Modelling of nanoparticle jet from leakage of conveying pipe - breakage of nanoparticle aggregate

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Abstract

This paper presents a numerical modelling of nanoparticles jet under pressure in which the breakage of nanoparticles aggregates and the drag force are simulated by Code_Saturne. Within a nanoparticles jet, the size distribution and number concentration of aggregates evolves due to the breakage of aggregates under the fluid turbulence. The breakage of aggregates has been modeled by implementing a Monte-Carlo method within Code_Saturne under Euler-Lagrange approach. The numerical results show that the breakage of aggregates is very strong in the turbulence field near the leakage. When aggregates leave this near field, the breakage decreases because of lower turbulence and in the same time the aggregate size decreases which enhances aggregate strength. The sensitivity of the breakage theoretical model to the resistance of aggregates under various conditions of turbulent fluid dissipation shows an expected trend. Those numerical results need to be compared with experimental data when available in the future.

Keywords : nanoparticles, aggregate, breakage, accidental jet.

1. Introduction

Nowadays, nanomaterials are more and more used in industrial process leading to a significant increase in terms of interest and budget (Kuhlbusch et al, 2011). In this context, it is very important to identify the risk scenario case related to use of nanoparticles. Within several accidental scenario cases, the case of leakage of conveying pipe happened in the pass, for example, in Blanzy, (France, 2012). Although, this scenario case has very few attentions in the literature. Some experimentations investigate the behavior of nanoparticles in different configuration such free fall (Ibaseta et al., 2008) or flow under pressure in a small device (Stahlmecke et al., 2009, Yaobo et al., 2016) but those experimentations did not propose a model to predict the dispersion and the size-evolution of the nanoparticles. In parallel with those experiments, some authors investigate numerically the formation of aggregates composed of nanoparticle (Iglberger et al., 2008, Vanni, 2015, Dietzel et al., 2016). Those numerical simulations are very computationally expensive and cannot be applied for industrial applications or for risk studies. In order to model the nanoparticles jet, a specific CFD numerical tool need to be developed.

After an analysis of physical phenomena related to nanoparticles jet (Le et al., 2016), the drag force on aggregates and the breakage of aggregates are considered as important in this configuration. The drag force on aggregates influences the dynamic of aggregates. The breakage of aggregates by fluid turbulence influence the size distribution and number concentration of aggregates which are both important parameter for different other studies. Many studies in the literature try to understand the breakage mechanism of aggregates by numerical simulation (Calvert et al., 2011) or by experiments (Ding and Riediker, 2015). The breakage of aggregates can be caused by different effects as the fluid turbulence, the collision between aggregates and a surface, inter- aggregate collisions, etc... In a nanoparticle jet, we consider that the fluid turbulence is the main effect for the breakage. In this study, we use the probabilistic approach from experimental results of Kuster (1991) to model the breakage of aggregates. Recently, Code_Saturne v3.0, developed by EDF, was well validated with experimental data for microparticle case (Le et al., 2015) and is ready to simulate the nanoparticle jet.

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2. Characterization and physics of aggregates of nanoparticles

This section introduces the main physics acting in nanoparticles jet and the model used in the present study.

2.1 Fractal model of aggregates

Aggregate is an ensemble of nanoparticles, called primary particles, linked to each other by weak force as van der Waals force. Although if primary particles are spherical, aggregate do not have spherical shape. The shape of an aggregate can be characterized by a fractal dimension which link the number of primary particle in aggregate with its diameter (Vanni, 2000):

$$N_{pp} = k_f \left(\frac{d_A}{d_{pp}}\right)^{D_f} \tag{1}$$

where $k_f = 0.414D_f - 0.211$ and d_A is the interception diameter of the aggregate (basically it is the longest distance of the primary particle and the mass center of aggregate). In (1), d_{pp} is the primary particle diameter. The discussion of other model of k_f with respect to the choice of d_A is discussed in Gmachowski (2005).

2.2 Drag model for aggregates

In the literature, the simple model of drag coefficient for aggregates, proposed by Vanni (2000) is based on a correction of the drag coefficient of a spherical particle :

$$C_{d,F} = C_d \times \Omega \tag{2}$$

where C_d is the drag coefficient of a spherical particle and Ω a correction taking into account the permeability, the porosity and the fractal dimension of the aggregate. The coefficient Ω is modeled as following :

$$\Omega = \frac{2\beta^2(\beta - tanh\beta)}{2\beta^3 + 3(\beta - tanh\beta)} \tag{3}$$

where $\beta = d_A/(2\kappa)$ and κ is the permeability of aggregate. The detail model of the drag coefficient can be founded in Vanni (2000). In our study, we use this simple relation to model the drag on aggregate.

2.3 Breakage model for aggregates

The breakage frequency of aggregates by the fluid turbulence has been investigated by Kuster (1991) who proposes the following expression :

$$\omega_{fr} = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \frac{\Delta u_f}{d_A} \exp\left(-\frac{V_{b,c}^2}{2\Delta u_f^2}\right) \tag{4}$$

where the term $\Delta u_f / d_A$ is modeled by the following relation :

$$\frac{\Delta u_f}{d_A} = \left(\frac{2\varepsilon_f}{15\nu_f}\right)^{1/2} \tag{5}$$

with ε_f the turbulent fluid dissipation and ν_f is the fluid kinematic viscosity.

The term $V_{b,c}$ represents the strength or the resistance of aggregates to a given shear. That resistance is related to the cohesion of aggregates with different forces between primary particle as van der Waals force or capillary force. In our study, by analogy with the study of droplet breakage (Delichatsios & Probstein, 1974), we propose to model this resistance as following :

$$V_{b,c} = \left(\frac{\sigma_{res}}{\rho_A}\right)^{1/2} \tag{6}$$

where ρ_A is the aggregate density and σ_{res} the aggregate strength. Reynolds et al, 2005 discussed the complexity to determine the aggregate strength with experimental method and different models proposed in the literature. In this study, aggregates are released in the air where the van der Waals force play an important role in an aggregate. The aggregate strength is modeled by Rumpf (1958) model :

$$\sigma_{res} = \frac{9}{8} \frac{k_c \, \phi \, F_{ad}}{\pi \, d_{pp}^2} \tag{7}$$

In (7), the parameters are following:

- k_c is the mean coordination number inside the aggregate (Kuster, 1991) :

$$k_c \approx 15\phi^{1.2} \quad (8)$$

- ϕ the mean solid volume fraction of aggregate (Vanni, 2000) :

$$\phi = k_f \left(\frac{d_A}{d_{pp}}\right)^{D_f-3} \quad (9)$$

- F_{ad} the adhesion force between primary particles (Marchisio, 2003) :

$$F_{ad} = \frac{A}{12}\frac{d_{pp}}{x_{12}^2} \quad (10)$$

where A is the Hamaker constant, $A = 15.10^{-20}$ J and $x_{12}^2 = 4.10^{-10}$ m for titanium dioxide (Ibaseta, 2007).

When breakage occurs, different fragments of different sizes can be formed with respect to the applied force, the fractal dimension and the strength of aggregates. Several studies have investigated this aspect by both numerical (Sator et al., 2007) and experimental approach (Ihalainen et al., 2014) but none of the model can well predict the results of the breakage of aggregates. Also by experimental approach, Yeung & Pelton (1996) show that the breakage in large pieces is prominent for aggregates of low fractal dimension of 1.8 and the attrition and detachment of primary particles from aggregate surface is prominent for high fractal dimension of 2.4. By chosen $D_f = 1.8$ in our study, we consider only binary breakage, i.e., each breakage gives only two fragments. The case of several fragments is considered as multiples breakages. Additionally, we consider in our study that the size of the fragment is calculated based on the uniform probability.

2.4 Monte – Carlo numerical method for breakage of aggregate

The Monte – Carlo method used to model the breakage of aggregates follows several steps :

1. Solve the trajectory equation for particle
2. Calculate the probability of breakage based on the frequency of breakage
3. Generate a random number α between 0 and 1. If the random number is smaller than the probability of breakage, the breakage occurs.
4. If the breakage occurs.
   - Generate a random number Pm and calculate the new properties of aggregate
   - Create a new parcel with properties of first fragment and modify the old parcel with properties of second fragment.

3. Numerical simulation of Code_Saturne v3.0

In this section, we present the results of numerical simulation for both gas and aggregate phases. Finally, an analysis of several parameters, introduced in section 2, is presented.

3.1 Description of simulation case

The numerical simulation considers an air flow loaded of nanoparticle aggregates. The mixture enters in the test chambers through a nozzle of injection located at the top of the computational domain. The study focuses on the instantaneous release of aggregates. The breakage of aggregates is caused only by the turbulence created by the air flow. In our study, the inter-particle collisions are not modelled yet. The turbulence model k- ε monophasic standard is used. The simulation is performed in two steps to save simulation time:

1. The first step consists in simulating the fluid phase motion without aggregates during 5 seconds in order to assess the velocity and the dissipation of the flow.
2. In the second step, the evolution of aggregates is simulated within a frozen flow.

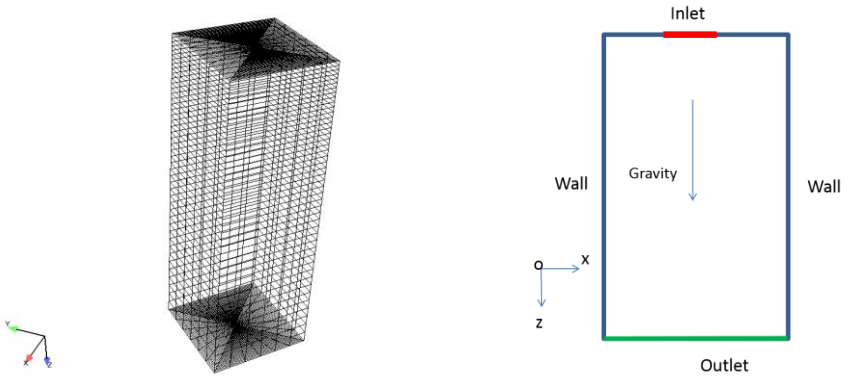
Table 1. Fluid and aggregates material properties

Fluid properties	Density	1.18 kg/m^3
	Dynamic viscosity	1.85.10^{-5} Pa.s

Aggregate properties	Density of primary particle	2500 kg/m^3
	Diameter of primary particle	20 nm
	Aggregate diameter	100 µm
	Fractal dimension	1.8

3.2 Mesh and boundary conditions

A 3D mesh with the size of $0.47m \times 0.47m \times 1.0m$ is used. This mesh contains 36180 cells. The mesh and the boundary conditions are presented in figure 1. The fluid velocity and the aggregates velocity at the nozzle are both equal to 11 m/s; 1000 aggregates are injected in the beginning of lagrangian simulation.

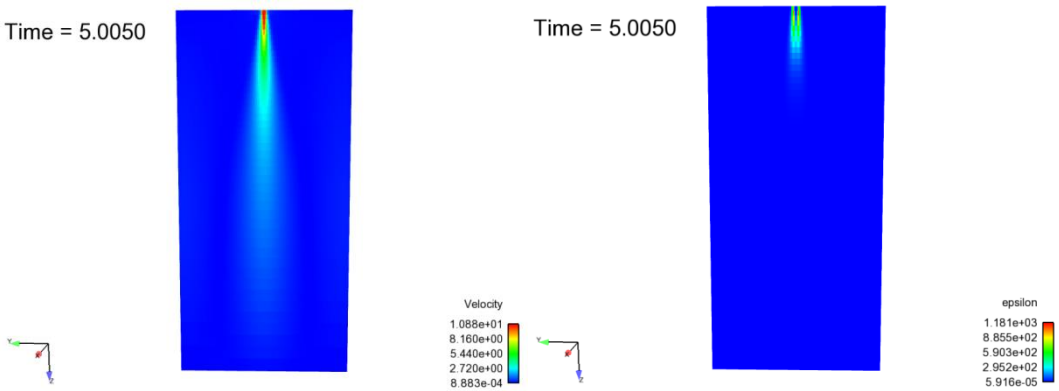


(a) 3D view of mesh *(b) Boundary conditions*

Figure 1. Mesh and boundary conditions used in the numerical simulation.

3.3 Numerical results

The results of gas phase after 5 seconds of simulation are presented in the figure 2 for the gas velocity field and dissipation field.

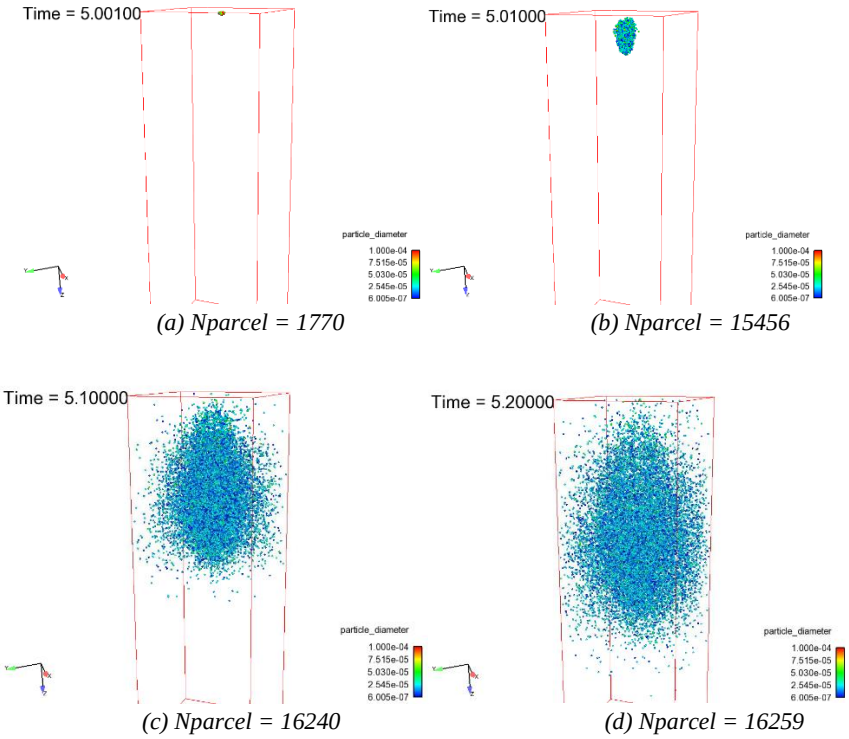


(a) Velocity field *(b) Dissipation field*

Figure 2. Qualitative result of fluid phase. (a) Velocity field. (b) Dissipation field. Time simulation is 5 s.

The velocity and dissipation fields of the fluid phase are consistent with the preliminary study (Le et al., 2015) that showed good comparisons with experimental data of Hadinoto et al, (2015). We observe that the dissipation of the fluid is stronger near the nozzle.

The qualitative results for aggregates are presented in the figure 3 for 0.2 seconds.



(a) Nparcel = 1770 *(b) Nparcel = 15456*

(c) Nparcel = 16240 *(d) Nparcel = 16259*

Figure 3. 3d instantaneous snapshot of the numerical simulation with aggregates. The number and size of aggregates changes because of the breakage. Time of lagrangian simulation is 0.2 second.

We can observe that initially, the number of aggregates increases very fast because they stay inside the strong dissipation field of the fluid. After this phase, a few aggregates have breakage. The size distribution of aggregates for different times in the simulation is presented in the figure 4.

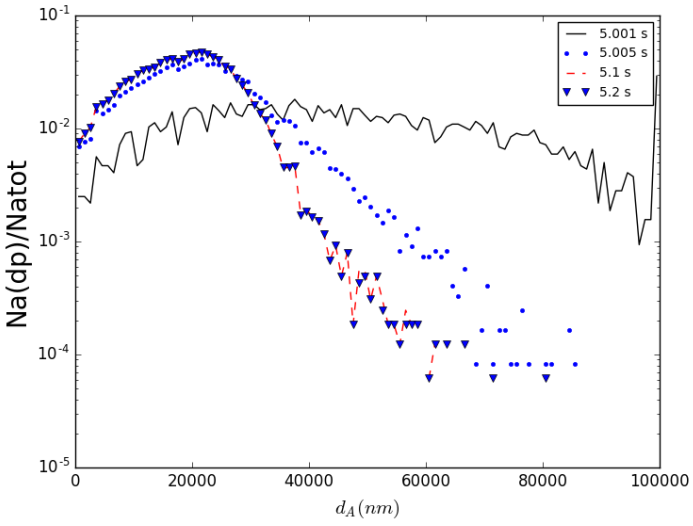
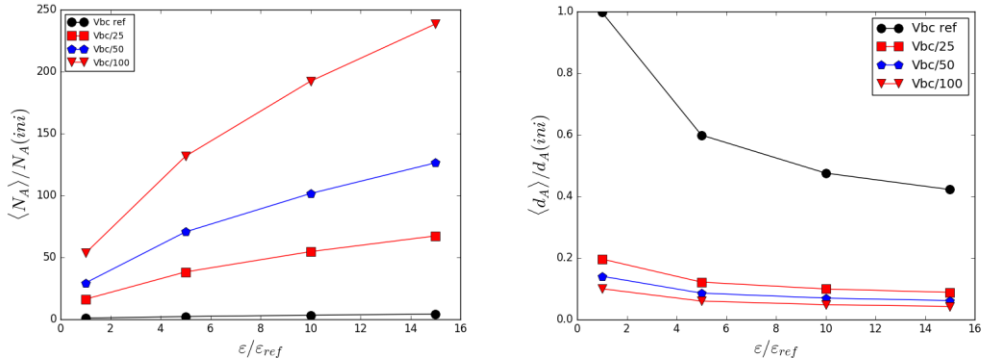


Figure 4. Distribution function of aggregate diameter for different times in the simulation within the whole domain

When aggregates move away from the strong dissipation field, the breakage becomes weak and the particle size distribution does not change as showed in figure 4. For this case, the mean diameter of aggregates is still in the microscale. However, we can observe that there are 1% of aggregates in the first intervals which are in nano-scale.

3.4 Parameters analysis

The two contributions of the breakage frequency are the resistance of aggregates ($\boldsymbol{V_{b,c}}$) and the turbulent fluid dissipation that is a result from the CFD computation of the fluid phase. For different cases, the dissipation is increased and the resistance of aggregate is decreased related to the reference case in order to observe the evolution of mean number and mean diameter of aggregates. As can be seen in Figure 4, in the reference case, the aggregate size distribution is stable after 5.2 second. In all simulations presented here, the mean aggregate number and the mean aggregate size are calculated between 5.2 and 5.5 second. The final results are presented in the figure 5.



(a) *(b)*

Figure 5. Number of aggregates normalized by initial number of aggregates (a) and diameter of aggregates normalized by initial diameter of aggregates (b) in function of fluid dissipation normalized by reference case.

When the resistance of aggregates decreases and the fluid dissipation increase, the breakage of aggregates will be more important. The results show that the number of aggregates increases and whereas the mean diameter of aggregates decreases. The trend obtained was expected.

4. Conclusion

The drag model for aggregates and the breakage model for aggregates have been implemented in Code_Saturne v3.0. The Monte-Carlo method was used to simulate the breakage of aggregates. The results show that the breakage of aggregates is very strong near the injection field. After that the breakage does not play an important role. The trend of the number concentration and distribution size are expected when the fluid dissipation and aggregate strength varies. In the future, the numerical results need to be compared with experimental data.

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Acknowledgments
Authors from INERIS would like to thank the French Ministry of Environment which financially supports this project.

Modélisation d'un jet chargé en nanoparticules à partir d'une fuite de transport pneumatique sous pression – fragmentation des agglomérats des nanoparticules

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Résumé

Ce papier représente la modélisation numérique d'un jet des nanoparticules sous pression dans lequel la fragmentation et la traînée des agglomérats sont simulées par Code_Saturne. Dans un jet des nanoparticules, la distribution de taille et la concentration en nombre des agglomérats évoluent en raison de la fragmentation des agglomérats par la turbulence du fluide. La fragmentation des agglomérats est modélisée par la méthode Monte-Carlo avec l'approche Eulérienne-Lagrangienne dans Code_Saturne. Les résultats numériques montrent que la fragmentation des agglomérats est très forte près de la fuite en raison de la forte turbulence du fluide. Lorsque les agglomérats quittent ce champ, la fragmentation diminue parce que la turbulence diminue et en même temps, la diminution de la taille des agglomérats augmente la résistance des agglomérats à être fragmentés. La sensibilité des variables de la fréquence de fragmentation montre une bonne tendance attendue. Pour la suite, ces résultats numériques nécessitent une comparaison avec les mesures expérimentales.

Mots-clés : nanoparticules, rejet accidentel, agglomérat, fragmentation.

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