APPLICATION OF THE MAXIMUM ENTROPY PRINCIPLE TO THE
ANALYSIS OF A DIESEL ENGINE FUEL SPRAY

Celso Argachoy
Centro Universitário da FEI
Departamento de Engenharia Mecânica
Av. Humberto A. C. Branco, 3972
09850-901 São Bernardo do Campo, SP - Brasil
celsoarj@fei.edu.br

Amilcar Porto Pimenta
ITA – Instituto Tecnológico de Aeronáutica
Divisão de Engenharia Aeronáutica – Departamento de Propulsão
Praça Marechal Eduardo Gomes, 50
12228-900 São José dos Campos, SP - Brasil
amilcar@ita.br

Abstract. The work presents a theoretical and an experimental analysis of the droplet size distribution in the spray
generated by the injectors of an internal combustion Diesel engine. The theoretical analysis has been made through a
simple droplet size distribution function derived by applying the Maximum Entropy Principle to the atomization
process, along the normalization of the probability distribution function and the mass conservation law. The
experimental analysis has been made through the laser diffraction technique, with the Malvern Mastersizer equipment.
A Diesel engine with electronically actuated injection pumps was used. One of the high-pressure tubes was derived
from the engine to feed the experimental injection nozzle, which is mounted in a high-pressure chamber filled with inert
gas and provided with transparent windows. The engine has been placed close to the structure in which the Malvern
Mastersizer is installed, so that the test chamber is positioned in the sampling area of the laser equipment, between
the transmitter and the receiver. The equipment analyzes the spray and then supplies its volume based droplet size
distribution function. Although predicted values from Maximum Entropy Principle do not perfectly match measured
ones, the principle was shown capable to define the form and the maximum peak of the droplet size distribution
function.

Keywords: Injectors, Fuel Spray, Diesel Engines, Maximum Entropy Principle, Laser Diffraction.

1. Introduction

In the Diesel engines, the theoretical and experimental evaluation of the droplets formed by the fuel spray have
fundamental importance in the point of view of the engine efficiency, in terms of the mechanical power generated in
relation to the amount of fuel employed, as for the exhaust emissions, mainly oxides of nitrogen and particulate matter.
According to Heywood (1988), the values of the air-fuel ratio in the combustion chamber are determined, among other
parameters, for the distribution and the path of the drops in the spray. Therefore, to study the combustion process in
two-phase flow in the engine combustion chamber, as well as to develop injection systems that contribute so that the
engines can be less pollutant with the same or perhaps with better performance, it is very important to have reliable
tools to analyze the fuel spray.

One of the proposals of this work is to analyze the laser diffraction as a technique for experimental analysis of the
spray droplets distribution. It is known that the experimental analysis is relatively hard, mainly due to the need of an
equipment, usually denominated combustion bomb, which reproduces some of the characteristics of the combustion
chamber in the fuel injection instant. It is also necessary the construction of the injectors prototypes to be analyzed,
what demands time and resources. Therefore, the work has the objective of analyzing the use of the Maximum Entropy
Principle for a prevision of the drops size distribution, to make possible a theoretical comparative evaluation of
injectors, or also to compose future models to aid in the study of the injection process, and consequently in the
modeling of the two-phase flow combustion. The work starts from the presupposition that the theoretical tool doesn't
substitute the use of the experimental analysis. It is known that each one of them is more appropriate to certain phases
of the injection systems development or in the engine combustion analysis, and that is important to distinguish these
phases correctly.

2. The Maximum Entropy Principle

The concept of entropy introduced in thermodynamics by Clausius (1862), received the statistical interpretation
showed in Eq. (1) from Gibbs (1928) apud Jaynes (1957a).
\[ S = -K \sum_i P_i \ln P_i \]  \hspace{1cm} (1)

Where \( P_i \) is the probability that a certain microscopic state of a system will occur. The summation will extend for every microscopic states those will generate a same macroscopic state.

It was Claude S. Shannon (1948) apud Jaynes (1947b), an electronic engineer that worked with communication systems for Bell Telephones, who got for the first time an statistical interpretation of the entropy, without any reference to physical particularities of the studied system. Originally, his purpose was to minimize the transmission errors, due the natural dispersion of the electromagnetic waves when propagating in a material. He noticed that a statistical approach of the problem was better than the application of the Maxwell’s Equations and the principles of the electrodynamics to the process. Using a statistical approach, the Eq. (2) appeared naturally in his calculations.

\[ H_X(y) = -\sum_{i,j} P(i,j) \ln P_i(j) \]  \hspace{1cm} (2)

The Eq. (2) describes a relationship between the probability of occurrence of an event \( y \) and the conditioned probability of the occurrence of \( y \) and the event \( x \). Shannon designated such expression as the entropy of the statistical distribution, as a consequence of the similarity between the form and the properties of the expression, and the properties and the form of the entropy described by the statistical thermodynamics. In the equation obtained by Shannon doesn't exist reference to specific physical quantity, just happening typical probability distributions of studied sampling range; therefore, he demonstrate that many of the mathematical properties of the entropy didn't depend on the physics but on the statistics, and this was the origin of the statistical entropy concept. Forward, Jaynes (1957b) demonstrated this point of view, applying it to the statistical thermodynamics of the systems in equilibrium, showing that the Shannon’s point of view can lead to a perfectly coherent description of the equilibrium thermodynamic systems, and in this formulation, it is not necessary to suppose the entropy as a function of the state of system, but the entropy appears as a statistical characteristic associated to absence of knowledge about the speeds and positions of the different molecules that compose the system. Jaynes showed also that the entropy could be a measure of the level of information that we have about the microscopic structure of the system, proving that the usual equations of the statistical thermodynamics could be derived by a standard mathematical procedure, supposing only the usual conservation laws of the physics and the hypothesis that the entropy of the system is maximum in the equilibrium. Jaynes showed that such formalism could be extended for any system of many elements where the basic physics of the elements interaction was known as well as some conservation laws.

In the spray analysis application of the Maximum Entropy Principle, the proposal of Li and Tankin (1987) establish that the sum of the masses of all droplets produced by unit of time should be equal the mass of injected liquid for unit of time. This presupposition is exactly the principle of the mass conservation, which can be expressed by the Eq. (3).

\[ \sum_i P_i v_i \rho_i \hat{n} = \hat{m}_i + S_m \]  \hspace{1cm} (3)

Where \( P_i \) is the probability (in terms of the numeric fraction in relation to volume fraction) of finding a drop in the spray with a volume \( v_i \) and density \( \rho_i \), \( \hat{n} \) is the total number of drops produced in the spray by time unit, and \( \hat{m}_i \) is the mass flow of the injected liquid. \( S_m \) represents the mass source term in the region within the nozzle exit and the position where droplets are formed. If some liquid portion is vaporized in this region, then the mass source term is negative, if condensation of the ambient vapor occurs, it is positive. For the injection conditions which the present control volume is submitted, when liquid velocity at the nozzle exit is very high and atomization starts immediately at the nozzle exit, the mass source term can be considered null. Another basic probability presupposition in the problem is that the sum of the probabilities \( P_i \) should be unity, as the Eq. (4).

\[ \sum_i P_i = 1 \]  \hspace{1cm} (4)

Using the Method of the Lagrange Multipliers, we have the Eq. (5).

\[ \frac{d}{dP_i} \left\{ -\sum_i P_i \ln P_i - (\lambda - 1) \sum_i P_i - \beta \sum_i v_i \rho_i \hat{n} \right\} = 0 \]  \hspace{1cm} (5)

Consequently:
\[ P_i = \exp \left(-\lambda - \beta \frac{\rho_i n}{\hat{m}_i} \right) \tag{6} \]

Where \( \lambda \) and \( \beta \) are Lagrangian multipliers that must be determined. Substituting the multipliers in a convenient form of the Eq. (6), it will supply the droplet distribution function, in terms of volume fraction, expressed by Eq. (7).

\[
\frac{dV}{dD} = 3 \left( \frac{\pi \rho_i n}{6 \hat{m}_i} \right)^{2} D^{5} \exp \left( - \beta \frac{\rho_i n}{6 \hat{m}_i} \right) \tag{7} \]

According to Li and Tankin (1987), the Sauter mean diameter \( D_{32} \) can be calculated by the Eq. (8).

\[
D_{32} = C \left( \frac{\hat{m}_i}{\rho_i n} \right)^{1/5} \tag{8} \]

Where:

\[
C = \left( \frac{6}{\pi} \right)^{1/3} \frac{1}{\Gamma \left( 5/3 \right)} = 1.374 \tag{9} \]

with \( \Gamma \left( 5/3 \right) = 0.90330 \) (Gamma function)

3. Experimental Evaluations

The experimental assembly at the laboratory of the Aeronautical Engineering Division of ITA can be observed in the Fig. 1. A Mercedes-Benz OM904 LA four cylinder Diesel engine, with electronic fuel management, was used in the experimental evaluations. The engine was mounted on a base with wheels, together with all systems necessary to his autonomous operation without load.

The engine speed without load can be only the low idle or the upper no-load speed, because the engine speed regulation system doesn't contemplate the operation in no loads intermediate speeds. On the condition of upper no-load speed, that corresponds approximately to 2.720 min\(^{-1}\) in this engine, would be extremely difficult to analyze just one injection event, therefore these experimental evaluations has been made in the idle speed of 600 min\(^{-1}\).

![Figure 1. General view of the experimental assembly.](image)

To make possible and secure the evaluation of the droplet diameter distribution in the spray, it was necessary to build a test chamber that reproduces the same air density in the combustion chamber, using pressurized nitrogen. This high density would be guarantee the same spray speed that would happen in the combustion chamber. The centerline of
the windows is aligned with the laser beam of the Malvern Mastersizer equipment. According to the studies of Arcoumanis and Gavaises (1998), the injector is positioned with a 70 mm distance between the nozzle exit and the centerline of the chamber windows. The distance from the face of the range lens to the injection plane, along the laser beam is 78 mm. The test chamber was made in welded steel, and the transparent windows were machined and polished from acrylic plates, with thickness of 18 mm. To guarantee the actual engine conditions, no special samples with just one orifice were used, but controlled samples of engine multi-hole injectors. To analyze the spray of just an orifice, the injector was mounted in a jet-break cavity with a narrow opening for the area of the chamber crossed for the laser beam. This narrow window allows the passage of just one of the six jets of the injector, while the fuel from the others hit the walls and flow to the bottom of the cavity. When the nitrogen of the camera is eliminated, through a valve, it carries out this accumulated fuel.

In the Figure 2, two views of the test chamber and the instrumentation can be observed, in which the following main elements are identified: 1. Malvern Mastersizer transmitter; 2. Malvern Mastersizer receiver; 3. Test chamber; 4. Telescopic base of the chamber (linked to the test engine base); 5. Nitrogen entrance; 6. Thermocouple (type K); 7. Transducer for the pressure inside the chamber; 8. Nitrogen and accumulated fuel exit; 9. Fuel pressure transducer; 10. Nozzle holder and delivery connection.

The nitrogen pressure inside the test chamber was established to reproduce, in the room temperature, the same air density inside the combustion chamber at the instant of injection beginning. The air pressure inside the combustion chamber was determined through a piezometric pressure transducer connected to an AVL Indiskop equipment, in engine test bench. Considering the air pressure of 94 kPa in the engine entrance, the pressure in the combustion chamber at the beginning of injection of 3800 kPa, the air temperature in the entrance of 303 K, the estimate chamber temperature at the beginning of injection of 890 K and the air density in the engine entrance of 1,1461 kg/m$^3$, using the general equation of the gases in Eq. (10):

\[
\frac{P_{1}}{\rho_{1} T_{1}} = \frac{P_{2}}{\rho_{2} T_{2}}
\]

(10)

The air density in the combustion chamber is 15.6 kg/m$^3$. Using another form of the general equation of the gases:

\[
\frac{P_{N_{2}}}{\rho_{N_{2}}} = R_{N_{2}} T
\]

(11)

For the nitrogen, at the room temperature of 303 K, it is obtained the pressure inside the test chamber of 1.4 MPa. The unit pump of the first cylinder is used to pressurize the fuel for the injector mounted inside the test chamber. This pump was disconnected from its respective nozzle holder, and its high-pressure line was prolonged to connect the nozzle in the test chamber. Therefore, the engine works with only 3 cylinders that guarantee the engine camshaft movement and also the first cylinder unit pump injection.

Keep in mind that in the normal engine operation we have successive injections, it is necessary to find a way to control the unit pump so that, in the spray analysis, just one injection occurs each measurement. Therefore, it was installed an additional unit pump (besides the 4 others), connected only to the engine electric wiring as if it was the first cylinder unit pump (no connection with the engine camshaft). The solenoid valve of this additional unit pump was
wired in parallel to the solenoid valve of the original first cylinder unit pump, that stay mounted in the engine, in conditions of pressurizing the injector. Between these units it was installed a switch that, when pressed, transfers the opening electric pulse from the additional unit pump, that works together with the other units of the engine, for the unit pump of the first cylinder. This way, when pressing the switch once, it is had immediately an injection in the test chamber.

The procedure to measurement setup is made through the Malvern equipment software. The first step is the alignment process of the transmitter laser beam with the central axis of the photo-diode elements. An alignment must be made whenever any of the optics (the cell, range lens beam expander, etc.) are removed or replaced or the equipment is moved. It is an automatic procedure executed through the equipment software. After the alignment process, it should be made an initial background measurement used to subtracting the ambient light signals from the total scattering received from the injection sample. On the present work, before the evaluation of each injector, it was made an alignment of the optic units and, before each measurement with the same injector, it was made a new background calibration to consider the residual particles left by the previous measurement.

4. Experimental Results

Two samples of Bosch injectors with 6 plane orifices, according the definition of Lefebvre (1989), were tested, with orifices diameters of 164 µm (Bosch model DLLA147P944) and 174 µm (Bosch model DLLA147P945), with eight measurements for each sample. The data were processed by the Malvern equipment software, generating histograms of the volumetric size distribution for each test. The software distributed the diameters in a histogram of relative frequencies with variable class width. The data are exhibited with diameter range from 0,5 to 600 µm, distributed in 32 diameter classes. The objective is a continuous distribution of probabilities, so the geometric average of each class limits is used as the abscissa to the corresponding frequency observed in each interval. The Fig 3 shows the comparison of the average droplet diameter distribution for each test injector.

The distribution of droplet size obtained for each injector is very similar. Considering that the only difference between the samples is the orifice diameter and that this difference is relatively small (164 µm and 174 µm), the results are shown consistent. To make easy a comparative evaluation, it is convenient to use a representative mean diameter of the distribution like the Sauter Mean Diameter (\(D_{32}\)), calculated by the Eq. (12).

\[
D_{32} = \frac{\sum N_i D_i^3}{\sum N_i D_i^2}
\] (12)

Through the test data, it was obtained the Sauter Mean Diameter corresponding to the average of 8 tests with each injector:

- Injector with orifice diameter of 164 µm: \(D_{32}^{164} = 19,08\) mm
- Injector with orifice diameter of 174 µm: \(D_{32}^{174} = 19,49\) mm

The values of the Sauter Mean Diameter of the injectors are very close and can be considered as only indicators of a tendency. Therefore, it is possible to say that the measurements show a tendency that the injector with orifice diameter of 174 µm produce a spray whose droplet size distribution has a larger Sauter Mean Diameter in comparison with the other produced by the injector with small orifices. According to Heywood (1988) and Bergmann et al. (1996), it should be emphasized that this tendency show that the injector with smaller Sauter Mean Diameter (\(D_{32}\)), of generated drops could produce smaller values of particulate matter, when applied in a Diesel engine, in comparison with the other injector. This tendency was confirmed in the engine emission test bench of DaimlerChrysler engine laboratory, considering the EURO III (CONAMA 5) version of the engine, as could be seen in the comparison showed in Tab. 1.

<table>
<thead>
<tr>
<th>Injector Model</th>
<th>NO(_X) emissions (%)</th>
<th>Particulate matter emissions (%)</th>
<th>Specific fuel consumption (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>DLLA 147 P 944 (164 µm)</td>
<td>100,0 (base)</td>
<td>100,0 (base)</td>
<td>100,0 (base)</td>
</tr>
<tr>
<td>DLLA 147 P 945 (174 µm)</td>
<td>100,2</td>
<td>123,7</td>
<td>98,7</td>
</tr>
</tbody>
</table>
5. Comparison of the Theoretical Function with the Experimental Data

It is important to say that it is not possible a direct comparison between the experimental volumetric droplet distribution, obtained by the laser scattering technique, and the theoretical droplet distribution, expressed by the Eq. (7). With the experimental technique, it is obtained the volume proportion, in each class of droplet size, of the total volume of droplets in the sample. Unlike the basic hypotheses established in the application of Maximum Entropy Principle, the distribution of droplet size obtained by the Malvern equipment is not based in the size of isolated drops. However, it can be verified some interesting aspects when analyzing the experimental data beside the data obtained by Maximum Entropy Principle. For this analysis, it is necessary firstly to determine the value of the parameters group that composes the Eq. (7). According to Li and Tankin (1987), the number of drops produced by the spray can be obtained through the Eq. (8), in which the Sauter Mean Diameter is determined experimentally. The value of the parameters group that composes the Eq. (8) can be described for the Eq. (13).

\[
\left( \frac{m_l}{\rho \cdot n} \right)^{3/2} = \frac{D_{32}^E}{1,374}
\]

Where the value of \( D_{32}^E \) is calculated by the Eq. (12). The droplets distribution functions generated by the Eq. (7) for the two types of injectors studied in this work are then:

\[
\left( \frac{dV}{dD} \right)_{p944}^{\text{calc.}} = (1,147 \cdot 10^{-7}) \ D^5 \exp(-1,955 \cdot 10^{-4} \ D^3)
\]

(14)

\[
\left( \frac{dV}{dD} \right)_{p945}^{\text{calc.}} = (1,010 \cdot 10^{-7}) \ D^5 \exp(-1,835 \cdot 10^{-4} \ D^3)
\]

(15)

According to Li (2000), the experimental data can also be expressed in the form of probability density function:

\[
\left( \frac{dV}{dD} \right)^{\text{meas.}} = \frac{V(D_{i+1}) - V(D_i)}{D_{i+1} - D_i} = \frac{\text{Relative Frequency (p.) in %}}{\text{Class Width (} \Delta \text{.) \cdot 100}}
\]

(16)
In the Fig. 4 can be observed the experimental distribution curves for the two injectors, as well as the distributions obtained by Maximum Entropy Principle in the same droplet size intervals, also for each injector. For more clearness, the graphs were simplified considering only the classes of droplet size smaller than 100 µm.

**Figure 4.** Comparison of theoretical and experimental droplet size distributions.

The comparison between experimental and theoretical distributions shows both with good defined picks occurring in the same point. The behavior for diameters largest than 30 µm are significantly different, as well as the values of the volume fractions in the picks. The comparisons between theoretical and experimental results presented by Li and Tankin (1987) also show these characteristics. These different behaviors, can be attributed mainly the difference among the nature of the modeling, based on the size of isolated drops, and the nature of the available experimental method, based on the volume proportion in each droplet size class, of the total sample volume. According to Lefebvre (1989) the volumetric distributions privilege the range of drops of larger diameter in comparison to the linear size distributions of isolated drops. That seems to explain why the fraction of relative volume the drops of larger diameter are not predicted by the calculated distribution. In the theoretical distribution, the pick is significantly larger, compensating the volume fraction relative to the drops of larger diameter.

6. Conclusions

The theoretical results, to obtain a probability density function of the droplets size distribution from the Maximum Entropy Principle, don't allow a comparative evaluation so consistent as the experimental evaluation. The calculated distribution takes in account that the moving droplets changes only mass among themselves and with the ambient. The model precision could be improved considering that the droplets change also momentum and energy among themselves and with the ambient, according to Archambault and MacCormack (1998). It should be noted once again, unlike the basic hypotheses established in the application of Maximum Entropy Principle, that the distribution of droplet size obtained by the Malvern equipment is not based in the measurement of isolated drops. In the experimental technique, they obtained the volume proportion in each droplet size class of the total volume of droplets. Although it is not possible a direct comparison, both distributions show a good defined maximum pick that occurs in the same point.

In the present work, an experimental method of analysis of Diesel engine injectors was also evaluated, using the laser diffraction technique to obtain the probability density function of a droplet size distribution. This method was shown representative, keeping in mind the consistence of the comparative results obtained with the tested injectors. The measurement zone of the equipment depends of the range lens that collects the laser light that has been scattered from
the sample. In the experiments was used the 300 mm lens, and the distributions are complete without cut off at the small or large size end. The laser diffraction technique was capable to indicate difference in the spray, even from injectors considered very similar (orifices with diameters of 0.164 mm and 0.174 mm).

7. Future Developments

In the future experimental evaluations it will be important to develop a test chamber to allow a comparative evaluation of injectors with more different characteristics, as jet angle, number of holes, construction of the nozzle holder, etc., always guaranteeing the same plan of incidence of the laser beam. It would be also important the installation of the engine in a test bench. Another experimental technique in the spray analysis is the high-speed image acquisition, which will be utilized in future experiments. In the theoretical analysis, it will be considering that the moving droplets changes not only mass, as it was considered, but also momentum and energy amongst themselves and with the ambient, these information, according to Archambault and MacCormack (1998), should be considered in the formulation of Maximum Entropy Principle, through a more detailed physical and mathematically sophisticated model. In near future, spray formation studies will be made also with some Brazilian biodiesel blends.

8. Acknowledgements

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9. References

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10. Responsibility notice

The authors are the only responsible for the printed material included in this paper.