

CFD Analysis of non-evaporating sprays using the DQMOM method

A. H. Nielsen^{**†}, B. H. Hjertager^{††}, and T. Solberg[†]

[†] Department of Biotechnology, Chemistry and Environmental Engineering
Aalborg University

Denmark, DK-6700 Esbjerg

^{††} Department of Mathematics and Natural Sciences

University of Stavanger

Norway, N-4036 Stavanger

Abstract

In this paper the recently formulated direct quadrature method of moments (DQMOM) is used for simulating a non-evaporating dilute turpentine round jet. The DQMOM method is implemented in the CFD code Fluent and compared against a standard Eulerian multi-fluid model. The predictions of the DQMOM method show that the full potential of this method is not realized because, neither coalescence nor breakup seem to occur. The DQMOM method is thereby reduced to a standard Eulerian multi-fluid model. Nevertheless the DQMOM method is still capable of predicting the correct trend in the experimental data.

Introduction

The demand for increasingly more competitive and environmental friendly chemical reactors e.g. sprays requires a detailed description of the occurring transport phenomena. The design and optimisation of chemical reactors have traditionally been based on experiments. However, computational fluid dynamics (CFD) models, which provide more details of the flow behaviour and more flexibility in changes to design and operating conditions, are being developed.

Focusing on gas-liquid multiphase systems or sprays, numerical simulations and measurements of non-evaporating sprays have been reviewed by Madsen et al. [1]. He investigated both numerically and experimentally the droplet size distribution in Y-jet and pressure-swirl atomizers. Evaporating sprays include spray drying and spray combustion. The challenges in CFD modeling of spray dryers have been reviewed by Nijdam et al [2]. Nijdam et al. validated their discrete droplet model against the phase Doppler anemometer (PDA) measurements of Nijdam et al. [3] in Nijdam et al [4] and [5] for a non-evaporating spray and for an evaporating spray [2]. Nijdam et al. [5] assessed an Eulerian multi-fluid model with 1 continuous gas phase and 9 dispersed droplet phases for a non-evaporating spray, while Nijdam et al. [4] did make a comparison of an Eulerian model vs. a Lagrangian. The discrete droplet phases had a fixed droplet diameter. Recently Bine & Jones [6] presented a DPM model for evaporating sprays using a LES turbulence model. They compared their predictions with the experiments of Chen et al. [7]. Spray combustion of liquid fuels is a large research field including both monodisperse and polydisperse liquid flows. Sadiki et al. [8] give a review of discrete droplet models used for both reacting and non-reacting polydisperse liquid-fuels sprays. A complicating factor with reacting sprays is the droplet evaporation due to radiation. Marchisio & Fox [9] gives a review of Eulerian multi-fluid models for polydisperse evaporating sprays.

Computational Multiphase Fluid Dynamics (CMFD) consists of interface tracking, particle tracking and averaging methods. In the interface tracking method Lakehal et al. [10], the shape and size of all particles are fully resolved because all interfaces between the continuous and dispersed phases are tracked. As a limited number of particles can be studied due to limitations in computer resources, interface tracking methods have theoretical interest studying interfacial forces as well as aggregation and breakage. In the particle tracking method R ger et al. [11], all particles are tracked individually. The interfacial forces acting on the particles as well as the collision dynamics of the particles must be modelled to account for the coupling between the continuous and dispersed phases. Likewise, the aggregation and breakage of particles must be modelled to describe the shape and size of the particles. As there is again a limited number of particles that can be tracked on present day's computers, the particle tracking methods are typically used for dilute multiphase systems. Particle tracking models are often referred to as Euler-Lagrange models or discrete particle models (DPM). The method most interesting to industrial applications is the averaging method where ensemble averaged transport equations are derived in terms of phase- and mass-averaged variables for momentum, mass and energy for each phase Drew & Passman [12]. This method has no limitations with respect to the volume fraction of the dispersed secondary phase and can, therefore, be

* Corresponding author: aholm@bio.aau.dk

applied to both dense and dilute multiphase systems. The interfacial forces which are dependent on the interfacial area of the particles must be modelled. Very often the particles are assumed to be spherical and to have a constant diameter. The averaging models are often referred to as Euler-Euler models or multi-fluid models. In order to include the particle size distribution, a population balance model must be included.

In a population balance model Ramakrishna [13], a transport equation is solved for the number density function. The particle size distribution is influenced by mechanical, thermal or chemical processes. The mechanical processes involve aggregation and breakage of interfaces by for instance turbulence and surface instabilities. The thermal processes involve nucleation and growth due to evaporation or condensation. Likewise, chemical processes involve nucleation and growth due to chemical reactions. The solution methods for the population balance equation most relevant for CMFD are the method of classes (CM) and method of moments (MOM). In the method of classes, the internal coordinate is divided into a number of classes over its size range. For each size class, the population balance equation then yields a number density equation. In CMFD, a uniform grid in the internal coordinate with fixed size classes is typically adopted i.e. the MUSIG (multi-size-group) model of Lo [14]. A disadvantage of the method of classes is that as many as 10-30 classes must be used to get a good representation of the particle size distribution Chen et al.[7] and Wang & Wang [15]. Accordingly 10-30 extra transport equations have to be solved just for the particle size distribution. In order to allow for different phase velocities Krepper et al. [16], the dispersed particle phase is first divided into N velocity classes. This method is known as the heterogeneous MUSIG model [16]. The particle size distribution of each velocity class is then next divided into M size classes.

In the past most polydisperse spray models have been based on either discretizing the liquid flow field into groups of equally sized droplets, as in the discrete droplet model (DDM) in which parcels of droplets are tracked in a Lagrangian framework, or by solving separate Eulerian conservation equations for a number of size ranges.

An attractive alternative is the moment methods that involve transportation of moments of the droplet size distribution (DSD). The advantage of the moment methods is that the number of moments required is very small (about four to six). The main issue is the so-called closure problem, related to the difficulties in writing the transport equations of the moments in terms of lower-order moments.

A recently developed method called the Direct Quadrature Method of Moments (DQMOM) developed by Marchisio & Fox [17] works by solving the moments rather than solving the particle size distribution itself like a class method does.

Fox et al. [18] presented Eulerian multi-fluid simulation of polydisperse liquid sprays where the Williams spray equation is solved using DQMOM.

The CFD model of Madsen et al. [1], [19] and [20] is using the DQMOM method developed by Marchisio and Fox [17]. The droplet size distributions were predicted using a multi-fluid model combined with the DQMOM and population balance model discrete droplet model in Fluent. The predictions were compared with his Phase Doppler (PDA) and interferometric particle imaging (IPI) measurements of Wu et al. [21].

This work will use the model Madsen et al. [1], [19] and [20] for modelling the experimental data obtain from a dilute non-evaporating turpentine round-jet [3].

Theory

Multi-Fluid and population balance Model

The basic idea behind the model is to solve the continuum Eulerian equations for the continuous gas phase and N dispersed droplet (liquid) phases. In this case, three droplet sizes are considered. For each phase the momentum and volume fraction equations are solved. For the interfacial momentum transfer between gas and droplet phases only drag (Schiller-Naumann) is included. The standard k-ε turbulence model is adopted for each phase.

The newly develop moment solver, the Direct Quadrature Method Of Moments (DQMOM) of Marchisio and Fox [17] involves the solution of an equation for each secondary phase for solving the droplet diameter to model the droplet size distribution (DSD).

The DQMOM model allows one to simulate the velocity fields of the gas-droplet flow. When studying the evolution of the DSD due to breakup and coalescence, the population balance equation (PBE) has to be solved. The PBE takes the form of Madsen et al. [19]

$$\frac{\partial}{\partial t} n(d) + \frac{\partial}{\partial x_j} [U_j(d) n(d)] = S(d) \quad (1)$$

where $n(d)$ is the droplet number distribution, d is the droplet diameter, $U_j(d)$ is the average velocity conditioned on d and $S(d)$ is the source term, that contains breakup and coalescence. The idea behind the DQMOM

solver is the solution of the closure problem related to the evolution of the moments of the DSD. It is done using a quadrature approximation of order N. This corresponds to the approximations of the DSD as follows:

$$n(d) = \sum_{q=1}^N \omega_q \delta[d - d_q] \quad (2)$$

where ω_q is the weights (droplet number density) and d_q is the abscissas (droplet diameter) of the quadrature approximation, and δ indicates the Dirac delta function. DQMOM works by solving transport equations for weight (ω_q) and weighted abscissa ($\delta_q = \omega_q d_q$) of the distribution:

$$\begin{aligned} \frac{\partial}{\partial t}(\omega_q) + \frac{\partial}{\partial x_j}(U_{j,q}, \omega_q) &= S_{\omega_q} \\ \frac{\partial}{\partial t}(\delta_q) + \frac{\partial}{\partial x_j}(U_{j,q}, \delta_q) &= S_{\delta_q} \end{aligned} \quad (3)$$

The two unknown source terms S_{ω_q} and S_{δ_q} are determined by requiring 2N moments to be exactly satisfied, giving the following matrix system

$$(1-k) \sum d_q^k S_{\omega_q} + k \sum d_q^{k-1} S_{\delta_q} = \bar{S}_{m_k} \quad (4)$$

where \bar{S}_{m_k} is the source term for the k^{th} moment defined by

$$\bar{S}_{m_k} = \int_0^{\infty} d^k S(d) dd \quad (5)$$

Equation (3) can be reformulated in terms of volume fraction and droplet diameter to be written as follows

$$\begin{aligned} \frac{\partial}{\partial t}(\alpha_q \rho_l) + \frac{\partial}{\partial x_j}(\rho_l \alpha_q U_{j,q}) &= \frac{\pi}{6} \rho_l d_q^2 [3 S_{\delta_q} - 2 d_q S_{\omega_q}] \\ \frac{\partial}{\partial t}(\rho_l \alpha_q d_q) + \frac{\partial}{\partial x_j}(\rho_l \alpha_q U_{j,q} d_q) &= \frac{\pi}{6} \rho_l d_q^3 [4 S_{\delta_q} - 3 d_q S_{\omega_q}] \end{aligned} \quad (6)$$

A more detail description of the DQMOM method can be found in [1],[19] and [20]

Coalescence and breakup kernels

The blob injection model is used for modeling atomization. In the blob model liquid blob are injected with a diameter equal to the sheet thickness. The primary breakup of these blobs and secondary breakup of droplets is done using the standard WAVE breakup model of Reitz [22], where the relative velocity is assumed to be proportional to the local droplet turbulence properties.

Symmetric fragmentation is adopted. An unstable droplet with diameter d produces two droplet of diameter $2^{-1/3}d_q$. The daughter distribution function of this breakup mechanism is:

$$b(d|dq) = \begin{cases} 2 & \text{if } d = 2^{-1/3}d_q \\ 0 & \text{otherwise} \end{cases} \quad (7)$$

The moment transform of the daughter distribution function then becomes

$$\bar{b}_q^{(k)} = 2^{(3-k)/k} d_q^k \quad (8)$$

The original WAVE model is formulated due to a rate approach for Sauter mean diameter (SMD) reduction of the parent drops within the discrete droplet model (DDM) of Reitz Chyba: zdroj odkazu nenalezen. This has been transfer to the breakup kernel by

$$\alpha_q = \frac{1 - d_{st}/d_q}{(2^{1/3} - 1)\tau_{bu}} = \frac{1 - d_{st}/q}{0.26\tau_{bu}}, \quad d_{st} < d_q \quad (9)$$

where τ_{bu} is the breakup time and d_{st} is the stable diameter. This ensures that the SMD is consistent with the original model.

The droplet-droplet collision model used is a semi-empirical and has two stages. The first stage is to determine the collision rate between droplets. Collision rates are expressed by a collision coefficient β_{pq} that is defined such that $\beta_{pq}n(d_p)n(d_q)$ is the number per unit volume and time between two sizes droplets having densities $n(d_p)$ and $n(d_q)$. According to the kinetic energy theory, Delichatsios & Probstein [23], the collision coefficient is given by

$$\beta_{pq} = \pi d_{pq}^2 U_{rel} \quad (10)$$

where $d_{pq} = (d_p + d_q)/2$ and U_{rel} is the relative velocity between two droplet classes. The following form for the average relative velocity $U_{rel} = |u_p - u_q|$, between colliding droplets is assumed:

$$U_{rel} = \sqrt{|\vec{U}_p - \vec{U}_q|^2 + 2(1 - \rho_{pq})(k_p + k_q)} \quad (11)$$

where \vec{U} is the mean droplet phase velocity and k is the droplet phase turbulent kinetic energy. ρ_{pq} is a correlation coefficient ($0 \leq \rho_{pq} \leq 1$), describing the correlation of the fluctuating velocity. If one consider two droplets in contact with other separated by d_{pq} , then the correlation coefficient is assumed to be

$$\rho_{pq} = 1 - \frac{3.6 \left(\frac{\varepsilon_p + \varepsilon_q}{2} d_{pq} \right)^{2/3}}{k_p + k_q} \quad (12)$$

where ε is the droplet turbulent kinetic energy dissipation.

The second stage of the model determines the outcome of the collisions. The model account for coalescence, bounce and collision-induced breakup (fragmentation). With the collision confident the expression for the coalescence kernel becomes

$$c_{pq} = \min(E_{boun}, E_{coal}) \beta_{pq} \quad (13)$$

where the probability of coalescence at low We_{coll} is Ko & Ryou [24]

$$E_{boun} = \min \left[1, \left(\frac{We_{coll}}{4.8 f(\gamma)} \right)^{1/3} \right] \quad (14)$$

and the probability of coalescence at higher We_{coll} is Brazier-Smith et al. [25]

$$E_{coal} = \min \left[1, \frac{4.8 f(\gamma)}{We_{coll}} \right] \quad (15)$$

and We_{coll} is the collisional Weber number defined as

$$We_{coll} = \frac{\rho_l U_{rel}^2 d_{small}}{\sigma} \quad (16)$$

here d_{small} is the diameter of the smaller of the interacting droplets and σ is the surface tension. The function $f(\gamma)$ is defined as Ko & Ryou [24]

$$f(\gamma) = \gamma^2 - 2.4 \gamma^2 + 2.7 \gamma \quad (17)$$

where $\gamma = d_{big}/d_{small}$ is the droplet ratio. One possible outcome of the droplet-droplet collisions is the breakup of the original droplets into smaller droplets. The collision-induced breakup kernel is then express as

$$e_{pq} = (1 - E_{coal}) \beta_{pq} \quad (18)$$

In Georjon and Reitz [26] proposed a model for “shattering” collisions between droplets. They assumed that when droplets collide they form a ligament, which is stretching due to the inertia of the collision. An estimation of the diameter of the droplets fractions d_{frag} is given by the correlation of Post and Abraham [27]

$$d_{frag} = \frac{1.89(d_p^3 + d_q^3)^{1/3}}{\sqrt{2.81 \cdot We_{coll}^{2/7} (1 + \gamma^3)^{2/21} + 1}} \quad (19)$$

The moment transform of the daughter distribution function then corresponds to the collision induced break-up mechanism

$$\overline{f_{pq}^{(k)}} = (d_p^3 + d_q^3) d_{frag}^{k-3} \quad (20)$$

Numerical configuration

The spray configuration considered here is the Laser- (LDA) Phase- Droplet Anemometry (PDA) measurements by Nijdam et al. [3].

The spray design has an aerodynamic design (long, tapered and sharp-edged) which was designed for preventing recirculation at the nozzle exit. The nozzle has an inside diameter of 9.8 mm and a length of 240 mm. The spray has an exit velocity of 23 m/s and a turbulent intensity of 1.4 %. The gas temperature at nozzle exit is 0 °C. The co-flow has a velocity of 2.4 m/s with an air flow temperature of 16 °C. Pressurized turpentine with a density of 810 kg/m³ was fed onto a commercial nebulizer (Sonotek) to produce a dispersion of droplets in the size range from 1 µm to 90 µm. The total turpentine droplet flow at the exit of the nozzle was 2 ml/min.

Boundary condition for the spray is given in Nijdam et al. [4]. The original 13 droplet sizes were reduced to three secondary phases using the PD-algorithm of Gordon R. G. [28], so that the distribution still contains the correct moments. The following volume fraction (diameter): 1.998e-05 (25.06 µm), 2.229e-05(53.59 µm) and 3.02e-06(76.54 µm) are used.

For this case an axisymmetric 2D mesh with dimension 0.49×0.098 meters containing 40000 cells was created.

Results and Discussion

The spray seems to be so dilute that droplet collisions and thereby coalescence of droplets are unlikely. Furthermore the Weber number is as low as 0.4 making even breakup unlikely. The fact that no coalescence or breakup is going on in the spray reduce the advantages of the DQMOM. In essence, DQMOM is reduced to a class method like the Eulerian multi-fluid model with which it is compared in this paper. It is therefore expected that the DQMOM and the Eulerian multi-fluid model will predict similar results.

The axial-velocity for the Eulerian multi-fluid model and the DQMOM method are presented in figure 1 together with the experimental data. The data are presented in normalized form by dividing the local axial velocity with the maximum velocity, and the radial distance are normalized dividing the radial distance from the centre axis, by the half width $R_{1/2U}$.

It is shown that the Eulerian model is capable of predicting the flat profile of the jet when leaving the nozzle and the transformation into a bell form downstream the nozzle from about ten diameters downstream. The DQMOM model predicts the experimental data the first five diameters downstream. From ten diameters downstream only the droplet diameter of node 1 is capable of predicting the experimental data. The calculations of dilute sprays require extremely low residuals for convergent solution. This is a problem in CFD code Fluent because; Fluent has a lower limit of 1e-08 for the volume fraction. If the volume fraction goes below the limit, then Fluent simply assume that there is no droplets in field and hereby sets the velocity equal zero, like a cut-off function. This behaviour is seen in figure 1 for the velocity profiles at the outer regions of the spray, where the droplet concentration drops below 1e-08.

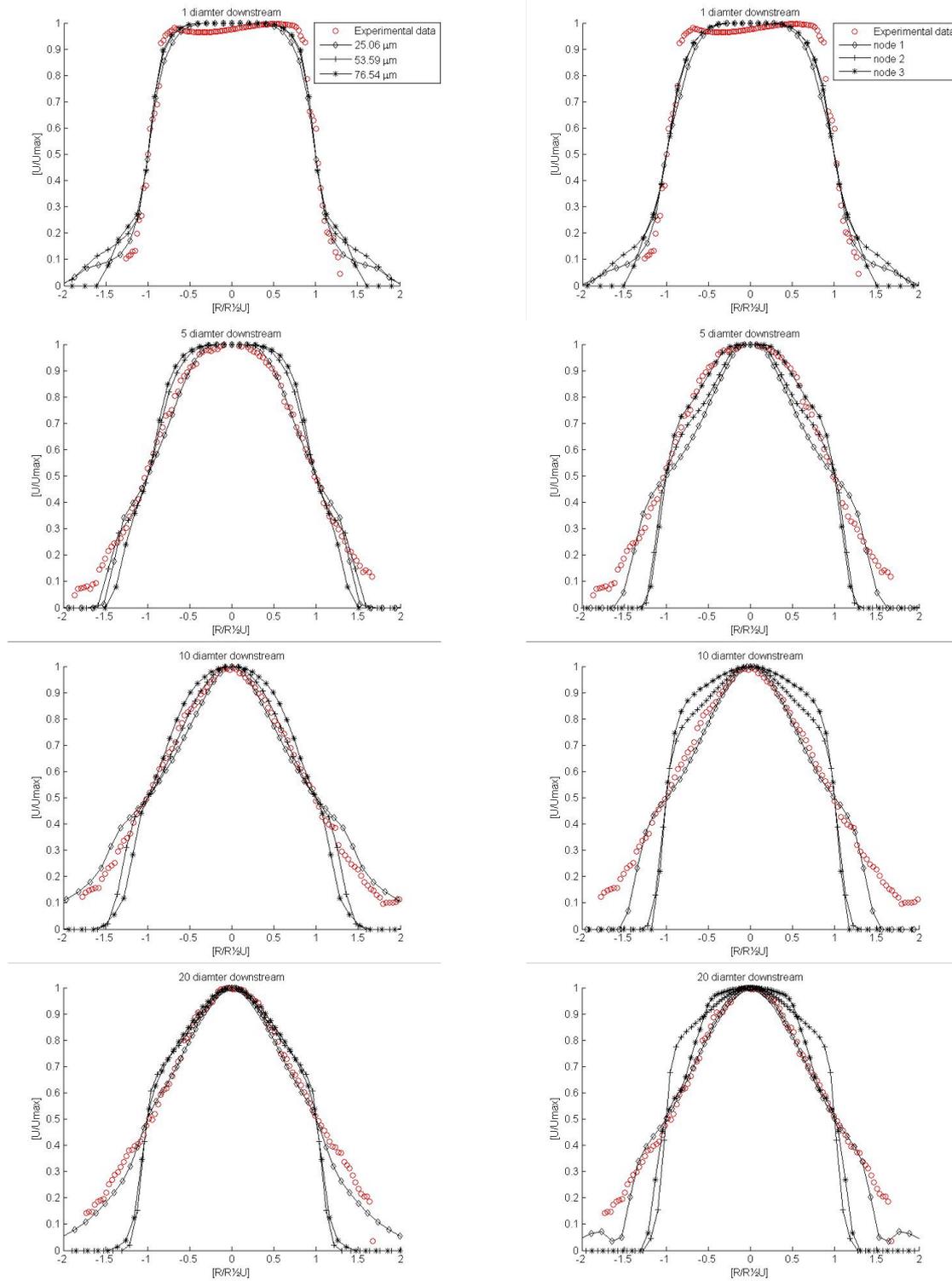


Figure 1. Eulerian multi-fluid model (left) and DQMOM (right) simulation for radial profiles of dimensionless excess axial velocity U/U_{max} versus dimensionless radius $R/R_{1/2U}$ for different droplet size classes at various locations

The volume-flux data for the Eulerian multi-fluid model and the DQMOM model are normalized and presented in a similar way the in figure 2. The experimental data shows that a bell transformation occurs downstream. This bell transformation is the result of slower moving air at the edge of the spray, while having a high velocity at the centre, which leads to a penetration of the core of the spray downstream.

Both the Eulerian multi-fluid model and the DQMOM model are capable of predicting the bell-shaped profile for all droplet diameters. The bell-shape indicates that a turbulent diffusion mechanism is going on for the dispersion of droplets.

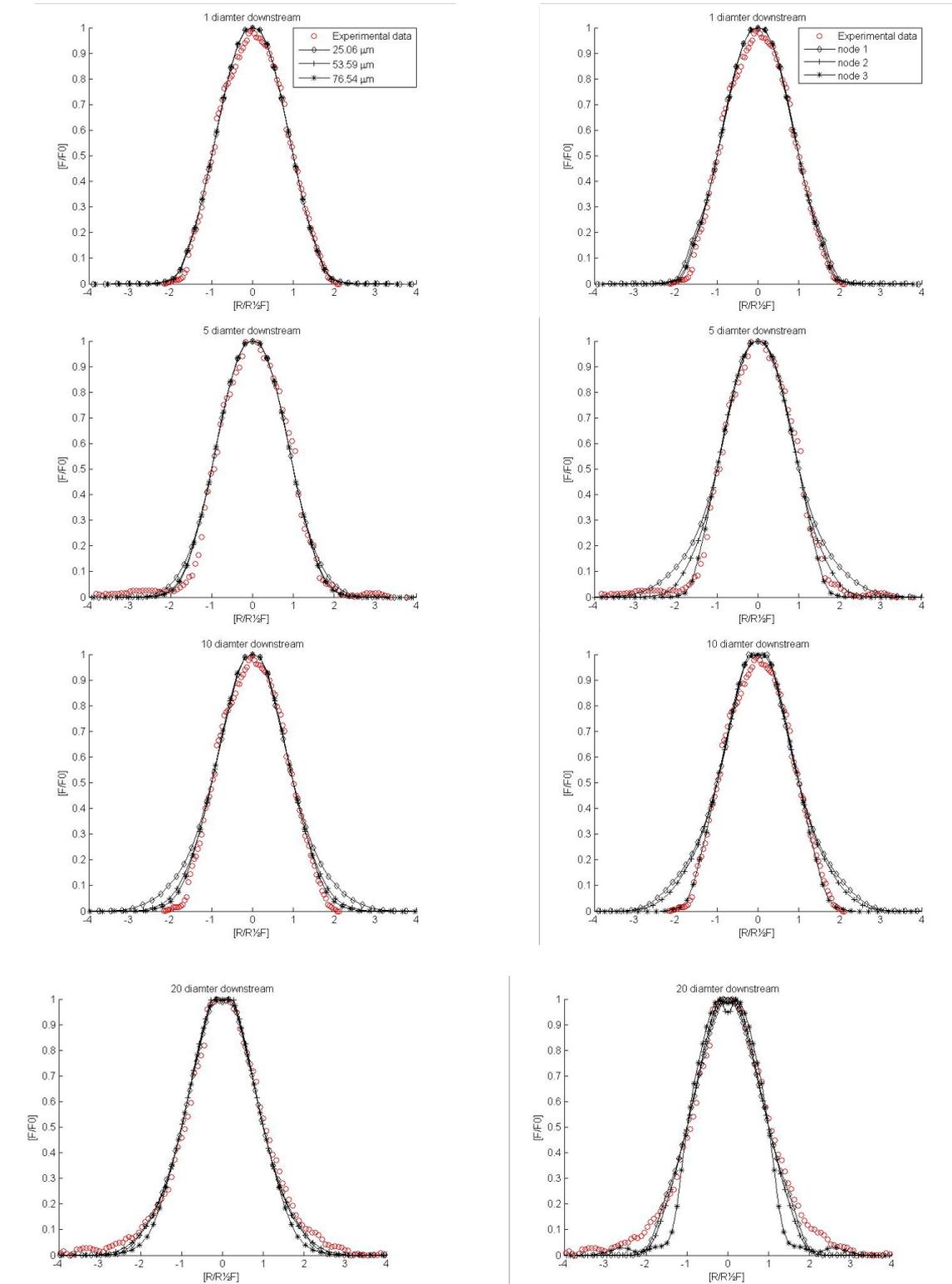


Figure 2. Eulerian multi-fluid model (left) and DQMOM (right) simulation for radial profiles of dimensionless excess flux, F/F_0 , versus dimensionless radius $R/R_{1/2U}$ for different droplet size classes at various locations

Figure 3 present the mean droplet diameter (D_{20}) as a function of the radial distance from the centre line. Simulation of the mean diameter (D_{20}) with the Eulerian multi-fluid model and the DQMOM model shows that the DQMOM method is the slightly better for predicting the mean diameter. Both models are capable of predicting a constant mean diameter at the nozzle exit.

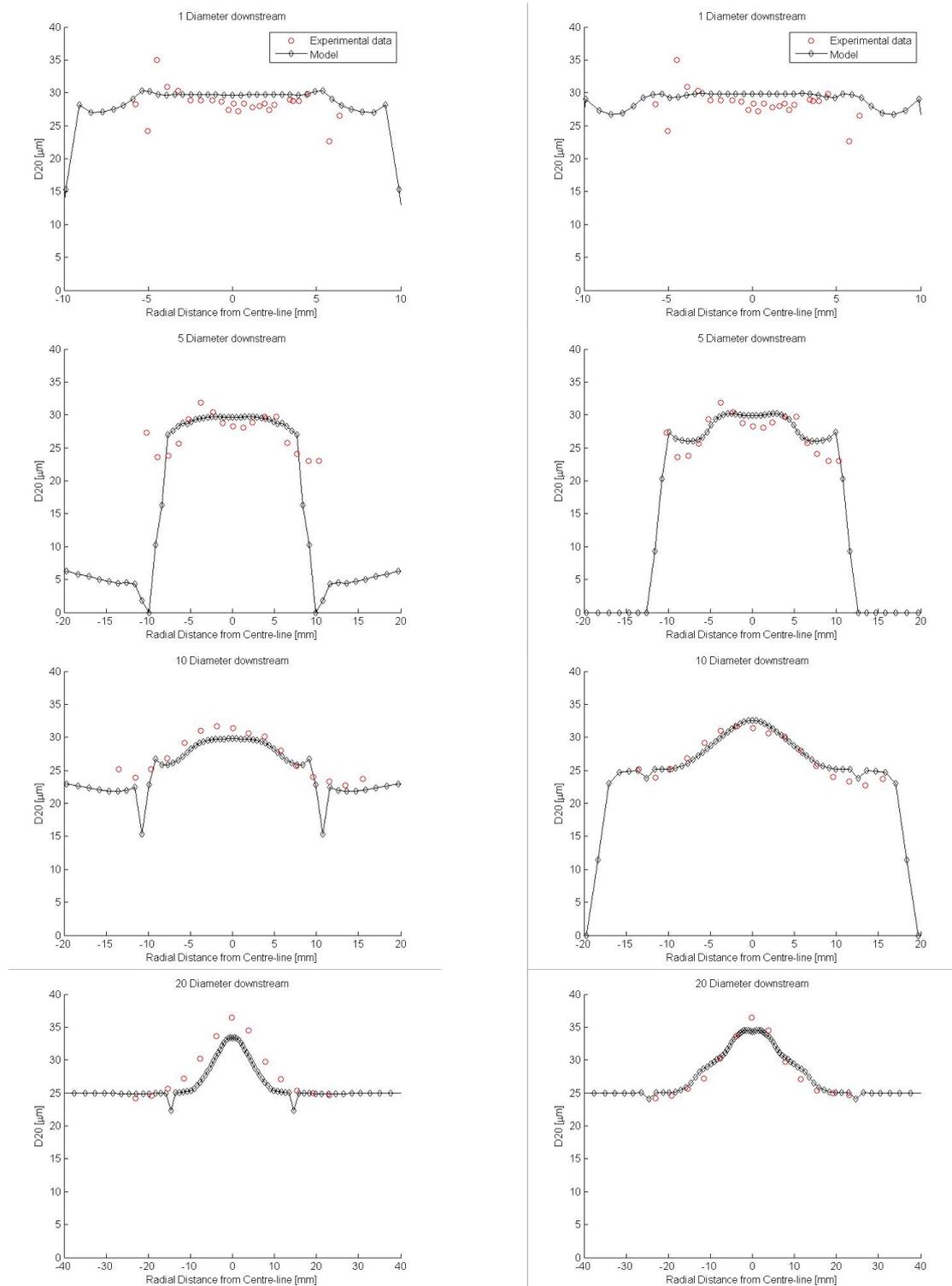


Figure 3. A comparison of the radial profiles of the area-based mean diameter (D_{20}) Eulerian multi-fluid model (left) and DQMOM model (right)

Conclusion

The DQMOM method has been used for modeling experimental data of a non-evaporating dilute turpentine round jet [3] with focus on velocity profiles, flux profiles and the mean diameter (D_{20}). The result shows that the DQMOM method is reduced to a standard class method because, the spray is too dilute for coalescence to occur. The Weber number for the spray has been calculated to 0.4, which indicates that no breakup is occurring either. Nevertheless DQMOM is still able to predict the correct trend in the experimental data.

Nomenclature

a_q	breakup kernel [s^{-1}]
$b(d d_q)$	breakup daughter distribution function [-]
$\bar{B}_q^{(k)}$	moment transform of $b(d d_q)$ [-]
C_{pq}	coalescence kernel
g	gravity [m/s^2]
d	abscissas (droplet diameter) [m]
E	coalescence efficiency [-]
e_{pq}	collision induced breakup kernel [m^3/s]
$\bar{f}_{pq}^{(k)}$	moment transform of $f(d d_p, d_q)$
k	gas turbulent kinetic energy [m^2/s^2]
k^{th}	moment of the DSD [m^k/m^3]
\dot{m}	Mass transfer
$n(d)$	droplet number distribution [m^{-3}]
N	number of droplet phases [-]
P	pressure
S	source term
U	velocity [m/s]
We	Weber number

Greek letters

α	volume fraction [-]
δ	weighted diameter [m/m^3]
ε	turbulent kinetic energy dissipation [m^2/s^3]
γ	droplet size ratio [-]
ρ	density [kg/m^3]
ρ_{pq}	correlation [-]
τ	breakup time [s]
ω_q	weight (droplet number density) [m^{-3}]

Subscripts

Boun	bounce
Coal	coalescence
Coll	collision
Frag	fragments
g	gas
l	liquid
p th	droplet phase
q th	droplet phase
rel	relative
st	stable

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