

# Unveiling the Potential of CFD for Nozzle Spray Prediction

## REVISIONS MADE TO THE PROPOSAL

Comments: The members feel that your proposal meets most of what is asked for in the brief, however they feel that it could be improved by providing more detail about the models you will use (e.g. turbulence models, droplet size distribution) ...

*Response: We will use the Large Eddy Simulation framework to capture the turbulence behavior of the flow. The droplet size distribution will not be empirically modelled, rather, it will be a results of the VOF-to-DPM framework implemented into model. We will be evaluating how different combinations of meshing strategies and VOF-to-DPM threshold settings affect the accuracy of the prediction. Building on top of the prediction on the primary atomization, we will also be evaluating the significance of secondary droplet breakup (using the Taylor analogy model) and coalescence (using the O'Rourke algorithm) on the overall droplet size prediction. One of our main goals will be to determine strategies to achieve a delicate balance between the level of complexity and the accuracy of the modelling framework.*

*We have now updated the description above in the last paragraph of Work Package 2&4 on Page 6 of the proposal.*

Comments: ... and the experimental justification of the relevance of ANSYS-Fluent in producing closures with accurate predictions on realistic system size.

*Response: There are numerous publications below lending evidence to the suitability of ANSYS-Fluent in capturing realistic atomization behavior for single fluid pressure swirl nozzles, which is the premise of this proposal.*

*[24] Yu, H., Jin, Y.C., Cheng, W., Yang, X., Peng, X., Xie, Y. 2021. Multiscale simulation of atomization process and droplet particles diffusion of pressure-swirl nozzle. Powder Technology 379, 127-143.*

*[25] Sun, Y., Alkhedhair, A.M., Guan, Z., Hooman, K. 2018. Numerical and experimental study on the spray characteristics of full-cone pressure swirl atomizers. Energy 160, 678-692.*

*[26] Nihasingaye, P.B., Zhou, G., Yang, X. 2021. Modelling spray performance of alternative aviation fuel. Energy 224, 120086.*

*We have strong familiarity with the ANSYS Fluent CFD package and the ease-of-use of its interface will be attractive for subsequent industrial applications. Nevertheless, we will*

*interpret our results with emphasis on the fundamental theoretical model and the numerical strategy used, so that our recommendations are applicable even if a different CFD package or open-sourced framework is used.*

*We have now revised the description of Work Package 1 on Page 5 of the proposal to include the above justification.*

Comments: A significant amount of the work that you propose is experimental, while the brief specifies a computational project. Would it be possible to use published data to validate your model instead? This might allow you to include non-Newtonian systems in your project.

**Response:** *We have undertaken an extensive search of the literature for suitable and reliable experimental data to complement our proposed simulation work. Experimental data from the two report below by Günter Brenn and co-workers will be adopted. Günter Brenn is the editor-in-chief (Europe) for the journal Atomization and Sprays. These sets of data cover Newtonian and non-Newtonian fluids. More interestingly is that they were generated in collaboration with Nestle under industry relevant conditions, suitable for this project.*

*We have now significantly revise and included justification in selecting these two sets of experimental data for this project on Page 5 of the proposal in describing Work Package 2 & 4. We have also revised the Gantt Chart on Page 4.*

[21] *Tratnig, A., Brenn, G., Stricner, T., Fankhauser, P., Laubacher, N., Stranzinger, M. 2009. Characterization of spray formation from emulsions by pressure-swirl atomizers for spray drying. Journal of Food Engineering 95, 126-134.*

[22] *Tratnig, A., Brenn, G. 2010. Drop size spectra in sprays from pressure-swirl atomizers. International Journal of Multiphase Flow 36, 349-363.*

Comments: Additionally, a number of members (representing most companies who use spray drying extensively) were disappointed that your plan doesn't include non-Newtonian fluids.

**Response:** *We have now revised the proposal to include non-Newtonian fluids. Simulation work on the non-Newtonian fluids will be undertaken in Work Package 4. We will complement the simulation work with experimentally data from the report below. Two emulsion based non-Newtonian fluids with well characterized shear thinning behavior will be explored.*

[21] *Tratnig, A., Brenn, G., Stricner, T., Fankhauser, P., Laubacher, N., Stranzinger, M. 2009. Characterization of spray formation from emulsions by pressure-swirl atomizers for spray drying. Journal of Food Engineering 95, 126-134.*

Comments: Finally, your budget is front-end loaded, which is inconsistent with how IFPRI pays for projects (i.e., three annual \$40,000 grants). Hopefully, this won't be a major inconvenience for you.

***Response:** The initial front-end loaded budget was mainly due to the experimental components in the initial proposal. We have now removed the experimental components and revised the proposal to use reported experimental data. Hence, the three annual \$40,000 grant model will work for the project.*

*We have now revised the budget on Page 6 of the proposal.*

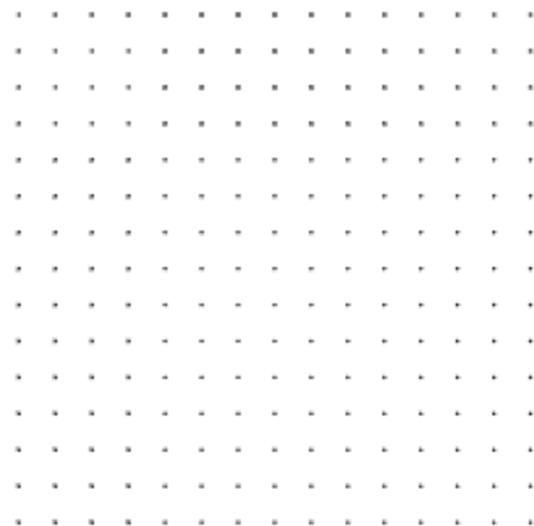


PROPOSAL TO:

**International Fine Particle  
Research Institute**

PREPARED BY:

**A/Prof. Meng Wai Woo**



# **Unveiling the Potential of CFD for Nozzle Spray Prediction**

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(Revised)

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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 numerical investigation will cover the pressure swirl atomization of *Newtonian* and *non-Newtonian* fluids. We will base the simulation exploration on experimental data from Günter Brenn and co-workers <sup>[21][22]</sup>, undertaken and reported in collaboration with Nestle. Hence, the numerical exploration in this work will have strong industrial relevance. This project is in alignment with existing spray characterization facility in the University of Auckland. The main outcome from this project will be strategies in using the VOF-DPM technique for nozzle atomization 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 <sup>[1]</sup>. 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.

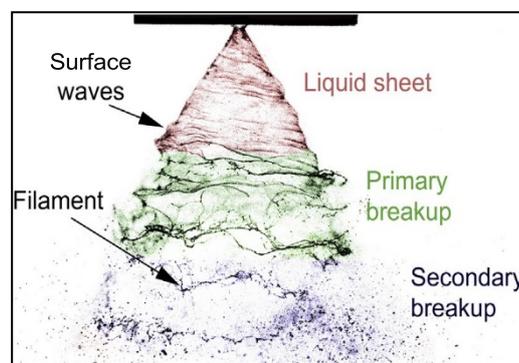


Figure 1. Breakdown of the atomization process <sup>[2]</sup>

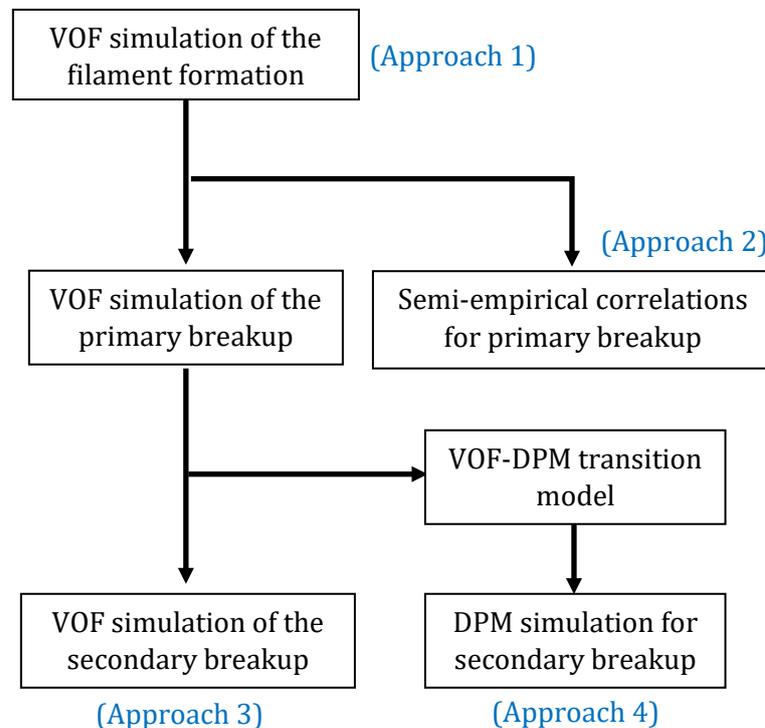


Figure 2. The state-of-the-art in CFD spray prediction

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 <sup>[3][4][5][6][7]</sup>. 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) <sup>[8]</sup>. The empirical correlation developed so far, employed in the reported framework, was developed based only on an idealized primary breakup process <sup>[9][10][11]</sup>. 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 <sup>[8]</sup>.

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 <sup>[12][13][14][15][16]</sup>. 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 <sup>[17][18][19]</sup>. 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 Newtonian and non-Newtonian fluids and across various nozzle sizes. It is uncertain how well the VOF-DPM technique predicts the atomized droplet sizes, capturing these parameters under industry relevant conditions. Most importantly,

there is a need to ascertain suitable VOF-DPM 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:

<p><b>Objective 1:</b> To evaluate the VOF-DPM technique for <u>Newtonian fluid</u> pressure swirl atomization prediction</p> <p><b>Objective 2:</b> To evaluate the VOF-DPM technique for <u>non-Newtonian fluid</u> pressure swirl atomization prediction</p>
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### 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 Newtonian and non-Newtonian fluids. We envisage two publications from this project, one publication from each objective (Milestones #3 and #5 in the table below).

### PROJECT PLAN

Work Packages		Year 1				Year 2				Year 3			
		Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
1	VOF-to-DPM modelling framework development	■											
2	VOF-to-DPM simulation (Newtonian fluid)				■								
3	Objective 1 completion							★					
4	VOF-to-DPM simulation (non-Newtonian fluid)								■				
5	Objective 2 completion											★	
6	Bi-quarterly project update		★		★		★		★		★		
7	PhD thesis completion											★	
8	Project final report											★	

## Work Package 1: 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 using the ANSYS-Fluent package before integration with the NESI network. There are numerous publications lending evidence to the suitability of ANSYS-Fluent in capturing realistic atomization behavior for single fluid pressure swirl nozzles, which is the premise of this proposal <sup>[24][25][26]</sup>. We have strong familiarity with the ANSYS Fluent CFD package and the ease-of-use of its interface will be attractive for subsequent industrial applications. Nevertheless, we will interpret our results with emphasis on the fundamental theoretical model and the numerical strategy used, so that our recommendations are applicable even if a different CFD package or open-sourced framework is used.

## Work Package 2 & 4: VOF-to DPM simulations

We have undertaken an extensive search of the literature for suitable experimental data to complement our proposed simulation work. Key criteria for the experimental data were:

1. Spray rates and droplet sizes relevant to industrial operation.
2. Sufficient atomizer geometry and spray operation data available for simulation.
3. Full set of fluid properties available for simulation.
4. Stretches across *Newtonian* and *non-Newtonian* fluids.
5. Atomized droplet size distribution data (not just data on the internal core and external film formation).
6. Reliable measurements from a reputable group.

Fulfilling the criteria above, we have decided to adopt the experimental data by Günter Brenn and co-workers (Graz University of Technology), published in two separate papers cited here <sup>[21][22]</sup>. These two sets of data were undertaken in collaboration with the Nestle Product Technology Centre and is of high relevance to the industry. In addition, both sets of data were generated using the same range of Delavan single-fluid swirl nozzles (with different housing and orifice plate combinations). This will allow us to systematically evaluate the capability of the model to capture various geometrical configurations and to systematically extend the evaluation across *Newtonian* and *non-Newtonian* fluids.

To be more specific, this work will cover the following range of fluid properties,

Newtonian fluids: Dynamics viscosity (8-166 mPas), density (1240-1315 kg/m<sup>3</sup>), surface tension (51-72 mN/m)

Non-Newtonian fluids: Two shear thinning fluids (EM1 & EM2) with Carreau-Yasuda model fitted shear thinning characteristics

EM1 - solid contents (45.2 %wt), density (1110 kg/m<sup>3</sup>), surface tension (0.0425 mN/m)

EM2 - solid contents (49.8 %wt), density (1090 kg/m<sup>3</sup>), surface tension (0.0425 mN/m)

We will compare the film forming characteristics and droplet size distribution from the primary breakup of the film. We will use the Large Eddy Simulation (LES) framework to capture the turbulence flow field of the atomization [23][24]. This has been reported as a suitable compromise, capturing sufficient turbulent characteristics for atomization prediction (compared to RANS and its variants) without excessive computational requirements (compared to DNS simulations). The droplet size distribution will not be empirically modelled, rather, it will be a result of the VOF-to-DPM framework implemented into the model. We will be evaluating how different combinations of meshing strategies and VOF-to-DPM threshold settings affect the accuracy of the prediction. Building on top of the prediction of the primary atomization, we will also be evaluating the significance of secondary droplet breakup (using the Taylor analogy model) and coalescence (using the O'Rourke algorithm) on the overall droplet size prediction. One of our main goals will be to determine strategies to achieve a delicate balance between the level of complexity and the accuracy of the modelling framework.

## PROJECT ALIGNMENT TO EXISTING FACILITIES

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

*ANSYS Workbench access:* We have access to the ANSYS Workbench academic license package. This package is also available in the NESI HPC Cluster that we will use for this project.

*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	9,540
<u>Equipment:</u>			
Computer	4,000	-	-
<b>TOTAL budget requested from IFPRI</b>	<b>42,040</b>	<b>38,040</b>	<b>38,040</b>

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

*Computer:* The amount requested is for a local workstation for the student in developing the model and to interface with the NESI HPC Cluster.

## 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.

## REFERENCES

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