A generalized population balance model for the prediction of droplet size distribution in sprays

Kirpalani, D. M.; McCracken, T. W.

Publisher's version / Version de l'éditeur:

Proceedings. The 10th International Congress on Liquid Atomization and Spray Systems(ICLASS-2006), 2006

ICLASS-2006
Aug.27-Sept.1, 2006, Kyoto, Japan

Paper ID ICLASS06-058

A GENERALIZED POPULATION BALANCE MODEL FOR THE PREDICTION OF DROPLET SIZE DISTRIBUTION IN SPRAYS

D.M. Kirpalani [1], T.W. McCracken[1]

[1] Institute for Chemical Process and Environmental Technology
National Research Council of Canada
Ottawa, ON K1A 0R6 Canada
deepak.kirpalani@nrc.ca

ABSTRACT Past research in spray modeling has been based on the discretization of the liquid flow field into equally sized parcels, as in the discrete droplet model, that are tracked using a Lagrangian framework or by solving the Eulerian conservation equations for different droplet size classes. An alternative also used is the method of moments (MOM) approach that involves the transport of moments of the droplet size distribution. The MOM approach offers a distinct advantage that the number of moments required is extremely small. However, the main issue is the closure problem, related to writing transport equations of the moments in terms of the lower order moments.

A population balance formulation to describe the evolution of droplets in sprays is proposed in this work. Using population balance equations (PBE), the dispersed phase is represented as a population and the size distribution of the population is approximated as a summation of N Dirac Delta functions, represented as droplet phases and each phase is characterized by a diameter and volume fraction. Also, new kernel functions that account for droplet coalescence and breakup are also presented in this work. Extended source term parameterizations for coalescence and breakup mechanism are coupled with continuity and momentum equations in a computational fluid dynamics (CFD) model. This model eliminates the limitation of fixed size class discretization. Experimental validation of the model indicates that an extended model may lead to an improved description of the droplet size distribution, spray plume dimensions and also the volume-averaged droplet velocity

Keywords: Liquid Atomization, Droplet, Numerical Simulation and Population Balance.

1. INTRODUCTION

The fundamental approach to modeling polydispersed sprays has been limited to the discretization of the liquid flow field into groups of equi-sized droplets as in the discrete droplet model in which the parcels of droplets are tracked in a lagrangian framework. The alternate approach used involves the solution of separate Eulerian conservation equations for a number of size ranges.

Computational approaches developed for spray modeling are often derived from the spray equation developed by Williams[1] for the droplet distribution function. The Lagrangian Monte Carlo procedure for spray modeling was proposed by Dukowicz[2] to develop a coupled solution between the spray equation and computation of the gaseous phase. To complete the spray formulation, a model of droplets production is required. The wave breakup model of Reitz[3] is the most widely used for modeling production of droplets. By assuming, in this model, that the breakup results from a hydrodynamic instability caused by surface tension, the newly formed droplets are characterized by a single Rayleigh mode[4] of atomization. At the same time, the Rayleigh's type of breakup takes place when the liquid jet is injected into quiescent environment at a relatively low velocity. When the liquid jet is injected into the flowing motion of gas at high relative velocity, large Weber number, the influence of interfacial forces is less pronounced and the mechanism of breakup becomes more complex. A wide range of turbulent eddies may impact on the liquid jet resulting in its breakup. The modeling of droplets formation under this type of breakup[5-8] often referred to as the air-blast atomization, is the main subject of this paper.

Several experimental studies[5-9] have demonstrated the difficulty in clearly defining a dominant air-blast atomization mechanism. Each spray region produces droplets with a large spectrum of size, which is often independent of the breakup pre-existing properties.

Accurate knowledge of fluid mechanics is required for the correct quantification of spray processes. In recent year computational fluid dynamics (CFD) has emerged as a powerful tool for the understanding of the fluid mechanics prevailing in the reactors. Its success in single phase processes is significant while the presence of multiple phases makes the description of the flow difficult. This requires the correct distribution of disperses phases (liquid droplets) with regards to both the size and number in spatiotemporal coordinates. This can be obtained by using the population balance modeling (PBM) The disperse phase distribution is governed by processes of convection and diffusion caused due to the continuous phase (atomizing gas, which is turbulent in nature) and coalescence and breakage of the dispersed phase, which again are essentially governed by the local flow characteristics. In view of this, both the PBM and CFD rely on the success of each other and hence either of them can not be used for the entire description of the multiphase flow behavior. Hence there is a need to couple these approaches for the accurate modeling of sprays at the cost of the lesser computational resources. Due to different nature of the governing equations involved in both the approaches, the methods to solve the resulting equations need to be developed.

An interesting approach that applies the Kolmogorov[10] scenario to the breakup of a liquid at large Weber numbers has been developed in the past. In this current work, a turbulence breakup and dispersion model is used to capture the effects of turbulence on droplet breakup as well as droplet trajectories.

2. POPULATION BALANCE MODEL

The spray system is considered as a two-phase flow using a full multi-fluid Eulerian model. In this approach mass and momentum balance equations are solved for each phase.

The coupling between phases is achieved through interphase exchange terms. The mass and momentum balance equations can be written as

$$\frac{\partial}{\partial t}\alpha_L\rho_L + \nabla.(\alpha_L\rho_L\overline{u_L}) = 0 \tag{1}$$

$$\frac{\partial}{\partial t}\alpha_G\rho_G + \nabla.(\alpha_G\rho_G\overline{u_G}) = 0 \tag{2}$$

$$\frac{\partial}{\partial t}\alpha_L\rho_L u_L + \nabla.(\alpha_L\rho_L\overline{u_L}u_L) = -\alpha_L\nabla P + \overline{\overline{\nabla.\tau_L}} \tag{3}$$

$$\frac{\partial}{\partial t}\alpha_G\rho_G u_G + \nabla.(\alpha_G\rho_G\overline{u_G}u_G) = -\alpha_G\nabla P + \overline{\overline{\nabla.\tau_G}} \tag{4}$$

The turbulence was modeled using standard $k - \varepsilon$ model (Launder and Spalding, 1972) suitably extended to spray flows.

The droplet phase is assumed to be composed of 6 discrete droplet bins and a discretized population balance equation is solved for the droplet number density along with birth and death terms due to breakup and coalescence. The equation for the i^{th} droplet class fraction f_i is written as

$$\frac{\partial}{\partial t}\alpha_L\rho_L f_i + \nabla.(\alpha_l\rho_l\overline{u_L})f_i = S_i \tag{5}$$

where f_i is defined as the ratio of total volume of droplets of class i to the total volume of droplets of all classes. These functions are expressed as

$$S_i = B_{breakup} - D_{breakup} \tag{6}$$

The droplet breakup kernel appearing in the integrals above are described below. Droplet breakup is analyzed in terms of droplet interactions with turbulent eddies. The turbulent eddies increase the surface energy of the droplet through deformation. Breakup occurs if the increase in surface energy reaches a critical value. A binary breakage is assumed. The kernel contains no adjustable parameters. The breakup rate (Luo[11]) of droplets of size v into particle sizes of $v f_{BV}$ and $v(1-f_{BV})$

2.1 Droplet Breakage Kernel for External Air Blast Type Applications

Droplet breakup parametrization consists of the product of the breakup probability and the collision frequency. Summarizing over the possible eddy sizes yields

$$\Omega_B(v_i, v_k) = \sum P_B(v_i, \lambda_j, v_k)\omega_B(v_i, \lambda_j) \tag{7}$$

The collision frequency between eddies of size between λj and λj + dλ and droplets of volume size v_i is a similar expression to the collision frequency between gas molecules and is given by

$$\omega_B(v_i, \lambda_j) = \frac{\pi}{4}(d_i + \lambda_j)^2 u(v_i, \lambda_j) n(v_i) n(\lambda_j) \tag{8}$$

The relative velocity between the colliding droplet and turbulent eddy is expressed as

$$u(v_i, \lambda_j) = (u_t(v_i)^2 + u_t(\lambda_j)^2)^{\frac{1}{2}} \tag{9}$$

With turbulent velocity

$$u_t(\lambda_j)^2 = \beta^{\frac{1}{2}}(\varepsilon\lambda_j)^{\frac{1}{3}} \tag{10}$$

This equation is also used for finding the turbulent velocity of the droplets by replacing the eddy length scale by the droplet diameter (Luo[11]). The probability of obtaining one specific droplet daughter class, as a result of breakup of a parent droplet size, colliding with an eddy size is given as the sum over different eddy energy levels $e1$.

$$P_B(v_i, \lambda_j, v_k) = \sum P_B(v_i, \lambda_j, e_1, v_k)\omega(\lambda_j, e_1)$$

Where $\omega(\lambda_j, e_1)$ is the fraction of is eddies of size λ_j having energy level e_l. It is assumed that the turbulent kinetic energy probability distribution is

$$p_e(\chi) = \exp(-\chi) \tag{11}$$

$$\chi = \frac{e(\lambda_j)}{\overline{e}(\lambda_j)}$$

Where

The mean turbulent kinetic energy of an eddy with size λ_j, $e(\lambda_j)$, was given as[11],

$$e(\lambda_j) = \frac{\pi\beta}{12}\rho L \varepsilon^{\frac{2}{3}}(\lambda_j)^{\frac{11}{3}} \qquad (12)$$

The function related to breakup due to the energy density causing breakage into a smaller daughter volume size k may be written as

$$F_d(d_k) = \max(e(\lambda_j) - \pi\sigma d_i^2[\frac{d_k^2}{d_i^2} + (1 - \frac{d_k^3}{d_i^3})^{\frac{2}{3}} - 1, 0) \qquad (13)$$

Hence the probability of breakup

$$P_B(dk, \lambda_j) = \frac{w_d(\lambda_j) - \frac{6\sigma}{d_k}}{\int_{dk,\min}^{dk,\max} (w_d(\lambda_j) - \frac{6\sigma}{d_k}) d(d_k)}$$

Where

$$w_d(\lambda_j) = \frac{e(\lambda_j)}{\frac{4}{3}(\frac{\lambda_j}{2})^3} \qquad (14)$$

The coupling between droplet breakup and CFD was achieved through the dynamic drag term based on the Sauter mean droplet diameter (SMD). Equations (1) through (14) were solved numerically using Fluent software- a commercial finite volume CFD solver.

2.2 Population Balance Model Using Wave Breakup

The blob injection model in which blobs of liquid are injected with a diameter equal to the orifice diameter can also be incorporated into population balance approach. The primary breakup of the liquid blobs and their subsequent breakup can be modeled using the standard WAVE breakup model. In this case, the breakup rate for the droplets is defined as;

$$\Omega_B = (1 - d_j / d_i)^{1/3} \omega_B \qquad (15)$$

Where ω_B is the breakup frequency.
And this approach can be been widely applied for spray modeling for internally mixed and external atomization processes.

3. RESULTS AND DISCUSSIONS

The population balance approach has been applied to spray analysis of air-blast atomizers. An outline for using this modeling approach to the WAVE breakup theory has also been proposed. Model validation has been carried out with respect to the air blast atomizer experimental data provided by Stepowski et. al.[12]. Computed half-geometry (axi-symmetric) spatial distributions of drops in the spray, are displayed in Fig. 2 . The inlet parameters are used from their experiments on air-blast atomization at atmospheric pressure Stepowski et al.[12] In this experiment, the round jet of water issues from the central tube (D_L = 1.8 mm) at low velocity and atomizes by a concurrent flow of air flowing at high velocity from an annular duct (D_G = 3.4 mm). The spatial distributions. The 2-dimensional computational grid used is an axi-symmetric. The flow geometry was discretized into 27,000 hexahedral cells. Due to symmetry only one-half of the spray geometry was modeled. The dimensions of the grid are 0.003 and 0.012 m, respectively. The spatial distributions of droplet in Fig. 2 shows that a broad spectrum of droplet size is presented in the spray at high gas to liquid momentum ratios. The distributions at 1 mm from injector orifice shows mainly large drops of the size of injector orifice accompanied by smaller droplets at the periphery of the spray., it is seen that, from distributions at 5 mm from the injector, droplets that are proportional to the size of the injector orifice are broken down and new droplets are produced with diameters of 100-200 microns. The model is validated for breakup length by comparing with experimental data[12]. These numerical distributions can be assessed only qualitatively since the existing experimental technique is not accessible to measurements of size distribution in the near-nozzle region. In Fig. 3, the existence of large droplets at low gas-to-liquid momentum ratios is shown indicating the irregular nature of the breakup. At high gas-to-liquid ratios, the breakup length is significantly reduced as shown in Fig. 2.

In this work, the numerical scheme of stochastic computing of droplet breakup was implemented using a population balance model along with an Eulerian approach for integration of governing equations in the gas phase. The effects of interaction between droplets and gas motion, the turbulent dispersion of droplets were also taken into account. The computation of a round water jet atomized by a high-speed annular air jet, was also performed. The liquid core length was estimated and was in qualitative agreement with measurements. As to the far field of spray, the downstream variation of the Sauter mean diameter was compared with experimental data. The predicted values were relatively in agreement with experimental data. The generation of large population of small droplets as a result of breakup with increasing distance from injector has been shown at high momentum ratios. The breakup model described in this work and can be easily implemented into any numerical code that computes two-phase compressible flows with Eulerian formulation of spray.

Nomenclature

B_B = *birth breakup, 1/(m3 s)*
D_B death breakup, 1/(m3 s)
d_i = droplet class diameter, m
$e(l)$ = eddy energy level, J
$e(ij)$ = energy in an eddy of diameter size ij, J
$F_d(d_k)$ = function for the breakup due to energy density into smallest daughter fragment d_k , J/m3
fi = fraction of droplets of class i
ni = droplet number density of class i
P = pressure, Pa
$P_B(v_i,\lambda_j)$ = breakup probability of droplet v_i being hit by an eddy of size λ_j
$P_B(v_i,\lambda_j,e_l,v_k)$ = breakup probability of droplet (volume) v_i being hit by an eddy of size λ_j with energy level e_l breaking up into smallest daughter fragment v_k
$P_B(v_i,\lambda_j,v_k)$ = breakup probability of droplet v_i being hit by an eddy of size λ_j breaking up into smallest daughter fragment v_k
u_i = velocity of phase i, m/s
$u(v_i,v_j)$) relative velocity between droplets of volume sizes v_i and v_j, m/s
$u(v_i,\lambda_j)$) relative velocity between droplets of volume sizes v_i and an eddy of diameter size v_j, m/s

Greek letters
α_i = volume fraction of phase i
β = constant, 2.41
λ_j = eddy diameter class j, m
χ = kinetic energy fraction for an eddy in turbulence
$\Omega_B(v_i,v_k)$) breakup rate of class v_i into smallest daughter class v_k, 1/(m³ s)

6. REFERENCES

1. F. A. Williams, "Spray combustion and atomization," Phys. Fluids, **1**, 541, 1958.
2. J. K. Dukowicz, "A particle-fluid numerical model for liquid sprays," J. Comput. Phys. **35**, 229, 1980.
3. R. D. Reitz, "Modeling atomization processes in high-pressure vaporizing sprays," J. Atomization Spray Tech. 3, 309, 1987.
4. W. S. Rayleigh, "On the instability of jets," Proc. London Math. Soc. 4, 10, 1878.
5. A. H. Lefebvre, *Atomization and Sprays,* Hemisphere, New York, 1989.
6. B. Liu and R. D. Reitz, "Mechanism of air-assisted liquid atomization,", J. Atomization and Sprays **3**, 55, 1993.
7. N. Chigier and R. D. Reitz, "Regimes of jet breakup mechanisms, physical aspects," in *Recent Advances in Spray Combustion: Spray Atomization Drop Burning Phenomena*, edited by K. K. Kuo, AIAA, Reston, 1996, Vol. 1, pp. 109–135.
8. J. C. Lasheras and E. J. Hopfinger, "Liquid jet instability and atomization in a coaxial gas stream," Annu. Rev. Fluid Mech. **32**, 275, 2000.
9. T. L. Georjion and R. D. Reitz, "A drop-shattering collision model for multidimensional spray computations," J. Atomization and Sprays **9**, 231, 1999.
10. A.N. Kolmogorov, "On the log-normal distribution of particles sizes during break-up process," Dokl. Akad. Nauk SSSR **31**, 99, 1941.
11. Luo, H., 1993. "Coalescence, breakup and circulation in bubble column reactors" *Ph.D. Thesis, Trondheim, Norway*, 1993.
12. D. Stepowski and O. Werquin, "Diagnostics of scalars in two-phase dense jets by plane laser," in *Combustion in Rocket Engine* CNES, Cepadues-Editions, Toulouse, France, 2001.

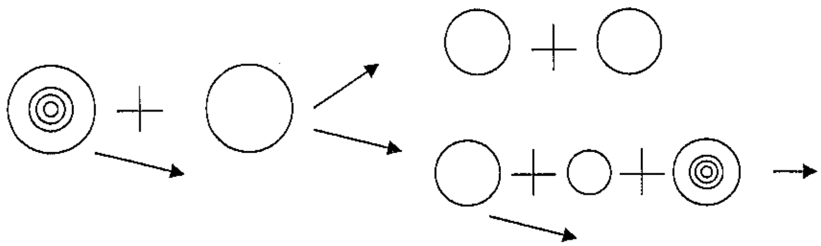

Figure 1. An eddy colliding with a droplet may result in a collision that transfers the turbulent kinetic energy of the eddy to the droplet (top right) or daughter droplets may be formed along with a used eddy

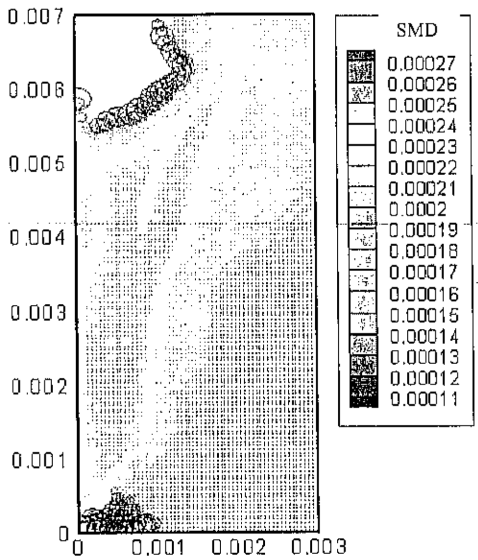

Figure 2. Computed spatial distributions of Sauter mean diameter of the spray of water atomizing by the coaxial air jet. The ratio of gas-to-liquid momentum at the exit of injector is equal to 26.4. Dimensions of the grid are given in mm.

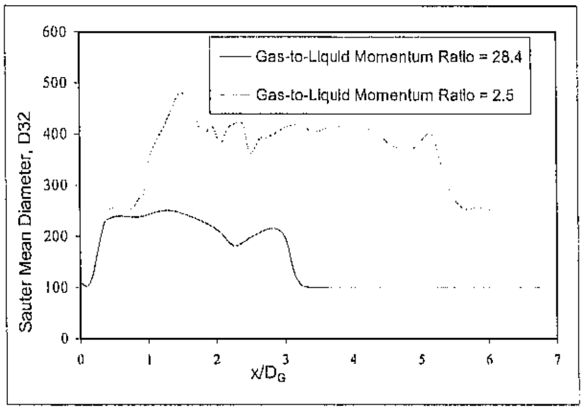

Figure 3. Computed Sauter mean diameter (SMD) of the spray of water atomizing by the coaxial air jet at different momentum ratios along the centerline of the spray indicating the regularity of breakup at higher momentum ratios.