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VoF-to-DPM 3D Model for non-reacting gas liquid two-phase flow characterization

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Abstract

The atomization of liquid jets plays a vital role in combustion systems, such as gas turbines and rocket engines. Understanding the behaviour of gas-liquid two-phase flows is crucial for enhancing the performance and safety of propulsion systems. This paper proposes the utilization of the Volume of Fluid (VOF) method in conjunction with the Discrete Phase Model (DPM) to accurately capture the characteristics of a non-reacting spray in a co-flow. The study involves a 3D cylinder with an air blast injector and an axial co-flow. The simulation results demonstrate the successful representation of the primary breakup and dispersion of droplets. The hybrid RANS-LES model employed achieves accurate results with reasonable computational cost. Future work will involve model validation using experimental data and parameter variation analysis.

1. Introduction

The atomization of liquid jet is widely studied both experimentally and numerically due to their extensive application. Among these applications, particular importance is given to the combustion system of gas turbine and rocket engines. Combustion relies on the efficient and precise control of gas-liquid two-phase flows injected in the combustion chambers. Therefore, understanding the characteristics and behaviour of these two-phase flow is crucial for enhancing the performance, reliability, and safety of propulsion systems.

Traditionally, non-dimensional parameters such as the Webber number We_g, liquid and gas Reynolds number Re_l and Re_g, and gas-to-liquid momentum ratio ALR have been used to describe the atomization process of a liquid jet [1]. These parameters depend by the physical characteristic of the nozzle and the properties of the fluids involved. Nevertheless, the injector performance, and the resultant injection are correlated to the ambient, i.e., microgravity for liquid rocket engines. The key characteristics of a spray include the particle size distribution PSD, the velocity distribution, the density or number of droplets for unit of volume, the volume fraction and the temperature [2]. The efficiency of the spray in relation to the involved application depends by these characteristics. Its optimization depends on the control of spray formation.

Sprays formations involve three main phases: liquid fluid ejection, primary breakup, and secondary breakup mechanisms. The primary breakup mechanism can be further described into two stages. The capillary instability, influenced by the air velocity, leads to the initial perturbation in the jet closest to the nozzle. The second stage is driven by aerodynamic forces that result in ligament formation, followed by ligament breakup [3]. The secondary breakup is mainly linked to the parameters and conditions cited above.

Numerous experimental studies have contributed to understanding the droplet formation. However, the challenging conditions under which these sprays are applied created uncertainty when predicting their behaviour. This uncertainty arises from limited access to determinate boundary condition in a laboratory setting or the inability to observe the phenomenon in the actual operating environment, such as a combustion chamber [4]. As a result, accurately characterising these flows becomes an intricate task, necessitating the development of specialized modelling techniques.

The numerical modelling of two-phase flows has made significant advancement in recent years, thanks to increased computational power enabling the utilization of advanced turbulence modelling techniques. However, it is important to note that these models may still exhibit numerical errors. Comparison between experimental data obtained under atmospheric pressure condition, and numerical modelling results in extreme condition may provide a qualitative assessment. Therefore, there is the necessity of a robust model at an acceptable computational cost.

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The Volume of Fluid (VOF) method has proven to be a valuable tool for simulating multiphase flows, providing a detailed representation of the phase interface [5] [6]. However, the VOF method faces limitations in capturing the dispersed phase dynamics accurately, especially in situation involving small droplets and complex geometries [7]. To overcome these challenges and improve the fidelity of simulations, this paper proposes the utilization of the Discrete Phase Model (DPM) in conjunction with the VOF method.

The DPM is a Lagrangian particle-tracking technique that enables the simulation of dispersed phases, such as droplets, in multiphase flows [8]. By incorporating the DPM into the VOF framework, it becomes possible to achieve a more comprehensive understanding of the gas-liquid two-phase flow characteristics. This integrated VOF to DPM model hold significant promise for accurately capturing the behaviours of these flows, allowing for improved predictions of critical parameters.

1.1 Objectives

The objective of this study is to present a qualitative investigation into the application of the VOF methods in combination with the DPM model to characterize a non-reacting spray in a co-flow. The numerical results obtained from this approach will be further compared with experimental data. A multiscale approach is adopted, utilizing a Stress-Blended Eddy Simulation (SBES) sub model. The simulations are conducted using the commercial software Ansys fluent V22, and the built-in VOF-to-DPM phase interaction is utilized for the model transition.

2. Physical and Numerical setup

The case study involves a simple 3D cylinder of 60 cm of diameter, in which a spray is injected. The spray is generated using an air blast injector with a co-axial configuration for both liquid and atomising air flow rates. The spray is then surrounded by an axial co-flow with a moderate velocity. The model features three different inlets. The liquid enters through the capillary central entrance with a gauge pressure of 150 000 Pascal. The air blast flow enters the system at the same level as the liquid, through a co-axial entrance, and at the same pressure gauge. Finally, the air co-flow enters through axially inlet again, but with ambient gauge pressure. These conditions align with those tested in a previous study [9], enabling us to validate our model and explore its applicability in real-world scenarios.

2.1 CFD approach

The commercial software Ansys Fluent V22 is utilized for the modelling and analysis of the spray and its characteristics. The governing equation to be solved include the mass continuity equation, given by eq. 1,

$$\frac{\partial \rho}{\partial t} + \nabla \rho \boldsymbol{u} = 0 \tag{1}$$

Here, ρ indicates the density, t denotes time, and $\mathbf{u}$ represents the velocity vector. The momentum conservation equation is expressed as equation 2,

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla p + \nabla^2 \boldsymbol{\mu}\boldsymbol{u} + \rho \boldsymbol{g} \tag{2}$$

Here, p indicates pressure, μ represents the dynamic viscosity, and $\rho\boldsymbol{g}$ represents the gravitational body force.

The Volume of Fluids method is employed to reconstruct the interface between phases solving the volume of fluid ϕ in each phase, using the following equation:

$$\frac{\partial \rho \phi}{\partial t} + \nabla(\boldsymbol{u}\rho\phi) = 0 \tag{3}$$

A hybrid LES RANS model is applied to solve the flow field. Menter [10] describes this model with a simple concept where RANS and LES are combined. This combination is performed at stress-level with a function f_s as shown in the following equation:

$$\tau_{ij} = \tau_{ij}^{RANS} f_s + (1 - f_s)\, \tau_{ij}^{LES} \tag{4}$$

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In this equation τ_{ij} represents the stress tensor calculated with the SBES model, f_s is the shielded function and τ_{ij}^{RANS} and τ_{ij}^{LES} are respectively the stress tensors computed with the RANS and LES models. In the case where both models are Eddy viscosity models the previous formulation simplifies as:

$$\mu_t = \mu_t^{RANS} f_s + \mu_t^{LES}(1 - f_s) \tag{5}$$

Here, μ_t, μ_t^{RANS} and μ_t^{LES} represent the turbulent viscosity for the SBES model, RANS model and LES model, respectively.

The function f_s is complex and does not provide further information on the solution, but the concept is simple. When the function is zero, pure LES is being solved, whereas a value of 1corresponds pure RANS.

2.2 Study domain, methodology and numerical method

The study domain of this work is the spray phenomenon, which is generated using the air blast injector technique. The liquid enters through a central capillary entrance, while the atomizing air enters coaxially to induce instability and primary breakup in the liquid jet. The spray is enveloped by an air co-flow, and the gas-liquid mixture exits the domain.

The primary objective of this work is to assess the predictive capability of the selected model in term of spray characteristics and representation of the spray formation throughout its various phases.

The 3D geometry is discretized using a structured mesh. To ensure reliable results, mesh independence is schieved by employing four different meshes throughout the domain. The mesh refinement process is conducted iteratively, considering the computational time required and the resulting improvement in accuracy, Table 1 shows these variations. In conclusion the G3 presents a good accuracy and an acceptable computation cost.

Regarding the boundary conditions, the inlet conditions consist of a velocity inlet (m/s) for the air co-flow, a mass flow rate (kg/s) for the liquid phase and the air blast flow rate. The walls are assigned no-slip boundary conditions and reflect in respect to the DPM phase.

For the simulation, the commercial software Ansys Fluent V22 is utilized, employing a transient approach with the SIMPLEC algorithm. The pressure gradient is discretized using the PRESTO! Scheme while the Geo-Reconstruct scheme is employed for the volume fraction of the liquid phase. The bounded central differencing scheme is utilized for momentum, and a second-order upwind scheme is employed for turbulent kinetic energy and the specific dissipation rate. K-omega is the turbulence model used and the substructure are resolved with the SBES model.

Table 1: Grid analysis

	G2	**G3**	**G4**	**G5**
Number of elements	1 768 000	3 762 000	5 600 000	8 384 000
Variation [%]	0[a]	6%	6.3%	6.6%
Increase in computational Time	0[a]	100%	400%	650%

[a] Starting case, all the evolutions are compared with the first case studied

3. Results and discussion

In this chapter, we evaluate the predictive capability of the used model from various perspective. Firstly, we analyse the evolution of the liquid jet from the onset of injection until primary breakup occurs. Subsequently, we examine the coupling between the VOF and DPM methods. Lastly, we delve into the behaviour and changes of the blended function f_s across the domain.

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3.1 Evolution of liquid jet after onset of injection

Figures from Figure 1 to Figure 4 illustrates the evolution of the liquid jet during injection. Figure 1 shows the situation after 0.01ms, the liquid jet is injected in the domain. The initial instability emerges within a few microseconds of the injection. In Figure 2 the instability caused by the co-axial air flow become evident as well as the formation of elongate structure. As time progresses the interpenetration of the air flow rate and the liquid jet leads to enhanced instability and rupture of the liquid jet (Figure 3). This process gives rise to the formation of ligaments, followed by their rupture, ultimately completing the primary breakup [3] (Figure 4).

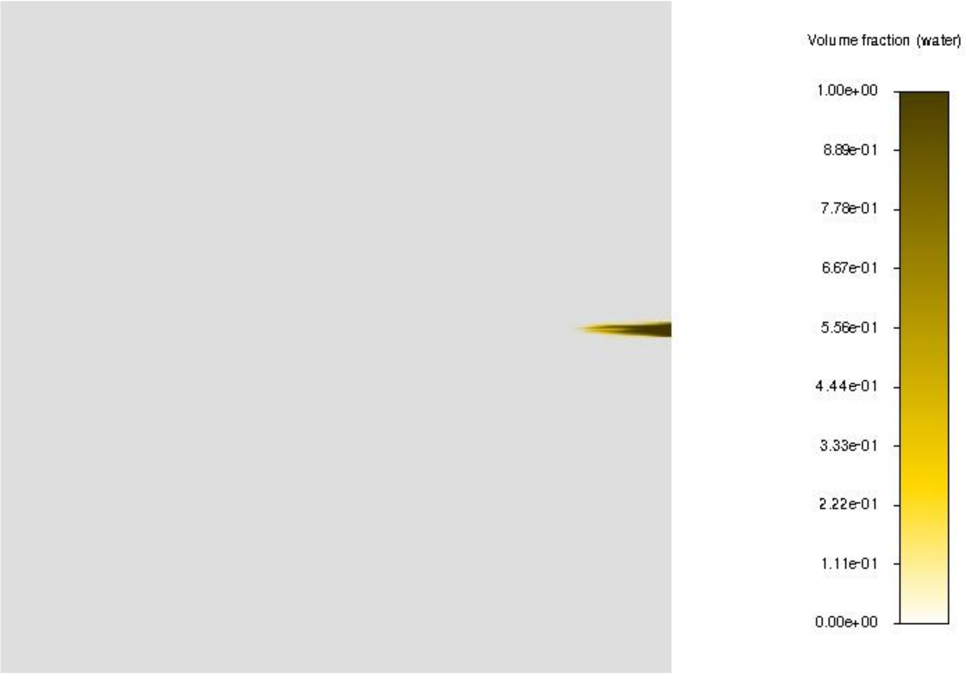

Figure 1: Liquid jet enters the domain at the time laps of 0.01ms. The jet shows the first effect of the perturbation introduced by the co-axial flow rate.

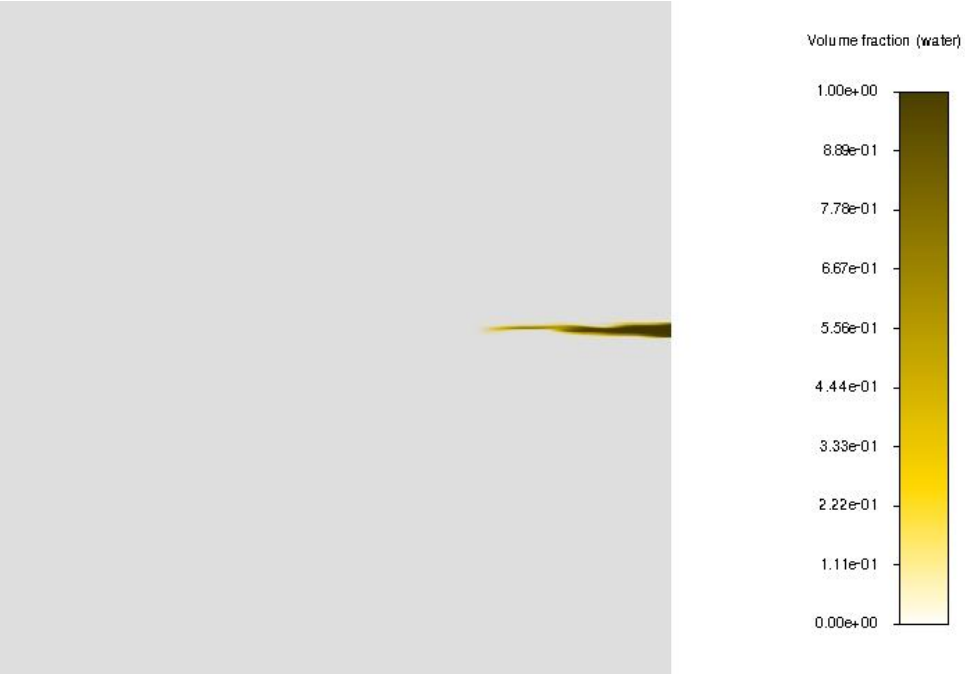

Figure 2: Liquid jet after 0.05ms after the onset of the injection. The instability arises clearly and leads to a elongation of the liquid jet.

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Figure 3: Liquid jet after 0.08ms after the onset of the injection. The interpenetration between gas and liquid phase enhances the instability creating the breakup.

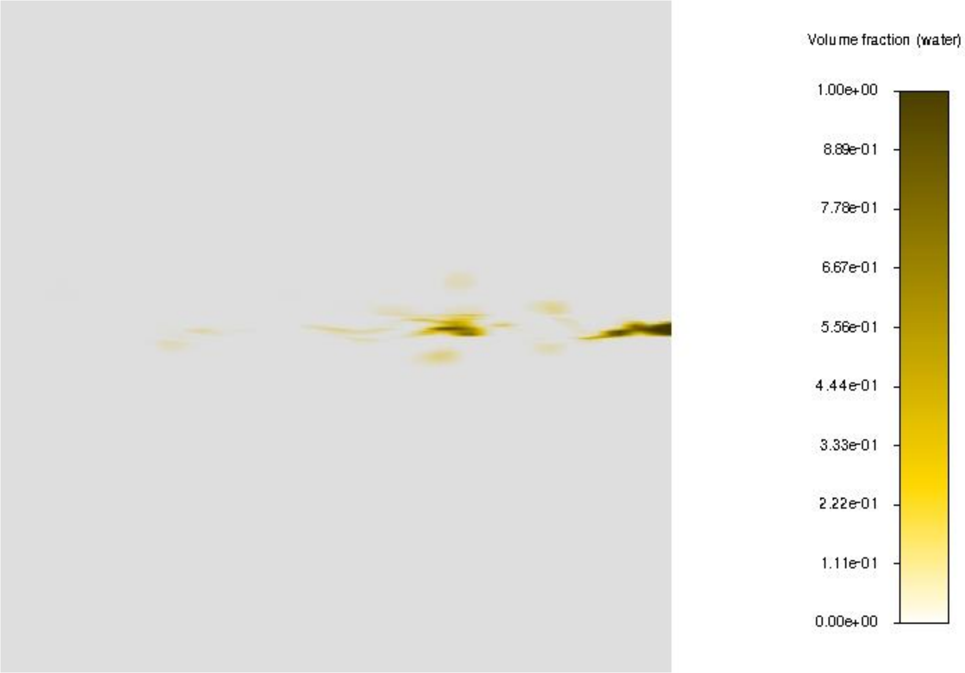

Figure 4: Liquid jet after 0.15ms after the onset of the injection. The primary breakup is achieved, and the liquid jests is separated in lump completing the primary breakup.

3.2 Coupling VoF to DPM methods

The coupled VOF to DPM model successfully captured the primary breakup and its evolution. In terms of tracking discrete phase particles within the domain, the model enables the tracing of droplets formed during primary breakup with reasonable computational efficiency. Figure 5 displays the droplets colorized by axial velocity, highlighting the highest velocity at the centre of the spray. Additionally, droplets with negative axial velocity can be observed, likely indicating their entrapment within recirculation zones caused by the varying flow velocities involved. Table *2* shows key parameters on the obtained distribution tracked with the DPM model.

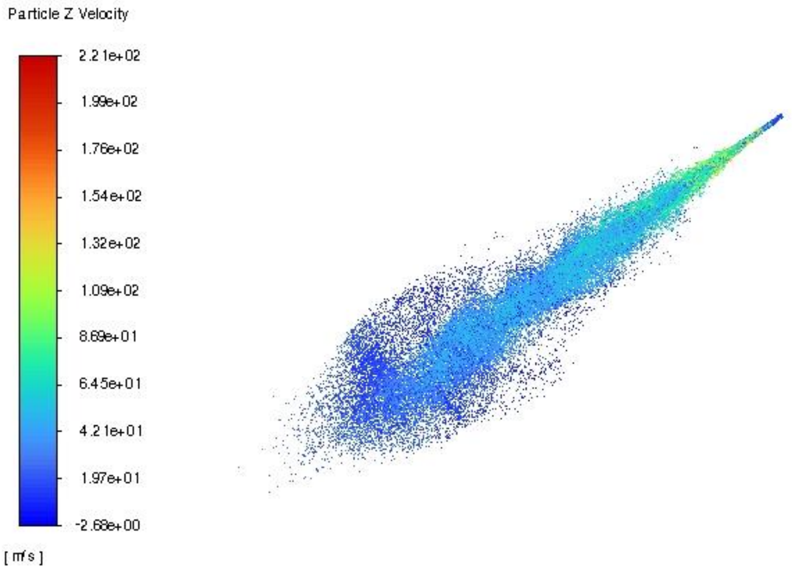

Figure 5: Droplet distribution coloured by axial velocity.

Table 2: Particle Size Distribution parameters

Number of particles	**Total mass [kg]**	**Mean diameter [m]**	**SMD [m]**
1.9705e6	1.482e-5	1.052e-5	6.302e-5

3.3 Evolution of coherent structures

Figures from Figure 6 to Figure 9 depicts the progressive development of the coherent structure within the solved flow field, with colorization representing the magnitude of velocity. In the initial stage of the injection, a spiral coherent structure is observed, enveloping the spray structure. These intricate structures signify the presence of instability. The evolution of these structures is closely linked to the prediction of spray penetration power[11].
In Figure 6, we can observe that the tortuous structure is not present at the top of the structure, indicating a minimal presence of perturbation observed in Figure 1. Starting from the instant represented in Figure 7, the tortuous structure rises up to the spray, inducing enhanced instability.

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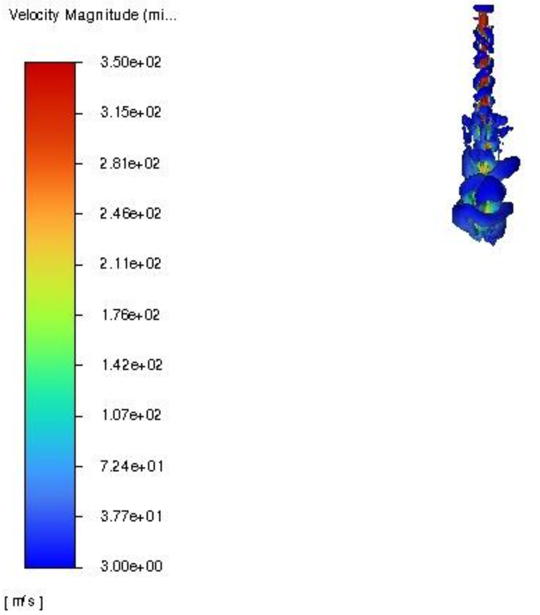

Figure 6: Coherent structure evolution after 0.01ms

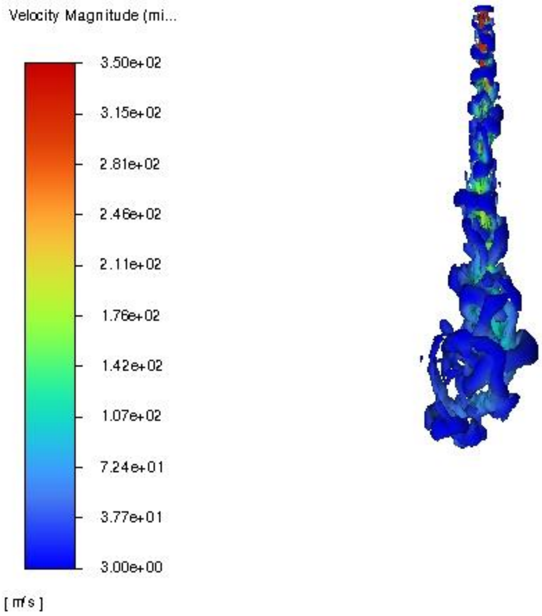

Figure 7: Coherent structure evolution after 0.05ms

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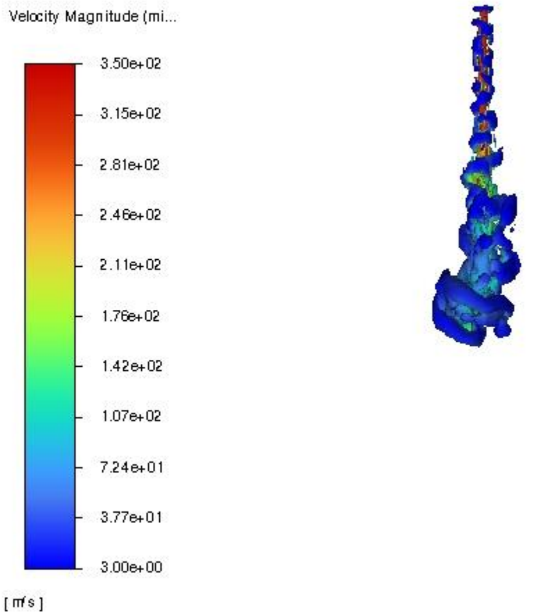

Figure 8: Coherent structure evolution after 0.08ms

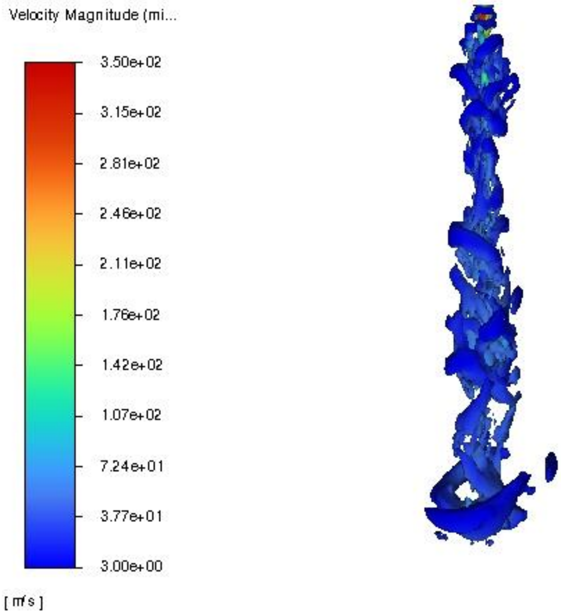

Figure 9 Coherent structure evolution after 0.15ms

4. Conclusions

The VOF to DPM model has demonstrated its capability to accurately simulate the complex dynamics of sprays, including the primary breakup process and subsequent droplet dispersion. By incorporating the VOF method, which reconstructs the interface between phases, and the DPM approach, which tracks individual droplets, the model has captured the intricate details of the spray behaviour. The instability observed in the liquid jet are correlated within the evolution of the coherent structures.

The successful utilization of a hybrid RANS-LES model has demonstrated its effectiveness in achieving accurate results while maintaining a low computational cost. By combining the strengths of both RANS and LES approaches, the model was able to capture the intricate flow phenomena with improved fidelity, while minimizing the computational resources required.

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Further studies on these models will involve the validation of the model using experimental data, focusing on key spray characteristics. Additionally, an in-depth analysis will be conducted to assess the impact of parameter variations, including air blast flow rates, co-flow, and gauge pressure.

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