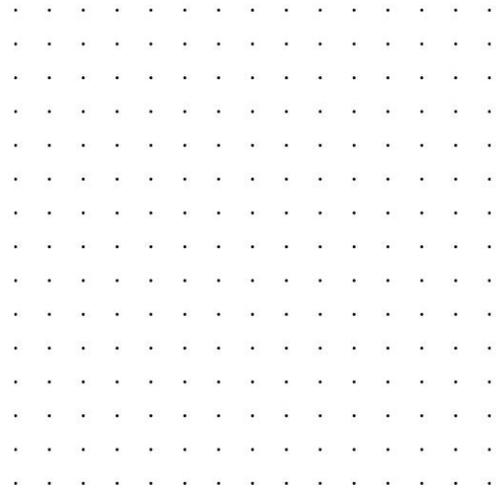




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**International Fine Particle
Research Institute**

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Unveiling the Potential of CFD for Nozzle Spray Prediction

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Unveiling the Potential of CFD for Nozzle Spray Prediction

EXECUTIVE SUMMARY

The state-of-the-art in using the Computational Fluids Dynamics (CFD) technique for spray prediction lies in the pursuit of a delicate balance between the computational requirements and the flexibility and accuracy of the prediction. We will investigate the potential of the VOF-DPM technique (volume of fluid-discrete particle modelling), which is a subset of CFD, to provide this delicate balance for routine engineering spray prediction. The scope of this investigation will cover single fluid hollow-cone and full-cone atomization, with fluid viscosity ranging between 1 to 260 mPa.s. This project is in alignment with existing spray characterization facility in the University of Auckland. We will experimentally characterize the filament formation and the primary and secondary droplet breakup behavior, complementing the VOF-DPM analysis. The main outcome from this project are strategies in using the VOF-DPM technique for hollow cone and full cone spray prediction.

BACKGROUND

Commercially available swirl nozzles is commonly developed and characterized with water. This poses significant uncertainties in nozzle selection and operation for spray dryer or spray granulator operators, as the sprayed solutions are typically very different from water (eg. high viscosity binders, concentrated solution in spray drying, organic solvent-based solutions in the pharmaceutical industry). Contract manufacturers, in particular, will find these uncertainties even more challenging as they regularly deal with new product or binder formulations.

Direct measurement and characterization of nozzles in the industry is not routinely feasible due to manufacturing compliances and the cost associated in setting up the measurement facility onsite. Manufacturers work around these uncertainties by relying on guessing work and experiences with specific nozzles and settings. There are also a vast number of empirical correlations available in the literature to help guide manufacturers in nozzle selection and operation ^[1]. Due to the rapid development in nozzle design and the typically limited conditions in which these correlations are developed, the accuracy of these correlations adds another layer of uncertainty to the problem.

For these reasons, there is a need for a flexible toolbox to guide manufacturers in nozzle selection and operation. The flexible toolbox should overcome the current limitations and should be able to provide a reliable indication on the droplet size distribution and spray angle accounting for different nozzle constructions, product formulations and operating conditions. This project will explore the use of the Computational Fluid Dynamics (CFD) simulation technique as a flexible atomization predictive toolbox.

STATE-OF-THE-ART IN CFD SPRAY PREDICTION

The atomization process from a pressure nozzle involves the initial formation of thin filaments. Primary breakup of the filaments forms the primary droplets, which undergoes further secondary breakup into finer droplets (also potential coalescence throughout the process). Figure 1 illustrates this process. Within the CFD simulation framework, the Volume-of-Fluid (VOF) technique (and its variant in meshing and surface detection algorithm), is the main method used to capture these various phenomenon composing the atomization process. Figure 2 summarizes the state-or-the-art in this area.

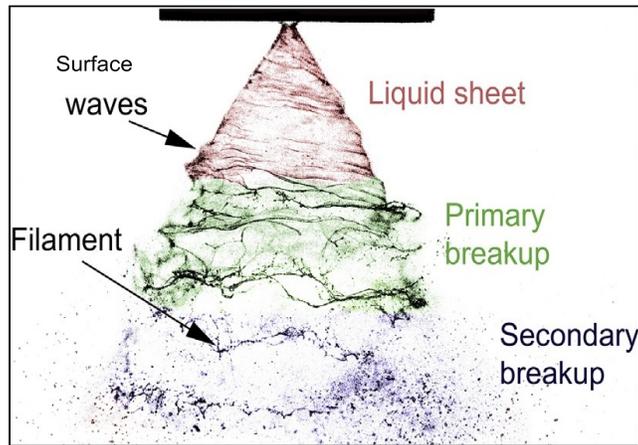


Figure 1. Breakdown of the atomization process [2]

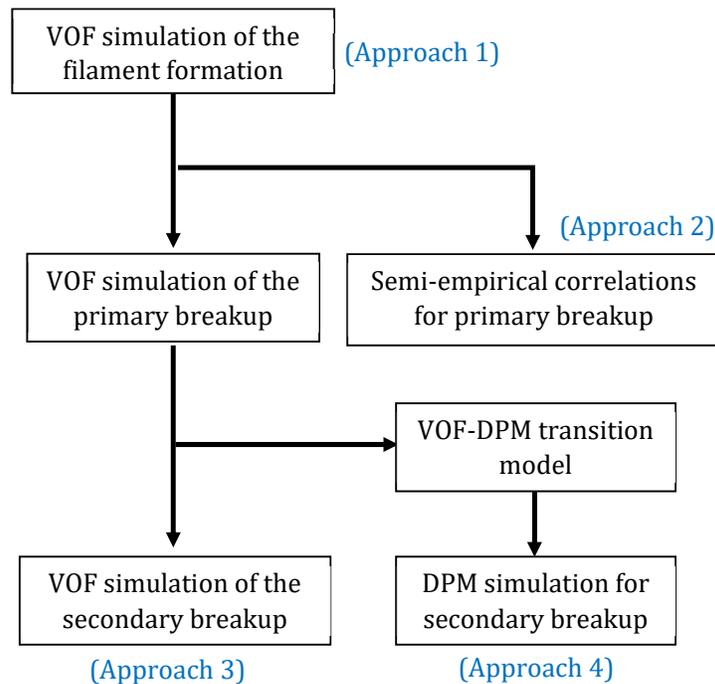


Figure 2. The state-of-the-art in CFD spray prediction

In essence, the VOF technique involves tracking the interface of the atomized fluid throughout the simulation domain. It is a very computationally expensive technique as excessively fine mesh is required to capture the characteristic length scale of the atomization process which stretches across several magnitudes: from centimeters (the nozzle size and the length scale of the whole spray), hundreds of microns (film formation), to tens of microns (primary and secondary droplets). The state-of-the-art in this area lies in the pursuit of a delicate balance between the computational requirements and the degree of flexibility and accuracy from the VOF simulation.

Most of the reported simulation work focuses on Approach 1 (Figure 2), as it provides a computationally inexpensive indication on the performance of the atomizer ^{[3][4][5][6][7]}. The application of just predicting the filament or cone formation is limited, because it does not provide a prediction of the final droplet size distribution. Some worker extended this approach by coupling the VOF predictions with empirical correlations linking the characteristics of the filament with the final droplet size distribution (Approach 2 in Figure 2) ^[8]. The empirical correlation developed so far, employed in the reported framework, was developed based only on an idealized primary breakup process ^{[9][10][11]}. While this approach may be low in computational cost, it is in essence empirical and there is significant random uncertainty in the accuracy of the prediction across a wide range of nozzle geometry and fluids ^[8].

At the other end of the spectrum, Approach 3 (Figure 2) utilizes the VOF technique to provide a full visualization of the atomization process, from the filament formation to the secondary breakup phenomenon ^{[12][13][14][15][16]}. The main drawback is that it requires very significant computational resources. Limiting the simulation to regions very close and adjacent to the nozzle may partly overcome this problem. However, this limits the predictive capability to capture the full effective characteristics of the spray. For this reason, this technique may not be useful for routine engineering application.

In the middle of the spectrum is Approach 4 (Figure 2), which involves the VOF-DPM technique ^{[17][18][19]}. This technique transforms the VOF predicted primary droplets and represents them as discrete points in the simulation (hence, DPM - Discrete Phase Modelling). This obviates the need for excessively high computational resources in modelling the secondary breakup of the primary droplets as imposed by Approach 3. This approach also does not have empirical limitations as imposed by Approach 2, because the VOF technique explicitly captures the primary breakup. Therefore, now, this technique provides the greatest potential for the application of CFD in atomization prediction for routine engineering applications; striking a balance between computational requirement and the level of details from the simulation. A survey of the literature on this approach revealed that there is currently limited systematic validation work for Approach 4. Most of the reported work focused on fuel injection atomization. There is currently no one single study systematically evaluating this approach across hollow and full cone swirl atomization, with fluids typically used in powder production or in the atomization of binders (for granulation). These two types of nozzles (hollow and full cone) will involve significantly different filament formation characteristics, hence, different distribution of the primary droplets and different propensity for secondary breakup or coalescence. It is uncertain how well the VOF-DPM technique captures these

scenarios. Most importantly, there is a need to ascertain suitable numerical strategies for the different spray conditions. This project will fill these gaps in knowledge.

On this basis, the following are the objectives of this project:

Objective 1: To evaluate the VOF-DPM technique for hollow cone single fluid swirl atomization prediction
Objective 2: To evaluate the VOF-DPM technique for full cone single fluid swirl atomization prediction

EXPECTED PROJECT OUTCOMES

We will gain a deeper understanding on how the various numerical parameters of the VOF-DPM technique affect the accuracy and the computational requirements of the atomization prediction. We will provide recommendations on strategies to achieve a balance between accuracy and computational requirements from an industry perspective. In most cases (particularly for contract manufacturers), the capability to realistically cover a range of possible operating conditions may bring more benefits than achieving very high accuracy within a limited range. We will develop strategies for both hollow cone and full cone atomization. We envisage two publications from this project, one publication from each objective.

PROJECT PLAN

Work Packages		Year 1				Year 2				Year 3			
		Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
1	Retrofitting rig for film formation measurement.	■											
2	Nozzle CAD geometry development	■											
3	VOF-to-DPM modelling framework development			■									
4	Atomization experiments (hollow cone)				■								
5	VOF-to-DPM simulation (hollow cone)				■								
6	Objective 1 completion							★					
7	Atomization experiments (full cone)								■				
8	VOF-to-DPM simulation (full cone)								■				
9	Objective 2 completion											★	
10	Bi-quarterly project update		★		★		★		★		★		
11	PhD thesis completion											★	
12	Project final report											★	

Work Package 1: Retrofitting measurement rig for film formation measurement

We have an existing Spraytec laser diffraction facility, with a compressed air driven atomization system for up to 15 Bar pressure. This setup allows for vertical height adjustment of the nozzle, which will be important for measuring the primary and secondary breakup process, respectively. For this project, we will retrofit the system to allow high speed and high-resolution camera measurement of the film formation. Extending a reported method [3], we will use planar laser illumination to allow video capture of the shape of the filament formed. We will undertake 2D planar analysis of the filament formation process with ImageJ image processing, to obtain filament thickness, cone angle, penetration distance data. In the absence of an LDA system, we will determine the filament velocity by high-speed video recording and analysis using the Trackmate plugin in ImageJ.

Work Package 2: Nozzle CAD geometry development

From our experience, it will be difficult to obtain detailed nozzle CAD from nozzle manufacturers. We will 3D scan the nozzles used in the experiments (internal inserts and housing) to develop the CAD geometry for the simulations. We will be exploring two sets of hollow and full cone BETE nozzles. For the full cone single welded nozzles, we will 'dissect' the nozzles in the workshop to enable scanning of the internal geometry.

Work Package 3: VOF-to-DPM modelling framework development

We have access to the New Zealand NESI high performance-computing cluster. We will develop the modelling framework locally before integration with the NESI network. We will use the ANSYS Fluent CFD package.

Work Package 4 & 7: Atomization experiments

We will use glycerin, water and ethanol mixtures to generate fluid with a range of viscosity (1 – 260 mPa.s), density (970 - 1200 kg/m³) and surface tension (41 – 72 mN/m) [20]. The advantage of the using mixtures with these components is that it is transparent and this will facilitate film measurements.

We will use the following set of nozzles and will undertake the experiments at various atomization pressures to cover a wide range of operating conditions. For each mixture, we will measure the filament characteristics as described earlier and will characterize the primary and secondary breakup phenomenon.

BETE Twist & Dry Low Flow Hollow Cone (TDL1-22, TDL4-22, TDL1-27, TDL4-27): This set of hollow cone nozzle will provide a combination of swirl velocity and orifice size for wide evaluation of the model.

BETE WL Low Flow Full Cone (WL1/4, WL1/2, WL3/4): This set of full cone nozzles will provide a set of orifice sizes for wide evaluation of the model.

Work Package 5 & 8: VOF-to DPM simulations

We will numerically simulate the extensive set of experimental runs. We will make comparison in terms of the prediction of the filament characteristics, droplet size

distribution from the primary breakup of the film and the droplet size distribution after the secondary breakup of the droplet. The bulk of the analysis will focus on analyzing how different meshing strategies, VOF surface tracking approaches and VOF-to-DPM numerical parameters affect the accuracy as well as the computational requirement of the model.

PERSONNEL

A/Prof. Meng Wai Woo has 15 years' experience in CFD simulations and have undertaken CFD projects with the spray drying, pharmaceutical and resource recovery industry. He will lead the project and will recruit a PhD student with strong CFD and CAD simulation background for the project. The student will be working on both objectives of the project.

PROJECT ALIGNMENT TO EXISTING FACILITIES

The project is in alignment with the following capabilities and facilities available to the team.

Spraytec: This will be the main equipment used for the sprayed droplet characterization. Meng has significant experience in using this equipment for high flow industrial scale spray characterization (current project with the NZ dairy industry).

Atomization rig: This compressed air driven rig developed for the current dairy based atomization characterization project will be used for the proposed work and will be able to handle up to 15 bar atomization pressure and can be retrofitted with different nozzles.

3D scanner for nozzle CAD development: We will have access to this facility as part of the University of Auckland Digital Research Hub.

ANSYS Workbench access: We have access to the ANSYS Workbench academic license package. The academic license is limited to simulations with 500k in the number of mesh. We will work within this boundary for the project. Achieving a suitable numerical strategy to work around this will provide a good incentive for industry adoption of the technique so that reasonable computation time and resources are feasible.

Access to NESI HPC Cluster: The University of Auckland is a partner of the NESI HPC cluster and we will have access to the cluster without any additional cost to the project.

BUDGET & JUSTIFICATION

Item	Year 1 (\$NZD)	Year 2 (\$NZD)	Year 3 (\$NZD)
<u>PhD Student:</u>			
Stipend	28,500	28,500	28,500
Fees	9,540	9,540	9540
<u>Measurement facility retrofitting:</u>			
High speed camera purchase	10,000	-	-
Compressed air curtain for camera	1,000	-	-
Planar laser illumination setup	8,000	-	-
Workshop cost	1,000	-	-
<u>Consumables and experimental needs:</u>			
Solutions for experiments	1000	1000	1000
Nozzles	4000	-	-
TOTAL budget requested from IFPRI	63,040	39,040	39,040

PhD student stipend and fees: The amount requested is the standard three-year full scholarship provided to students in the University of Auckland.

Measurement facility retrofitting: The requested support goes towards retrofitting the existing facility for atomizer film or ligament formation measurement. The amount requested is for a Kron Technologies high-speed camera (Kronos 2.1 HD model) and includes the positioning adjustment tripod. The planar laser illumination setup includes the cost for the planar laser source. The compressed air curtain is to protect the camera from mists and splashes generated by the spray. We have significant experience managing this when undertaken measurements with high flow rate sprays.

Consumables and experimental needs: We will purchase two sets of nozzles suitable for low manageable spray rates in the laboratory and for covering the experimental range as described earlier. This cost includes purchasing additional (full cone nozzles) units for 'dissecting' to allow full 3D scanning of the nozzles internals. We will purchase glycerin and ethanol for the atomization experiments. Corresponding to the flowrates of nozzles described, we estimate that 25L of glycerin and 5L of ethanol will be sufficient each year for the experiments.

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