A New Approach for the Application of the Maximum Entropy Formalism on Sprays

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The present paper reports a new method for the application of the maximum entropy formalism for the prediction of spray drop size distributions. This formalism is a tool that allows the prediction of the least biased statistical state of a system when some partial information related to the system is known.
As far as sprays are concerned, this formalism has been applied in the past for the prediction of continuous drop size distributions by using a mathematical method called the Lagrange's multipliers method. Unfortunately the brought information, expressed in terms of constraints, needs to be written under very limited mathematical forms.
The present paper is intended to present a new method based on a discrete description of the distribution. This method based on non linear programming theories is more general and allows the writing of any type of constraints. After a detailed presentation of this new method, some examples highlight this new original approach.

1. Introduction

The maximum entropy formalism is a statistical tool used for the prediction of probability density functions when partial information related to the sought pdf is known. This information is written under a set of constraints and the formalism suggests that the least biased, or most objective, pdf which satisfies the set of constraints, is the one with maximum uncertainty that is to say the one that maximizes statistical entropy. This notion of uncertainty of a probability distribution was initially introduced by Shannon [1].
In the last 25 years, some authors attempted to apply the maximum entropy formalism to reconstruct drop size distributions of sprays. Most of these approaches are detailed in the recent paper of Babinsky and Sojka [2]. All the studies that use this formalism are conducted with the same mathematical methodology but with different objectives. For instance Li *et al* ([3] to [9]), Sellens *et al* ([10] to [13]) and Cousin *et al* [14] attempted to use this formalism in order to predict drop size distributions of sprays. Works of Li *et al* and Sellens *et al* are based on the writing of conservation laws as brought information. Cousin *et al* propose a method to couple the maximum entropy formalism with the linear theory that brings partial information about the primary breakup of liquid systems. More recently, Malot *et al* [15] and Boyaval *et al* [16] propose a different way to use the maximum entropy formalism. Depending on the studied spray, they propose a two [16] or a three [15] parameters distribution that is derived from the maximum entropy formalism. The objective is then to reduce the distribution to a set of limited characteristics that are physically relevant and that contain all the information available in the distribution.

In all papers about the maximum entropy formalism applied on sprays, the Lagrange's multipliers method is the only approach to derive an expression of the sought probability density function. Unfortunately this method forces to use very limited type of constraints, that is to say the definition of mean diameters having the form D_{p0}. This paper proposes a new method to apply the formalism. This approach is more general and allows the use of less restrictive constraints. The present paper briefly introduces the classical method and details the new approach. The application of this method on sprays is illustrated by considering either one or two constraints. In addition the proposed test cases allow to highlight some limitations of the maximum entropy formalism that have been observed in the past but never discussed.

2. The classical approach

As far as sprays are concerned, a drop size distribution is generally characterized either by a number-based or a volume-based distribution. The choice is essentially conditionned by the performance of the measurements diagnostic. In this paper, we limit the application of the maximum entropy formalism to the prediction of the number-based probability density function (pdf) f_n. Then, in the classical approach, the sought distribution needs to verify the normalization law :

$$\int_0^{\infty} f_n(D)dD = 1 \tag{1}$$

and is subject to nh constraints only under the following form:

$$D_{p_i 0}^{p_i} = \int_0^{\infty} f_n(D) D^{p_i} dD \quad \text{where } i = 1, 2, \ldots, nh \tag{2}$$

The constraints are either derived from a partial modeling or based on experimental results. The most objective pdf is the one that maximizes the so-called statistic relative entropy defined as :

$$S = -\int_0^{\infty} f_n(D) \ln\left(\frac{f_n(D)}{m(D)}\right) dD \tag{3}$$

The function m is called the prior distribution. As far as the number-based pdf is concerned, authors set this function m to a constant value. This means that in the absence of constraints, the most objective pdf is the one that gives iso-probability (f_n is constant). In the present paper, the same assumption is made.

Then the use of the Lagrange's multipliers method provides an analytical expression for f_n :

$$f_n(D) = \exp\left[-a_0 - \sum_{i=1}^{nh} a_i D^{p_i}\right] \tag{4}$$

where a_0, a_1, …, a_{nh} are called the Lagrange's multipliers and their values are deduced from equations (1) and (2).

The use of the Lagrange's multipliers method imposes to write the constraints under the form of the definition of the classical moments of a distribution as written in equation (2) (see Sowa [17] for extensive details on moments of a spray distribution). In the case of spray distribution, the orders of these moments can be either integer or real.

3. The new method

The use of the Lagrange's multipliers method imposes a very limited type of constraints. For instance, the definition of the Sauter mean diameter or the representative diameter $D_{v,90}$ can not be used as constraints in this formalism. This paper is intended to propose a new method that allows to write the constraints under any mathematical forms. This new method is made possible thanks to non linear programming methods. As a matter of fact, Spelluci [18] proposes a computer code to find extrema of a multivariate function that is subject to equalities and inequalities. In order to avoid extensive details, the capability of such an approach applied on maximum entropy formalism is summarized here.

With this new method, a discrete description of the drop size distribution needs to be considered. Thus the range of the observable drop diameter has to be fixed between a minimum (D_{min}) and a maximum (D_{max}) value. This introduces two new variables in the approach but these two diameters bring a more realistic description than the continuous approach where D_{max} is assumed to be infinite. In addition, these two extreme diameters may be deduced from a partial modeling of the primary breakup.

In order to simplify the present method, we assume for convenience that the minimum diameter is zero and distributions are presented as a function of a reduced diameter defined by :

$$D^* = \frac{D}{D_{max}} \tag{5}$$

The drop diameter range is divided into n classes having the same width. Each class "i" is characterized by an occurrence probability x_i and a probability vector $X(x_1, x_2, \ldots, x_n)$ is then built. The method consists in finding the most objective vector X that is to say the one that verifies the normalization law :

$$h_0(X) = \sum_{i=1}^{n} x_i - 1 = 0 \tag{6}$$

the nh constraints :

$$h_j(X) = 0 \text{ or } \geq 0 \quad \text{where } j = 1, 2, \ldots, nh \tag{7}$$

and that maximizes the entropy defined as :

$$S(X) = S(x_1, x_2, ..., x_n) = -\sum_{i=1}^{n} x_i \ln(x_i) \tag{8}$$

Thanks to a modified numerical code, the present problem can be solved. In addition, constraints can be non linear and written either under the form of equalities or inequalities. For instance, this new method makes possible the use of representative and mean diameters. At the present time it is possible to consider 300 distinct classes (n=300) and 1800 constraints (nh=1800) can be written. This clearly shows that this new approach is well adapted to spray drop size distributions.

4. Application of the new approach in the case of a single constraint

4.1. Introduction

In the present part of the paper, let us consider the case where one constraint is written only. The chosen constraint is the definition of one mean drop diameter D_{pq} where p and q can take any value contrary to the previous studies where q needed to be set at zero. For convenience the results will be presented by using the reduced diameter D^* defined in equation (5). Then in the present case, equation (7) is written under the following form :

$$h_1(X) = \sum_{i=1}^{n} x_i D_i^{*p} - D_{pq}^{*p-q} \sum_{i=1}^{n} x_i D_i^{*q} = 0 \tag{9}$$

where D_i^* is the reduced mean diameter of the class “i”. According to equation (9), p+q is called the constraint order.

In addition, we ensure all occurrence probabilities to be positive :

$$h_j(X) = x_j \geq 0 \text{ for } j = 2,3,....n \tag{10}$$

4.2. Effect of the number of diameter classes

As the present approach is based on a discrete description, the number of classes of the distribution may be an important parameter. The first results are intended to show the effects of the number of classes on the method. For the present case, we choose p = 3 and q = 2 meaning that the written constraint is the definition of the Sauter mean diameter. In addition we impose : $D_{32}^* = 0.5$. As the original results of this new method are obtained with a discrete description, these results are mathematically manipulated to be presented under the preferred form of probability density functions. However in the case of small number of classes (n small), the normalization law may be not perfectly verified under the continuous form. However in the discrete description, the normalization law is always ensured. Figure 1 shows the effect of the number of classes on the calculated number based-distribution. Figure 2 corresponds to the derived volume-based distribution deduced from the relation :

$$f_V(D) = \frac{D^3}{D_{30}^3} f_n(D) \tag{11}$$

where droplets are assumed to be spherical.

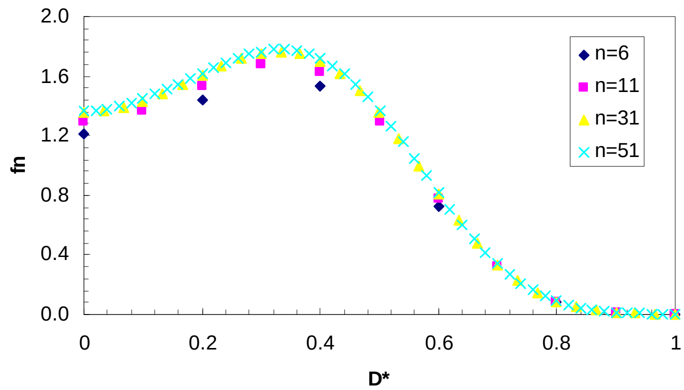

Fig. 1 Effect of the number of classes on the calculated number-based pdf

One has to keep in mind that f_V is not a probability density function in the pure mathematical sense, but a volume fraction distribution of the drop according to its diameter. Figure 1 shows that the number of classes does not need to be very high and a value for n higher than 31 seems sufficient for the investigated case. As it can be also observed in this figure, the number-based pdf has a positive value for D* = 0. This behavior is not physically valid. This directly comes from the choice of the constraint. As a matter of fact, in the absence of constraints, as the prior function m is constant, the maximum entropy formalism provides a constant pdf meaning that all classes of diameters have the same probability to occur. If a constraint with a positive constraint order as the one written in equation (9) is added, probability for having big droplets is then reduced by maintaining the possibility to get small droplets. Finally, when the volume-based distribution is deduced from equation (11) as shown in Fig. 2, a more realistic pdf is obtained due to the fact that small droplets carry a negligible volume of the spray.

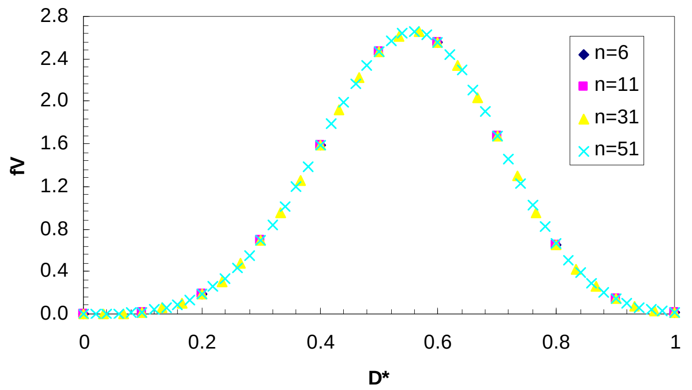

Fig. 2 Effect of the number of classes on the deduced volume-based pdf

4.3. Effect of the value of the constraint

Let us consider a case with n=51 classes and the definition of the Sauter mean diameter is the only written constraint. Figure 3 shows the calculated volume-based pdf for different values of the relative Sauter mean diameter. f_V is deduced from f_n thanks to equation (11). For values of D_{32}* smaller than 0.5, the use of the maximum entropy formalism allows the prediction of a volume-based pdf physically acceptable. As a matter of fact the calculated pdf tends to zero for both minimum and maximum diameters. However in the case of higher values of D_{32}*, the application of the MEF leads to a not physically valid pdf. This result is similar as the one found with the number-based pdf presented in Fig. 1.

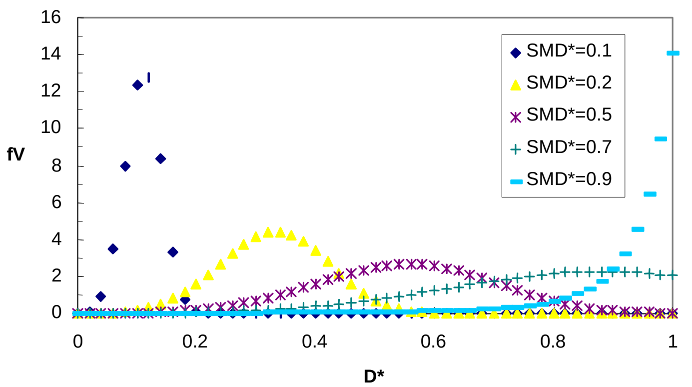

Fig. 3 Effect of the value of the reduced Sauter mean diameter on the drop size distribution

4.4. Effect of the constraint on the spread of the drop size distribution

As far as spread of spray drop size distributions is concerned, it is preferred to use the relative span factor defined by :

$$\Delta_V = \frac{D_{v0.9} - D_{v0.1}}{D_{v0.5}} \tag{12}$$

where $D_{V0.1}$, $D_{V0.5}$, $D_{V0.9}$ are the classical representative diameters.

It can be observed in Fig. 3 that the higher the D_{32}^*, the more spread f_V is. In the application of the maximum entropy formalism in the continuous case, Boyaval and Dumouchel [16] wrote a single constraint equivalent to the definition of a mean diameter D_{p0}. As shown in Fig. 4, they found that the span factor is independent of the absolute value of D_{p0} but depends on the order of the constraint p only.

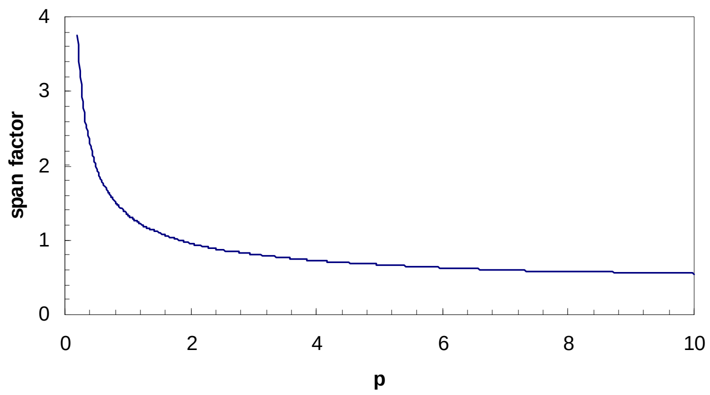

Fig. 4 Evolution of the order of the constraint with the relative span factor (courtesy of Dumouchel)

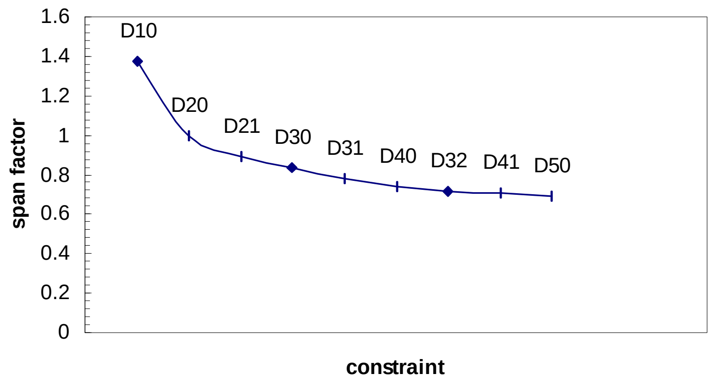

Fig. 5 Effect of the definition of the constraint on the relative span factor

This behavior is verified with the new method. As a matter of fact, by writing only the definition of the mean diameter D_{pq} as constraint, we found that the span factor depends on the value of p and q only and does not depend on the value of D_{pq}. Contrary to the previous approaches, q can take values different from zero. This result is illustrated in Fig. 5 for integer values of p and q ranging from 0 to 5. The curve we obtain is perfectly the same as the one obtained by Boyaval and Dumouchel (Fig. 4) but with complementary points. In particular we can clearly see that a constraint having the same order, i.e. p+q, does not provide the same calculated relative span factor. For instance with an order set to 3, the use of the constraint "D_{21}" brings a different Δ_V than with the use of the constraint "D_{30}".

5. Example of the application of the new approach in the case of two constraints

The present part of the paper is intended to show some limitations of the maximum entropy formalism if at least two constraints are written. This is illustrated with one example only.
In the Ahmadi and Sellens's approach [13], the prediction of the number-based pdf is based on the writing of three constraints. The first constraint that uses a negative constraint order is called the partition constraint and is the definition of the mean diameter D_{-10}. This constraint forces the number-based pdf f_n to tend to zero when diameter reaches zero. This effect is similar as the one obtained for big droplets with a positive constraint order. The second constraint that expresses the surface energy conservation is the definition of the surface mean diameter D_{20}. The third constraint, based on the mass conservation law, is the definition of the volume mean diameter D_{30}. By using these three constraints, thanks to the use of the Lagrange's multipliers method, Ahmadi and Sellens obtain a number based pdf that has the following form :

$$f_n(D) = \exp\left(-a_0 - a_1 D^{-1} - a_2 D^2 - a_3 D^3\right) \qquad (13)$$

Depending on the input values of D_{-10}, D_{20} and D_{30}, the coefficient a_3 can be negative and leads to a calculated diverging pdf for the big drop population. Despite that this behavior can be detected on some figures, this result has never been commented in the literature. The present part of the paper is intended to bring a reason of this behavior thanks to the use of the new method by considering a simplified case. Let us write two constraints that are the definition of D_{10}^* and D_{20}^* that is to say the two first moments of a distribution. In this test case, n = 101 classes are considered, the reduced mean diameter D_{10}^* is set to 0.5 and D_{20}^* is a tunable parameter.

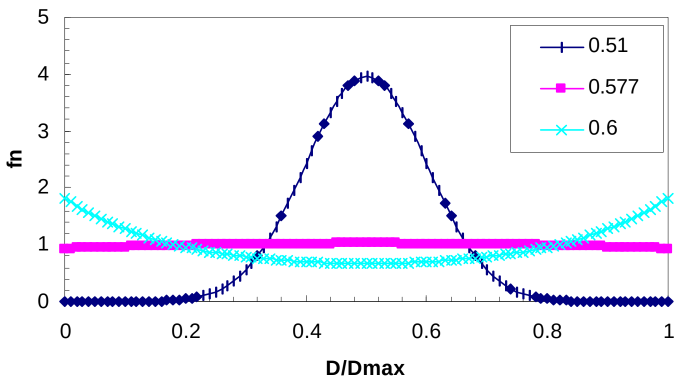

Fig. 6 Effect of the value of D_{20}^* on the calculated pdf ($D_{10}^* = 0.5$)

Figure 6 shows the calculated number-based pdf in the case of three different values for D_{20}^*. For the smaller value ($D_{20}^* = 0.51$), the two mean diameters are very close and lead to a narrow distribution ensuring that the calculated pdf tends to zero for both minimum and maximum diameters. For the value $D_{20}^* = 0.577$, the maximum entropy formalism leads to the prediction of a constant pdf. This corresponds to the chosen prior probability density function that is to say f = m (see equation (3)). This result is in perfect agreement with theory. As a matter of fact, in the present discrete formulation, we assume that the prior function m is constant. Thus in order to respect the normalization law, for all diameter classes, the occurrence probability associated to the function m equals 1/n. It can be shown that the mean of the distribution m is 0.5 and its standard deviation is $(1/3)^{1/2}$ (i.e. 0.577 approximately). This means that with the constraints $D_{10}^* = 0.5$ and $D_{20}^* = 0.577$, no new information is brought to the system and the application of the maximum entropy formalism leads to f = m.

Finally, as shown in Fig. 6, when D_{20}^* is set to a higher value, the result provided by the formalism is not physically valid anymore. This comes from the fact that the maximum entropy formalism is not able to predict distributions more spread than the prior distribution. This is exactly what happens in some Ahmadi's calculated pdf leading to a diverging pdf for large diameters.

6. Conclusion

This paper presents a new method for the application of the maximum entropy formalism to predict drop size distribution in sprays. This method, based on recent results in non linear programming, needs to be carried out with a discrete description of the drop size distribution. In addition, contrary to the classical Lagrange's multipliers method, this new approach allows to write any type of constraints and is not mathematically limited anymore. This paper details the new method and its capabilities and an illustration is given with some examples.
It was shown if the definition of any mean drop diameter D_{pq} is the only written constraint, the relative span factor of the volume-based drop size distribution deduced from the MEF is not a function of the value D_{pq} but depends on both p and q.
Moreover it is also observed that when the two first moments of the distribution are used as constraints, the maximum entropy formalism leads to a non physically valid pdf if the second moment of the distribution has a value higher than the one of the prior function. This result illustrates well some unrealistic calculated pdf found in the literature.

7. References

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