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PREDICTION OF DROPLET SIZE AND VELOCITY DISTRIBUTION IN SPRAY USING MAXIMUM ENTROPY METHOD

ABSTRACT:
The prediction of droplets diameter and velocity distribution in a spray is so difficult since its process and mechanism is not completely known and depends too many parameters. The early stage of the atomization process (Primary Breakup) is clearly deterministic, whereas the final stage of spray formation (Secondary Breakup) is random and stochastic. In the second region, which deals with the stochastic aspect of droplet size and velocity distributions, analysis is done by using the maximum entropy principle (MEP). The MEP predicts atomization process while satisfying constrain equations of mass, momentum and energy. Finally, an experimental investigation is done to verify the theoretical model. For this means, a specific nozzle is designed and manufactured so the breakup length and the droplet size and velocity distributions are measured using high-speed camera and laser based technique (Phase Doppler anemometry).

KEYWORDS:
Spray, Maximum Entropy, Modeling, Distribution, Velocity, Diameter

INTRODUCTION

In the past years, numerous investigations are concentrated on making appropriate model to describe jet fracture and droplet formation.

Classic model to predict diameter distribution and velocity of the droplets are derived mainly from experimental data. In this procedure, a curve is fitted on different data obtaining from various conditions of nozzle operations. This procedure is the main basis for distributions like Rosin & Rambler, Nukiyama-tanasawa, log-kornel and root-kornel and Log hyperbolic.

In an alternative method of empirical procedures, an analytical model using entropy maximization procedure (MEP) is developed for computing the size distribution of droplets in the past two decades.

At the end of 1980, maximum entropy principle is observed for calculating size and velocity distribution of the droplets in the sprays. This viewpoint predicts the distribution using a set of rules and principles implying general information related to the system.

This approach assumes that in addition to conservation of mass, momentum and energy, the droplet size distribution function satisfy a maximum entropy principle.

This approach suggests the most plausible size distribution in which conservation equations are satisfied and system entropy is maximized. Using MEF model and the initial value for average diameter, it is possible to acquire size distribution and droplet velocity in a spray or probability density function (PDF).

This approach are presented, at the first, by Sellens and Brzustowski in 1986 [5,6] and then developed by Tankin and Li in 1987 [9] in which initial conservation and energy of partial surface equations are used.

Then, Ahmadi and Sellense [4] could estimate droplet size distribution independent from their velocity distribution. In 1996, Cousin [2] observed the correct application of entropy maximization principle and announced that this formulation can predict any distributing in the spray. He used different average diameter and concluded that the relation between diameter and volume of particle should be considered in the formulation in order to obtain a suitable volume distribution.

In 2003, X. Li & M. Li [8] proposed an innovative model for estimation of droplet size distribution based on maximization of entropy during the spray process. This idea forecasts the distributions by implementing a set of rules and principles implying general information related to the system. Entropy maximization principle for modeling the size and velocity of droplet is applicable only for the adiabatic system in which thermodynamics equilibrium is prevailed.

MATHEMATICAL MODEL AND GOVERNING EQUATIONS

To extract governing equations and determine size and velocity distribution for particles, a control volume on the outlet of injector is assumed. Control volume is considered in such a way that the inlet is coincident with outlet of injector and the outlet is continued to the droplet formation location. Figure 1 shows the control volume considered in a conical spay of an injector. According to the figure, a droplet, which is formed separated from its neighborhood fluid, is assumed to be out of the control volume and hence the interaction of a droplet with surrounding is out of the control volume.

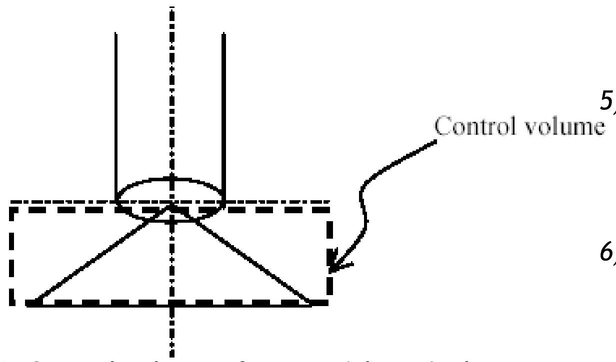


Figure1. Control volume of spray with conical pattern

Droplet formation process in the control volume can be considered as a transformation from one to another equilibrium state. According to the thermodynamics laws, during changing in state mass, momentum and energy is conserved as well as entropy maximization occurs. Therefore, the basis in mathematical modeling of spray systems is the consideration and derivation of appropriate mass, momentum and energy conservation equations for analyzing the spray systems. Regarding to the formulation of entropy maximization, conservation equation can be stated in terms of probability density function. P_{ij}, which is the probability of finding a droplet with volume v_j and velocity u_i. Hence, the mass, momentum and energy conservation equation can be restated as:

1) Mass balance:

$$\sum_i \sum_j p_{i,j} V_i \rho \dot{n} = \dot{m}_o + s_m$$

2) Momentum balance:

$$\sum_i \sum_j p_{i,j} V_i \rho \dot{n} u_j = \dot{J}_o + s_{mu}$$

3) Energy balance:

$$\sum_i \sum_j p_{i,j} \dot{n} (V_i \rho u^2{}_j + 2\sigma A_i) = \dot{E}_o + s_e$$

In these equations, $\dot{n}$ is the droplet generation rate in the spray. $\dot{m}_o$ ، $\dot{J}_O$ ، $\dot{E}_O$ are mass flow rate, momentum and energy which get into the control volume from injector outlet. S_m, S_{mu} and S_e are the source terms for mass, momentum and energy equations respectively which are used to compensate the existence of additional parameter waived in the equations.

In addition to the kinetic energy, a droplet has a surface energy, which is necessary for its formation. Therefore, $2\sigma A_i$ terms are considered in the energy equation. To obtain a more proper form of equations, it is possible to normalize the equation with $\dot{m}_o$ ، $\dot{J}_O$ ، $\dot{E}_O$. Regarding to the definition of momentum average velocity and droplet average volume in spay, mass, momentum and energy equations can be rewritten as follow:

4) Mass balance:

$$\sum_i \sum_j p_{ij} (\frac{V_i}{V_m}) = 1 + \frac{s_m}{\dot{m}_o}$$

5) Momentum balance:

$$\sum_i \sum_j p_{ij} (\frac{V_i}{V_m})(\frac{u_j}{\bar{u}_o}) = 1 + \frac{s_{mu}}{\dot{J}_o}$$

6) Energy balance:

$$\sum_i \sum_j p_{ij} (\frac{V_i}{V_m}) \frac{1}{H} \left[(\frac{u_j}{\bar{u}_o})^2 + B' k_i \right] = 1 + \frac{s_e}{\dot{E}_o}$$

In these equations, k_i is the division of area to volume of a droplet which belongs to the group size $k_i = \frac{A_i}{V_i}$, $B' = \frac{2\sigma}{\rho \bar{u}_o^2}$. H is the shape factor for velocity profile and can be defined as:

$$H = \frac{\left(\frac{\dot{E}_O}{\dot{m}_o}\right)}{\dot{u}_o^2} = \frac{\left(\frac{\dot{E}_O}{\dot{m}_o}\right)}{\left(\frac{\dot{J}_O}{\dot{m}_o}\right)^2} \qquad (7)$$

When outlet velocity profile is uniform, the shape factor (H) is equal to 1 and volume, velocity and dimensionless source terms can be described as:

$$\bar{V}_i = \frac{V_i}{V_m} \ , \ \bar{u}_j = \frac{u_j}{\bar{u}_o} \ , \ \bar{s}_m = \frac{s_m}{\dot{m}_o} \ ,$$

$$\bar{s}_{mu} = \frac{s_{mu}}{\dot{J}_O} \ , \ \bar{s}_e = \frac{s_e}{\dot{E}_O}$$

In addition to the three above mentioned equations, according to the probability concept, total summation of probabilities should be equal to unity:

$$\sum_i \sum_j p_{ij} = 1 \qquad (8)$$

As it is mentioned before, there are infinite probability distributions P_{ij} to satisfy the equations 4 through 8, therefore the most appropriate distribution is the one in which Shannon entropy is maximized.

$$S = -k \sum_i \sum_j p_{ij} Lnp_{ij} \qquad (9)$$

Using Lagrange coefficient procedure, the probability distribution in which entropy is maximized is presented as follow:

$$p_{ij} = \exp[-\lambda_0 - \lambda_1 \overline{V}_i - \lambda_2 \overline{V}_i \overline{u}_j - \lambda_3 (\frac{\overline{V}_i \overline{u}_j^2}{H} + \frac{B' k_i \overline{V}_i}{H})] \quad (10)$$

To obtain coefficient λ_i, *equations 4 to 8 and 10 should be solved simultaneously. Probability of finding the droplets which their volumes are between* $\overline{V}_{n-1}$ *and* $\overline{V}_n$ *and their velocities are between* $\overline{u}_{m-1}$ *and* $\overline{u}_m$ *is presented as follow:*

$$_{n-1} \le \overline{u} \le \overline{u}_m \} = \sum_{V_{n-1}} \sum_{u_{m-1}} p_{ij} =$$

$$\lambda_1 \overline{V}_i - \lambda_2 \overline{V}_i \overline{u}_j - \lambda_3 (\frac{\overline{V}_i \overline{u}_j^2}{H} + \frac{B' k_i \overline{V}_i}{H})] \quad (11)$$

Generally, in the spraying problems, the size and velocity of droplets are varied continuously. Therefore, it is possible to uniformly descriptive the analytical domain and instead of using $\sum$ *; the equations can be stated in the integral form over size and velocity of droplets. It is also feasible to convert analytical domain from volume and velocity of droplets to their diameter and velocity. Hence, Probability of finding droplets which their diameters are between* $\overline{D}_{n-1}$ *and* $\overline{D}_n$ *and their velocities are between* $\overline{u}_{m-1}$ *and* $\overline{u}_m$ *is presented as follow:*

$$p\{\overline{V}_{n-1} \le \overline{V} \le \overline{V}_n, \overline{u}_{m-1} \le \overline{u} \le \overline{u}_m\} = \sum_{V_{n-1}} \sum_{u_{m-1}} p_{ij} =$$

$$= \sum_{\overline{V}_{n-1}}^{\overline{V}_n} \sum_{\overline{u}_{m-1}}^{\overline{u}_m} \exp[-\lambda_0 - \lambda_1 \overline{V}_i - \lambda_2 \overline{V}_i \overline{u}_j - \lambda_3 (\frac{\overline{V}_i \overline{u}_j^2}{H} + \frac{B' k_i \overline{V}_i}{H})] \quad (12)$$

In these equations, $\overline{D}_{n-1}$ *and* $\overline{D}_n$ *are the droplet diameters related to the volumes* $\overline{V}_{n-1}$ *and* $\overline{V}_n$ *and f is the probability density function for size and velocity of a droplet (PDF).*

$$f = 3\overline{D}^2 \exp[-\lambda_0 - \lambda_1 \overline{D}^3 - \lambda_2 \overline{D}^3 \overline{u} - \lambda_3 (\frac{\overline{D}^3 \overline{u}^2}{H} + \frac{B\overline{D}^2}{H})]$$

$$we = \frac{\rho \overline{u}_o^2 D_{30}}{\sigma}, \; B = \frac{12}{we} \quad (13)$$

The relative velocity of liquid and gas is near liquid velocity in the analytical domains (location of droplet formation). Droplet generated from spraying is relatively small and usually their shape is considered to be spherical due to the surface tension effects. Equations 4 to 8 can be restated in integral forms and in analytical domains of velocity and diameter of the droplet. Hence, regarding above mentioned statement, to obtain Lagrange coefficient (λ_i *) in PDF (f), it is necessary to solve the following sets of equations.*

$$\begin{cases} \int_{\overline{D}_{min}}^{\overline{D}_{max}} \int_{\overline{u}_{min}}^{\overline{u}_{max}} f\overline{D}^3 d\overline{u} d\overline{D} = 1 + \overline{s}_m \\ \int_{\overline{D}_{min}}^{\overline{D}_{max}} \int_{\overline{u}_{min}}^{\overline{u}_{max}} f\overline{D}^3 \overline{u} d\overline{u} d\overline{D} = 1 + \overline{s}_{mu} \\ \int_{\overline{D}_{min}}^{\overline{D}_{max}} \int_{\overline{u}_{min}}^{\overline{u}_{max}} f(\frac{\overline{D}^3 \overline{u}^2}{H} + \frac{B\overline{D}^2}{H}) d\overline{u} d\overline{D} = 1 + \overline{s}_e \\ \int_{\overline{D}_{min}}^{\overline{D}_{max}} \int_{\overline{u}_{min}}^{\overline{u}_{max}} f d\overline{u} d\overline{D} = 1 \\ f = 3\overline{D}^2 \exp[-\lambda_0 - \lambda_1 \overline{D}^3 - \lambda_2 \overline{D}^3 \overline{u} - \lambda_3 (\frac{\overline{D}^3 \overline{u}^2}{H} + \frac{B\overline{D}^2}{H}) \end{cases} \quad (14)$$

As it can be seen from the equations, the analytical domain is changed from $\overline{D}_{min}$ *to* $\overline{D}_{max}$ *and from* $\overline{u}_{min}$ *to* $\overline{u}_{max}$. *The variations of* $\overline{D}$ *and* $\overline{u}$ *in the domain are independent that is, the probability of existence for every droplet (with arbitrary velocity* $\overline{u}$ *and diameter(* $\overline{D}$ *) is considered*

SOURCE TERMS

Not considering the flow which enter from the nozzle of control volume and droplets which after formation depart the control volume, if there is any inlet or outlet of mass flow rate, it should be considered in a source terms. As an example, the evaporation and distillation of liquid during spraying process should be considered in a source term. If within the control volume, there is a momentum exchange between the flow and continuous phase, this momentum transformation should be considered as a source term. For instance, the effects of drag force on liquid body can be stated. The drag force is proportional to the relative velocity between liquid and gas.

In the present formulation of entropy maximization, all the sources and sinks of energy (source and sinks of kinematics energy, surface energy, turbulence energy etc will be accumulated in the energy source term (Se). If there is any energy conversion whiting the control volume, it is not considered as a source term. Therefore, the entire energy, entering and exiting from control volume and not considered in the equations is computed as a source or sink term. As an example, the energy conversion from heat and the energy exchange from evaporation and distillation can be pointed out.

When the liquid enter from the nozzle to the gas environment, some of its kinetic energy is consumed by free surface formation and consequently droplet constitution. This energy which is called surface energy is a state of energy conversion within the control volume and hence, is not computed in the source terms.

NUMERICAL ANALYSIS

To obtain this function, it is imperative to determine Lagrange coefficient λ_i in equations 13 which can be computed from solving the equations set of 14 simultaneously. In this paper, to solve this set of equations, Newton-Raphson method is used. At first, some initial value for the $\lambda_0, \lambda_1, \lambda_2, \lambda_3$ is assumed. Then, using this values and Newton-Raphson procedure, new value for λ_0 and then $\lambda_1, \lambda_2, \lambda_3$ is obtained and this procedure is continued until final answer is computed.

To solve these equations, it is noted that, function G_i and their derivatives are integral functions. Therefore, to compute their value, double integrals function should be solved numerically in all iterations. Another important point is that G_i functions and their derivatives are integral functions and the terms in these integrals are exponential, hence if the selection of an initial guessed of λ_i turns out to be close to the answer, the value starts to diverge away from the answer immediately.

MODELING

To assess maximum entropy principle for determination of PDF, the procedure is evaluated for a special operating condition. Therefore, a spray resulting from a conical hollow nozzle is modeled. The prescribed condition is the one which was previously used by Li and Tankin [7, 8] in their research.

In this condition, a fluid (water at 20^0C) is sprayed to a stationary continuous environment (air at 20^0C and 1atm pressure). The injector characteristics are presented in table 1.

If the velocity profile at the injector outlet is assumed uniform, the shape factor of velocity profile (H) will be unity. But if the outlet flow from the injector is assumed to be fully developed and turbulent, this factor will be equal to 1.01647 if the fluid is relatively developed, the shape factor will be between 1 and 1.01647 [8]. Regarding the fact that Li and Tankin, in their investigation, assumed a uniform velocity profile at the injector outlet, in this research shape factor of velocity profile is considered unity. According to the supposed value in table 1, table 2 parameter can be computed.

Table1. Spray characteristic [7]

Fluid characteristic	Density	998.2 (Kg/m^3)
	Surface Tension	0.0736 (N/m)
Ambient air characteristic	Density	1.22 (Kg/m^3)
	Absolute viscosity	1.915*10^{-5} (N/m.s)
Injector specification	Output Diameter	0.002 (m)
	Gap thickness	1.097*10^{-5} (m)
Injection condition	flow	2.809*10^{-3} (Kg/s)
	Average Velocity	40.8 (m/s)
	Initial rotation velocity	0
	Initial angular injection	24.4
	Average mass diameter	1.37*10^{-5} (m)
	Coefficient of figure	1

Table2. Momentum and energy flow rate into the control volume

Weber Number	We	311
Control volume flow rate	$\dot{J}_O$	0.1147 (N)
Control volume energy rate	$\dot{E}_O$	4.684 (Nm/s)

To solve the governing equation, analytical domain is considered as follow:

$$\overline{D}_{\min} = 0 \quad , \quad \overline{D}_{\max} = 3$$
$$\overline{u}_{\min} = 0 \quad , \quad \overline{u}_{\max} = 3$$

The source term of all the conservation equations except momentum equation are assumed zero because by considering zero source term for momentum equation, this equation and kinetic energy behaves in such a way that the velocity variation approach zero which contradict the reality. Besides, in the present simulation, the effects of evaporation, collision and merging of droplets are not considered. To evaluate the air effects on the droplets, all of them are supposed to have spherical shape.

One of the occasion in which momentum exchange between liquid and continuous phase occurs is the influence of drag force on the droplet body. To evaluate drag force, conical layer from outlet of the nozzle to the fracture inception of the fluid layer is opened and estimated as a triangular shape. As an approximation, it is considered that this layer is a flat and stationary layer on which the air is passed with a relative velocity of liquid gas. Considering a laminar boundary layer flow passing on a flat plate, it is possible to compute C_f so the momentum source term can be evaluated as shown in table 3. The Reynolds number in calculation of the source term is based on the jet velocity at the outlet of injector [7].

Table3- Computed source term for momentum equations

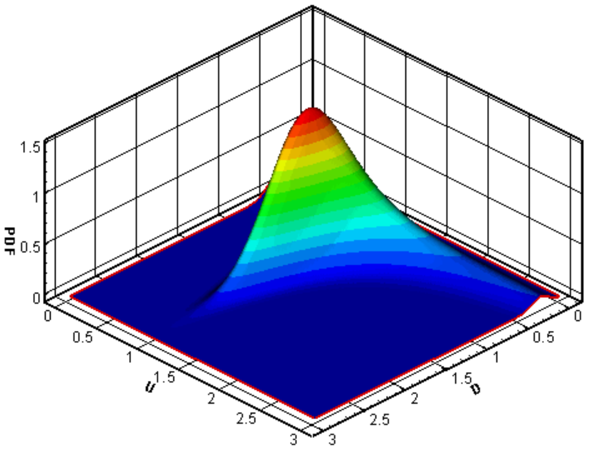
Air Velocity	Drag Force	Non dimensional number of terms sources
Corrected average velocity	1.953*10^{-3} (N)	-0.01702

Air velocity also considered as an average of minimum film velocity (velocity at the outlet of injector) and film velocity at the location of friction force calculation. In this procedure, an integral of average velocity is computed to some extent.

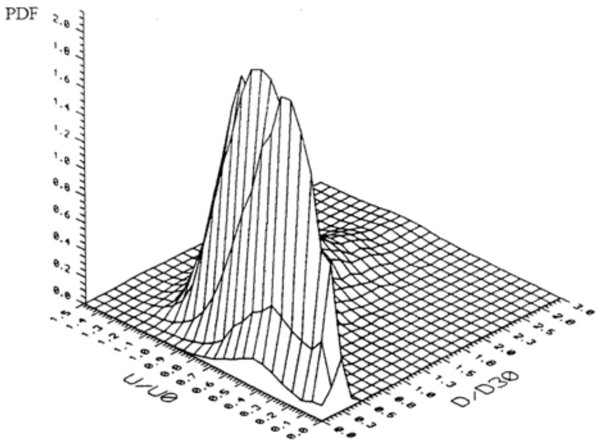
NUMERICAL RESULTS

The three dimensional probability distribution for size-velocity and measurements are demonstrated in figures 2. Computations are shown in figure 2-a while experimental data of Li and Tankin results [7] are presented in figure 2-b.

The calculated probability contour and measurements are also exhibited in figure 3. The difference between contours distributions is affected by measurement accuracy for the momentum source term which is also affected by the drag forces exerted on the droplet after jet fracture because, as it is mentioned, in the present spray, the fracture of conical jet occurs at 7 *cm apart from the nozzle, while the region which velocity and size of droplets are measured at the distance of 10 cm apart and during this interval, the droplets are generated from the fluid jet and drag forces exerted on the droplet are not consisted in computation of momentum source term.*



2-a: The computed velocity-size probability distribution



2-b: The measured velocity-size probability distribution [7]

Figure 2. Comparison of theoretical and experimental velocity-size probability

In figure 4, the measured and computed probability distributions of size are demonstrated. This function is acquired from the integration of velocity-size probability distribution function over the velocity interval. As it is apparent from the figure, there is a satisfactory agreement between theoretical and experimental results.

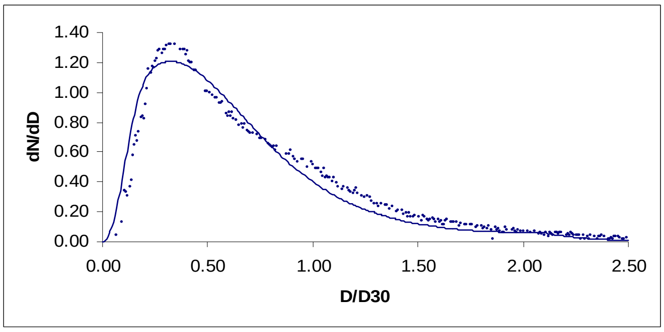
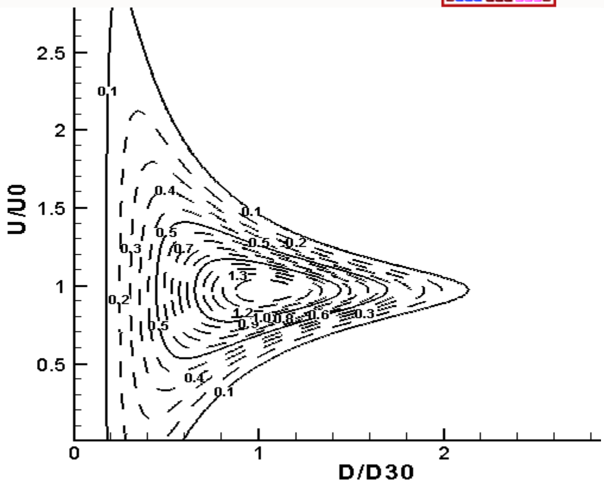
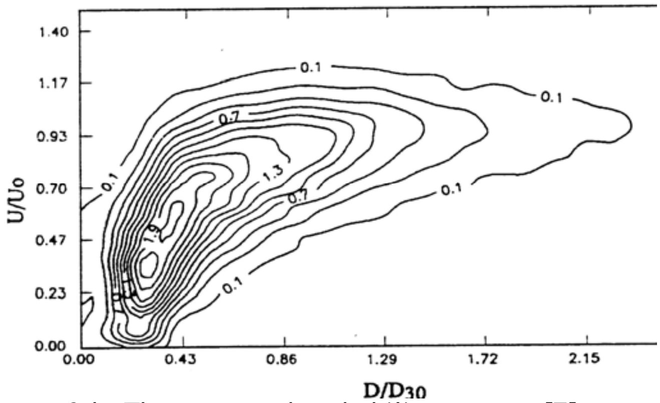


Figure 4. Comparison of theoretical and experimental droplet size distribution



3-a. The predicted probability contour



3-b. The measured probability contour [7]

Figure 3. Comparison of theoretical and experimental contour

WEBER NUMBER EFFECT

In this section, the influence of increasing Weber number on the velocity and size distribution of droplets, in a spray, are investigated. Rising Weber number always results in increasing instability of the fluid jet. It is also leads to the earlier formation of droplets and jet fracture. In figures 5 and 6 the diameter and velocity distributions of droplets at the distance of 10cm from the nozzle and after jet fracture inception and droplet generations versus Weber number are shown. According to the figure 7, by increasing the Weber number, the curves of droplet size distribution become more flat and its maximum decreases hence, droplet size distribution become uniform. However, after Weber number reaches to a specific number, the variations of distribution curves decreases even its trend can be reversed. This point can be seen more clearly in the droplet velocity distribution in next figure. In figure 8, by increasing the Weber number, from a small value to a specific value, the velocity distribution curves shrinks and expands. As a result, the peak of velocity distribution curves becomes greater.

By Increasing Weber, number beyond the critical point, the trends reversed and the velocity distribution of droplets expand and their maximum decrease. Therefore, the velocity distribution becomes uniform.

Therefore, as it can be seen, there is a critical Weber number, which has influence in the velocity distribution; for the prescribed conditions, its value is obtained 200 approximately.

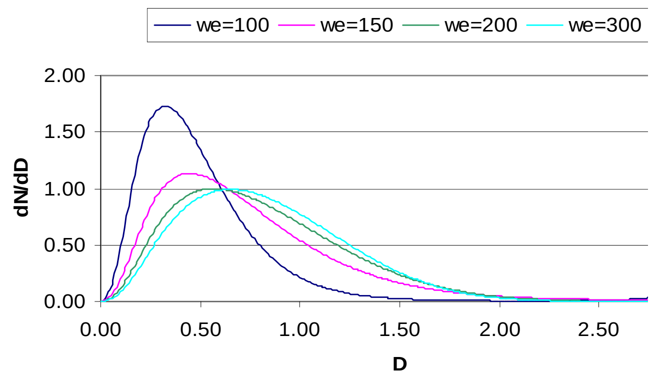


Figure 5: Curves of the dimensionless size of the sprayed droplets at the distance of 10cm from the nozzle versus Weber number

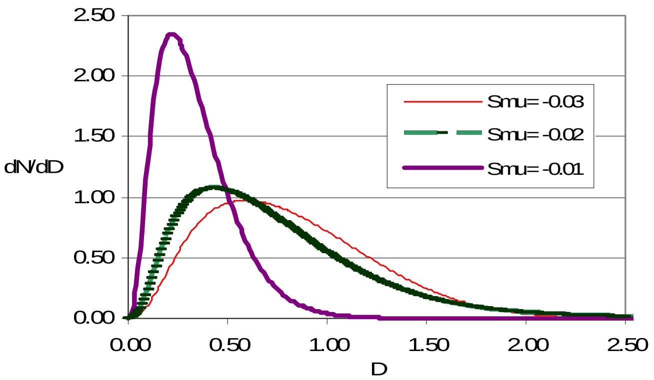


Figure 6- Curves of the dimensionless diameter of the sprayed droplets at the distance of 10cm from the nozzle versus momentum source term

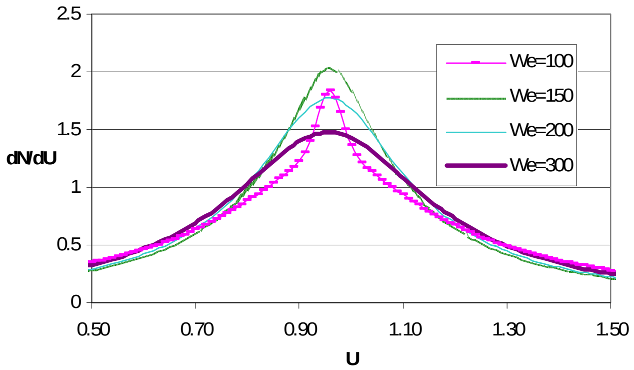


Figure 7- Curves of the dimensionless velocity distribution of the sprayed droplets versus Weber number

ENERGY SOURCE TERM EFFECTS

All the sources and sinks of energy (like kinematics sources and sinks, surface energy, turbulence energy) are collected in the energy source term (S_e). The inlet and outlet energy of the control volume are assumed as the energy source or sink. However, the energy conversion within the control volume is not computed in the source terms. In the turbulence flows, the velocity fluctuations produce additional kinematics energy within the control volume, which is not considered in the equations.

This turbulence energy, which can be consumed for the jet deterioration and droplet formation, is an energy source term and should be considered in the energy source term to increase accuracy [1].

Hence, it is expected that by increasing the magnitude of energy source term, the quality of atomization increases which leads to generating more uniform velocity and diameter distributions of the droplets. This effect is demonstrated in the figure 9 and 10, in which the velocity and diameter distribution of the droplets is plotted.

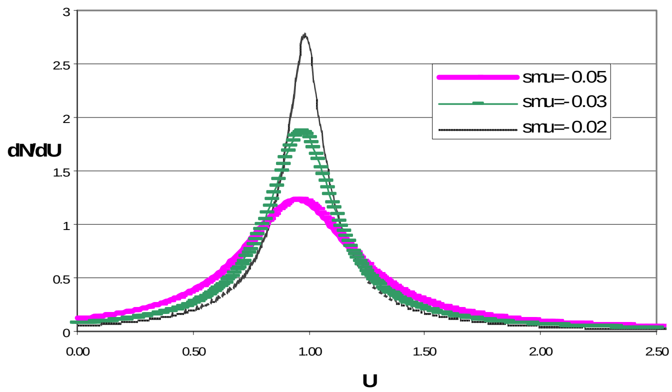


Figure 8- curves of the dimensionless velocity of the sprayed droplets at the distance of 10cm from the nozzle versus momentum source term

CONCLUSION

In the present paper, the random process of distributing diameter and velocity of the droplets is modeled implementing maximum entropy principle (MEP) after jet fracture and droplets formation.

This approach is applicable for predicting the size and velocity distribution of droplets in the systems which thermodynamics equilibrium prevails. However, the process of spray formation is irreversible and no adiabatic and there is always interaction between atomized liquid and surrounding gas. Therefore, establishing a harmony between the results of modeling using MEP and experimental data is a difficult achievement. Although, simplified assumptions used to solve the equations, the results demonstrated a satisfactory conformity with the experiments, which revealed the model ability to account the effects of processes occurs in the spray control volume. Since the functions and their derivatives in the governing equations are in the integral form and function in the integral are exponentials, the solution is sensitive to the initial guess λ_i and by using a wrong initial value, and the solution diverged immediately.

A precise estimation of the source terms is very important so that to acquire exact results the relative velocity variation between liquid and gas in estimating the drag forced should be considered. It is also crucial to observe the drag forced exerted on the droplet after fracture inception. For computation of turbulence effect, at the outlet of the nozzle and heat transformation between two phases, energy source term should be calculated.

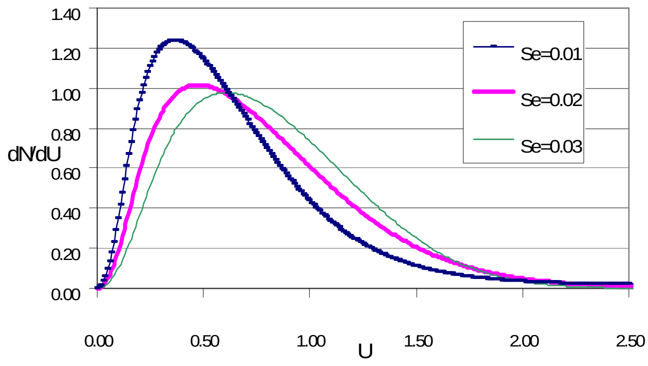


Figure 9 - Curves of the dimensionless diameter distribution of the sprayed droplets at the distance of 10cm from the nozzle versus momentum source term

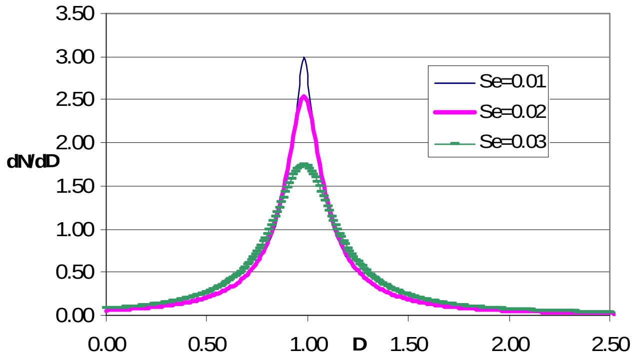


Figure 10 - Curves of the dimensionless velocity distribution of the sprayed droplets at the distance of 10 cm from the nozzle versus momentum source term

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