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

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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.

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

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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