Numerical Description of a Pressure-Swirl Nozzle Spray

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Submitted to **Chemical Engineering and Processing: Process Intensification**

Revisions are shown in red (June 12th, 2016)

Abstract

Pressure-swirl nozzles are widely used in both industrial and experimental processes. However, the spray flow fields are difficult to predict due to the complexities of the dense break-up region. Herein, an inflow boundary condition approach is employed whereby droplets are computationally injected at 9 mm downstream of the orifice based on experimentally derived descriptions of the mean droplet and gas velocities, combined with empirical relations for turbulent kinetic energy and dissipation. The gas flow is then predicted with a Reynolds-Averaged Navier-Stokes solution while the particle trajectories are computed with a discrete random walk model. This approach was found to reasonably describe downstream spatial distribution of gas and droplet velocity, with moderate mesh resolution and CPU time. In addition, the evolution of the droplet velocity fluctuations was found to be consistent with turbulent diffusion theory based on the local Stokes numbers and turbulent kinetic energy.

Keywords: pressure-swirl nozzle, spray structure, numerical study, CFD, turbulence

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1. Introduction

Pressure-swirl atomizers (simplex nozzles) have many applications in both industrial and experimental processes, such as combustion, spray cooling, and tracer seeding. The downstream mass distribution of the droplets is generally critical for such applications and this distribution is dependent on the droplet sizes and the interaction of the spray with the surrounding turbulent gas.

In order to investigate the detailed structure of a spray generated by a pressure-swirl atomizer, velocities of continuous and disperse phases, and sizes of spray droplets can be acquired theoretically, experimentally, or numerically. Theoretical and experimental studies have been completed by Lefebvre's research group [2-5] in terms of spray angle, mean drop size, and radial liquid distribution, all of which are a function of fluid properties and nozzle dimensions. Similarly, Chin's group [6, 7] and Som's group [8] experimentally and analytically investigated general spray characteristics downstream of a pressure-swirl atomizer for a larger range of conditions. These studies allowed general structure of the flow but more details have been obtained recently, using Phase Doppler Particle Analyzer (PDPA) by Santolaya *et al.* [9] for a pressure swirl spray nozzle. These studies provided detailed spatial information about gas flow velocities, droplet velocities for different size classes, and spatial distribution of liquid mass flow rates.

However, numerical predictions of these sprays are less common. This is because, of the complicated phenomena near the orifice which involves dense multiphase flow with high aerodynamic coupling. In particular, physics such as liquid sheet break-up, droplet formation, two-way coupling between turbulent flow and disperse phase, and contact interaction between droplets require intensive computationally resources to fully resolve all the spatial details. Difficulties especially come from capturing fluid instabilities and the interphase physics that cause liquid sheet to break-up into different sizes of droplets, while being subjected to anisotropic

non-homogeneous turbulence. Many numerical studies have focused on tracking of the liquid/gas interface inside the atomizer in order to provide a prediction of air core and liquid sheet [10-12]. Similarly, Yeh [13] conducted turbulent flow simulations of liquid jet emanating compared different turbulent models and provided turbulent intensity at the atomizer exit for the pressure-swirl atomizer. Belhade *et al.* [14] studied pressure-swirl atomization using an Eulerian method that treated the turbulent mixing as a single phase of liquid-gas mixture. Due to limits of this method, only mean droplet size and liquid axial mean velocity were predicted. In general, none of the above methods allowed a fully validated description of the two-phase flow ranging from the orifice to hundreds of orifice diameters downstream.

In this study, a two-phase computational fluid dynamic (CFD) simulation is implemented just downstream of the liquid sheet break-up region of a pressure-swirl nozzle to allow the simulation to focus on the more computationally practical spray structure evolution. Herein, previous PDPA experimental data after the break-up region are employed as input boundary condition data. Turbulent characteristics of continuous phase are modeled at the same boundary based on empirical correlations of jet flow. Thus, spray structure and droplet spatial distribution resulting from coupling of both disperse and continuous phases can be simulated in the far downstream domain. This novel approach to simulating a pressure-swirl nozzle spray allows moderate mesh resolution and CPU time while avoiding the complicated break-up region details. It is the first such computational study to the authors' knowledge. Importantly, by adapting inflow boundary conditions, this methodology may be applied to other pressure-swirl nozzle spray cases to predict downstream spray structure, which may allow broad implementation of this technique. Furthermore, this study also examines the hypothesis that droplet velocity fluctuations can approach the theoretical rms ratios based on inertial theory.

2. Flow Physics and Numerical Methodology

In the present study, the Eulerian numerical approach is chosen for the gas phase and the Lagrangian approach for the liquid phase. To ensure both numerical stability and low computational cost, the continuous phase (ambient gas) is solved using the Reynolds-averaged Navier-Stokes (RANS) equations with a standard k- ε model, while the dispersed phase (droplet) is solved by trajectory discretization with a discontinuous random walk (DRW) model to incorporate turbulent fluctuations.

In the standard k- ε model [15], the turbulent kinetic energy k and its rate of dissipation ε are solved in two transport equations:

$$\frac{\partial}{\partial t}(\rho_g k) + \frac{\partial}{\partial x_i}(\rho_g k u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu_g + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho_g \varepsilon - Y_M \quad (1)$$

$$\frac{\partial}{\partial t}(\rho_g \varepsilon) + \frac{\partial}{\partial x_i}(\rho_g \varepsilon u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu_g + \frac{\mu_t}{\sigma_k} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{1\varepsilon} \frac{\varepsilon}{k} (G_k + C_{3\varepsilon} G_b) - C_{2\varepsilon} \rho_g \frac{\varepsilon^2}{k} \quad (2)$$

The turbulent viscosity μ_t appearing on the right-hand side expressions is calculated by:

$$\mu_t = C_\mu \rho_g \frac{k^2}{\varepsilon} \quad (3)$$

In equation (1) and (2), ρ is density, u refers to gas velocity, and the subscript g indicates a gas-phase property while the turbulent kinetic energy generation and distraction terms (G_k , G_b , and Y_M) are described in Ref. 15. Herein, conventional values are used for the constants and non-dimensional numbers: $C_{1\varepsilon} = 1.44$, $C_{2\varepsilon} = 1.92$, $C_\mu = 0.09$, $\sigma_k = 1.0$, $\sigma_\varepsilon = 1.3$. Note that the spray flow field is assumed to not impact the gas-phase turbulence, i.e. there are no inter-phase coupling terms for Eqs. 1-2 consistent with recent work by Huang *et al.* [16]. However, the impacts between mean continuous phase and discrete phase velocities are coupled by momentum exchange, where the latter is described below.

To describe trajectory of a discrete phase particle dominated by drag and gravity forces, the equation of motion for droplets with centroid velocity v_i is expressed in a Lagrangian reference frame [17] as:

$$\frac{dv_i}{dt} = F_D (u_i - v_i) + \frac{(\rho_d - \rho_g)}{\rho_d} g_i \quad (4)$$

In this expression, the subscript d indicates a droplet property and F_D is the drag force per particle mass per relative velocity defined as

$$F_D = \frac{3\mu_g C_D \text{Re}}{4\rho_d d^2} \quad (5)$$

The value in the numerator Re is the relative Reynolds number, which is defined in terms of the magnitude of relative velocity w as

$$\text{Re} \equiv \frac{\rho_g dw}{\mu_g} \quad (6a)$$

$$w = \sqrt{w_i w_i} \quad (6b)$$

$$w_i = v_i - u_i \quad (6c)$$

The last expression for w_i is the component of relative velocity in the i direction. A spherical droplet assumption is reasonable herein since the Weber numbers are less than unity, since a unity Weber number corresponds to droplet diameters of 400 microns [17]. Thus, the drag coefficient C_D for spheres is used and taken from Morsi and Alexander [18].

The instantaneous gas velocity in Eqs. 4 and 6 can be obtained in terms of mean and fluctuation values:

$$u_i = \overline{u_i} + u_i' \quad (7)$$

The mean value (first term on right-hand side) is obtained from RANS solution. For the fluctuation velocity (second term on right-hand side), synthetic turbulence must be used to properly capture turbulent diffusion. Herein, the discrete random walk (DRW) model of Ref. 19 is employed, which requires a random number (σ), an eddy lifetime (τ_Λ), and a velocity perturbation strength (u_{rms}). For small droplets with small relative velocities, the characteristic lifetime of eddies can be based on the integral time in DRW model. Thus, in DRW model, the gas velocity fluctuations can be computed in each integral time as

$$u'_i = u_{rms} \sigma_i \quad (8a)$$

$$u_{rms} = \left(\frac{2}{3} k \right)^{1/2} \quad (8b)$$

$$\tau_\Lambda = C_\tau \frac{k}{\varepsilon} \quad (8c)$$

In Eq. 8a, σ represents three independent Gaussian random numbers and C_τ of Eq. 8c is the eddy timescale coefficient, whose calibrated value is 0.21 [19]. A new random number is generated when the droplet path duration exceeds τ_Λ (eddy life time) or τ_{tra} (eddy traversal time), where the latter is obtained as

$$\tau_{tra,i} = \frac{\Lambda_i}{w} \quad (9)$$

where Λ is turbulence integral length scale, which is based on the local turbulent kinetic energy and dissipation values [19].

To validate this approach in terms of predicting turbulent flow decay and particle lateral diffusion, Snyder and Lumley's classical experiment [20] was utilized. In this experiment, nearly homogenous turbulent flow was generated by grids and the spatial diffusion of four different kinds of particles were measured. The RANS-based CFD employed an inflow boundary

condition based on measurements of $\bar{u}$, k and ε at 60 mm downstream of the grid. The CFD predictions of the evolution and decay of these turbulent flow properties are compared to the experimental data in Fig. 1, and the agreement can be regarded as excellent. The experimental and predicted lateral dispersions of four different particles released in this flow are shown in Fig. 2a. These particles include: hollow glass with a diameter of 46.5 μm and a density of 260 kg/m^3 , solid glass with a diameter of 87.0 μm and a density of 2500 kg/m^3 , corn pollen with a diameter of 87.0 μm and a density of 1000 kg/m^3 , and copper with a diameter of 46.5 μm and a density of 8900 kg/m^3 . As noted in the caption, the particle inertias can be characterized in terms of a response time scale (τ_p) defined as

$$\tau_d = \frac{\rho_d d^2}{18\mu_g} \quad (10)$$

It can be seen in Figs. 2a and 2b that radial diffusion increases as response time (and inertia) decreases. The hollow glass particles have the smallest response time scale due to its small diameter and small density, so these particles diffuse quickly and widely in downstream. On the contrary, the copper particles are large and heavy, so they are less affected by the turbulent flow and hence the lateral diffusion is narrow. The present DRW-based CFD results indicated good agreement for short-time and long-time turbulent particle diffusion. Based on the above, this validated numerical approach is utilized below to predict pressure-swirl liquid spray structure and droplet dispersion.

In the simulations, all the droplets are tracked simultaneously and an algorithm is used to determine collisions between droplets. In particular, the stochastic estimate of collisions is based on the model discussed by O'Rourke [21] and Rüger *et al.* [22]. The model considers collision probability, and according to O'Rourke, the probability distribution of the numbers of collision is based on a Poisson distribution equation. Details and derivations on employing the concept of a collision volume to calculate the possibility of collision can be found in Ref. 21. Once it is

decided that two parcels of droplets collide, the outcome of the collision must be determined. The critical offset is defined and calculated by O'Rourke using below expression with the collisional Weber number and the relative radii of the collector (larger droplet, subscripted with the number 1) and the smaller droplet (subscripted with the number 2).

$$b_{crit} = (r_1 + r_2) \sqrt{\min\left(1.0, \frac{2.4f}{We}\right)} \quad (N1)$$

where the collisional Weber number is defined with the relative velocity between two parcels v_{rel} , the arithmetic mean diameter of the two parcels $\bar{d}$ and the surface tension σ as

$$We = \frac{\rho_d v_{rel}^2 \bar{d}}{\sigma} \quad (N2)$$

and f is a function of r_1/r_2 , defined as

$$f\left(\frac{r_1}{r_2}\right) = \left(\frac{r_1}{r_2}\right)^3 - 2.4\left(\frac{r_1}{r_2}\right)^2 + 2.7\left(\frac{r_1}{r_2}\right) \quad (N3)$$

Meanwhile, the actual collision parameter b is defined as

$$b = (r_1 + r_2) \sqrt{Y} \quad (N4)$$

where Y is a random number between 0 and 1. The calculated value of b is compared to b_{crit} , and if b_{crit} is greater than b , the result of the collision is coalescence. The number of smaller droplets that coalesce with the collector is calculated using Poisson distribution and the properties of the coalesced droplets are updated considering the basic conservation laws.

In the case of a grazing collision, the new velocities are calculated and updated in the simulation based on momentum and kinetic energy conservations. It is assumed that some fraction of the kinetic energy of the droplets is lost due to viscous dissipation and angular momentum generation.

This fraction is expressed in a energy loss term of b , the collision offset parameter. Herein, O'Rourke derived the following expression for the new velocity

$$v_1' = \frac{m_1 v_1 + m_2 v_2}{m_1 + m_2} + \frac{m_2 (v_1 - v_2)}{m_1 + m_2} \left(\frac{b - b_{crit}}{r_1 + r_2 - b_{crit}} \right) \quad (N5)$$

Note that Eq. N5 is used for each of the components of velocity. No other droplet properties are altered in grazing collisions.

This collision model assumes that the frequency of collisions is much less than the particle time step. Thus, the particle time step needs to be carefully chosen (sometime need to adjust the particle length scale accordingly) to make sure the results are time-step-independent. Additionally, the model is most applicable for low-Weber-number collisions where collisions result in bouncing and coalescence [21]. Above a Weber number of about 100, the outcome of collision could be shattering.

Sometimes the collision model can cause mesh-dependent artifacts to appear in the spray. O'Rourke's algorithm assumes that two droplets may collide only if they are in the same continuous-phase cell. This assumption can prevent droplets that are quite close to each other, but not in the same cell, from colliding. In two dimensions, a finer mesh and more computational droplets can be used to reduce these effects. The overall accuracy of the scheme is second-order in space [21]. Thus, the cell size as well as time step were also carefully chosen in the simulation (discussed in next section) to have grid and time independence.

3. Axisymmetric Simulation

To simulate structure of liquid spray after the break-up region, an axisymmetric zone is defined based on the experimental flow field [9] as shown in Fig. 3, and the boundary conditions are listed in Tab. 1. Thus, the geometry is simply a long rectangle and the mesh is uniform structured mesh. A cylindrical coordinate system is chosen with the nozzle orifice as the origin with r for

radial and x for axial distance. Inflow and outflow boundary conditions are set at $x = 9$ mm and $x = 80$ mm respectively, while a wall boundary is set at $r = 170$ mm. Note that in the experiment, the spray was operating in a square cross-section tank of 340 mm by 340 mm cross-section rather than cylinder, but this geometry difference may be reasonable neglected because the spray structure is generally contained to be within $r = 40$ mm as shown in Fig. 3. In the simulation, radial spatial distributions of both the continuous and disperse phase flow properties are introduced at inflow boundary ($x = 9$ mm), including velocity and turbulence of the gas as well as mass flux, velocity, and turbulence of the drops. Details of these distributions are described below.

For the continuous phase, the experimental gas axial velocity at $x = 9$ mm was fitted with a hyperbolic sech function as shown in Fig. 5, and the gas radial velocity was similarly fitted with an exponential bounded quintic polynomial. These velocity profiles satisfied a 0.15-m/s gas co-flow velocity, consistent with the experimental test conditions. The profiles of gas turbulent kinetic energy and dissipation rate are calculated based on turbulent jet curve fits of experimental data [24] with a form:

$$p(\eta) = (C_0 + C_2\eta^2 + C_4\eta^4 + C_6\eta^6)e^{-A\eta^2} \quad (11a)$$

$$\eta = \frac{r - r_0}{x - x_0} \quad (11b)$$

In this expression, η is a normalized position, and r_0 and x_0 are orifice radius and location respectively. It was found that the gas mean axial velocity of the pressure swirl nozzle at $x = 9$ mm was nearly identical to that for the turbulent jet flow of Ref. 24 at $x = 32$ mm. Thus, the profiles of turbulent kinetic energy and dissipation rate at 32 mm downstream of the jet in Ref. 24 were employed as inflow boundary condition at $x = 9$ mm downstream of the pressure swirl nozzle. This was accomplished by using the C_i and A listed in Ref. 24.

For the disperse phase, the Rosin-Rammler equation [1] fitted with the experimental data is chosen to represent the polydisperse distribution. Using previous experimental data [9], the overall droplet size distribution was measured across the spray at 9 mm downstream of the nozzle and was fitted to a Rosin-Rammler distribution. At a given radius, the mean droplet size and the volume percentage of three different droplet sizes were known in the experiment, so the local Rosin-Rammler distribution can be fitted. As a result, the mass fraction for a given radius and a given droplet size can be calculated using the combination of both overall and local Rosin-Rammler fits. For this study, a MATLAB codes was developed to calculate the droplet distribution and to generate the droplet input files for the simulation. In Fig. 4, the droplet mass flow rate distribution is shown as function of radius and droplet size at 9 mm downstream of the nozzle orifice, which is the inlet boundary in simulation.

Three droplet size classes are considered in the later analysis: small from 5 to 10 μm , medium from 20 to 30 μm , and large from 50 to 60 μm . This preserves a 30.6- μm Sauter mean diameter (SMD), consistent with the measured SMD at $x = 9$ mm. Also, collision physics have been included in the CFD predictions as this allowed improved predictive performance when comparing with experiments. In particular, smaller droplets which collide near the centerline to make larger droplets will tend to increase the mass flux of larger droplets in this region. The droplet mean axial velocity profiles for the CFD for all three classes are obtained by fitting the experimental data at $x = 9$ mm as shown in Fig. 5. However, it was noted that the flow simulations yielded higher fidelity if a random velocity perturbation was also included, especially for large droplets, to reflect initial turbulence. Because the droplet velocity fluctuations were not measured, it was assumed that droplet velocity fluctuation are equal to that of gas velocity at $x = 9$ mm, yielding the instantaneous velocities as shown in Fig. 6.

To specify the radial variation of the droplet mass flow rate at this computational inflow plane, an assumption was needed regarding the distribution among the three sizes. In the measurements,

the mass flux based on the sum of the three classes at $x = 9$ mm was $0.509 \text{ cm}^3/\text{s}$, which is a 34.4% deficit of unaccounted flux relative to the total injected liquid volumetric flow of $0.77 \text{ cm}^3/\text{s}$. Therefore, it is herein assumed that the relative flow rate percentages of three classes are the same as measured (small class at 2%, medium class at 57%, and large class at 41%), and the mass fluxes for each case were then scaled so that the total flow rate was $0.77 \text{ cm}^3/\text{s}$, consistent with the experimental total volumetric flow. Based on particle velocity profile, liquid flow rate, the radial distribution of a particle mass flow rate at inflow boundary is shown as Fig. 7. Thus, all particles are injected at 9 mm with a specified droplet velocity profile (Figs. 5 and 6) and radial mass flow rate distribution (Fig. 7).

In CFD simulation, mesh sizes of $\Delta x = \Delta r = 10^{-3} \text{ m}$ and time step of 10^{-3} s are chosen based on grid and temporal resolution studies. In each time step, 2410 parcels (groups of droplets that move at the same speed) are injected into simulation domain. These conditions are chose such that a two-fold improvement in grid, timestep and parcel resolution resulted in less than 1% variation in downstream gas or droplet mean velocity. The computational resources required for this approach are therefore rather modest while ensuring accuracy and computational efficiency. In order to predict the mean spray structure, the droplet trajectories were time-averaged (after the initial transient phase for which the first droplets exited the computational domain) using a volume integral of particle concentration. To achieve statistically stationary results, this sampling was averaged over 1000 time steps, which corresponds to a time interval of one second. The coupled gas flow solution had also converged at that time to a steady-state flow.

4. Results

Predictions of the axisymmetric gas flow after convergence, are shown in terms of the velocity field (Fig. 8a) and turbulent kinetic energy field (Fig. 8b). The velocity field of continuous phase indicates a high speed core in the center, where gas is accelerated by injected particles, and this

velocity decays in both the downstream and outward (radial) directions as expected due to turbulent diffusion of a jet. Similarly, Fig. 8b shows that the turbulent kinetic energy is high in the core region due to high shear rates and interphase coupling, since the particle concentration is relatively high in this region. The radial gas velocity profiles are shown in Fig. 9 for three different streamwise positions, where the above trends can be observed directly and where there is reasonable agreement with the experimental results of Santolaya *et al.* [9]. However, the centerline velocity tends to be under-predicted at $x=72$ mm (Fig. 9c), suggesting that the turbulent kinetic energy may be over-predicted in this region.

Figure 9 also shows the particle axial velocities at different axial positions. In general, the particle velocities are similar to the gas velocities, but the larger particle velocities tend to have the highest velocities. This is due to the higher inertia and response times of these droplets that prevents them from slowing down as quickly as that of the smaller drops and that of the gas. The medium and smaller droplets tend to more closely follow the gas velocity, especially at the far downstream locations. There is a good agreement between CFD results and experimental data sets for droplet velocity, though again the centerline velocity tends to be under-predicted, especially at $x=72$ mm (Fig. 9c). In addition, Fig. 9d shows the velocity profiles at $x=72$ mm but the particle collision is turned off in the simulation. It can be seen that collision effect on small and medium size particles is not strong. However, without collision, it over-predicts the velocity for large particles compared to experimental data because large particle has large inertia and response time. But collision changes their velocity direction and reduces the magnitude, thus the axial component of velocity is reduced. This is reason that CFD results with collision (Fig. 9c) show a better agreement with experiments than results without collision (Fig. 9d).

To investigate the lateral diffusion of the drops, the mass flow rates are shown in terms of radial distribution at different downstream locations (Fig. 10). In general, the small droplets tend to stay closer to the centerline while the largest droplets tend to be more spread out (especially when the

collision is turned off in Fig. 10d). Their increased radial can be attributed to their initial radial velocity and their high inertias coupled with turbulent diffusion. The predicted mass flow radial distributions are quite similar in shape to the experiments but tend to over-predict the radial spread of the droplets. This again suggests that the simulations are over-predicting the turbulent kinetic energy of the gas. An effect which may have caused this difference is the lack of inter-phase coupling to the gas turbulence evolutionary equations (Eqs. 1 and 2) since it is known that droplets much smaller than the integral eddy sizes (as is the case here) tend to dampen turbulence as discussed by Sundaram & Collins [25]. Unfortunately, such coupling is not well understood [26] so that there is no robust model for this for CFD and thus is typically ignored [16]. Such turbulence coupling is an outstanding challenge for these flows, which should motivate further research in this area.

The overall droplet size distributions at four different axial stations are shown in Tab. 2 and are compared with the experimental data. In the experiment of Santolaya *et al.* [9], the percentages of liquid volumetric flow rate for medium and large size droplets were given, as well as droplet mean diameter of the volume size distribution (D_{43}). Herein, the volumetric flow rates are converted to mass flow rate ($\dot{m}_{dot}$) and the CFD predictions are listed by side. It can be seen that, for the medium droplet size, the percentage decreases when going downstream. On the contrary, for the large droplet size, the percentage increases because droplets collide and they merge into larger droplets. Due to droplet collisions, the droplet mean diameter increases a lot in both experiments and simulations. The simulations provide a reasonable prediction and show a good agreement with the experiment data on the axial droplet size distribution and development.

Finally, the droplet kinetic energy was investigated to gain insight into the controlling physics. Since no experimental results were available, the CFD predictions of droplet turbulence were compared to modeled results which employ a combination of particle kinetic theory and the

predicted gas flow turbulence. In order to describe lateral velocity fluctuation of the droplets, the particle radial velocity fluctuation is defined as

$$v'_{r,rms} = (v_r - \overline{v_r})_{rms} \quad (12)$$

where v_r indicates particle radial velocity, $()'$ indicates a fluctuation from the mean value and $()_{rms}$ indicates the root-mean-square value. This radial particle kinetic energy can be compared to the gas turbulent kinetic energy based on theory in Ref. 23 which employs the integral-scale particle Stokes number, which is the ratio of the particle inertia (Eq. 10) to turbulent integral time-scale (Eq. 8c):

$$\frac{v'_{r,rms}}{u'_{r,rms}} = \frac{1}{\sqrt{1 + St_\Lambda}} \quad (13a)$$

$$St_\Lambda = \frac{\tau_d}{\tau_\Lambda} \quad (13b)$$

The ratio of particle to gas velocity fluctuations (Eq. 13a) tends to unity when the Stokes number trends to zero, i.e. the particle turbulence will tend to the gas turbulence as the droplet size and inertia becomes very small so that it simply follows and mimics the gas motion. As shown in Fig. 11, the simulations of the droplet velocity fluctuations are consistent with this inertial theory and the predicted gas velocity fluctuations. The results also show that the small droplets are in close equilibrium with the fluctuating gas flow at this far downstream location while the large drops have substantially reduced fluctuations (relative to the gas) in the core region but tend to equilibrium conditions at large radial locations.

5. Conclusions

The present investigation demonstrates a numerical approach to predict droplets and gas flow distributions for a pressure-swirl nozzle, by employing initial conditions just after the liquid sheet

break-up and droplet formation. This approach can save both mesh resolution and CPU time by avoiding simulation details of the complicated break-up region. In the present approach, inputs of both continuous and disperse phases (including velocity, flow rate, and turbulence) are introduced at the inflow boundary ($x = 9$ mm) of an axisymmetric domain. The spherical droplets were simulated by using Rosin-Rammler equation to represent the polydisperse size distribution. The time-averaged simulation results show good agreement of the axial velocity of both the gas and the droplets with the experimental data in terms of both radial and streamwise spatial distributions. This included an average error of 8.5% and a peak error of 37.4% for droplet velocity. The development of the average spray structure is reasonably predicted, with all droplet sizes showing a smooth radial distribution of mass flux with a peak flux away from the centerline. The trends of increasing radial penetration for the larger droplets relative to the smaller ones was well predicted by the experiments, but there was an over-prediction of the radial diffusion for larger size drops. This may be attributed to a lack of inter-phase coupling to the gas turbulence, which is challenge for these flows and should motivate further research in this area. For radial mass flux prediction, the average error was 23.5% and the peak error of 33.3% at $x = 72$ mm. For overall droplet size distribution at different axial stations, it shows a good agreement between the experimental data and the CFD predictions. In general, the numerical approach used herein allowed for highly efficient simulations with detailed velocity characteristics quantitatively consistent with experiments and radial mass flux predictions that are qualitatively correct. In addition, the predicted ratios of particle velocity fluctuations agree with inertial theory, indicating that they are governed by their local Stokes numbers and the underlying gas flow turbulence.

Acknowledgements

The spray simulation is based upon work performed within “EFRI-RESTOR/GOALI: Novel Compressed Air Approach for Off-shore Wind Energy Storage” project, supported by the National Science Foundation under Grant No. NSF/EFRI-1038294.

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Fig. 1 Comparison of numerical results to the experiment of Snyder and Lumley [20]
for a) turbulent kinetic energy and b) dissipation rate

Fig. 2a Numerical results of dispersion of four kinds of particles (with increasing particle response time): a) hollow glass (0.00174sec), b) corn pollen (0.0223sec), c) solid glass (0.0557sec) and d) copper (0.0594sec).

Fig. 2b Diffusion comparison of numerical results to the experiment of Snyder and Lumley [20]

Fig. 3 Sketch of simulation domain based on figure from Santolaya *et al.* [9]

Tab. 1 Boundary conditions used in present simulation

Boundary Type	Position	Condition
Axis	$r = 0$ mm	N/A
Velocity inlet	$x = 9$ mm	Specify velocity profile, turbulent kinetic energy profile, and dissipation rate profile
Wall	$r = 170$ mm	No slip, adiabatic, droplet escapes when hit it
Pressure outlet	$x = 80$ mm	Zero gauge pressure

Fig. 4 Droplet mass flow rate distribution at 9 mm downstream of the orifice

Fig. 5 Axial velocity input for both gas and particles at 9 mm

Fig. 6 Large particle axial velocity input by adding randomness at 9 mm

Fig. 7 Droplet mass flow rate input

Fig. 8 Simulation result (left: without particle; right: with particles): a) contours of gas velocity magnitude (m/s), and b) contours of turbulent kinetic energy (m^2/s^2)

Fig. 9 Droplet axial velocity comparison between CFD and experiment

a) at $x = 18$ mm, b) at $x = 36$ mm, c) at $x = 72$ mm,

and d) at $x = 72$ mm turn-off collision

Fig. 10 Droplet mass flow rate comparison between CFD and experiment

a) at $x = 18$ mm, b) at $x = 36$ mm, c) at $x = 72$ mm,

and d) at $x = 72$ mm turn-off collision

Tab. 2 Comparison of the overall droplet size distribution at different axial station

x [mm]	Medium Size %m _{dot}		Large Size %m _{dot}		D ₄₃ [μm]	
	Exp.	CFD	Exp.	CFD	Exp.	CFD
9	22.1	21.0	11.1	15.4	37.89	36.32
18	17.1	19.3	13.8	16.7	39.95	37.39
36	13.3	15.4	20.3	20.0	42.71	39.64
72	9.1	11.4	21.6	23.7	49.67	44.69

Fig. 11 Droplet kinetic energy radial distribution at $x = 72$ mm