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# On the Contribution of Drag and Turbulent Stresses in the Fragmentation of Liquid Droplets: A Computational Study

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Abstract

In a recent publication *(Aly et al., Intl. Comm. Heat and Mass Transfer, 37(6) pp 618-623),* the authors have developed a new mathematical model for predicting spray and atomization characteristics in an Eulerian-Eulerian framework. The model takes into account both the drag and turbulence induced fragmentation stresses. In the present paper, the authors investigate the relative contribution of the two different stresses in the break-up process using the new model for a case of a co-axial air-blast atomizer. The results show that turbulent stresses play the dominant role in the fragmentation of liquid droplets.

*Keywords: CFD; Population balance; Atomization; Droplet break-up; Turbulence.*

## 1. Introduction

Computational fluid dynamics (CFD) of single and multiphase flows has been a rapidly developing research topic over the last years. At this point, advanced CFD codes are a valuable complement to experimental investigations, since they allow a detailed local analysis of the flow. Engineering flow prediction of single-phase flows is standard application of CFD and is widely used nowadays. However, there remain a number of challenges that arise in multiphase CFD analysis beyond those present in single phase methods. One of these most important obstacles is the adequate physical modeling of the break-up of the discrete phase bubbles/droplets due to stresses arising from the interfacial dynamics between phases. In the case of a liquid discrete phase and a gas continuous phase, these stresses are the drag and turbulent stresses [1].

Many multiphase break-up models can be found in the literature. Coulaloglou & Tavlarides [2] proposed a break-up model for liquid-liquid dispersion systems in which the break-up frequency is defined by the fraction of particles breaking divided by a characteristic time scale. Luo & Svendsen [3] devised a kinetic theory-type model for bubbles break-up. In their model, the break-up frequency is calculated as a collision frequency between eddies and particles multiplied by a collision efficiency. Martinez et al. [4, 5] proposed a break-up model for bubbles based on

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kinematic ideas (energy balance). An extensive review of such models can be found in [6]. All these break-up models were devised for modeling bubbles in liquids or droplets in liquid-liquid systems and therefore none of them is appropriate for modeling liquid droplets in gas systems; such as spray systems. Moreover, they all take into account the turbulent deformation stresses only and neglect the contribution of drag forces. For spray systems with high inlet air velocities such as air-blast atomizers, this assumption shall not be introduced without prior quantitative analysis. For these reasons, a new mathematical model was devised by the authors for predicting liquid droplets break-up in spray systems without neglecting the contribution of the drag stresses [7].

In the present study, the new model is used to quantitatively compare the roles of turbulent and drag stresses in the break-up process. A case study of a co-axial air-blast atomizer is chosen for the numerical simulation. Before presenting the results of the quantitative analysis, the model is validated through a comparison with experimental data. The break-up model used in this study and the CFD methodology in which the model is implemented will be described briefly in the next sections followed by a presentation of the details of the numerical simulation.

## 2. Droplet Break-up

Droplet break-up depends on the balance between the shear stresses acting to destroy the particles and the surface stresses acting to retain the particle form. The dimensionless Weber number is the ratio between shear stress and the surface tension stress. Hence, break-up will occur only if the Weber number locally exceeds a certain critical value. The deforming shear stresses are categorized into two distinct mechanisms: turbulent stresses and drag induced interfacial stresses.

### *2.1. Droplet Break-up Due to Turbulence*

Assuming isotropic turbulence, Kolmogorov [8] and Hinze [9] formulated that a droplet immersed in a continuous phase would experience an average deforming turbulent stress equals to:

$$\tau_t = \rho_c \overline{\delta u^2(d)} \tag{1}$$

Where $\rho_c$ is the density of the continuous phase and $\overline{\delta u^2(d)}$ is the mean square of a velocity difference over a distance equal to the droplet diameter.

According to Kolmogorov's 1941 theory of isotropic turbulence, $\overline{\delta u^2(d)}$ is represented by:

$$\overline{\delta u^2(d)} = \beta(\varepsilon d)^{2/3} \tag{2}$$

Where $\varepsilon$ is the turbulence dissipation rate and $\beta$ is a dimensionless constant

For the case of droplets in a gas, where the density of the dispersed phase $\rho_d$ is much higher than the density of the continuous phase $\rho_c$, Kocamustafaogullari and Ishii [10] theoretically argued that Eq. (2) should be modified such as:.

$$\overline{\delta u^2(d)} = \frac{\rho_d - \rho_c}{\rho_d}\left(\frac{\rho_d}{\rho_c}\right)^{2/3}\beta(\varepsilon d)^{2/3} \tag{3}$$

For the case of water droplets in air, the value of $\frac{\rho_d - \rho_c}{\rho_d}$ approaches 1 and can be neglected. Hence:

$$\overline{\delta u^2(d)} = \left(\frac{\rho_d}{\rho_c}\right)^{2/3}\beta(\varepsilon d)^{2/3} \tag{4}$$

Substituting Eq. (4) in Eq. (1), the deforming turbulence stress is represented by:

$$\tau_t = \left(\frac{\rho_d}{\rho_c}\right)^{2/3} \beta(\varepsilon d)^{2/3} \rho_c \quad (5)$$

Since Weber number is the ratio between the deforming shear stress and the surface tension stress. Droplet break-up will occur at a critical Weber number corresponding to a critical droplet diameter equals to $d_{cr}$. Representing the surface tension by $\tau_s = \sigma/d$, the critical Weber number can be represented by:

$$We_{cr} = \frac{\tau_t}{\tau_s} = \frac{\left(\frac{\rho_d}{\rho_c}\right)^{2/3} \beta(\varepsilon)^{2/3} \rho_c (d_{cr})^{5/3}}{\sigma} \quad (6)$$

Rearranging Eq. (4.6), the critical droplet diameter at which break-up will occur can be calculated from:

$$d_{cr} = \left[\frac{We_{cr}\sigma}{\beta\rho_c}\right]^{3/5} \varepsilon^{-2/5} \left(\frac{\rho_d}{\rho_c}\right)^{-2/5} \quad (7)$$

If a value of the critical Weber number is provided, Eq. (7) can be then used to determine the maximum stable droplet diameter. Experiments showed that for low viscosity liquids, the critical Weber number is bounded by:

$$5 < We_{cr} < 25 \quad (8)$$

Within this range, the critical Weber number was found to depend on the droplet Reynolds number $\mathrm{Re}_d$ .Kolev [1] correlated the experimental observations of many authors into:

$$We_{cr} = 55\left[\frac{24}{\mathrm{Re}_d} + \frac{20.1807}{\mathrm{Re}_d^{0.615}} - \frac{16}{\mathrm{Re}_d^{2/3}}\right] \quad \text{For} \quad 200 < \mathrm{Re}_d < 2000 \quad (9)$$

And,

$$We_{cr} \approx 5.48 \quad \text{For} \quad \mathrm{Re}_d > 2000 \quad (10)$$

In this study, the droplet break-up time will be approximated as the turbulence time scale. Applying Kolmogorov's theory of turbulence with the correction of Kocamustafaogullari and Ishii [10] for the case of $\rho_d >> \rho_c$, the droplet break-up time can be calculated from:

$$t_{br} = \frac{d}{\sqrt{\overline{\delta u^2(d)}}} = \left(\frac{\rho_c}{\rho_d}\right)^{1/3} \frac{d^{2/3}}{\sqrt{\beta}(\varepsilon)^{1/3}} \quad (11)$$

### *2.2. Droplet Break-up Due to Drag*

For the case of drag induced break-up, the maximum stable droplet diameter can be computed from an expression similar to Eq. (7). However, the mean square of the velocity difference $\overline{\delta u^2(d)}$ must be replaced by the square of the relative velocity between the phases $(V_c - V_d)^2$. Hence, the critical diameter can be computed from:

$$d_{cr} = \frac{We_{cr}\sigma}{\rho_c (V_c - V_d)^2} \quad (12)$$

Pitch et al. [11] developed a correlation to compute the break-up time for the case of drag induced break-up. The correlation reads:

$$t_{br} = t_{br}^{*} \frac{d}{|V_c|} \sqrt{\frac{\rho_d}{\rho_c}} \tag{13}$$

Where $t_{br}^{*}$ is a dimensionless time and can be computed from:

$$t_{br}^{*} = c\left(We\ -12\right)^{m} \tag{14}$$

Where *c* and *m* are constants that depends on the Weber number. See[1].

After calculating the maximum stable diameter and the break-up time corresponding to drag and turbulence induced droplet break-up, a condition has to be set to decide whether turbulence or drag will be the criterion of break-up. Kolev [1] theoretically proposed that the decision should be made based on the maximum droplet diameter in both cases. i.e. if break-up will result from turbulent stresses; otherwise drag will be the criterion of break-up.

$$\frac{We_{cr}\sigma}{\rho_c\left(V_c - V_d\right)^2} > \left[\frac{We_{cr}\sigma}{\beta\rho_c}\right]^{3/5} \varepsilon^{-2/5} \left(\frac{\rho_d}{\rho_c}\right)^{-2/5} \tag{15}$$

## 3. CFD Methodology

In the Eulerian multi-fluid model, the gas and droplet phases are treated as interpenetrating continua in an Eulerian framework. The gas phase is considered as the primary phase, whereas the droplet phases are considered as dispersed or secondary phases. The gas and droplet phases are characterized by volume fractions, and by definition, the volume fractions of all phases must sum to unity:

$$\alpha_g + \sum_{q=1}^{N} \alpha_q = 1 \tag{16}$$

Where $\alpha_g$ is the gas volume fraction, $\alpha_q$ is the volume fraction of the $q^{th}$ droplet phase, and N is the total number of droplet phases.

The governing equations of the multi-fluid model can be derived by conditionally ensemble averaging of the local instant conservation equations of single phase flow [12]. For the spray problem under investigation, the flow is assumed to be isothermal; hence, the energy equation will not be included. Furthermore, since evaporation is not included in the current study, there is no interfacial mass transfer between the gas and droplet phases.

The continuity equation for the gas phase is

$$\frac{\partial}{\partial t}\left(\alpha_g \rho_g\right) + \frac{\partial}{\partial x_i}\left(\alpha_g \rho_g U_{i,g}\right) = 0 \tag{17}$$

Where $U_{i,g}$ and $\rho_g$ are the velocity and density of the gas phase respectively.

The continuity equation for the qth droplet phase is

$$\frac{\partial}{\partial t}\left(\alpha_q \rho_l\right) + \frac{\partial}{\partial x_i}\left(\alpha_q \rho_l U_{i,q}\right) = \sum_{p=1}^{N} \dot{m}_{pq} \tag{18}$$

Where $\dot{m}_{pq}$ characterizes the mass transfer from the $p^{th}$ to the $q^{th}$ droplet phase due to break-up and coalescence.

The momentum equation for the gas phase is

$$\frac{\partial}{\partial t}\left(\alpha_g \rho_g U_{i,g}\right)+\frac{\partial}{\partial x_i}\left(\alpha_g \rho_g U_{i,g} U_{j,g}\right)=-\alpha_g \frac{\partial p}{\partial x_i}+\frac{\partial}{\partial x_j}\left(\alpha_g \tau_{ij,g}\right)+\alpha_g \rho_g g_i+\sum_{q=1}^{N} F_{i,qg} \quad (19)$$

Likewise, for the droplet phases, the momentum balances are

$$\frac{\partial}{\partial t}\left(\alpha_q \rho_l U_{i,q}\right)+\frac{\partial}{\partial x_i}\left(\alpha_q \rho_l U_{i,q} U_{j,q}\right)=-\alpha_q \frac{\partial p}{\partial x_i}+\frac{\partial}{\partial x_j}\left(\alpha_q \tau_{ij,q}\right)$$

$$+\alpha_q \rho_l g_i+F_{i,gq}+\sum_{q=1}^{N} \dot{m}_{pq} U_{i,pq} \quad (20)$$

Where $\tau_{ij,g}$ and $\tau_{ij,q}$ are the stress tensors for the gas and droplet phases, respectively. P is the pressure shared by all phases and $g_i$ is the gravity in the i$^{th}$ direction. The last term of Eq. (21) takes into account momentum transfer due to mass transfer between the droplets phases. Since the liquid phase in this study is treated as one dispersed phase rather than multiple droplet phases, this term is set to zero in all the simulations. The term $F_{i,qg}$ is the interfacial momentum transfer from the droplet phase to the gas phase. This term accounts for the drag, virtual mass effect, and lift forces. For the problem under investigation, both the lift forces and the virtual mass effect are insignificant compared to the drag force and thus only the drag force will be considered. The drag contribution is calculated based on the Schiller-Naumann model [13-15]

In order to track the droplets diameter in the Eulerian solver, a conservation equation for the droplet numbers that governs the distribution function of the droplets must be solved. Such equation is known as the population balance equation [16] and can be written in the following form:

$$\frac{\partial}{\partial t} n\left(d,U_i\right)+\frac{\partial}{\partial x}\left[U_i n\left(d,U_i\right)\right]+\frac{\partial}{\partial U_i}\left[F_i n\left(d,U_i\right)\right]=S\left(d,U_i\right) \quad (21)$$

Where $n\left(d,U_i\right)\,\mathrm{d}\,d\,\mathrm{d}\,U_i$ is a multivariate number distribution function that denotes the average number of droplets in the diameter range $\mathrm{d}\,d$ about $d$, with velocities in the range $\mathrm{d}\,U_i$ about $U_i$. $F_i$ is the force acting to accelerate the droplets, and $S\left(d,U_i\right)$ represents the rate of change of the distribution function caused by droplet formation or destruction processes such as nucleation, droplet breakup, or collisions. For the spray problem under consideration, only the effect of break-up will be included.

In this study, the population balance equation is solved using the Quadrature Method of Moments (QMOM). The details of such method will not be presented here for brevity and the reader is referred to ref.[17-19].

## 4. Numerical Simulation

Numerical simulations were performed for a case study of a two-dimensional coaxial air-blast atomizer. The numerical results of the Sauter Mean Diameter SMD were compared with the empirical correlation given by Liu et al. [20] for the same type of atomizer and boundary conditions. The correlation which is based on the experimental data is expressed as:

$$SMD=685{,}8\left(u_g-3.297u_l\right)^{-0.4813} m^{0.3665}+0.1824 d_l m \quad (22)$$

where $u_g$ and $u_l$ are the gas and liquid velocity; respectively. $d_l$ is the inlet jet diameter in millimeter, SMD in micrometer, and *m* is the ration of the liquid to gas mass flow rate.

A mesh consisting of 24120 grid cells was constructed in a rectangular solution domain 100 mm in width and 160 mm in height. Liquid water enters the domain from a 1 mm inlet boundary on the top bounded by two air inlets; each is 5 mm in width.

In the current study, water enters the domain as a continuous phase and then transition into fragments and droplets occur at some point either downstream or upstream of the nozzle exist in a process called phase inversion. The dynamics and interfacial interactions of phase inversion are not yet well understood and assumptions had to be made in order to proceed with the numerical simulation. Therefore, in the current model, phase inversion is assumed to take place as soon as the gas volume fraction reaches $\alpha^{\max} = 0.8$.

## 5. Results and Discussions

The new break-up model coupled with Eulerian multiphase model was used in the numerical simulation of a co-axial air-blast atomizer using three variants of the $k\ \varepsilon$ model. The simulation was performed at four different air inlet velocities and compared to the empirical correlation Eq. (22). The comparison is shown in Figure 1

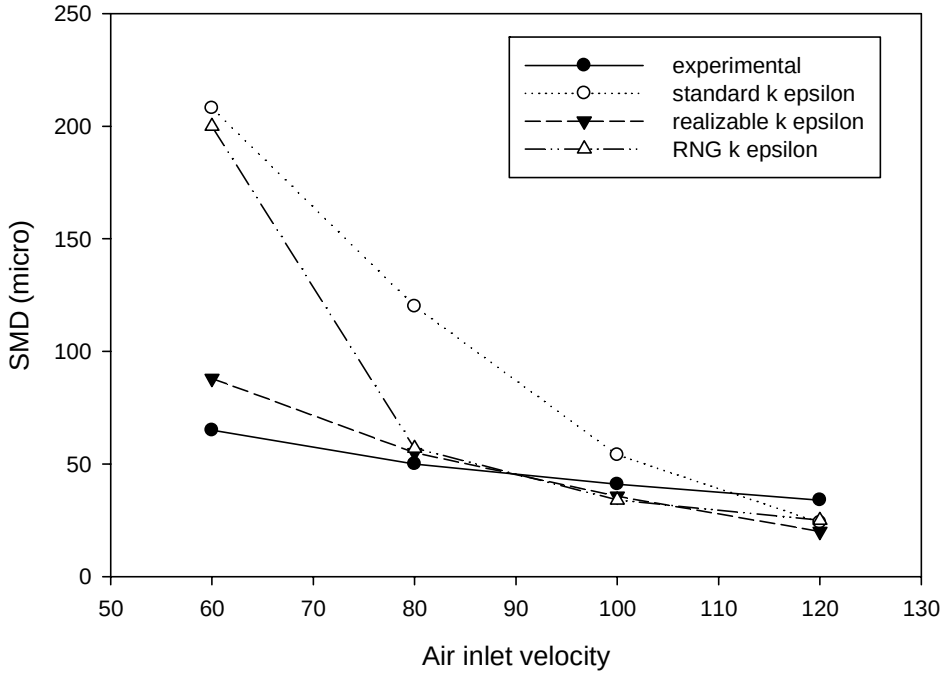
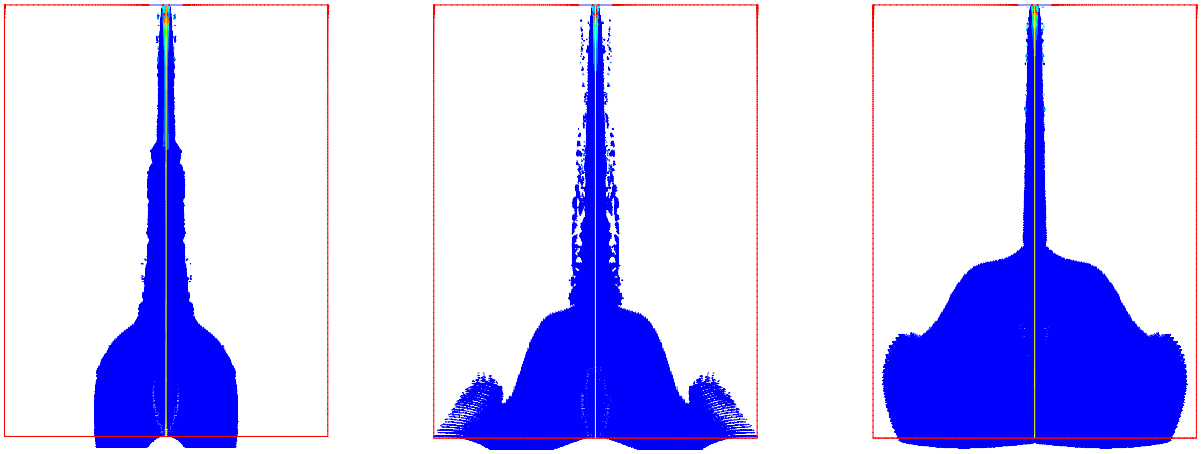



Figure 1. Comparison of three turbulence models with experimental data at four different air inlet velocities

It is clear from Figure 1 that the realizable $k\ \varepsilon$ model obtained better agreement with the experimental data than the other two models. This is thought to be the result of making $C_\mu$ in the eddy viscosity equation variable and sensitizing it to the mean flow variables rather than being a constant as in the other two models. Owing to its superiority over the other models, the realizable $k\ \varepsilon$ model was used in all the coming simulations

Values of droplet diameter have a significant effect on the spray dispersion, and hence, spray angle. It is expected that as the SMD values decrease, the spray angle increases due to a lesser momentum resistance to the dispersion forces. This dependence is revealed in Figure 2 which shows the spray pattern of the dispersed phase for three different air inlet velocities.



(a) (b) ©

Figure 2. Spray patterns at different air inlet velocities (a) v=80 m/s, (b) v=100 m/s, and (c) v=120 m/s

One of the main objectives of this study is to qualitatively and quantitatively investigate the relative contribution of both the turbulence and drag induced stresses in the atomization process. The significance of such investigation stems from the fact that most simulations of spray systems ignore the effect of drag forces without prior analysis. Figure 3. presents a qualitative analysis of the contribution of both forces in the atomization process. The colored spots in this figure represents areas were the critical diameter computed from Eq. (12) is smaller than the critical diameter computed from Eq. (7) and hence drag is the criterion of break-up, while the grey area is where turbulence stresses are the criteria of break-up.

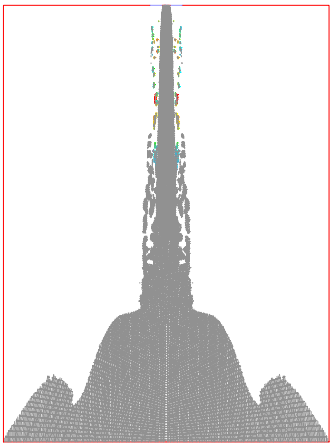


Figure 3. differences between drag and turbulence critical diameter

A quantitative analysis was also performed to determine the contribution of drag forces in the atomization process relative to turbulent stresses. The analysis was performed by eliminating the role of drag forces from the break-up model; thus making a model for turbulent stresses only, and comparing the results with the complete model. This analysis was repeated at four different air inlet velocities and the results are shown in Figure 4.

It is clear from Figure 4. that the results obtained from the two codes are very similar and hence the quantitative drag contribution to the atomization process is minimal. However, this may not be a general case and these results can vary for different types of atomizers or different flow conditions.

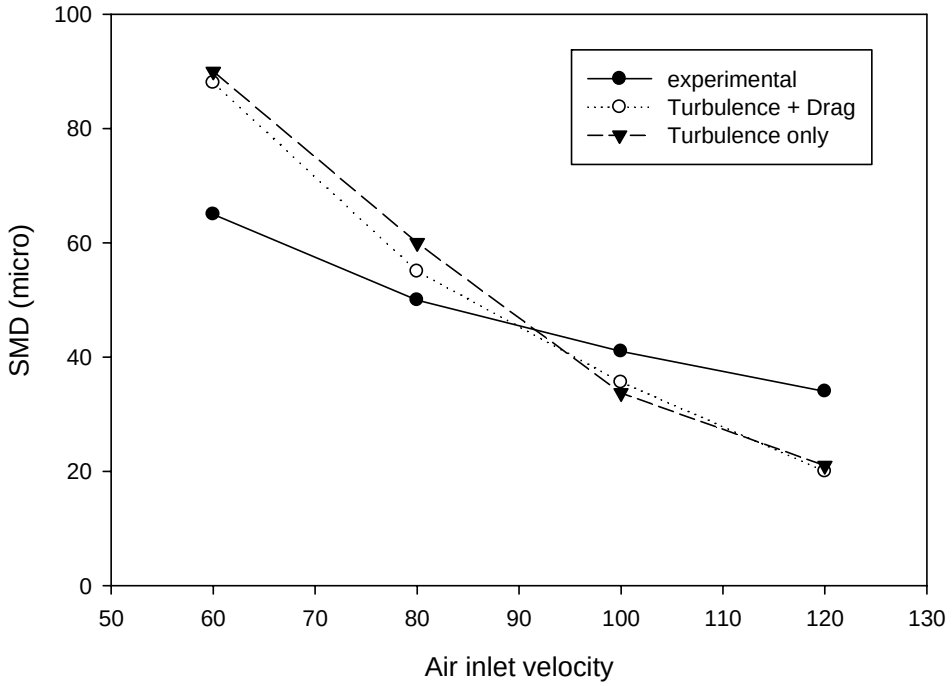



Figure 4 Comparison between the pure turbulence code and the combined turbulence and drag code with experimental data

## 6. Conclusion

In this study, a new mathematical model that describes droplet break-up in liquid spray systems was presented. The model takes into account the effects of both drag and turbulence induced fragmentation stresses on droplet break-up. The model is coupled with an Eulerian-Eulerian CFD model that solves the governing Navier-Stokes equations for all the phases. A reasonable agreement has been reached with experimental data of SMD values for a case study of a coaxial air-blast atomizer. Aside from the computational significance of the new model, the new physical finding of this study is the qualitative and quantitative analysis of the contribution of drag stresses to the atomization process. This contribution was found to be minimal for the specific case of air-blast atomizer compared to the turbulent stresses.

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