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## **Atomization modelling : An Eulerian approach**

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**Keywords:** two-phase flow, liquid dispersion, hollow cone nozzle, Fluent CFD software.

### **Abstract**

**Reducing pesticide drift requires particularly a better understanding of atomization process. An Eulerian model was therefore developed to model the atomization of a liquid sheet generated by a hollow cone nozzle. First, three-dimensional calculations were performed to model the turbulent swirled flow inside the nozzle. Second, two-dimensional axisymmetric calculations were carried out to model liquid dispersion into the air and to calculate droplet Sauter Mean Diameter and droplet velocity. 3-D calculations were used as boundary conditions for the 2-D calculations. A “one-fluid-two-phase” approach was developed. A fluid with variable density was considered. The mean density was dependant on the Favre averaged liquid mass fraction. Liquid dispersion into air was calculated thanks to a transport equation for the mean liquid mass fraction. As the flow was highly anisotropic, the Reynolds Stress Model was used for turbulence. Moreover, a transport equation for the mean liquid/air surface area was developed. Production of the mean surface area was linked to the mean flow stretching, turbulence and droplet break up effect. Destruction of the mean surface area was related to droplet coalescence effect and took into account surface tension coefficient. Combining liquid mass fraction with surface area led indeed to the assessment of a Sauter Mean Diameter all over the calculation domain. The model was implemented in Fluent 6 Computational Fluid Dynamics software, using User Defined Functions. Experimental droplet axial velocity and droplet diameter were measured using Phase Doppler Anemometry. Comparisons between modeling and experimental data showed good agreement.**

### **INTRODUCTION**

During pesticide spraying, the way the droplets reach or not the target depends in particular on their size and velocity (Nuyttens et al., 2010). Atomization process consists in producing discontinuous liquid fragments from a continuous sheet or jet. This is a mechanism also called first break up in contrast with secondary break up that concern the subsequent break up of the ligaments into droplets. The well-known Eulerian–Lagrangian numerical approximation is frequently adopted for prediction of the multi-phase flows. Liquid phase is described as stochastic particles with a given radius and velocity injected into the air within a prescribed spray angle. However, this approach does not model the atomization process itself as it considers droplets already formed. Moreover, close to the nozzle, there are liquid ligaments rather than spherical drops.

Therefore, an Eulerian “one-fluid-two-phase” approach was proposed. Investigation of the two-phase flow inside and outside a hollow cone nozzle was performed. The ultimate goal of this research was on the one hand to describe liquid

dispersion into the air, and on the other hand, to calculate droplet characteristics (diameter and velocity) issued from the nozzle.

## MATERIALS AND METHODS

### Eulerian Model

The two-phase flow was considered as a turbulent flow of a fluid with a variable density composed of a liquid and a gas mixture. High Weber and Reynolds numbers were considered, so that capillarity and laminar viscosity were neglected for the large-scale liquid dispersion calculation. On the other hand, capillarity was taken into account to carry out the small-scale liquid/air surface area calculation.

Conventional conservation equations for the total mass and the mean momentum of the stationary turbulent flow were calculated following:

$$\frac{\partial \bar{\rho} \tilde{u}_j}{\partial x_j} = 0$$

$$\frac{\partial \bar{\rho} \tilde{u}_i \tilde{u}_j}{\partial x_j} = - \frac{\partial \bar{p}}{\partial x_i} - \frac{\partial \overline{\bar{\rho} u_i'' u_j''}}{\partial x_i}$$

where  $\bar{\rho}$  is the mean density,  $\tilde{u}_j$  and  $u_j''$  are the  $j$ th Favre averaged velocity component and velocity fluctuation component respectively and  $\bar{p}$  is the mean pressure. The Reynolds stress tensor  $\overline{\bar{\rho} u_i'' u_j''}$  was calculated by a transport equation for each of the six components. Indeed, the well-known (k,ε) model was not suited to our study.

The mean density  $\bar{\rho}$  was related to the Favre averaged liquid mass fraction  $\tilde{Y}$  by:

$$\frac{1}{\bar{\rho}} = \frac{\tilde{Y}}{\rho_l} + \frac{1 - \tilde{Y}}{\rho_g}$$

where  $\rho_l$  and  $\rho_g$  are the constant liquid and gas densities respectively.

Liquid dispersion was modeled thanks to a transport equation for the mean liquid mass fraction. Neglecting the laminar diffusion flux, this equation was written as follow:

$$\frac{\partial (\bar{\rho} \tilde{Y} \tilde{u}_i)}{\partial x_i} = - \frac{\partial \overline{\bar{\rho} u_i'' \tilde{Y}}}{\partial x_i}$$

$$\overline{\bar{\rho} u_i'' \tilde{Y}} = - \left[ \frac{\mu_t}{Sc_t} + \frac{C_p \bar{k}^2 \bar{\rho}^2}{\bar{\varepsilon}} \left( \frac{1}{\bar{\rho}_g} - \frac{1}{\bar{\rho}_l} \right) \right] \frac{\partial \tilde{Y}}{\partial x_i}$$

From the mean mass fraction, it was possible to calculate the mean volume mass fraction  $\bar{\tau}$  following:

$$\bar{\tau} = \frac{\bar{\rho} \tilde{Y}}{\rho_l}$$

Moreover, the transport equation for the mean surface area  $\Sigma$  was developed:

$$\frac{\partial \Sigma \tilde{u}_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \frac{\mu_t}{\bar{\rho} Sc_\Sigma} \frac{\partial \Sigma}{\partial x_i} \right) + (A + a) \Sigma - V_a \Sigma^2$$

where the first term of RHS represented diffusion term with  $Sc_\Sigma = 0.7$ . The second term was composed of two production term, with:

$$A = -\alpha_0 \frac{\overline{u_i u_j}}{\tilde{k}} \frac{\partial \tilde{u}_i}{\partial x_j}$$

$$a = \alpha_1 \frac{\tilde{\epsilon}}{\tilde{k}} + \alpha_2 f(\tilde{Y}, \Sigma, \tilde{\epsilon})$$

where  $A$  stood for the production due to the mean velocity gradient and  $a$  stood for the production of surface area due to turbulence and to collisions.

The last term represented the destruction of surface area. It was linked to surface tension effects and coalescence of liquid fragments. More details can be found in reference (Belhadef 2012).

From both transport equations for the mean mass fraction  $\tilde{Y}$  and the mean surface area  $\Sigma$ , one could estimate the Sauter Mean Diameter from the algebraic following equation:

$$\overline{SMD} = \frac{6\overline{\rho Y}}{\Sigma \rho_l}$$

### Numerical procedure

In the present paper, the flow inside and outside a hollow cone nozzle (ATR 80 lilas, Albuz, CoorsTek Solcera, USA) was modeled. The numerical modeling was performed using the commercially available Fluent 6 CFD software with User Defined Functions. This package was based on a finite volume method, in association with the SIMPLE algorithm and the second order scheme. As the flow inside the hollow cone nozzle was swirled, it was not possible to carry out directly 2D calculations. Therefore, 3D calculations were performed to calculate the flow of water into air from the inside of the nozzle up to 2 cm from the nozzle exit. Left of the Figure 1 shows the sketch of the computational domain with the boundary conditions. The upper part represents half of the nozzle itself, whereas the bottom part represents the outlet domain in order to calculate the flow outside the nozzle. The inlet boundary condition was an injection pressure equal to 4 bar. 1,800,000 tetrahedral cells were used, with a minimum length of 0.03 mm along the discharge hole and coarser length scale far from the exit. As the results showed that the mean liquid mass fraction and mean axial velocity were axisymmetric on the plane located at the inlet of the discharge hole exit, 2D calculations were then performed. Indeed two-dimensional axisymmetric swirl calculations were carried out with a calculation domain that was longer in the axial direction up to 5 cm (see right of the Figure 1). The plane located at the inlet of the discharge area of the 3D calculations was used to define boundary 2D inlet conditions. The 2D computational domain was composed of 26,000 triangular cells.

### Experimental Set-up

The same swirl nozzle ATR 80 as for calculations was used to generate water droplets. Droplet velocity and droplet diameter measurements were carried out using Phase Doppler Anemometry (PDA). PDA is widely used for studying two-phase flows as

it provides both velocity and particle size at a single point. The post-process gave the velocity and the diameter statistics.

## RESULTS AND DISCUSSION

Figure 2 illustrates the 2D field of the mean liquid mass fraction up to 5 cm from the nozzle. Mass fraction lay between 0 and 1. It was equal to 1 inside the nozzle and 0 outside. Liquid dispersion into the air decreased the value of the liquid mass fraction. On the spray axis, the mean liquid mass fraction decreased downstream.

Figure 3 illustrates the profiles of the mean liquid volume fraction for various axial distances from the nozzle exit. Hollow cone spray was easily visible, low values of the mean liquid volume fraction being found close to the spray axis (i.e. for radial position =0). Moreover, this figure showed the liquid dispersion, as the spray was wider downwards and the peak of the volume fraction decreased downstream (i.e. for increasing y values). As far as the velocity was concerned, PDA provided mean liquid velocity, whereas the model supplied velocity of the mixture. Therefore, the mean liquid velocity  $\overline{u_{i/l}}$  was calculated from the mean velocity  $\tilde{u}_i$  following:

$$\overline{u_{i/l}} = \tilde{u}_i + \frac{\overline{\rho u_i Y''}}{\overline{\rho Y}}$$

Figure 4 illustrates comparison of axial profiles of the mean liquid axial velocity obtained on the spray axis both experimentally and by modeling. Good agreement between predictions and measurements was found. Note that mean axial liquid velocity had negative values from the nozzle exit up to 11 mm for PDA and 10 mm for model. The hollow cone spray presented indeed a recirculation zone, whose length was quite well estimated by the model.

## CONCLUSIONS

A one-fluid-two-phase Eulerian model was developed to model the atomization of a liquid sheet generated by a hollow cone nozzle. First, three-dimensional calculations were performed to model the turbulent swirled flow inside the nozzle. Secondly, using 3D results as boundary conditions, two-dimensional axisymmetric calculations were carried out to model liquid dispersion into the air and to calculate droplet characteristics. The mean density of the fluid was dependant on the Favre averaged liquid mass fraction. Liquid dispersion into air was calculated thanks to a transport equation for the mean liquid mass fraction. The Reynolds Stress Model was used for turbulence. Moreover, a transport equation for the mean liquid/air surface area was developed. Combining liquid mass fraction with surface area led indeed to the assessment of a Sauter Mean Diameter all over the calculation domain. The model was implemented in Fluent 6 Computational Fluid Dynamics software, using User Defined Functions. Experimental droplet axial velocity and droplet diameter were measured using Phase Doppler Anemometry. Comparisons between modeling and experimental data showed good agreement. This approach is applicable for studying nozzle geometry influence on droplet characteristics, as well as surface tension coefficient or injection pressure for instance.

### Literature Cited

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Nuyttens, D., De Schampheleire, M., Verboven, P., & Sonck, B. (2010). Comparison between indirect and direct spray drift assessment methods. *Biosystems Engineering*, 105, 2-12.

### Figures

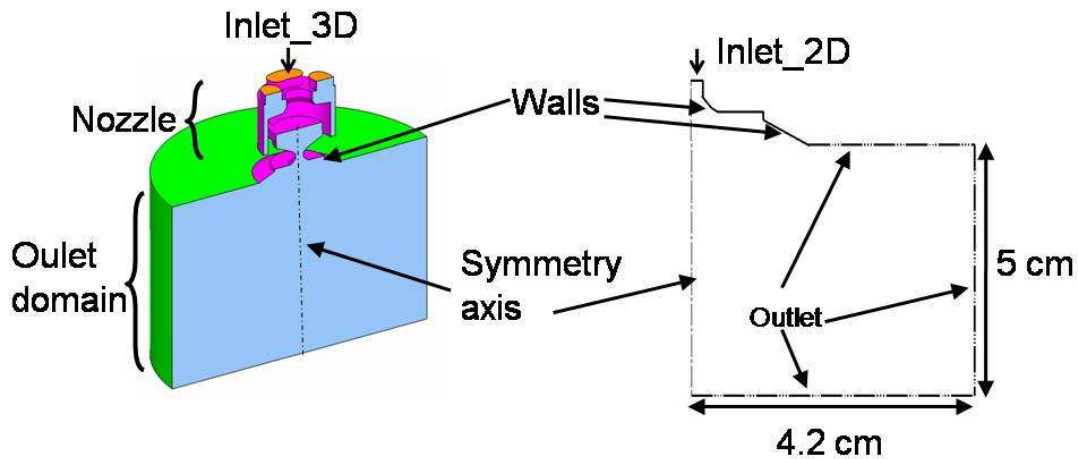


Figure 1. Sketch of the 3D and 2D computational domains

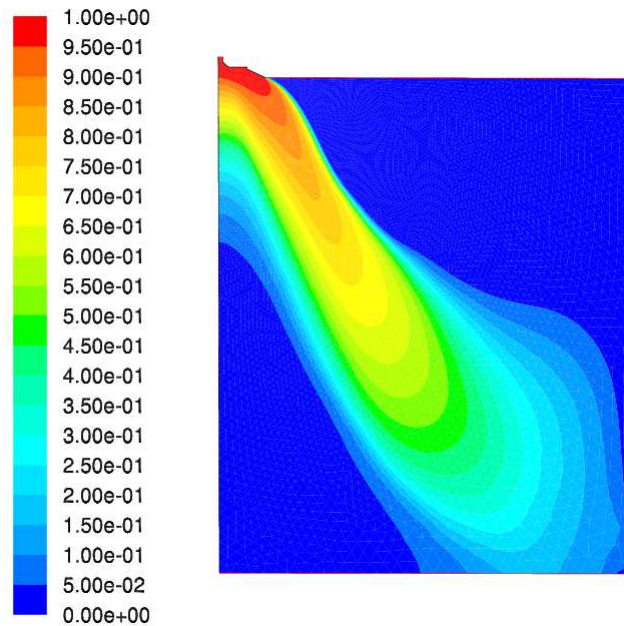


Figure 2. Field of the mean mass fraction - 2D calculations

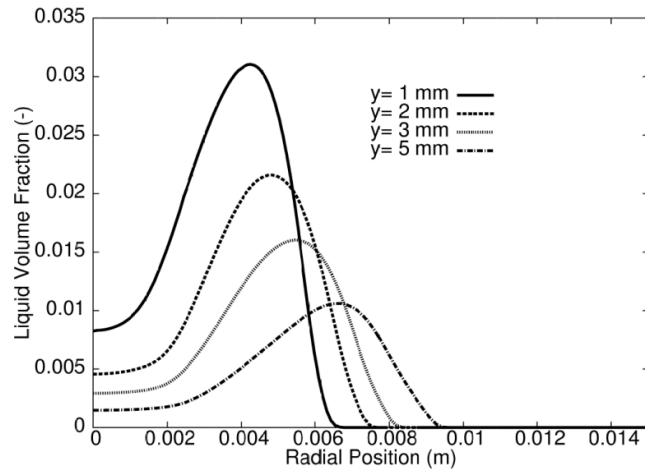


Figure 3. Profiles of the liquid volume fraction for various axial distances  $y$  from the exit

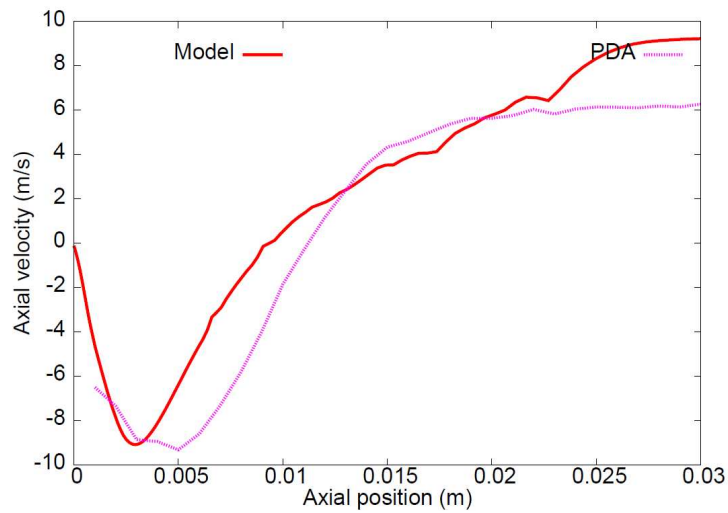


Figure 4. Comparison of the mean liquid axial velocity measured by PDA and modeled