Atomization Modeling for an Agricultural Hollow Cone Nozzle

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Abstract

The aim of the present study has been to propose an Eulerian model in order to investigate the atomization of a liquid sheet issued from a hollow cone nozzle. The model has been based on studies developed in the automotive and rocket engine fields, and has been adapted to agricultural sprays.

A fluid with variable density has been considered, ranging from the air density to the liquid density. Classical conservation equations have been solved for the fluid: a transport equation for the mean liquid mass fraction, and three other for the three velocity components. An original aspect of the model has concerned turbulence modeling. Turbulence has not been modeled using the classical (k-ϵ) model, as the flow involved was anisotropic. It has been modeled using transport equations for the six Reynolds Stress Tensor components.

Three-dimensional calculations have been carried out to study the flow of water in air from the inside of the nozzle to up to 1.5 cm outside the exit. The model has been applied to a hollow cone nozzle (ATR80 Lilas, Albuz) particularly used in orchards or wine growing. The computations have been performed using the CFD code Fluent using User Defined Functions.

Numerical calculations have shown a hollow cone liquid sheet expanded outside the nozzle, and a recirculation zone in the spray centre. Comparisons with experimental data have showed good agreement between the volume liquid fraction values, but bad agreement between the spray angles. Improvements concerning the liquid flux modeling are in progress. In the near future, the model could be used as initial conditions in drift models.

Introduction

Agricultural pesticide spraying commonly involves ejecting a water mixture made up of active molecules and adjuvants. Small droplets lead to an optimal coverage but may contribute to drift contaminating air, water and soils. Large droplets are less prone to drift but may stream down. The way the droplets reach the target or not depends partially on the size and velocity of the droplets at the nozzle exit.

Experimental studies in the agricultural field are complex to conduct as pesticide sprays are subjected to external conditions such as wind, variable temperature or hygrometry, whereas the modelling approach can use invariable conditions.

For 30 years, the United States Department of Agriculture (USDA) Forest Service has developped models to calculate the pesticide dispersion applied by aerial application above forests. In the 1990's the north american consortium of chemical registrants developped with USDA Forest Service and USDA Agricultural Research Service a Lagrangian model to calculate the pestide drift at time of application [5]. The authors insist indeed on the great importance of the initial distribution of the drop sizes [9] in the calculation of spray drift. Other studies on pesticide drift have been developped. A 2D model has been proposed to describe the drift of sprays resulting from flat fan nozzle [8]. Droplets are assumed to form at a distance equal to the sheet coherent length and have the same velocity as the liquid sheet. This study emphasizes in particular the importance of the correct definition of sheet velocity. Zhu et al. proposed a simplified and user-friendly version of a computer model, DRIFTSIM, to estimate drift distances for individual water droplets or classes of droplets [12].

Studies have also been conducted using CFD codes with an Eulerian/Lagrangian approach, considering isolated drops [3], [10]. Near the exit nozzle, this hypothesis was probably wrong. Moreover, this kind of model did not really model the atomization process as it consider spherical drop with a prescribed diameter and velocity.

Finaly, it must be stressed that swirling liquid spray have received little attention in the literature despite their interesting characteristics [6].

During present work, an Eulerian model was developped to assess the liquid dispersion outside an agricultural hollow cone nozzle.

Material and Methods

An Eulerian one phase model has been developped in the automotive and rocket engine fields [11], [7]. It has been adapted to agricultural nozzles [4]. The two phase flow was considered as a single phase turbulent flow composed of a liquid and a gas mixture with a highly variable density $\bar{\rho}$. $\bar{\rho}$ was bounded by the constant gas density ρ_g and the

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constant liquid density ρ_l.
The transport equation for the Favre averaged velocity $\tilde{u}_i$ did not contain any momentum exchange terms, as the mixture of liquid and gas was considered here. Neglecting the laminar term as the flow considered was highly turbulent, the equations (for i = 1, 2, 3) were:

$$\frac{\partial \bar{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial \left(\bar{\rho}\widetilde{u}_i\widetilde{u}_j\right)}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_j}\delta_{ij} - \frac{\partial}{\partial x_j}\left(\bar{\rho}\widetilde{u_i''u_j''}\right) \tag{1}$$

The Reynolds Stress Model (RSM) has been chosen as it has greater potential to give accurate predictions for complex flows. Abandoning the isotropic eddy-viscosity hypothesis, the RSM closes the equation (1) by solving transport equations for the Reynolds Stress tensor $\bar{\rho}\widetilde{u_i''u_j''} = \bar{\rho}\widetilde{R_{ij}}$ together with an equation for the dissipation rate $\widetilde{\epsilon}$.

$$\frac{\partial \bar{\rho}\widetilde{R_{ij}}}{\partial t} + \frac{\partial \left(\bar{\rho}\widetilde{R_{ij}}\widetilde{u}_k\right)}{\partial x_k} = D_{ij} + P_{ij} + \Phi_{ij} - \frac{2}{3}\bar{\rho}\widetilde{\epsilon}\delta_{ij} \tag{2}$$

where D_{ij} is the turbulent diffusion, P_{ij} the stress production , Φ_{ij} the pressure strain and $\bar{\rho}\widetilde{\epsilon}$ the dissipation.

$$D_{ij} = -\frac{\partial}{\partial x_k}\left(\bar{\rho}\widetilde{u_i''u_j''u_k''} + \overline{p'u_i''\delta_{jk} + p'u_j''\delta_{ik}}\right)$$

$$P_{ij} = -\bar{\rho}\widetilde{u_i''u_k''}\frac{\partial \widetilde{u}_j}{\partial x_k} - \bar{\rho}\widetilde{u_j''u_k''}\frac{\partial \widetilde{u}_i}{\partial x_k}$$

$$\Phi ij = \overline{p'\left(\frac{\partial u_i''}{\partial x_j} + \frac{\partial u_j''}{\partial x_i}\right)}$$

Neglecting laminar diffusion, the transport equation for the mean liquid mass fraction $\widetilde{Y}$ was :

$$\frac{\partial \bar{\rho}\widetilde{Y}}{\partial t} + \frac{\partial \left(\bar{\rho}\widetilde{Y}\widetilde{u}_i\right)}{\partial x_i} = -\frac{\partial}{\partial x_i}\left(\bar{\rho}\widetilde{u_i''Y''}\right) \tag{3}$$

The liquid turbulent diffusion was treated using a classical gradient law:

$$\bar{\rho}\widetilde{u_i''Y''} = -\bar{\rho}\frac{\nu_t}{Sc_t}\frac{\partial \widetilde{Y}}{\partial x_i} \tag{4}$$

where Sc_t is the turbulent Schmidt number, $Sc_t = 0.7$, $\nu_t = C_\mu \widetilde{k}^2/\epsilon$, C_μ=0.09 and $\widetilde{k} = (\widetilde{u_i''u_i''})/2$.
The mean density was related to the mean liquid mass fraction by:

$$\frac{1}{\bar{\rho}} = \frac{\widetilde{Y}}{\rho_l} + \frac{1-\widetilde{Y}}{\rho_g} \tag{5}$$

The mean liquid volume fraction $\overline{\tau}$ was obviously linked to the mean mass fraction $\widetilde{Y}$ by:

$$\overline{\tau} = \frac{\bar{\rho}\widetilde{Y}}{\rho_l} \tag{6}$$

The liquid dispersion was entirely calculated using eqs. (1), (2), (3), (4), (5).
In order to get the mean droplet diameter, a transport equation for the mean liquid/gas interface density (i.e. the quantity of the mean interfacial surface area per unit of volume) was solved. As this equation is still under development, no result concerning it will be presented here.

Results and discussion

The model was applied to a hollow cone nozzle ATR 80 Lilas (Albuz, France) used in arboriculture and wine growing for fungicide and insecticide treatment, considering water injected in quiescent air. Although the real liquid preparations involved in the pesticide spraying contain surfactants which reduce the dynamic surface tension coefficient, this effect is not considered here. The calculation zone considered in this study was actually very close to the nozzle exit, and we supposed that the surfactant had not enough time to reach the droplet surface. In other words, we considered a turbulent flow with high Weber and Reynolds numbers.

The computations were obtained on a half three dimensional grid with periodic conditions. The calculation domain was composed of two parts (see Figure 1): the nozzle itself bordered by walls (top of the figure) and the outlet domain (half of cylinder with 12.5 mm radius and 15 mm in height). A tangential canal leads the liquid into the conical swirl chamber. It exits through a hole of D = 0.92 mm diameter. The injection pressure was fixed at 5 bar as in arboriculture treatment, downstream a pressure outlet condition was imposed.
The computations were performed using the CFD code Fluent version 6.3.26 [1]. The geometry was generated with the Gambit 2.04 software package. The numerical grid constructed was consisting of 840, 000 cells. The narrower diameter of the nozzle D was composed of 30 cells. A steady approach has been considered, so the local time derivative terms of the set of equations (1), (2), (3) have been neglected. The total computational time was of the order of 30 hours on an 2.4 GHz Intel Pentium Xeon Processor.
Figure 2 shows the radial profiles of the mean liquid mass fraction $\widetilde{Y}$ at 1, 2, 3, 5 and 10 mm outside the nozzle exit.

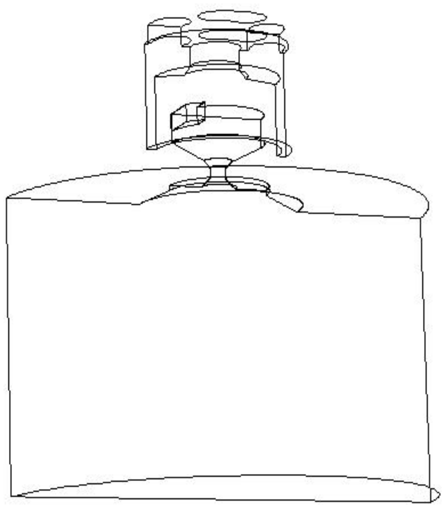

Figure 1: Computational domain

Radial dispersion of the liquid can be seen as the axial distance increases. For the maximum radial distances, the mass fraction is equal to 0 (except at 1 cm from the nozzle), as the liquid spray is surrounded by air.

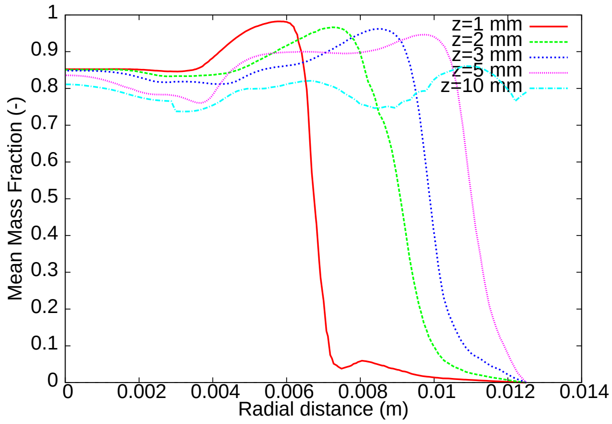

Figure 2: Radial profiles of the calculated mass liquid fraction at five axial positions

Figure 3 represents radial profiles of the mean liquid volume fraction τ defined by the eq. (6) at 1, 2, 3, 5 and 10 mm outside the nozzle exit. Hollow cone spray can be seen in accordance with experimental results [2]: the liquid sheet is visible. We can suppose that the sheet exists for τ greater than 1% for example. In the spray centre, the non-zero volume fraction may represent the volume fraction of the small droplets carried by the air flow.

Figure 4 shows the radial profiles of the axial velocity component at the same five axial distances outside the nozzle.

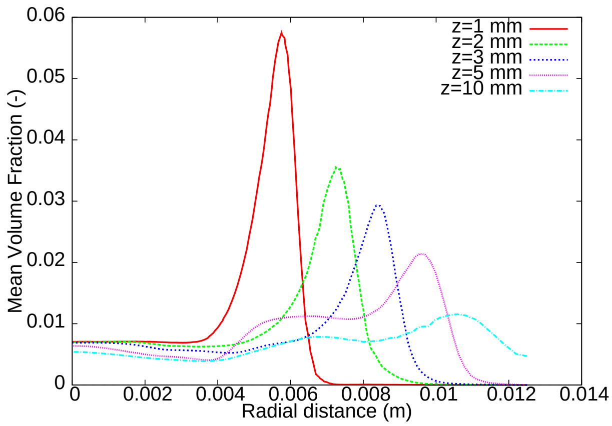

Figure 3: Radial profiles of the calculated volume liquid fraction at five axial positions

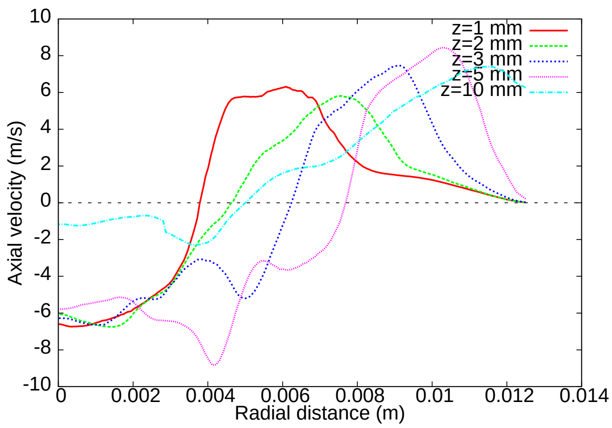

Figure 4: Radial profiles of the calculated axial velocity component at five axial positions

One can take notice of the recirculation zone in the spray centre, where the axial velocity is negative, i.e. the flow is upstream.

An experimental study has been conducted by A2 Photonic Sensors (Grenoble, France) in collaboration with Cemagref in order to measure the liquid presence rate at 1, 2, 3, 5 and 10 mm outside the nozzle exit. Water has been injected through the same nozzle ATR 80 Lilas at 5 bar. The phase detection probe consisted in a 50 μm optical fiber. The probe pierced the droplet sheet. The ratio between the time the probe was in the liquid phase and the total elapsed time led to the liquid presence rate, which is also the mean liquid volume fraction.

Figure 5 presents radial profiles of the liquid presence rate measured by the optic sensor in the liquid sheet. No measurement has been made in the spray centre, as there was not enough droplets to get reliable results. Comparing this figure with figure 3, we can see that orders of magnitude of the liquid volume fraction are roughly comparable. However, it is clear that the spray angle is badly calculated by the model, as droplets were found experimentaly at radial distances very lower than numerically. For example, at a distance of 5 mm from the nozzle, numerical results show a maximum of the volume liquid fraction at 1 cm from the spray axis, whereas experimental results show a maximum

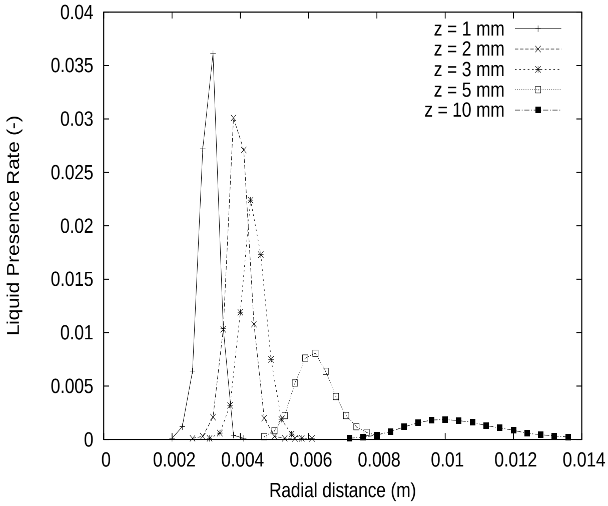

Figure 5: Radial profiles of the measured Liquid Presence Rate for five axial positions

at 6 mm from the spray axis. That is the reason why another expression for the liquid turbulent flux is currently being in order to take into account the anisotropy of the Reynolds Stresses.

Conclusion

The predictive capability of the Eulerian atomisation model has been assessed for an agricultural hollow cone nozzle. A one phase turbulent flow has been considered. Turbulence has been modeled using the Reynolds Stress Model. A hollow cone sheet has been found numerically, in accordance with experimental results. A recirculation zone containing little liquid has been seen numerically, suggesting the presence of small droplets having an upstream movement in the spray centre. Numerical liquid fraction values have been in good agreement with experimental results, but the spray angle has been still badly calculated. Improvements concerning the turbulent mass flux modeling are currently being. The long term perspective for this study will concern the coupling between this Eulerian model with a drift model in order to describe the entire trajectory of pesticide droplets.

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Nomenclature

D	nozzle diameter	m
$\widetilde{k}$	turbulent kinetic energy	m^2/s^2
$\bar{p}$	mean pressure	Pa
R_{ij}	Reynolds Stress tensor	m^2/s^2
$\widetilde{u_i}$	mean velocity	m/s
u”	fluctuating velocity	m/s
$\widetilde{Y}$	mean liquid mass fraction	-
Y”	fluctuating liquid mass fraction	-
$\widetilde{\epsilon}$	turbulent dissipation rate	m^2/s^3
$\bar{\rho}$	mean density	kg/m^3
τ	mean volume liquid fraction	-

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