration as follow:

$$\rho(x,r) = \frac{\rho_f}{C(x,r)\left(1 - \frac{\rho_f}{\rho_a}\right) + \frac{\rho_f}{\rho_a}}$$
(7)

with ρ_f the fuel density, ρ_a the air density and C(x,r) the local (mass-based) fuel concentration, defined as:

$$C(x,r) = \frac{m_f(x, r)}{m_a(x, r) + m_f(x, r)}$$
(8)

It should be noted that C(x,r) value can be significantly different from the local volume concentration, which is also frequently used in sprays studies.

For the developed region in the spray, fuel concentration and axial velocity can be considered to follow a Gaussian radial profile:

$$U(x,r) = U_{axis}(x) \exp\left(-\alpha \left(\frac{r}{R(x)}\right)^2\right)$$
(9)

$$C(x,r) = C_{axis}(x) \exp\left(-\alpha Sc\left(\frac{r}{R(x)}\right)^2\right)$$
(10)

with *Sc* the Schmidt number, and α the shape factor of the Gaussian distribution. The spray radius, *R*, is considered as the radial distance from the axis, where axial velocity concentration reaches 1% of the value at the spray axis. This kind of profiles have previously shown to be adequate to reproduce radial distributions of velocity and concentration in a diesel spray [10],[14],[34],[38].

Substituting Eqs. (8), (9) and (10) in Eq. (5), the momentum in any section of the spray can be expressed as:

$$\dot{M}_{o} = 2\pi\rho_{f}U_{axis}^{2} \times \int_{0}^{\infty} \frac{r\exp\left(-2\alpha\left(\frac{r}{R(x)}\right)^{2}\right)}{C_{axis}(x)\left(1-\frac{\rho_{f}}{\rho_{a}}\right)\exp\left(-\alpha Sc\left(\frac{r}{R(x)}\right)^{2}\right) + \frac{\rho_{f}}{\rho_{a}}}dr$$
(11)

where , as can be seen, the terms depending on the axial coordinate are $C_{axis}(x)$, $U_{axis}(x)$ and R(x).

Integrating Eq. (11) and taking into account that the radius of the spray R can be expressed as a function of spray velocity angle as:

$$R(x) = x \tan\left(\frac{\theta_u}{2}\right) \tag{12}$$

the following expression is obtained (details of all the steps followed in integration can be found in Appendix section of *Desantes et al.* [17]):

$$\dot{M}_{o} = \frac{\pi}{2\alpha} \rho_{a} \tan^{2} \left(\frac{\theta_{u}}{2}\right) x^{2} U_{axis}^{2} \sum_{i=0}^{\infty} \frac{1}{\left(1+i\frac{Sc}{2}\right)} \left[C_{axis}(x) \left(\frac{\rho_{f}-\rho_{a}}{\rho_{f}}\right)\right]^{i}$$
(13)

In this expression, the spray velocity angle θ_u is defined as the angle at which velocity reaches 1% of its value at the spray axis. This angle is assumed to be constant along the spray. The term *i*, is the index for the summation which approximates the solution of the integration seen in Equation (11). This model has been developed under the following assumptions:

- Cylindrical symmetry and Gaussian profiles are assumed for spray microscopic characteristics.
- The environment is quiescent, and so, no axis deflection exists.
- Air density in the injection chamber is constant during the whole injection process.
- Momentum flux and thus injection velocity and mass flow rate at the orifice outlet are constant during the whole injection process.
- Slip between gas and liquid phases is negligible.

Several comments can be made about these assumptions. Firstly, cylindrical symmetry assumption is more appropriate for single-orifice axi-symmetric nozzles, for which the

orifice axis is parallel to the injector axis. Nevertheless, in a multi-orifice nozzle the flow enters to the discharge orifices mainly from the upper part, and so, a slight asymmetry is expected in the spray characteristics. With respect to the second and the third assumptions (quiescent environment and constant air density), they can be considered as acceptable when the spray is injected into a constant volume chamber, where pressure and temperature can be controlled and the discharge gas velocity can be considered as negligible. On the contrary, in engine environment, changes in air movement, pressure and temperature along the engine cycle are expected and so they should be considered. Constant injection velocity is a typical assumption when studying stationary sprays, and can be considered as adequate for long injection pulses, at which the needle has reached its maximum lift. Finally, the no slip condition implies that the velocities of the spray and the discharge gas in the spray edge (r = R) are equal. Considering the low velocities of the spray at this radial position described by the Gaussian profiles, it is expected that this assumption is accurate enough for describing spray dynamics. At this point, it is also important to consider that the Gaussian profiles assumed for the current model are more realistic as getting further from the nozzle exit. For this reason, the model can be satisfactory to reproduce the spray characteristics in the near-nozzle field, but could not be adequate to study the region corresponding to the intact core of the spray.

This model has been extensively validated both in terms of local velocity and local mass concentration in previous studies [10],[17]. In Desantes *et al.* [17], for a given set of conditions, Schmidt number variations between 0.6 and 1.4 did not have any significant influence on the calculated on-axis velocities for the spray region beyond approximately $20\phi_{eq}$, with ϕ_{eq} being the equivalent diameter ($\phi_{eq} = \phi_o \sqrt{\rho_f / \rho_a}$) and ϕ_o the outlet diameter of the nozzle. Nevertheless, the influence of Schmidt number became very

important in the near-nozzle field. The consequence is that when Sc is not known, which is normally the case, a simplified equation for Sc=1 can be expected to give very good estimations far from the nozzle exit, as it will be demonstrated in next section, but the characteristics of the spray estimated in the near-nozzle spray are not accurate enough. For this reason, an estimation of the Schmidt number range value in realistic diesel injection conditions can be useful for obtaining more accurate predictions in this region, especially for those people devoting on diesel spray modeling.

3. Analysis of X-ray mass distribution measurements

3.1. Measurement basis

During the last years, Argonne National Laboratories have developed a technique for quantifying mass distribution inside sprays by means of X-ray absorption. Basically, this technique consists in passing a monochromatic X-ray beam through the spray at a determined position (see figure 2a). The X-ray source emits monochromatic beams with photon energy of 8.16 keV and a 2% bandwith ($\Delta E/Ev \sim 10^{-2}$). Each X-ray beam includes a total of $3x10^9$ incident photons/s. Using this configuration, the fuel used has an absorption coefficient of approximately $2.5x10^{-3}$ m²/g, which is considerably higher than the absorption coefficient seen for other electromagnetic radiations.

The Beer-Lambert law can be used to relate the intensity loss of the X-ray beam and the mass concentration [33]:

$$\frac{I}{I_0} = \exp(-\mu_m M') \tag{14}$$

I being the x-ray beam intensity transmitted through the spray and measured by a photodiode, I_0 the incident X-ray intensity, and μ_m the extinction coefficient (per mass/area). *M*' is the projected fuel mass per unit area along the X-ray beam path, which can be defined as:

$$M' = \int \rho_L(z) dz \tag{15}$$

where ρ_L is the local fuel density, defined as $\rho_L(x, r) = \frac{m_f(x, r)}{V_a(x, r) + V_f(x, r)}$, and z is the

x-ray beam direction, perpendicular to the spray axis. The reason for using local fuel density instead of local spray density seen before $\rho(x,r)$ is that X-ray absorption produced by the air entrained into the jet is negligible.

The advantage of using a technique based on X-rays in comparison with other nonintrusive optical measurement techniques is that, in the dense primary break-up region close to the nozzle outlet, the spray core is generally surrounded by a cloud of small droplets that is opaque to visible light, whereas with X-rays, the absorption replaces scattering as the dominant interaction mechanism between fuel particles and incoming photons [32][33][34]. Attenuation of a monochromatic X-rays only depends on the total fuel mass contained within the beam path and transmitted intensities can be captured even in the vicinity of the nozzle, where fuel concentration is equal or near unity.

As it can be seen, X-ray absorption technique allows to obtain an integrated value of the local fuel density along the beam path. Nevertheless, information about the local spray distribution can be reconstructed using the Gaussian profile described in equation (10). For this purpose, local fuel mass density $\rho_L(x,r)$ must be expressed in terms of local mass concentration C(x,r):

$$\rho_L(x,r) = \frac{\rho_f}{\left(1 - \frac{\rho_f}{\rho_a}\right) + \frac{1}{C(x,r)}\frac{\rho_f}{\rho_a}}$$
(16)

Where spray concentration can be obtained from equation (10) as:

$$C(x,r) = C_{axis}(x) \exp\left(-\alpha Sc\left(\frac{r}{x \tan\left(\theta_u/2\right)}\right)^2\right)$$
(17)

where spray velocity angle θ_u is defined as the angle at which concentration reaches 1% of its value at spray axis. Additionally, this Gaussian profile can be expressed in terms of spray mass angle instead of spray velocity angle by means of the following equation:

$$\tan\left(\frac{\theta_u}{2}\right) = \sqrt{Sc} \tan\left(\frac{\theta_m}{2}\right) \tag{18}$$

So that local concentration can be calculated as:

$$C(x,r) = C_{axis}(x) \exp\left(-\alpha \left(\frac{r}{x \tan\left(\theta_m/2\right)}\right)^2\right)$$
(19)

Introducing this expression of C(x,r) into Equation (16), and defining $R_m = x \tan(\theta_m/2)$, local fuel density can be expressed as:

$$\rho_L(x,r) = \frac{\rho_f}{\left(1 - \frac{\rho_f}{\rho_a}\right) + \frac{1}{C_{axis}(x) \exp\left(-\alpha \left(\frac{r}{R_m}\right)^2\right)} \frac{\rho_f}{\rho_a}}$$
(20)

Thus, M' can be calculated as seen in equation (17):

$$M'(x, r_{1}) = \int_{-\infty}^{+\infty} \frac{\rho_{f}}{\left(1 - \frac{\rho_{f}}{\rho_{a}}\right) + \frac{1}{C_{axis}(x) \exp\left(-\alpha \left(\frac{r_{1}^{2} + z^{2}}{R(x)^{2}}\right)\right)} \frac{\rho_{f}}{\rho_{a}}} dz$$
(21)

where r_1 is the radial position at which the X-ray beam is located in the z = 0 plane (see figure 2b), and can be defined as

$$r_1 = \left(r^2 - z^2\right)^{\frac{1}{2}}$$
(22)

3.2. Experimental data.

For the current analysis, M' axial distribution data will be used. These data have been obtained and reported by Argonne National Laboratories in a previous publication [32]. The experiments have been conducted using a standard diesel fuel doped with cerium. The resulted mixture has a density of 890 kg/m³ and a kinematic viscosity of 10^{-6} m²/s at 40 °C. The X-ray beam is made by a rectangular window of around 0.1x0.015 mm². Two multi-orifice mini-sac nozzles have been tested (see Figure 3), with identical nominal geometry (diameter of 130 µm and k-factor of 1.5) but different number of orifices (3 orifices for nozzle A and 5 orifices for nozzle B). Nevertheless, only one orifice from each of these nozzles has been characterized. Injection pressure of 80 MPa and backpressure of 1.85 MPa (leading to a chamber density of 21 kg/m³) have been selected.

The experimental data available for the following analysis has been summarized in Figure 4. It includes axial measurements up to 15 millimeters, with 29 points for nozzle A and 32 for nozzle B (Figure 3.a). Additionally, information about spray width characterized by FWHM (Full Width Half Maximum) is available for eight of these measuring locations until an axial position of 12 millimeters (Figure 3.b). This information has been obtained by carrying out tests at different radial r_1 positions in the range $-R < r_1 < R$.

4. Schmidt number estimation.

The theoretical model already presented in Equation (13) allows to calculate C_{axis} evolution for a given set of conditions. These conditions include the nozzle geometry and the pressure conditions through the Momentum flux at the orifice outlet, M_o , which depends on both [23], as well as spray cone angle and Schmidt number. Additionally, it has been already seen that M' results obtained by X-ray absorption technique can be directly related with the values of C_{axis} if spray cone angle is known (equation 21).

Thus, a combination of the model and the experimental data can be used to obtain the Schmidt number value that better represents spray measured characteristics. For this purpose, the first step will consist in evaluating spray cone angle by means of the FWHM data available.

4.1. Determination of spray angle.

Spray width has been defined by Leick *et al.* [32] using the FWHM criterion. This parameter quantifies the total spray width at the point at which the radial profile of M' reaches the 50% of its maximum value, *i.e.* FWHM(x) is the double of the radial position r_1 which satisfies that

$$M'(x,r_{\rm l}) = \frac{M'(x,0)}{2}$$
(23)

According to this definition, this radial position r_1 can be calculated for each axial position as $r_1(x) = FWHM(x)/2$.

Using the definition of M' from equation (21), the following expression can be obtained:

$$M'(x, r_{1}) = \int_{-\infty}^{+\infty} \frac{\rho_{f}}{\left(1 - \frac{\rho_{f}}{\rho_{a}}\right) + \frac{1}{C_{axis}(x) \exp\left(-\alpha \left(\frac{\left(FWHM(x)/2\right)^{2} + z^{2}}{\left(x \tan\left(\theta_{m}/2\right)\right)^{2}}\right)\right)} \frac{\rho_{f}}{\rho_{a}}}$$

$$= \frac{1}{2} \int_{-\infty}^{+\infty} \frac{\rho_{f}}{\left(1 - \frac{\rho_{f}}{\rho_{a}}\right) + \frac{1}{C_{axis}(x) \exp\left(-\alpha \left(\frac{z^{2}}{\left(x \tan\left(\theta_{m}/2\right)\right)^{2}}\right)\right)} \frac{\rho_{f}}{\rho_{a}}}$$
(24)

Equation (24) implies eight equations corresponding to the axial positions at which spray width information is available (Figure 4.b), and nine free parameters: spray mass angle θ_m , which is assumed to be constant along the spray axis, and C_{axis} value for each one of the eight axial measuring points *x*. As this equations system cannot be solved analytically, a numerical optimization procedure must be defined. This procedure consists of the following steps:

- Spray angle is fixed to a determined value θ_m .
- For each position at which FWHM parameter has been measured, *C_{axis}* values between 0.1 and 1 (with a step value of 0.001) are evaluated. The ability of the combination of spray cone angle and axial concentration to reproduce the FWHM experiments is evaluated using equation (25):

$$\delta M'(x) = M'(x, r_1 = FWHM(x)/2) - \frac{M'(x, r_1 = 0)}{2}$$
(25)

- The optimal C_{axis} value for each axial position x is calculated as the one which minimizes $|\delta M'(x)|$.
- Global mean squared deviation in the estimation of the FWHM axial evolution for the given spray angle is calculated as:

$$MSD_{\theta_m} = \sqrt{\frac{\sum_{j=0}^{n_x} \left[\delta M'(x_j)\right]^2}{n_x}}$$
(26)

where n_x is the number of axial positions.

This procedure is followed for a total number of 121 spray cone angle values between 5° and 35° (step value of 0.25°). The evolution of *MSD* in terms of spray cone angle for the two nozzle studies is shown in Figure 5. There is a global minimum in the evolution of *MSD* reached at 18.25° and 16.25° for nozzles A and B, respectively.

As it can be seen, although the two nozzles have the same nominal outlet diameter and k-factor, there is a non-negligible difference in spray cone angle value between them. This fact could be also appreciable paying attention to the spray width data available in Leick *et al.*'s study [32]. This difference can be probably due to the effect of the hydrogrinding process, whose information is not available. The hydro-grinding intensity (and, consequently, the curvature radius at the nozzle inlet) has shown to have a significant influence on spray cone angle in previous studies, so that small variations in this parameter can justify the variations seen in the current analysis [47],[48]. Additionally, silicone mould methodology has proved that there is non-negligible deviation of internal nozzle geometric parameters between different orifices of the same nozzles [49], leading to a significant uncertainty in the actual nozzle geometric parameters. Also Lee *et al.* [50] have found important differences in nozzle outlet diameter between the nominal values and the results of a metrology study developed using a X-ray visualization technique.

Along this analysis, a constant spray mass angle has been considered. As it has been discussed previously, this assumption does not describe precisely diesel spray characteristics, since different spray angle values have been reported in the literature close to the nozzle exit than in further axial positions. Nevertheless, it is expected that the influence of this assumption is confined very close to the intact length of the spray, while most of the experimental data used for current study correspond to the main region, at which spray angle is known to be constant. For this reason, constant spray angle assumption seems to be adequate for the current study, despite it implies possible uncertainties when getting close to the intact length zone.

4.2. Analysis of the axial distribution

As it has been seen previously, information of the axial evolution of M' up to 15 millimeters is available for the two nozzles analyzed. Once spray mass angle has been characterized for the tested conditions (18.25° and 16.25° for nozzles A and B respectively), Equation (21) can be used to extract C_{axis} values which best fit the

experimental M' data. For this purpose, as equation (21) cannot be solved directly, M' has been obtained using a range for C_{axis} between 0.1 and 1, with a step value of 0.001. These M' values have been compared with the experimental ones, leading to an optimal C_{axis} for each axial position and each nozzle. Nevertheless, it is important to consider at this point that there is no quantitative information about the possible uncertainties involved with the measuring process and so over the M' data. Anyway, the information available in the X-ray studies [32][33] show that the signal-to-noise ratio in this kind of measurements is considerably low, so that the M' values available can be assumed to reproduce spray characteristics with high precision..

In order to estimate the influence of the Schmidt number value on the characteristics of the spray, axial evolution of C_{axis} previously obtained can be compared with the values predicted by the theoretical model presented in section 2. In this model, as seen in Equation (13), axial spray behavior is described in terms of momentum flux, axial velocity and axial concentration. Momentum flux at the nozzle exit can also be defined as:

$$\dot{M}_o = \rho_f A U_o^2 \tag{27}$$

where *A* is the area of the nozzle exit orifice. So that Equation (13) can then be easily transformed into:

$$\rho_f A = \frac{\pi}{2\alpha} \rho_a \tan^2 \left(\frac{\theta_u}{2}\right) x^2 \left(\frac{U_{axis}}{U_o}\right)^2 \sum_{i=0}^N \frac{1}{\left(1+i\frac{Sc}{2}\right)} \left[C_{axis}(x) \left(\frac{\rho_f - \rho_a}{\rho_f}\right)\right]^i$$
(28)

where N is the number of terms for the truncation of the series defined in Equation (13). Previous studies have shown that axial concentration and velocity can be related in terms of Schmidt number [51] as:

$$\left(\frac{U_{axis}(x)}{U_o}\right) = C_{axis}(x)^{Sc}$$
⁽²⁹⁾

If this definition is introduced in Equation (13), an implicit equation for the Sc in terms of C_{axis} can be stated:

$$1 = \frac{\pi}{2\alpha} \frac{\rho_a}{\rho_f} \frac{1}{A} \tan^2 \left(\frac{\theta_u}{2}\right) x^2 \left(C_{axis}(x)\right)^{2Sc} \sum_{i=0}^N \frac{1}{\left(1 + i\frac{Sc}{2}\right)} \left[C_{axis}(x)\frac{\rho_f - \rho_a}{\rho_f}\right]^i$$
(30)

Finally, Equation (18) can be used to express Equation (30) in terms of mass angle:

$$1 = \frac{\pi}{2\alpha} \frac{\rho_a}{\rho_f} \frac{1}{A} Sc \tan^2 \left(\frac{\theta_m}{2}\right) x^2 \left(C_{axis}(x)\right)^{2Sc} \sum_{i=0}^N \frac{1}{\left(1+i\frac{Sc}{2}\right)} \left[C_{axis}(x)\frac{\rho_f - \rho_a}{\rho_f}\right]^i$$
(31)

where θ_m is the optimal spray mass angle previously calculated for the two nozzles, which is assumed to be constant for any axial position.

This expression has been numerically solved with a step value for the axial position x of 0.1 mm and a number of terms N of 11. The truncation error of the series would represent around 1.5-2% for typical values of Sc and C_{axis} , so that it can be concluded that the resolution with 11 terms is adequate.

Figures 6 and 7 show the evolution of C_{axis} in terms of axial position for the two tested nozzles respectively. The filled circles represent the values reconstructed from M'experimental data, obtained as explained at the beginning of this section. The lines show the evolution of axial concentration predicted by the model described in equation (31) for a range of Schmidt numbers between 0.5 and 1.

As it can be seen, Schmidt number has an important influence on C_{axis} evolution until an axial position of ~10-12 millimeters (around 75-80 D_o), where the difference between the curves becomes almost negligible. This behavior was also observed in a previous study [17]. Furthermore, two different zones can be defined attending to the behavior of C_{axis} depicted in the figure. Beyond an axial position of around 4 mm (*i.e.* ~30 D_o),

which includes the most important amount of experimental data, the behavior of the axial concentration is properly reproduced by the theoretical model for a *Sc* value near 0.5. This value is lower than those observed by Prasad and Kar [27], but it must be considered that injection parameters values were quite different from current typical conditions ($P_{in} < 20$ MPa, $\phi_o > 0.4$ mm, $P_{back} = 0.1$ MPa).

On the contrary, for axial positions up to approximately 4 mm (including the intact length), the behavior of $C_{axis}(x)$ does not correspond with any theoretical curve. This could be due to different reasons:

- As stated previously in the text, different investigation works based on visualization techniques have pointed out that spray angle near the nozzle exit (in the region corresponding to the intact length zone) is significantly different from the expected cone angle defined at higher axial positions
 [28],[29],[38],[52]. This fact could lead to a loss in the precision of the axial concentration estimation near the intact length of the spray.
- The hypothesis used to construct the model (mainly the gaseous jet analogy) are known to be adequate after spray has been decomposed in droplets small enough to behave in a similar way to a gas jet. This implies that the very first millimeters of the spray (corresponding to zone close to the intact length) are probably not well described by this model, as complex phenomena as primary atomization is not taken into account. Nevertheless, the good agreement between the model and the experimental results further from 3.5-4 mm can be taken as a proof of the capability of the model to reproduce spray characteristics in the near-nozzle field if Schmidt number value is well chosen.

5. Conclusions

A theoretical analysis combined with experimental mass distribution with X-ray radiography has been used with the aim of characterize near-nozzle spray behavior. For this purpose, a procedure has been proposed in order to relate projected mass density results available in the literature from X-ray absorption tests and spray local mass concentration. Once this procedure is applied, a one-dimensional model is applied in order to estimate the Schmidt number range at which spray internal characteristics of the spray, once primary atomization has taken place, are properly predicted. This simplified model, based on gaseous jet analogy, has shown to be useful to describe spray mass distribution for axial positions larger than 4 mm in the current analysis with a significant low calculation cost in comparison with CFD methods.

From this work, the following conclusions can be drawn:

- As a result of a theoretical reasoning based on momentum flux conservation in the axis direction of the diesel spray, a mathematical model has been obtained which relates the momentum flux with the profiles of velocity and concentration, local density and spray cone angle.
- X-ray projected mass distribution measurements have shown to be useful in order to characterize spray behavior in the near-nozzle field, where the influence of Schmidt number is more severe. Information of axial evolution of projected density from two different nozzles was available.
- The analysis of spray width obtained from X-ray measurements in terms of FWHM has allowed to calculate spray cone angle for the two nozzles used at a chamber density of 21 kg/m³. The differences observed in terms of spray angle are probably due to slight differences in nozzle geometry. In this sense, curvature radius at the inlet section, which is not known in the present work, has shown to have a strong influence on spray cone angle.

M' axial evolution has been used to reproduce axial concentration values which best fit with the experiments. These values have been compared with the curves obtained from the theoretical model at different Schmidt numbers. Beyond approximately 3.5 or 4 millimeters, spray characteristics are properly reproduced by a Schmidt number of 0.5. Nevertheless, for lower axial positions, any theoretical curve shows a good agreement with reconstructed *Caxis* values. The expected variation of spray angle during this region, not contemplated in this study, could explain this phenomenon.

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FIGURE CAPTIONS

Figure 1. General jet structure.

Figure 2.a. Scheme of x-ray measuring setup.

Figure 2.b. Description of integration for calculating M'.

Figure 3.Scheme of the internal geometry of a multi-orifice nozzle.

Figure 4. Summary of experimental X-ray results used for the Schmidt number estimation.

Figure 5. Mean Squared Deviation in the spray angle calculation derived from FWHM measurements.

Figure 6. Analysis of axial concentration evolution for Nozzle A.

Figure 7. Analysis of axial concentration evolution for Nozzle B