



A mathematical model for predicting spray atomization characteristics in an Eulerian–Eulerian framework[☆]

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ARTICLE INFO

Available online 17 March 2010

Keywords:

CFD
Population balance
Atomization
Droplet break-up
Turbulence

ABSTRACT

A new mathematical model is developed for calculating droplet break-up frequency based on both drag and turbulence induced fragmentation stresses. The droplet break-up model is introduced into a CFD methodology that is based on the Eulerian–Eulerian approach. The CFD solver couples the population balance equation along with the Navier–Stokes equations for predicting the droplets diameter. Finally, preliminary results using this CFD model are presented for the case of a coaxial airblast atomizer and a good agreement with the experimental data is achieved.

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1. Introduction

This study is conducted as a part of the project entitled “Development of a Database for Biofuel Combustion Properties”, initiated by the Universiti Teknologi Malaysia (UTM) in collaboration with Cambridge University and Rolls Royce Plc. The project aims to investigate the feasibility of using various palm oil blends in gas turbine combustors and to provide the industrial community with a database for the combustion properties of the blends. The first phase of the project is concerned with investigating the atomization properties of palm biofuel blends in gas turbine combustors. To that end, an efficient mathematical model capable of revealing spray atomization characteristics has been developed in the current study to meet the objectives of the project.

Sprays consist of a large number of droplets; each droplet has unique properties and undergoes complex interactions with the gas phase. Such interactions include: low Mach number fluid mechanics, droplet dynamics (break-up, atomization, mixing), turbulent transport of mass, momentum, and energy. The controlled dispersion of droplets in a turbulent flow is an important aspect of many industrial processes. The break-up of liquid fuel droplets influences the placement, mixture uniformity and evaporation of sprays.

CFD modeling of spray dynamics has been a rapidly developing research area in the last years. As a result, many CFD models have been formulated in order to describe the physics occurring in such processes. Most of these models can be categorized, according to the modeling approach and the level of details revealed from the simulation, into two categories. The first category is the Eulerian–

Lagrangian model [1,2] which is often referred to as the Discrete Phase Model (DPM). In this model, while the continuous phase is described by the standard Eulerian conservation equations (Navier–Stokes), the transport of the dispersed phase is calculated by tracking the trajectories of a certain number of representative parcels (particles). The second category of multiphase models is the Eulerian–Eulerian approach [3–5]. This approach treats both phases as interacting and interpenetrating continua, thus, in contrast to the Eulerian–Lagrangian model, the tracking of individual particles is avoided and the transport equations are solved for the dispersed phase as well. This implies that, by using an Eulerian–Eulerian framework, the dispersion and atomization of the liquid phase are predicted using the conservation equations for all the phases. Consequently, the use of empirical equations which requires experimentally measured spray characteristics to be provided prior to the solution, as in the case of Eulerian–Lagrangian models, is avoided. Comprehensive comparisons between the two approaches can be found in [6–8].

In order to calculate the droplets diameters throughout the atomization process, a conservation equation for the particle number density function of the dispersed phase has to be solved along with the Navier–Stokes equations. Such an equation is called the population balance equation (PBE). The population balance equation was first introduced in 1964 by Hulburt and Katz [9], and has recently gained an unprecedented attention because of its applicability to a wide variety of particulate processes [10–15]. In order to solve the population balance equation, a break-up kernel function has to be provided. Such break-up kernel has to include a break up frequency model that adequately represents the physics of the problem in hand. Many break-up models have been developed for modeling droplets in liquid–liquid systems and bubbles for gas–liquid systems. A review of such models can be found in [16]. However, it is believed by the authors that no such model has been developed and evaluated for

[☆] Communicated by W.J. Minkowycz.

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droplets in spray systems. Consequently, in contrast to other multiphase flow problems, very few studies involving the investigation of spray systems using the population balance equation can be found in the literature. The only study revealed to the authors was done by Madsen et al. [17]. In this study, the authors solved the population balance equation using the direct quadrature method of moments in order to simulate a Y-jet water spray. However, this study was restricted only to the WAVE break-up model which predicts droplet atomization based on a linear stability analysis. The major drawback of this model is its dependence on adjustable empirical constants. Moreover, this model does not include the effect of turbulent eddies and aerodynamic drag on droplet atomization.

In this paper, a new mathematical model is developed for calculating droplets break-up frequency based on both drag and turbulence induced fragmentation stresses. Preliminary results obtained by the new model for a case study of a coaxial airblast atomizer are then compared to experimental data to evaluate the model.

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 was first introduced by Heinrich Weber as 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.

Assuming isotropic turbulence, Kolmogorov [18] and Hinze [19] 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 ρ_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 d .

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 ε is the turbulence dissipation rate and β is a dimensionless constant. Although Landau [20] has argued that β should not be a universal constant, the authors found that a value of $\beta = 8.2$ as given by Batchelor [21] gives good results for a wide range of flows in spray problems. Moreover, the same value was used by Martinez-Bazan et al. [22] for modeling bubbles in liquids and by Eastwood et al. [23] for the case of liquid–liquid systems.

For the case of droplets in a gas, where the density of the dispersed phase ρ_d is much higher than the density of the continuous phase ρ_c , Kocamustafaogullari and Ishii [24] 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:

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

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:

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

Rearranging Eq. (6), the critical droplet diameter at which break-up will occur can be calculated from:

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

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:

$$5 < We_{cr} < 25 \tag{8}$$

Within this range, the critical Weber number was found to depend on the droplet Reynolds number Re_d . Kolev [25] correlated the experimental observations of many authors into:

$$We_{cr} = 55 \left[\frac{24}{Re_d} + \frac{20.1807}{Re_d^{0.615}} - \frac{16}{Re_d^{2/3}} \right] \text{ For } 200 < Re_d < 2000, \tag{9}$$

and,

$$We_{cr} \approx 5.48 \text{ For } Re_d > 2000, \tag{10}$$

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 [24] for the case of $\rho_d \gg \rho_c$, the droplet break-up time can be calculated from:

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

It is noteworthy to state that, for the best of the authors' knowledge, the proposed model is the first instance that the Kocamustafaogullari and Ishii correction is used in defining the turbulence time scale in modeling a turbulent multiphase problem. It is evident that the use of such correction in Eq. (11) has a significant effect on the results for spray problems in which $\rho_d \gg \rho_c$. Moreover, the authors suggest that Eq. (11) can be used to extend general break-up models, such as Martinez-Bazan et al. model [22] for bubbles in liquid and Eastwood et al. model [23] for liquid–liquid systems, to enable them of accurately modeling spray problems.

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

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

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

$$t_{br}^* = c(We_{cr} - 12)^m \quad (14)$$

Where c and m are constants that depend on the Weber number. See [25,26].

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 [25] theoretically proposed that the decision should be made based on the maximum droplet diameter in both cases. i.e. if

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

break-up will result from turbulent stresses, otherwise drag will be the criterion of break-up. The authors believe that the present study is the first numerical verification of Kolev's theoretical argument.

Finally, break-up frequency is calculated as a function of the droplet critical diameter and break-up time. Such as:

$$f_{br} = \frac{\left(\left(\frac{d}{d_{cr}} \right)^3 - 1 \right)}{t_{br}} \quad (16)$$

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:

$$\alpha_g + \sum_{q=1}^N \alpha_q = 1 \quad (17)$$

Where α_g is the gas volume fraction, α_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 a conditionally ensemble averaging of the local instant conservation equations of single phase flow [27]. 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

$$\frac{\partial}{\partial t} (\alpha_g \rho_g) + \frac{\partial}{\partial x_i} (\alpha_g \rho_g U_{i,g}) = 0 \quad (18)$$

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

The continuity equation for the q th droplet phase is

$$\frac{\partial}{\partial t} (\alpha_q \rho_l) + \frac{\partial}{\partial x_i} (\alpha_q \rho_l U_{i,q}) = \sum_{p=1}^N \dot{m}_{pq} \quad (19)$$

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

$$\begin{aligned} \frac{\partial}{\partial t} (\alpha_g \rho_g U_{i,g}) + \frac{\partial}{\partial x_i} (\alpha_g \rho_g U_{i,g} U_{j,g}) = & -\alpha_g \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} (\alpha_g \tau_{ij,g}) \\ & + \alpha_g \rho_g g_i + \sum_{q=1}^N F_{i,qg} \end{aligned} \quad (20)$$

Likewise, for the droplet phases, the momentum balances are

$$\begin{aligned} \frac{\partial}{\partial t} (\alpha_q \rho_l U_{i,q}) + \frac{\partial}{\partial x_i} (\alpha_q \rho_l U_{i,q} U_{j,q}) = & -\alpha_q \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} (\alpha_q \tau_{ij,q}) \\ & + \alpha_q \rho_l g_i + F_{i,qg} + \sum_{p=1}^N \dot{m}_{pq} U_{i,pq} \end{aligned} \quad (21)$$

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 the 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 [28–30].

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 [10] and can be written in the following form:

$$\frac{\partial}{\partial t} n(d, U_i) + \frac{\partial}{\partial x} [U_i n(d, U_i)] + \frac{\partial}{\partial U_i} [F_i n(d, U_i)] = S(d, U_i) \quad (22)$$

Where $n(d, U_i) dddU_i$ is a multivariate number distribution function that denotes the average number of droplets in the diameter range dd about d , with velocities in the range dU_i about U_i . F_i is the force acting to accelerate the droplets, and $S(d, U_i)$ 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. [31–33]. Turbulence was modeled using the realizable k - ε turbulence model [34]. In addition, since the problem involves two phases, a set of k and ε transport equations is solved for each phase.

4. Simulation of a coaxial airblast atomizer

In order to evaluate the new mathematical break-up formulation, numerical simulations were performed for a case study of a 2-dimensional coaxial airblast atomizer using the CFD methodology described earlier. The numerical results were compared with the empirical correlation given by Liu et al. [35] for the same type of

atomizer and boundary conditions. Five numerical simulations were performed for different air inlet velocities in order to simulate the effect of increasing air velocity on the spray characteristics. In all simulations, water was chosen as the dispersed phase in order to ensure the consistency of the flow conditions with the experimental results. A mesh consisted of 35,188 grid cells was constructed. The solution domain dimensions and a portion of the generated grid are shown in Figs. 1 and 2, respectively.

The Semi Implicit Method for Pressure Linked Equations (SIMPLE) algorithm [36] was used for pressure/velocity coupling of the governing flow equations. This algorithm satisfies the mass conservation equation by using a relationship between velocity and pressure corrections. A time step of 1e-5 was chosen for all the simulations to ensure the solution conversion within each time step.

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 proposed model, phase inversion is assumed to take place as soon as the gas volume fraction reaches $\alpha^{max} = 0.8$. This assumption is consistent with numerous studies in the literature. For instance, Wang et al. [37] used the value of 0.8 to describe the transition from the churn-turbulent flow regime in the bubble column reactor. In addition, the experimental results of Deichsel and Winter [38] suggest that for high speed critical flow in pipes, the transition from the churn-turbulent regime is delayed up to a volume fraction of 0.92.

Although the assumption of the phase inversion location based on only the local volume fraction value appears to be a vague assumption that may compromise the accuracy of the solution, it should be noted that most Lagrangian spray models do not include phase inversions by any means. Instead, the secondary phase enters the domain as individual parcels (droplets) that are tracked throughout the domain using a trajectory type equation. Thus, including the phase inversion of the secondary phase in the current model, even with some level of uncertainty about its exact location, is believed to have a fundamental advantage over conventional Lagrangian spray models.

5. Results and discussion

The numerical and experimental results of the Sauter Mean Diameter (SMD) values are plotted in Fig. 3 for five different air

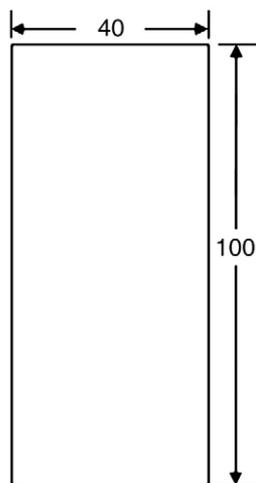


Fig. 1. Solution domain (dimensions in mm).

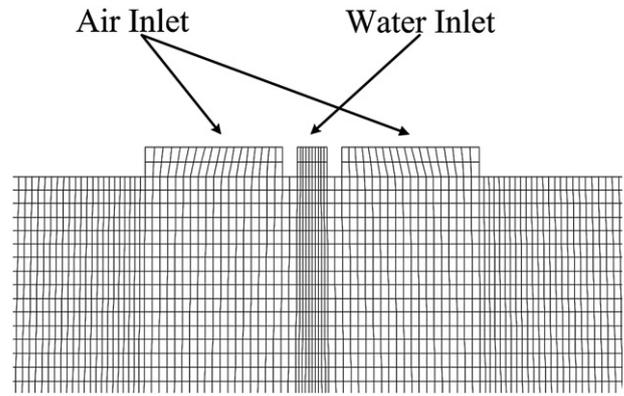


Fig. 2. Schematic of the grid and inlet boundaries.

inlet velocities. It is clear that a reasonable agreement has been reached using the new model for the whole range of air velocity.

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 Fig. 4 which shows the spray pattern via the constant diameter contours of the dispersed phase for three different air inlet velocities.

The mathematical model presented in this paper includes the effects of both drag and turbulence induced fragmentation stresses on droplet break-up. The decision of whether drag or turbulent stresses are the criteria of break-up was made based on the theoretical argument by Kolev [25] represented by Eq. (15). Fig. 5 demonstrates that indeed both types of stresses will contribute in the break-up process. It is shown in Fig. 5 that drag is often the criterion of break-up in the interface between the two phases near the nozzle exit, where the relative velocity between the two streams is at a maximum value.

6. Conclusion

In this study, a new mathematical model is formulated to describe droplet break-up in liquid spray systems. 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 case study of a coaxial airblast atomizer was numerically investigated using the new model and preliminary results show a reasonable agreement with experimental data for SMD

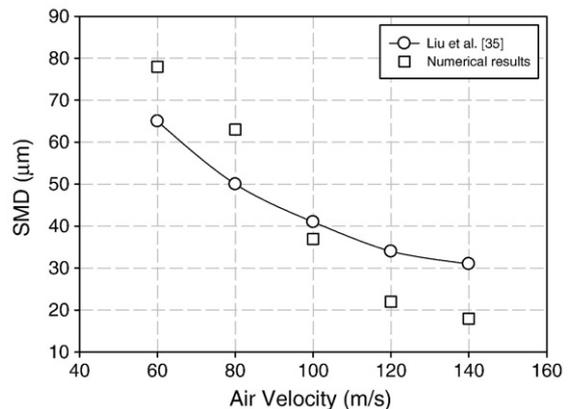


Fig. 3. Numerical and experimental SMD values for different air inlet velocities.

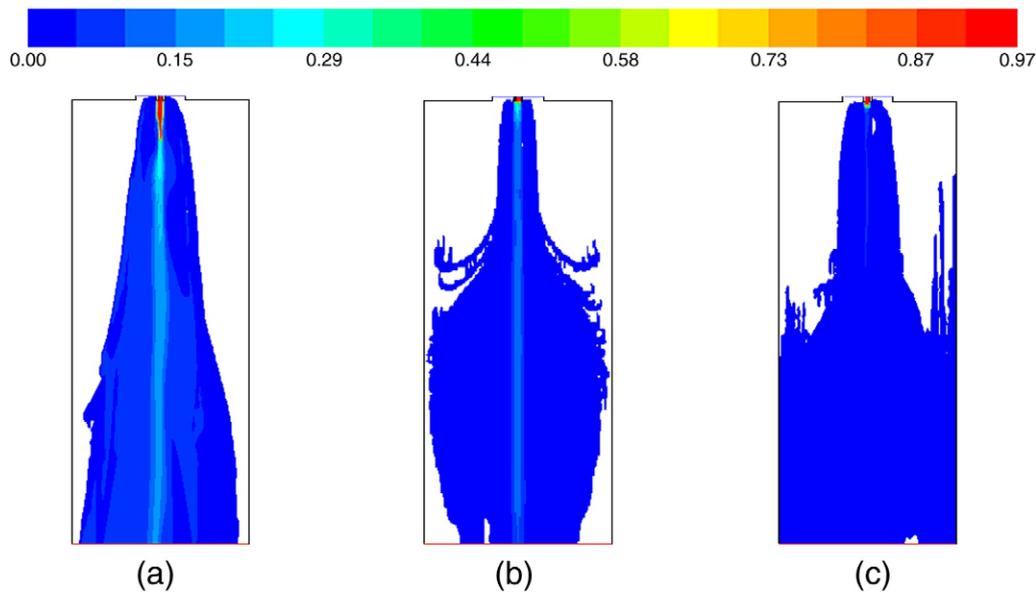


Fig. 4. Constant diameter contours of the dispersed phase for three different air inlet velocities. (a) air velocity = 60 m/s, (b) air velocity = 100 m/s, and (c) air velocity = 140 m/s.

values. The new physical findings revealed from the use of the proposed model can be summarized as follows:

- The definition of turbulence time scale, and hence break-up time, for spray problems has to include the Kocamustafaogullari and Ishii correction for high density ratios. This correction can be used to extend general break-up models to enable them of accurately modeling spray problems.
- Fig. 5 evidently shows that both drag and turbulent stresses contribute in the atomization process.
- The Kolev theoretical argument for the criteria of break-up, which was numerically verified in this paper for the first time, seems to give adequate results for the case of airblast atomization.

Acknowledgments

This study is a part of a joint project among the Universiti Teknologi Malaysia (UTM), Cambridge University, and Rolls Royce Plc. The authors acknowledge the support provided by the Malaysian Ministry of Science, Technology and Innovation (MOSTI) under the Science Fund grant 79253.

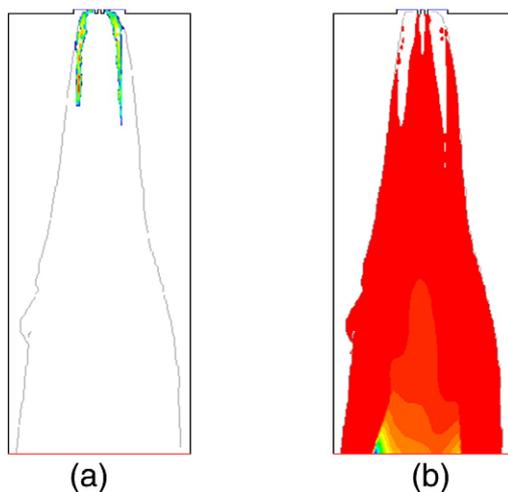


Fig. 5. Contours of the difference between drag and turbulence critical diameter at air inlet velocity = 60 m/s. (a) areas where $d_{cr}^{drag} < d_{cr}^{turb}$ i.e., drag is the criterion of break-up, (b) areas where $d_{cr}^{drag} > d_{cr}^{turb}$ i.e., turbulence is the criterion of break-up.

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