Numerical Simulation of Deposition of Fine Particles on Building Internal Surfaces

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Abstract
The deposition of fine particles in closed spaces has become more and more alarming, especially if we associate the theory of the capture of nonmetric viruses by pollutants. The certainty associated with the suspension of particles used to pose a serious risk to those who suffer from respiratory and cardiac diseases. Unfortunately, today, the deposit represents a threat of coronavirus contamination.

This study aims to present a numerical simulation of the deposition of fine particles on the internal surfaces of buildings. It is a continuation of an experimental study that was carried out in 2007 on a 125-litre test chamber that was built to evaluate the particle loss rate coefficients of 0.35, 0.53, 0.7, 1 and 2 µm on the coatings commonly found in buildings, and under three air flow intensities.

However, this numerical simulation presents the deposition of particles at two speeds 0.52 and 1.53 m/s, and in the presence of a propeller configured at three different rotational speeds, 1044, 1278 and 2000 rpm. The numerical results agreed with the experimental results which showed that the particle deposition clearly increases with the speed of the airflow near the walls. The results are presented through the calculation code ANSYSFLUENT 2020 R2.

Key words:
Input here the part of 4-5 keywords.
Air pollution, Dispersion, fine particle, velocity, FLUENT, CFD.

I. Introduction

Air pollution research has reached a strong focus in recent decades resulting in a growing demand for accurate modeling of pollutant concentration, both experimentally and numerically. Although the study of fines dispersion in complex urban environments is essential and directly related to the quality of life and safety of people living and working in such areas.

It is essentially a physicochemical type of pollution linked to human activities. While stationary sources of pollution such as district heating, industrial activities and waste incineration are now better controlled, the same cannot yet be said for pollution sources related to transportation, particularly automobile traffic. Outdoor air pollution has daily, weekly and seasonal cycles, depending on weather conditions. [1].

Several research studies have shown the performance of CFD codes for flow simulation [2], [3]. Consequently, we opted to carry out a numerical simulation of a study carried out in 2001 [4], and after on 2008 [5], continues on the same work to evaluate particle deposition on real surface coatings in a small chamber.

Specifically, the analysis is focused on the effects of airflow intensity on particle deposition. In addition, in our numerical simulation, the geometric design, mesh and configuration are well defined, taking into consideration the characterization of the cover surface, the airflow characteristics (turbulence velocity and intensity) as well as the air temperature and humidity. The particle deposition is then given in representative images, for three air flow intensities. Finally, the results of the measured deposits are obtained through the ANSYSFLUENT 2020 R2 code.2. Tables, Figures and Equations

II. Presentation of the experimental room

The experiments were realized in the air quality facilities of the LEPTIAB laboratory (University of La Rochelle, France). A small cubic chamber with a volume of 125 liters was designed for this study (Fig.1). The walls, floor and ceiling of the chamber are made of wooden panels mounted in aluminium frames. The interior surfaces of the panels can be covered with various cladding materials that were stored in the laboratory where the temperature and relative humidity were maintained between 18 and 20 C and approximately 50%. A small box constantly filled with clean air is placed near the hole on the outer surface of the ceiling to supply the air volume of the chamber with unpolluted air to replace the polluted air extracted from the volume by the particle counter.

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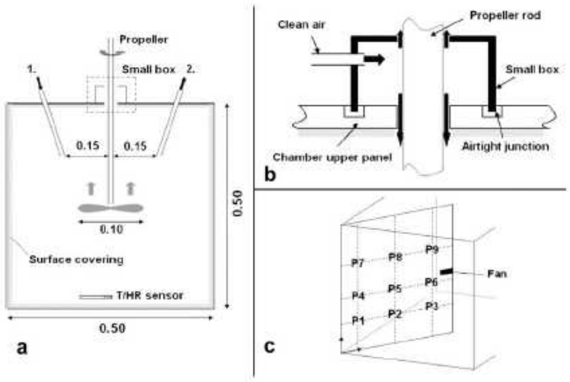


Fig 1: Experimental room

2.1 Experimental protocol

The particles are injected into the volume as soon as the particle concentration falls below the detection limit, the particle injection is stopped when the desired particle concentration is reached.

If we consider that after injection the particles are well mixed, the mass balance of the pollutant is given by the following equation:

$$\frac{dC_i}{dt} = f \times \lambda_r \times C_0 - \lambda_r \times C_i + \frac{1}{V} \times S_i + \frac{S}{V} \times \lambda_R \times D_i - \lambda_{D_e} \times C_i \quad (1)$$

Where C_i is the concentration of particles inside (m^{-3}), t is time (s), f is the particle penetration factor , λ_r is the rate of air renewal (S^{-1}), C_0 is the particle concentration of the incoming air (m^{-3}), V is the volume of the studied area (m^{-3}), S_i is the flow rate of the particle source (S^{-1}), S is the surface where the particles are deposited (m^2), λ_R is the re-suspension coefficient of the particles (S^{-1}), D_i is the mass of the particles (m^{-2}) and λ_{D_e} is the deposition particle constant (s^{-1}).

2.2 Digital protocol

Computational Fluid Dynamics (CFD) is an amazing tool of flexibility, accuracy and extent of application. And in this work, we use the ANSYS FLUENT code, powerful CFD software used to model flow, turbulence, heat transfer and reactions for industrial applications.

The implementation of numerical simulation imposes to follow a number of steps listed below:

1. Create the geometric configuration (Fig.2) and generate the mesh:

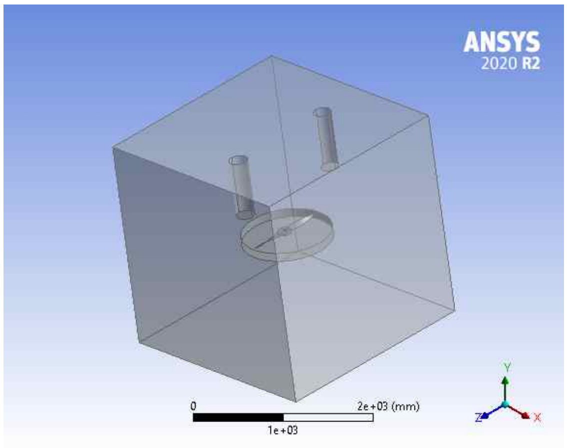


Fig 2: Geometric Conception

2. Run the appropriate solver for three-dimensional modeling,
3. Import and size the mesh (Fig.3),

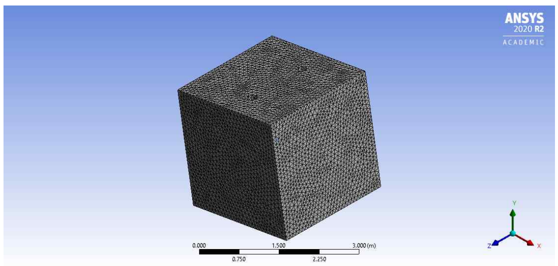


Fig 3: Mesh

4. Select physical models,
5. Setting material properties,
6. Setting the calculation conditions,
7. Define boundary conditions,

8. Provide an initial solution,
9. Set solver parameters,
10. Adjusting the convergence monitors,
11. Calculate and monitor the solution,
12. Post-Processing :
    a. Interaction avec le solver,
    b. Analysis of results: This is the most important part. It is necessary to check the physical coherency of the results obtained (speed profiles and/or global quantities),
    c. Exploitation of the results: We have at the end of the simulation, profiles of speed, energy dissipation, pressure...etc.

III. Results and discussion

In this part, we gather the results from the CFD ANSYS Fluent 2020 R2, to represent the simulation of the dispersion of fine particles on the walls of the experiment room. The results are obtained following an injection of particles whose diameter varies between 10^{-6} µm and 10^{-4} µm from the input determined on the meshing phase, with a feasible Rans K-Epsilon model where the turbulent viscosity is calculated using an improved method. The exact transport equation of the fluctuating component of voracity is used to derive the dissipation rate equation. The model k-ε which is considering to be more accurate than the achievable model. k-ε for the prediction of the distribution of the dissipation rate of flat and round jets [6]. The transport equations in this model are written as:

$$\frac{\partial k}{\partial t} + \frac{\partial k u_i}{\partial x_i} = \frac{\partial}{\partial x_i}\left(Dk_{eff}\frac{\partial k}{\partial x_i}\right) + G_K + \varepsilon \qquad (2)$$

$$\frac{\partial \varepsilon}{\partial t} + \frac{\partial \varepsilon u_i}{\partial x_i} = \frac{\partial}{\partial x_i}\left(Dk_{eff}\frac{\partial \varepsilon}{\partial x_i}\right) + \sqrt{2C_{1\varepsilon}S_{ij}\varepsilon} - C_{2\varepsilon}\frac{\varepsilon^2}{k-\sqrt{v\varepsilon}} \qquad (3)$$

with the turbulent viscosity determined by:

$$v_t = C_\mu \frac{k^2}{\varepsilon} \qquad (4)$$

Where C_μ is computed by:

$$C_\mu = \frac{1}{A_0 - A_S\frac{KU^*}{\varepsilon}} \qquad (5)$$

$$U^* = \sqrt{S_{ij}S_{ij} + \overline{\Omega_{ij}}\,\overline{\Omega_{ij}}} \qquad (6)$$

$$\overline{\Omega_{ij}} = \overline{\Omega_{ij}} - 3\varepsilon_{ijk}\omega_k \qquad (7)$$

Where $\overline{\Omega_{ij}}$the mean rate of rotation tensor and k is is the angular velocity. The constants A_0 and A_s are determined as below:

$$A_0 = 4,\ A_s = \sqrt{6}Cos\varphi \qquad (8)$$

$$\varphi = \frac{1}{3}ArcCos\,(\min\,(\max(\sqrt{6}W, 1)\,, 1) \qquad (9)$$

$$W = \frac{S_{ij}S_{jk}S_{ki}}{S^2} \qquad (10)$$

$C_{1\varepsilon}$ is defined as:

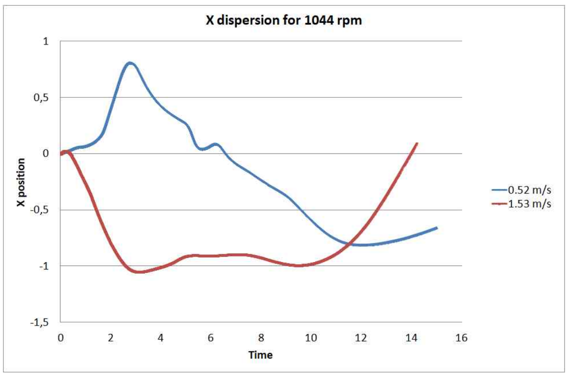
$$C_{1\varepsilon} = \max\,(\frac{\eta}{\eta+5}, 0.43) \qquad (11)$$

$$\eta = S(\frac{k}{\varepsilon}) \qquad (12)$$

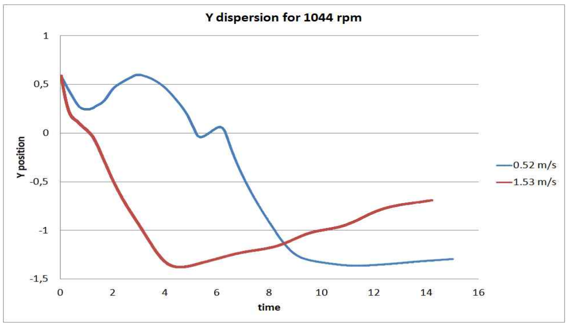
Note that the digital injection (5000 particles/liter) is done on two different velocities, 0,52 m/s and 1,53 m/s, while taking into consideration the 3 propeller speeds, 1044 rpm, 1278 rpm and 2000 rpm.

A comparison of the deposition of fine particles over time is necessary to highlight the effect of velocity on their behavior, and below are the graphical results and the simulation of dispersions on surfaces.

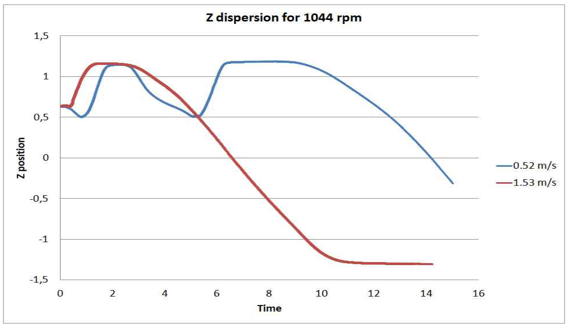
3.1 Results



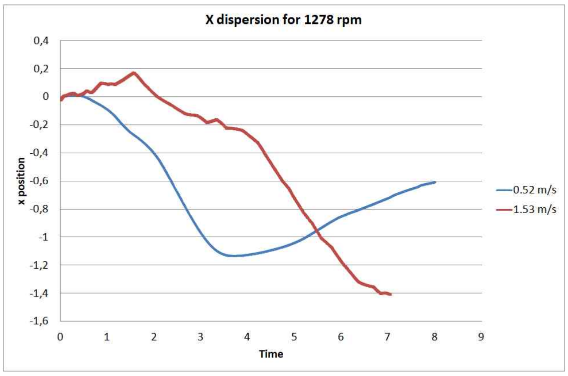
x position for 1044 rpm



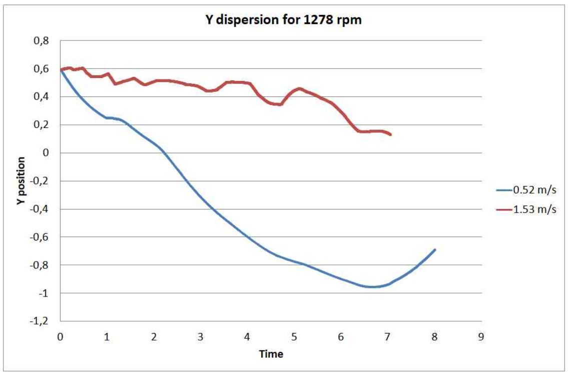
y position for 1044 rpm



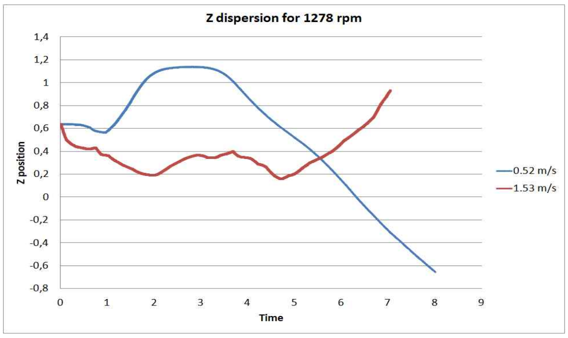
z position for 1044 rpm



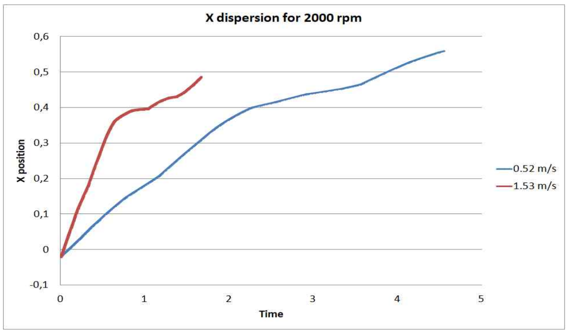
x position for 1278 rpm



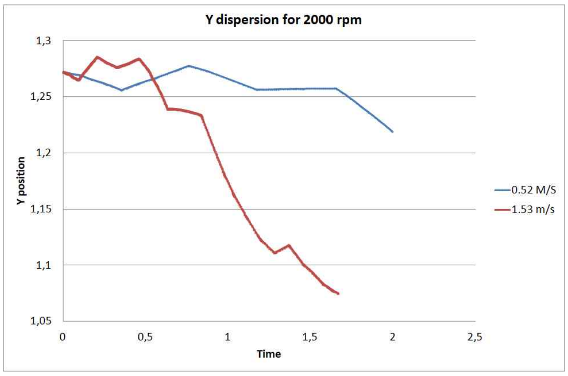
y position for 1278 rpm



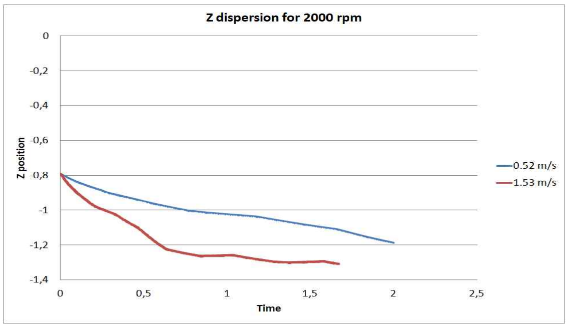
z position for 1278 rpm



x position for 2000 rpm

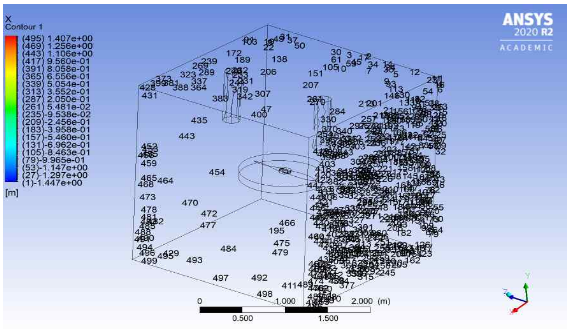


y position for 2000 rpm

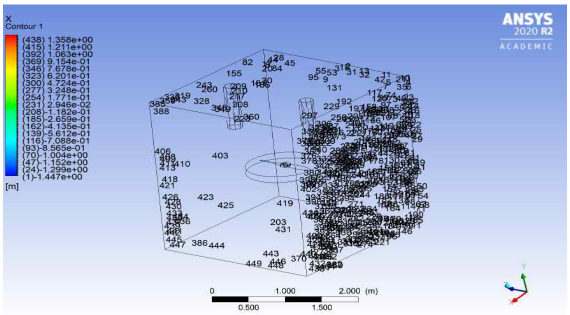


z position for 2000 rpm

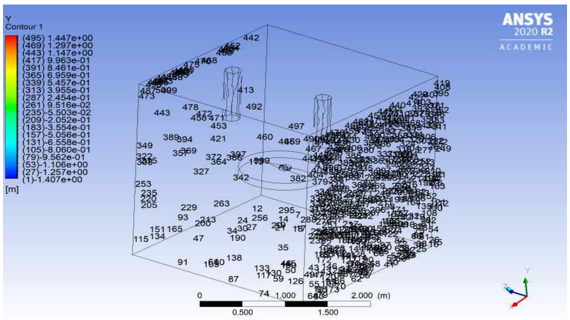
The numerical results clearly show how the particles disperse differently on the internal surfaces of the study chamber according to the entry velocity and the angular velocity of the helix, and the three-dimensional simulation shown in the figures above on the fluent ansys shows a more concrete view on the dispersion of the fines.



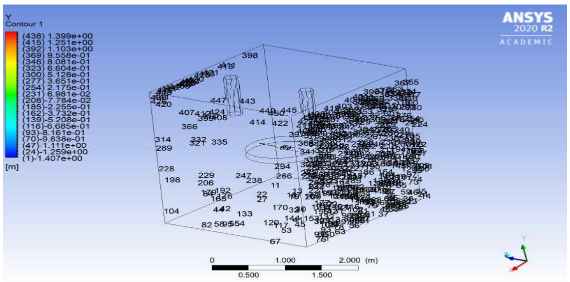
x dispersion for 1044 rpm and velocity 0.52 m/s



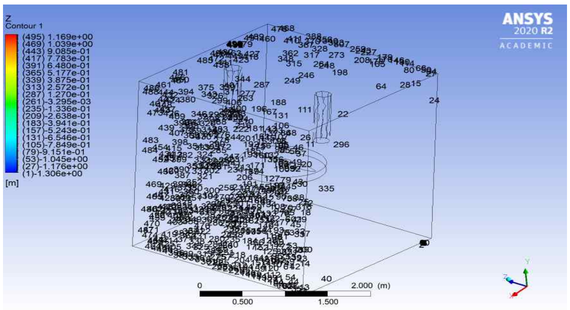
x dispersion for 1044 rpm and velocity 1.53 m/s



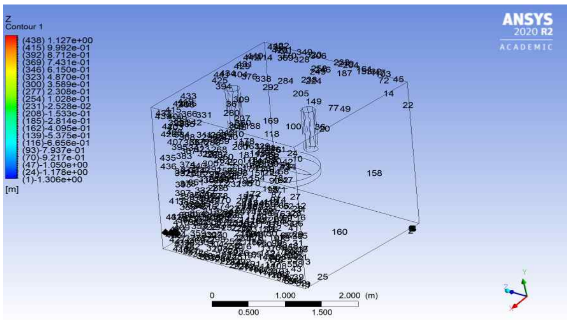
y dispersion for 1044 rpm and velocity 0.52 m/s



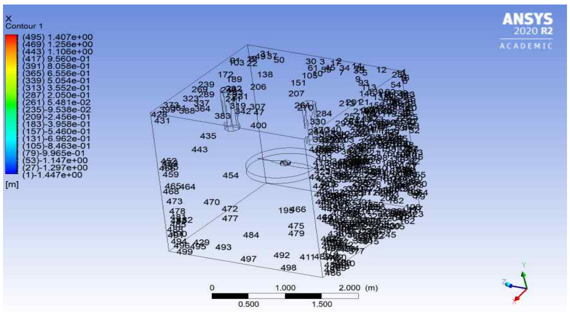
y dispersion for 1044 rpm and velocity 1.53 m/s



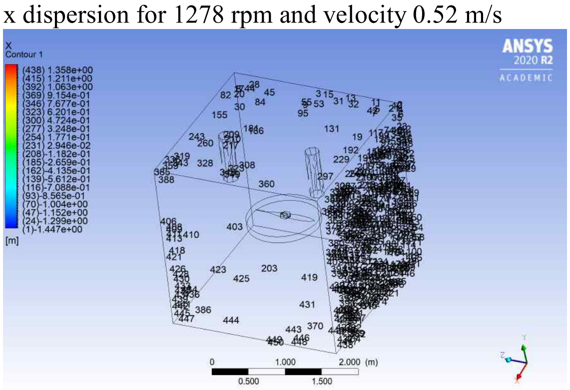
z dispersion for 1044 rpm and velocity 0.52 m/s



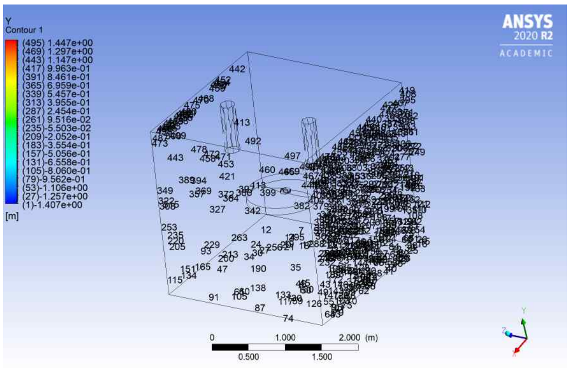
z dispersion for 1044 rpm and velocity 1.53 m/s



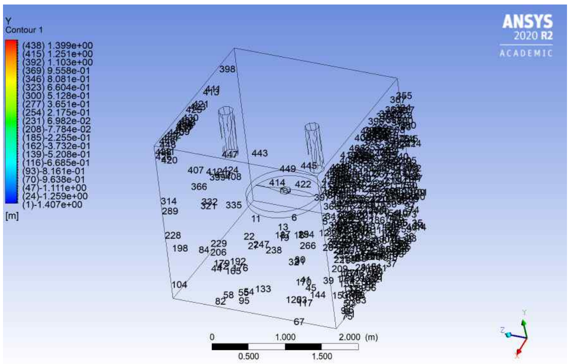
x dispersion for 1278 rpm and velocity 0.52 m/s



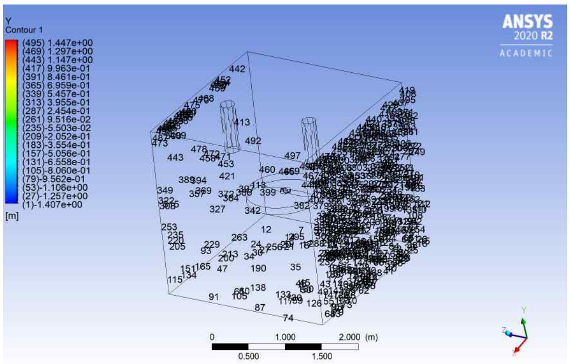
x dispersion for 1278 rpm and velocity 1.53 m/s



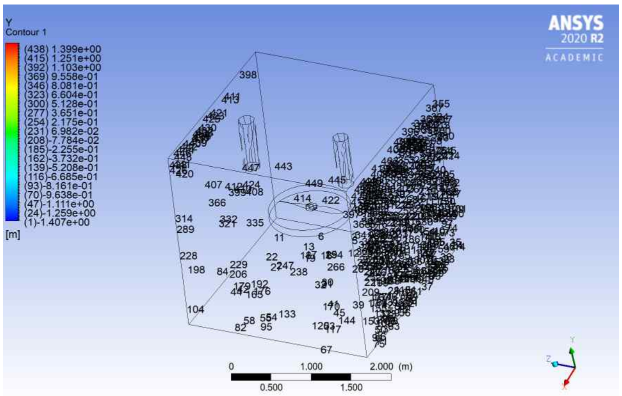
y dispersion for 1278 rpm and velocity 0.52 m/s



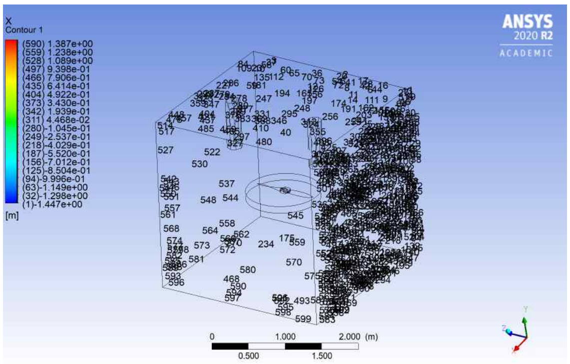
y dispersion for 1278 rpm and velocity 1.53 m/s



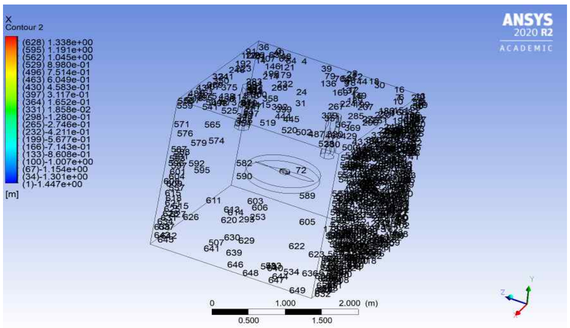
z dispersion for 1278 rpm and velocity 0.52 m/s



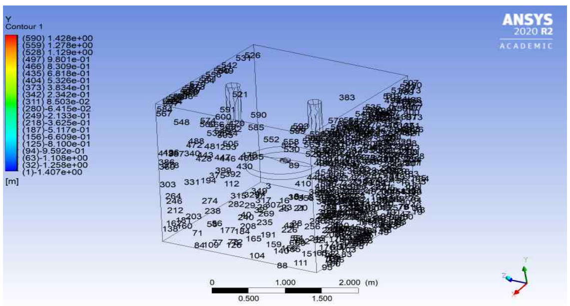
z dispersion for 1278 rpm and velocity 1.53 m/s



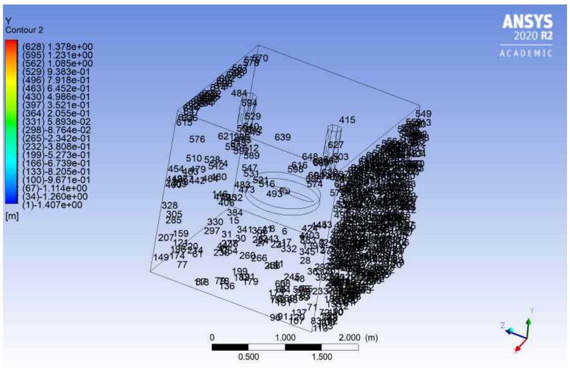
x dispersion for 2000 rpm and velocity 0.52 m/s



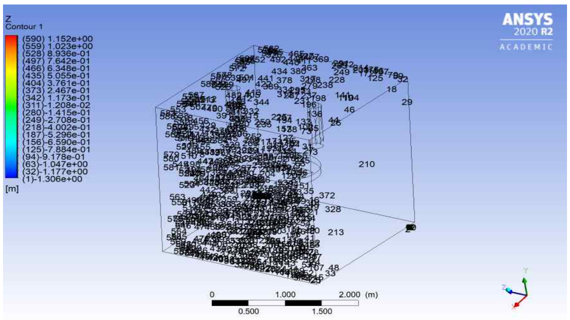
x dispersion for 2000 rpm and velocity 1.53 m/s



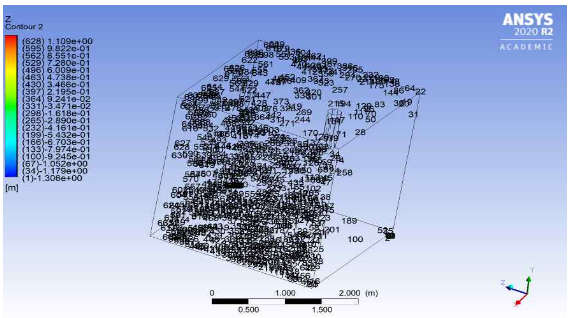
y dispersion for 2000 rpm and velocity 0.52 m/s



y dispersion for 2000 rpm and velocity 1.53 m/s



z dispersion for 2000 rpm and velocity 0.52 m/s



z dispersion for 2000 rpm and velocity 1.53 m/s

IV. Conclusion

In the present numerical study, we complete the experimental study by highlighting the velocity as well as the angular velocity and their effect on the deposition of fine particles with diameters ranging from 10^{-6} and 10^{-4} µm. The results clearly show that velocity plays a very particular role on the dispersion of fines, as well as on their suspension in the air, which illustrates the importance of taking into account the different parameters in future studies in order to show the behaviour of fine particles under several climatic conditions.

One hypothesis to be considered after this study is the suspension of the coronavirus in the area of the premises and the time required for its deposition on surfaces. Subsequently, a theoretical reflection and a numerical approach are underway to study the suspension of viruses captured by the fine particles.

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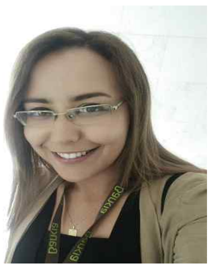

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