APPLICATION OF THE MAXIMUM ENTROPY FORMALISM ON DISCRETE DROP SIZE DISTRIBUTIONS

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ABSTRACT

The present paper is intended to get a better understanding of the application of the Maximum Entropy Formalism (MEF). The maximum entropy formalism is a statistical tool that allows the prediction of the most objective probability distribution when a limited information on the studied system is known. Regarding the actual state of art, one of the most challenging objective is to know the type of information to brought as a function of the physics involved. This preliminary study focuses on the effects of the aerodynamic drag forces on the evolution of the drop size distribution in space. As a matter of fact, when the droplets of a spray are subject to these forces, the drop size distribution evolves as a function of space because the smallest drops are more decelerated than the bigger drops. This paper proposes to determine the information to write through the constraints in order to perform a reconstruction of the drop size distributions thanks to the recent mathematical method to apply the maximum entropy formalism on sprays. By considering different initial drop size distributions (uniform, gaussian and Nukiyama-Tanasawa), the present paper shows that the best adapted constraint to write is the definition of the mean drop diameter D(0.8,0).

INTRODUCTION

In many industrial applications, sprays are mainly characterized thanks to data related to drop size distributions. The characterization consists either in the determination of a limited number of diameters (the Sauter mean diameter, D_{v90} for instance) or in the analysis of the whole drop size distribution. In the latter case, this brings a finer description of the drop size dispersion. For instance, this description becomes necessary when drop size distributions are multi-modal. In addition, it is often preferred to get the drop size distribution as close as possible to the location of the liquid system breakup in order to carry out spray simulations. As a matter of fact, the characteristics of the droplets that are released into the computational domain have to be perfectly known in such simulations.

The maximum entropy formalism was found to be a promising approach in the spray domain. This formalism is a statistical tool used for the prediction of a probability distribution when a partial information related to the studied system is known. This information is written under a set of constraints and the formalism suggests that the least biased, or most objective distribution, which satisfies the set of mathematical constraints, is the one that maximizes the statistical entropy that was introduced by Shannon [1].

In the last 25 years, some authors applied this approach to reconstruct drop size distributions of sprays. Babinsky and Sojka [2] detailed most of the published studies ([3] to [6]).

Regarding the actual state of art in the application of the maximum entropy formalism on sprays, one can wonder how to choose the constraints and on which physical basis. This paper is intended to bring clues to answer this question.

In the present study, the MEF approach is applied on artificial sprays issuing from one-dimensional simulations where the droplets are subject to aerodynamic forces only. The objective here is to find the most appropriate form of the constraints to write in order to reconstruct the drop size distribution that evolves as a function of the downstream distance. This study was conducted with the recent method of the application of the MEF developed by Cousin and Desjonquères [7]. This method has the advantage to allow the writing of any type of constraints contrary to the Lagrange's multipliers method that is always used in the application on sprays. In the present paper, a single constraint will be considered.

THEORETICAL ASPECTS

The Maximum Entropy Formalism Approach

The mathematical approach for the application of the Maximum Entropy Formalism is the one suggested by Cousin and Desjonquères [7]. In this paper, the drop size distribution is defined with a discrete description: the range of drop diameter is delimited by a minimum (D_{min}) and a maximum (D_{max}) value. The drop size spectrum is divided into n = 100 classes that have the same width. This number of classes was found sufficient to avoid a dependency of the results on this parameter. Each class i is characterized by an occurrence probability x_i and a probability vector $X(x_1, x_2,\dots,x_n)$ is built. The method consists in finding the most objective vector X that is to say the one that verifies the normalization law:

$$h_0(X) = \sum_{i=1}^{n} x_i - 1 = 0 \tag{1}$$

the nh constraints that can take the following forms:

$$h_j(X) = 0 \text{ or} \geq 0 \;\text{ where j = 1, 2, …, nh} \tag{2}$$

and that maximizes the relative entropy defined as :

$$S(X) = S(x_1, x_2,..., x_n) = -\sum_{i=1}^{n} x_i \ln\left(\frac{x_i}{m_i}\right) \tag{3}$$

where m is a reference or a priori probability distribution and corresponds to the reference state when no constraint is written. In the literature, when the number-based distribution is studied, this reference function does not appear explicitly because it is assumed to be a uniform distribution.
In addition, in the present study, a single constraint is written: the definition of the mean drop diameter D(p,q) where p and q are real numbers:

$$\sum_{i=1}^{n} x_i D_i^p - D(p,q)^{p-q} \sum_{i=1}^{n} x_i D_i^q = 0 \tag{4}$$

where D_i denotes the median diameter of the class i.

Spray modeling

This paper is limited to the analysis of the number-based distributions. Moreover the drop size distributions are temporally and spatially integrated. This choice comes directly from the fact that this type of representation is the one that is often deduced from measurements.

In the following parts, different initial drop size distributions (uniform, gaussian and Nukiyama-Tanasawa) are considered. All the droplets are released with a same constant velocity U_0 = 100 ms^{-1}. Each droplet evolves in a single direction by assuming that it does not interact with the other droplets. In addition the particles are subject to aerodynamic drag forces only. These drag forces are mathematically taken into account with the use of the following expression for the drag coefficient C_D :

$$C_D = 1 + \frac{24}{Re} \;\text{ with }\; Re = \frac{\rho_g UD}{\mu_g} : \tag{5}$$

where ρ_g and μ_g are the density and the dynamic viscosity of the ambient air respectively. In this study, the values of these two parameters are kept constant (ρ_g = 1.2 kgm^{-3} and μ_g = 1.8 10^{-5} kgm^{-1}s^{-1}). U is the velocity differential between the air and the droplet that is to say the drop velocity because air is supposed to be at rest. The choice of this drag law is subjective and may be revisited in future studies.

Based on the results provided by Chin et al [8], after mathematical manipulations, it can be shown that if the initial number-based distribution is called dN/dD, the distribution at a given distance dN’/dD becomes:

$$\frac{dN'}{dD} = \frac{\dfrac{dN}{dD}\dfrac{1}{U(D)}}{\displaystyle\int_{D_{min}}^{D_{max}} \frac{dN}{dD}\frac{dD}{U(D)}} \tag{6}$$

where U(D) is the velocity of the droplet that has a diameter D at the given location. In such a case, the variations of the drop size distribution with the distance are due to aerodynamic effects only. As a matter of fact, as illustrated on Figure 1, even if droplets have the same initial velocity as it is assumed here, air drag forces cause the smaller drops to loose momentum faster than the bigger drops.

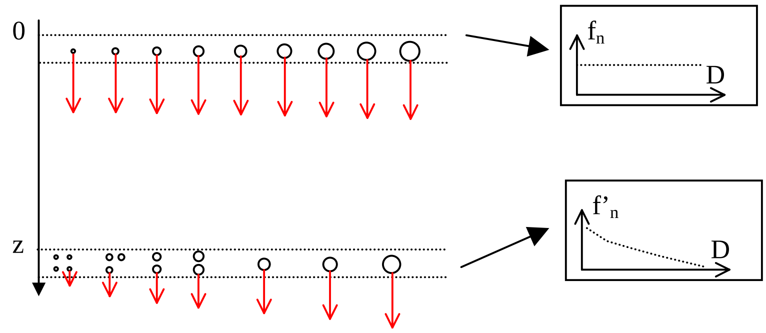

Fig. 1. Schematic description of the drop size distribution evolution

For instance, if we consider an initial gaussian number-based distribution, the distribution evolves as a function of the downstream distance z. This is the case on Figure 2 where all the droplets are released with a constant velocity set to 100 ms^{-1}. By increasing z, the relative number of small drops is increased. The conditions of the calculation were chosen in order to ensure that the droplets are never stopped because this could generate an infinite number of drops. This large number of small droplets can be clearly seen at z = 50 mm. Figure 3 shows the deduced volume-based distributions. With this representation, the increase of the small droplets population is less clear because these droplets are representative of a small relative amount of liquid. In addition, the volume-based distribution does not reach zero for large values of diameter because the initial distribution does not present a tail that tends to zero for large diameters.

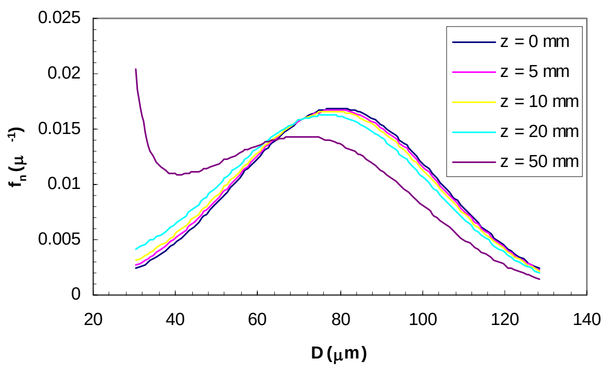

Fig. 2. Evolution of the number-based distribution

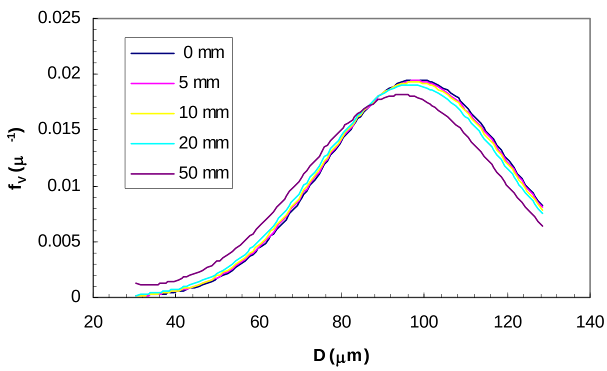

Fig. 3. Evolution of the volume-based distribution

APPLICATION

In the present paper, three different initial number-based distributions are considered: a uniform, a gaussian and a Nukiyama-Tanasawa distribution. For all these cases, the range of drop diameter is limited from 30 to 130 micrometers and all the droplets are released with a constant velocity set to 100 ms^{-1}. As this study is prospective, this choice is completely subjective and not related to any particular application. It is the reason why the considered drop size distributions are not necessarily realistic like the uniform distribution for instance. With the investigated distributions, the technique to employ the maximum entropy formalism is described as follows. For each distance z, it is possible to calculate any mean drop diameter D(p,q) from the spray simulations. The drop size distribution is then reconstructed with the maximum entropy formalism by considering a single constraint that is to say the definition of the mean drop diameter D(p,q) (see Equation 4). The objective of this study is to find the most appropriate constraint (that is to say the best couple (p,q)) and to see how the constraint that has to be written depends on the initial distribution. In order to limit the data in this short paper, the written constraints investigated are the definitions of the following drop diameters: D(0.6,0), D(0.7,0), D(0.8,0), D(0.9,0), D(1,0), D(2,0), D(3,2). The definition of the Sauter mean diameter is the only one that needs the particular technique developed by Cousin and Desjonquères [7]. However, this technique has always been used in the present paper. In order to carry out this study, the distributions issuing from the spray simulations are compared with the one deduced from the application of the MEF. These comparisons are either performed qualitatively on the graphical representations or quantitatively by calculating the relative entropy whose expression is given in Equation 3. In this case, x represents the probability distribution deduced from the MEF and m is the distribution we try to reconstruct. Then, a maximum value of the relative entropy is representative of a reconstructed distribution close to the real one.

Uniform initial distribution

The first considered initial distribution is uniform; it is the simplest distribution although it is not the most representative distribution that can be found in real sprays. However, when the Maximum Entropy Formalism is employed to reconstruct the number-based drop size distribution, authors from the literature use this distribution as the reference distribution. Figure 4 shows clearly that increasing z leads to a strong increase of the small droplet population. Figure 5 shows the reconstructed distributions at the highest distance z = 50 mm by considering different constraints. This figure shows that the use of constraints with relative high orders (D(3,2) or D(2,0) for instance) is not well adapted. The choice of a constraint close to the definition of the arithmetic diameter seems to be adapted. This can be quantitatively verified on Table 1 where the relative entropy is calculated for the different tested constraints. One can see that the definition of D(0.7,0) is the one that maximizes the relative entropy.

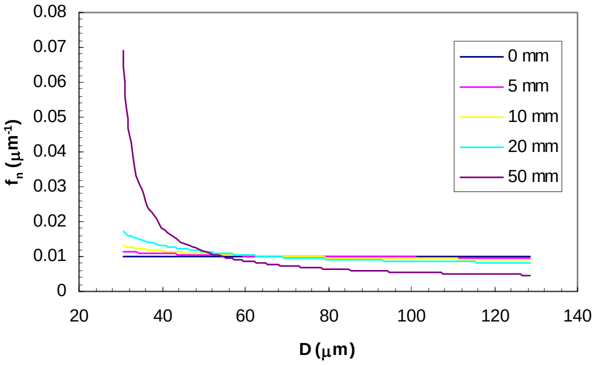

Fig. 4. Evolution of the number-based distribution

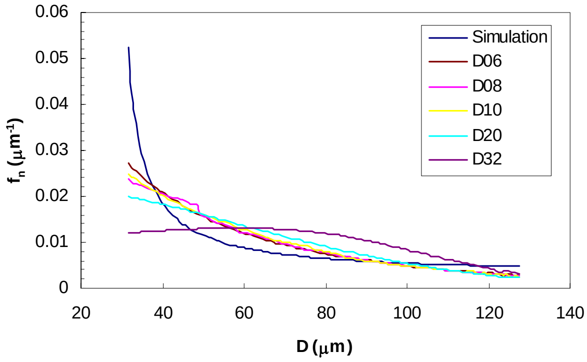

Fig. 5. Reconstruction of the drop size distribution (z = 50 mm)

Constraint	D(0.6,0)	D(0.7,0)	D(0.8,0)	D(0.9,0)	D(1,0)	D(2,0)	D(3,2)
Relative entropy	-0.0620	-0.0560	-0.0688	-0.0873	-0.0782	-0.1104	-0.1998

Table 1. Relative entropy as a function of the chosen constraint (z = 50 mm)

Gaussian distribution

Figure 6 shows the evolution of the drop size distribution as a function of z with an initial gaussian distribution. Figure 7 shows the reconstructed distribution by considering different constraints at the distance z = 50 mm from the release location of the droplets. The chosen distance corresponds to the trickiest case. Regarding the special shape of the distribution to reconstruct, a single constraint seems to be not sufficient. However Table 2 shows that the constraint expressing D(0.8,0) is the most appropriate.

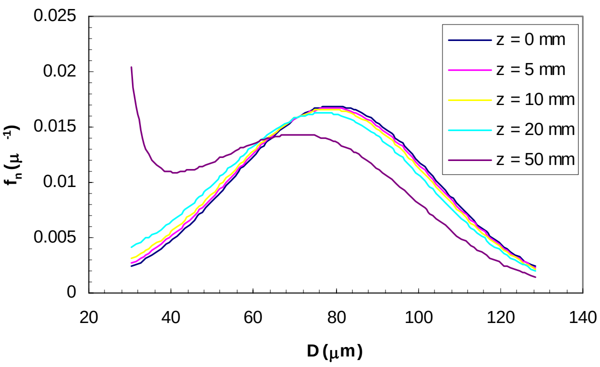

Fig. 6. Evolution of the number-based distribution

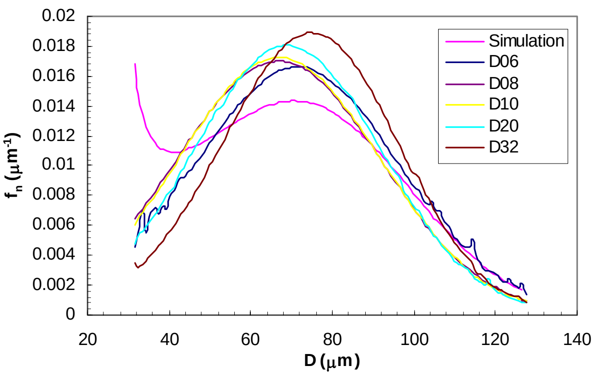

Fig. 7. Reconstruction of the drop size distribution (z = 50 mm)

Constraint	D(0.6,0)	D(0.7,0)	D(0.8,0)	D(0.9,0)	D(1,0)	D(2,0)	D(3,2)
Relative entropy	-0.0346	-0.0300	-0.0274	-0.0288	-0.0325	-0.0478	-0.0862

Table 2. Relative entropy as a function of the chosen constraint (z = 50 mm)

Nukiyama-Tanasawa distribution

Similar results are obtained by considering an initial Nukiyama-Tanasawa distribution as illustrated in Figure 8, Figure 9 and in Table 3. Once again, the use of the definition of the diameter D(0.8,0) seems to be the best single constraint to write.

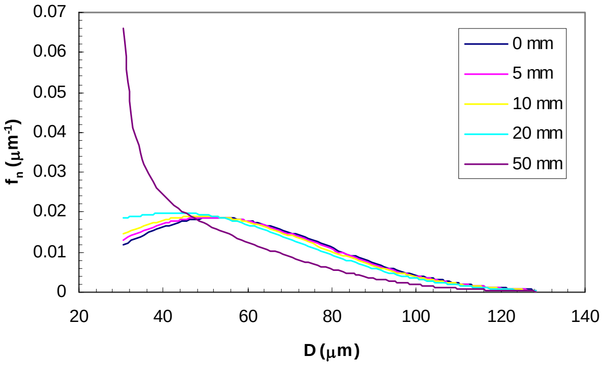

Fig. 8. Evolution of the number-based distribution

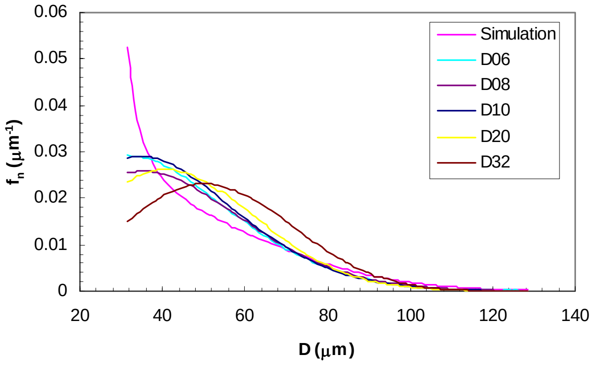

Fig. 9. Reconstruction of the drop size distribution (z = 50 mm)

Constraint	D(0.6,0)	D(0.7,0)	D(0.8,0)	D(0.9,0)	D(1,0)	D(2,0)	D(3,2)
Relative entropy	-0.0321	-0.0093	-0.0057	-0.0367	-0.0648	-0.0910	-0.1763

Table 3. Relative entropy as a function of the chosen constraint (z = 50 mm)

CONCLUSION

This paper presents an application of a new method for the application of the maximum entropy formalism on sprays. The motivation of such a study is to get a better understanding of this type of application. As a matter of fact, regarding the actual state of art, the knowledge of the constraints to write as a function of the physical phenomena remains unsatisfactory.

This paper was intended to highlight this question and to bring preliminary answers. As a matter of fact, the maximum entropy formalism was applied on numeric sprays where droplets were subject to a single physical phenomenon that is to say the aerodynamic forces. Such an approach takes the advantage to limit the complexity of the phenomena involved in the spatial and temporal evolution of a spray. However this method led to consider truncated distributions for small values of diameters because with such an approach, droplets whose diameter is smaller than 30 micrometers would conduct to droplets having a zero velocity for large distance from the drop release location. In this case, this would lead to diverging drop size distributions. In order to overcome this problem, it would be interesting to inject droplets into a gaseous medium that keeps a constant velocity as it can be found on a standard experimental set-up equipped with an extracting system.

In the present study, three different initial drop size distributions were investigated: the uniform distribution that is the simplest one and two other distributions (gaussian and Nukiyama-Tanasawa) which are more realistic.

Thanks to the notion of the relative entropy, it was shown that the best adapted constraint to write is the definition of the mean drop diameter D(0.8,0). For all the investigated situations, the type of constraint to write was found to be independent of the form of the initial distribution. This seems to show that the constraints to write is only related to the physical phenomenon and not on the value of the mean drop diameters as illustrated in Figure 10 where D(0.8,0) strongly depends on the choice of the initial distribution.

These results should be verified by extending the study on other initial distributions and other ranges of drop diameters. In addition, a finer analysis could be also investigated by refining the choice of the constraint to write. As a matter of fact, when the definition of the mean diameter D(p,q) is written, finer steps on both p and q could be carried out.

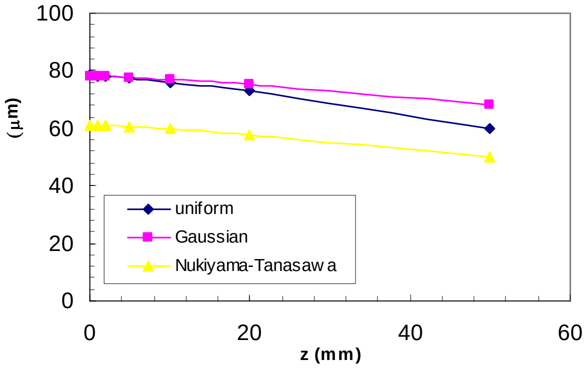

Fig. 10. Evolution of D(0.8,0) with distance for the three tested initial distributions

Finally, this preliminary study was found very promising; it encourages investigating the other physical phenomena present in the applications on sprays. For instance, it would be interesting to investigate phenomena such as droplet breakup, evaporation or coalescence. As it was done in this study, these phenomena should be considered independently in order to reduce the complexity of the problem. Thus, the following challenging step will consider the coupling of the different physical phenomena.

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