THE MAXIMUM ENTROPY METHOD APPLIED TO LIQUID JET ATOMIZATION

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ILASS-Europe '99 *5th - 7th July 1999*

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ABSTRACT

A method is proposed to obtain by theoretical considerations the size distribution of sprays for a thick layer in the presence of gaseous flow. First, a maximum disturbance wave length is deduced from linear theory. This wave length is injected into a Stuart vortex in which the deformation of an initially planar liquid surface leads to the formation of a ligament. Droplets are formed by breakup of this transversal detached - or longitudinal attached - ligament and a theoretical mean diameter can be determined. Maximum entropy principles are then applied to deduce the size distribution.

1. INTRODUCTION

Droplet size and velocity distributions of sprays can be predicted from a theoretical formulation based on maximum entropy principles [1,2]. The entropy of Shannon [1] is written for subsystems that may be in the states 1, 2, ...,n with the probabilities p_1 , p_2 , ...,p_n as :

(1) $$S(\underline{p}) = -k \sum_{i=1}^{n} p_i \ \mathrm{Log}\, p_i$$

In the continuous formulation and when only the reduced diameter $\overline{D}$ is important, this entropy becomes :

(2) $$S = -k \int_0^{\infty} f(\overline{D}) \mathrm{Log}\left(f(\overline{D})\right) d\overline{D}$$

In the classical modelizations, the joint droplet distribution function is derived subject to the constraints of mass flow rate, momentum flux and energy fluxes (kinetic and surface) in noncontinuous [3] or in continuous formulation [3, 4, 5]. This formalism requires the definition of a control volume [3, 6, 7] and experimental informations such as the measured mean drop diameters [7, 8]. The calculated distributions are in relatively good agreement with the experimental results for a lot of injectors producing thin planar, cylindrical, or conical liquid sheets [9]. More recently, Cousin et al. [10, 11] have investigated a method which gives the drop size distribution from a formalism based on the maximization of the entropy where the required information is principally provided by theoretical considerations. Indeed, a theoretical mean diameter is deduced from a two stage process which is assumed to lead to primary atomization [12] :
1) a linear instability followed by breakup and ligament formation ;
2) a breakup of the ligaments into drops by a Rayleigh process [13].
However, the width of the distribution must be given in addition to the theoretical results, which has been found constant for a given disintegration scheme.

Unfortunately, for thick layers (this is certainly the case of LOX jet atomization in cryogenic rocket combustion chambers [14, 15]) the breaking into half wave lengths, valid for thin liquid sheets, does not occur.
Starting from experimental observations, a five stage three-dimensional atomization process has been proposed [16], although these equations have not yet been solved. A numerical method has also been proposed [17] for simulation of high Reynolds number breakup of the liquid-gas interface. This method has been applied to two-dimensional situations and is extended now to three-dimensional cases.

We suggest here to extend the Cousin and Dumouchel method to thick layers, with a breakup process in three stages as follows :
1) in the first stage (§**2**), one deduces a maximum disturbance wave length from the linear theory ;
2) this characteristic length is injected as the wave length into a Stuart vortex (**§3**), then the deformation of an initially planar surface is studied ;
3) the last stage is the breakup of the obtained nonlinear wave and the formation of droplets (§**4**).
A mean theoretical diameter can then be found and a method of Cousin-Dumouchel can be applied (§**5**).

2. DETERMINATION OF THE WAVELENGTH OF THE MAXIMUM GROWING DISTURBANCE

A relatively thick liquid layer can be considered as infinite. The process of destabilization and atomization is not the same for a thick layer and for the well known thin layer problem. Many of linearized problems have been solved [18]. For inviscid fluids of densities ρ_1 and ρ_2 and velocities U_1 and U_2 respectively, and for small perturbations, in the presence of surface tension σ [19] and with no gravity effect, one obtains an amplification factor ω_i which satisfies the equation :

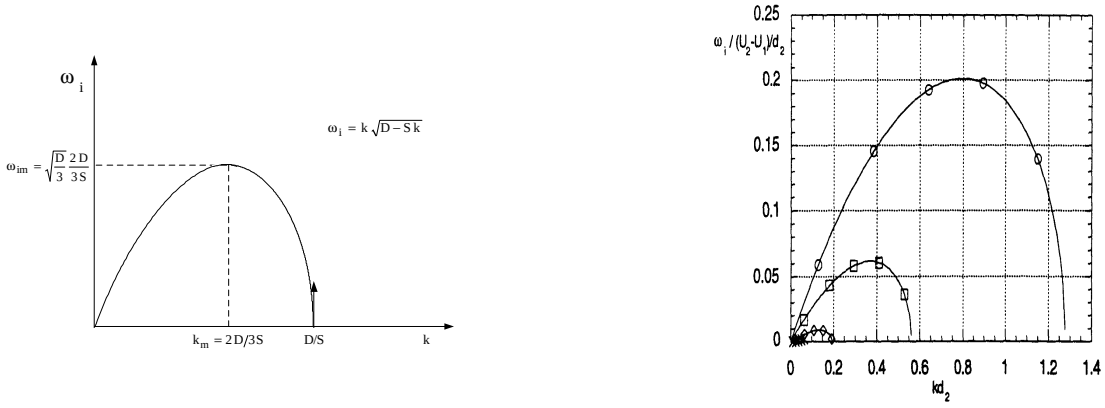
(1) $$\omega_i^2 = -\frac{\sigma}{\rho_1+\rho_2}k^3 + \frac{\rho_1\rho_2}{(\rho_1+\rho_2)^2}(U_1-U_2)^2 k^2$$

where k is the wave number (Fig. 1a).
If the viscous effects are no longer neglected, the problem becomes more complex especially due to the existence of boundary layers. A modelization has been performed by Raynal [16] who assumes linear velocity profiles inside the boundary layers and proves that only the gazeous boundary layer of thickness d_2 needs to be considered.

For small Richardson numbers ($Ri = \frac{(\rho_1-\rho_2)g d_2}{\rho_2(U_2-U_1)^2}$) and high Weber numbers ($We = \frac{\rho_2(U_2-U_1)^2 d_2}{\sigma}$), the obtained relation between the reduced growing factor Ω_i ($\Omega_i = \frac{\omega_i d_2}{U_2-U_1}$) and the reduced wave number K ($K = k\ d_2$) is the following :

(2) $$e^{-2K} = \frac{\left(2\left(K\frac{r_2}{r_2-1}-\Omega\right)-1\right)\left(\left(\frac{K}{r_2-1}-\Omega\right)\left(1+\frac{1}{S_2}\right)+1\right)}{\left(\frac{K}{r_2-1}-\Omega\right)\left(1-\frac{1}{S_2}\right)-1}$$

with $r_2 = \frac{U_2}{U_1}$, $S_2 = \frac{\rho_2}{\rho_1}$. The shapes of the obtained curves are approximatively the same in the two cases (i.e., inviscid fluids with surface tension and boundary layer with no surface tension), but the values of k_m and ω_{im} depend strongly on S_2 (Fig 1b).



a) b)

Fig. 1 Amplification factor for two semi infinite superimposed fluids

a) Inviscid fluids with surface tension: $S = \sigma/(\rho_1 + \rho_2)$, $D = \rho_1 \rho_2 (U_1 - U_2)^2 / (\rho_1 + \rho_2)^2$

b) With no surface tension but a linear velocity profile through the gazeous boundary layer [16] $r_2=\infty$
O $S_2=1$; [] $S_2=10^{-1}$; ◊ $S_2=10^{-2}$; × $S_2=10^{-3}$

3. NONLINEAR DEFORMATION IN A STUART VORTEX

For thick layers, atomization results from a nonlinear process, which seems to be three-dimensional [16] with the formation of attached ligaments. The proposed simplified method takes into account the nonlinear character of liquid cylinder formation, which leads, in a last stage, to droplet formation (§4). Stuart vortices[20, 21] that are introduced are exact analytical solutions of the equations of fluid mechanics. They provide a relatively good representation of shear flows. The stream function ψ of such a vortex is :

(3) $$\Psi = -\frac{\lambda U_\infty}{2\pi} \mathrm{Log}\left(\mathrm{ch}\frac{2\pi y}{\lambda} - \kappa \cos\frac{2\pi x}{\lambda} \right)$$

where x and y are natural coordinates of the space, λ is a wave length, U_∞ the half difference $(U_2-U_1)/2$ of the two superposed flows and κ a specific quantity of the local flow structure (for κ=0, one has a hyperbolic tangent velocity profile, for κ=0.25 one obtains cat eyes and κ=1 gives a vortex line).
Some characteristics of the studied problem, such as surface tension or density jump, are neglected in the Stuart vortex model, although these quantities can be considered to be present a priori in λ and κ. The wave length λ is assumed to be the most amplified wave length $\lambda_m=2\pi/k_m$ and κ corresponds to the local thickness of the vortex street which is an increasing function of the distance from the injector exit and can be determined by experimental observations or by simple rules (for example κ may be considered as a linear function of the distance to the injector exit).
The initially linear deformation of the plane surface y=0 becomes nonlinear rapidly with the velocity field induced by the stream function defined by equation (3) and leads to the formation of an attached liquid cylinder as can be seen in Fig. 2.

4. DROPLET FORMATION

If the liquid cylinder is detached and carried by the flow, perpendicular to it and at the wave velocity, then the process of droplet formation will be a Rayleigh process [12, 13, 21, 22]. If the liquid cylinder stays attached with two branches as suggested by Raynal [16], then its atomization will result from the surrounding flow which is travelling at nearly the gas velocity U_2 [23, 24, 25, 26] (Fig 3).
In the case where the ligaments are broken up following the Rayleigh mode, the pressure field due to capillary effects initiates a fluid motion. Any small perturbation causes variations of the cylindrical ligament cross

section and the resulting flow tends to accumulate the liquid into the larger cross section regions until the formation of

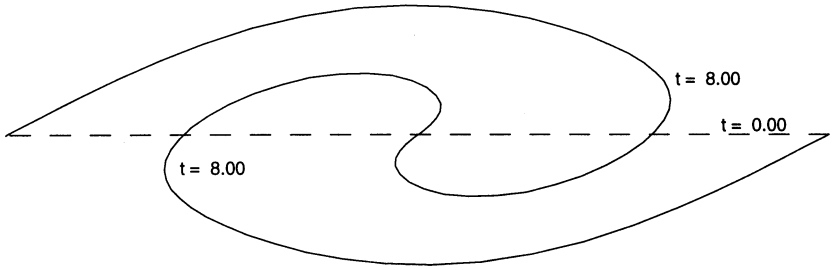


Fig 2. Nonlinear wave in a Stuart vortex at two reduced times t=0 (initially plane surface), t=8.

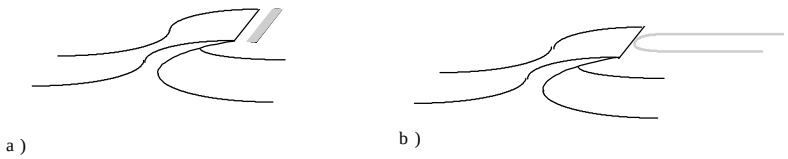


Fig 3. Formation of a liquid ligament
a) detached transverse cylinder
b) attached pair of ligaments

drops occurs. The obtained wave length, deduced from the linear analysis of Rayleigh, is 4.51 d_L, where d_L is the ligament diameter. Conservation of liquid volume gives the droplet mean diameter (droplets are assumed to be spherical) :

(4) $$d_G = 1.89\ d_L$$

In the second case, the ligaments stay attached to the wave crest, change their direction and become parallel to the mean flow direction, keeping their initial velocity. The velocity jump between the ligament branches and the outer gaseous flow will be estimated. If one takes for the wave velocity, the value given by Dimotakis [27], who considers a stagnation point with velocity $U_c = \left(\sqrt{\rho_1}\,U_1 + \sqrt{\rho_2}\,U_2\right)\Big/\left(\sqrt{\rho_1} + \sqrt{\rho_2}\right)$, one has $U = U_2 - U_c$. The classical perturbation method can then be applied to the cylinder in the presence of an external flow at a relative velocity U. Results have been obtained by Taylor [28] in the case of a very small density ratio $S_2 = \rho_2/\rho_1 \langle\langle 1$. Krülle et al. [24] consider also a viscous liquid, an inviscid gas and a non zero surface tension with no shear stress at the liquid-gas interface but the density ratio is no longer small. The growth rate of the perturbation is then a function of wave number and has a maximum value leading to the characteristic wave

number k_m in the same way as in **§2**. Assuming the stripped droplets have diameters proportional to the maximum unstable surface wave length λ_m it is then possible to deduce a mean diameter.

5. THE MAXIMUM ENTROPY METHOD

The mean theoretical diameter d_G found above will be used to define a diameter D_{q0} . Only mean diameters of the form D_{q0} can be used as constants, which, together with the normalization, lead to the two equations [10, 11] :

(5) $$\int_0^\infty D^q \, f_n(D) \, dD = \left(D_{q0}\right)^q$$

(6) $$\int_0^\infty f_n(D) \, dD = 1$$

Usually, a drop diameter D_{max}, large enough to obtain a good approximation of the integrals, takes the place of infinite upper limit.

The droplet diameter distribution function $f_n(D)$ is inserted into equation (2) in place of $f\left(\overline{D}\right)$ to obtain the entropy formula to be maximized taking the constraints (5) and (6) :

(7) $$S = -k \int_0^\infty f_n(D) \, \mathrm{Log}\left(f_n(D)\right) dD$$

The following distribution function is finally obtained :

(8) $$f_n(D) = \frac{q^{\frac{q-1}{q}}}{D_{q0} \; \Gamma\left(\frac{1}{q}\right)} \exp\left(-\frac{D^q}{q \, D_{q0}^q}\right)$$

where $\Gamma(x)$ is the Eulerian function : $\Gamma(x) = \int_0^\infty t^{x-1} \, e^{-t} \, dt$

A mean diameter D_{m0} can be deduced from the formula :

(9) $$\left(D_{m0}\right)^m = q^{\frac{m}{q}} \left(D_{q0}\right)^m \; \frac{\Gamma\left(\frac{m+1}{q}\right)}{\Gamma\left(\frac{1}{q}\right)}$$

For spherical particles, the distribution function used here $f_v(D) = \left(\frac{D}{D_{30}}\right)^3 f_n(D)$ is given by :

(10) $$f_v(D) = q^{\frac{q-4}{q}} \frac{D^3}{D_{q0}^4 \Gamma\left(\frac{4}{q}\right)} \exp\left(-\frac{D^q}{q D_{q0}^q}\right)$$

Finally, knowing q and the diameter D_{q0} , one is able to obtain $f_v(D)$. However the constraint order q is completely unknown. It is not given by the linear theory nor by mass conservation. The constraint to be written here must be chosen with care to ensure a correct width of the distribution. The corresponding value of the diameter D_{q0} can be deduced from the known diameter through a relation similar to eq. (9).

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