Numerical Simulation of Indoors Fine Particles Deposition

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Abstract

Fine particles suspended in the indoor air are deposited on all surfaces. This deposition process not only changes the concentration of particles indoors, but also affects the particle size distribution indoors. In addition, a variety of air pollutants bind to particles suspended in indoor air. Air velocity is one of the key factors influencing the deposition rate of particles on surfaces and is also an important parameter for indoor thermal comfort. This study focused on the deposition of fine particles on the walls of a room, using the calculation code ANSYS-FLUENT 2019 R3, and the results showed that for the particles studied, the deposition velocity on different surfaces increased from 0.53 to 0.0001 m/s. This study could well be useful in other studies on virus propagation estimation, analysis of the distribution of particles indoors and the design of uniform airflow.

Keywords: Air pollution, Dispersion, Modeling, Discretization, Turbulence, Kinetic energy, Dissipation, FLUENT, CFD
1 Introduction

Air pollution research has reached a strong focus in recent decades resulting in a growing demand for accurate modeling of pollutant concentration and dispersion, both experimentally and numerically. Although the study of fine particles 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.

The study of the transport and deposition of fine particles within the premises is therefore a research topic of great interest. Indeed, many applications in a wide variety of fields, such as geotechnics, the environment, hydraulics or the medical field, call for the transport of fine particles in a closed environment. Knowledge of the size, shape and other characteristics of the environment and fine particles is essential to understand the various processes that take place during the migration of fines. The surface plays an important role in the migration and the capture of fines through its influence on the process of fine particle movement and capture.

Several research works have shown the performance of CFD codes for flow simulation [3], [5], [6], [7]. Subsequently, the study of fine particle dispersion is necessary to understand the behaviour of fine particles under changing climatic conditions (inlet velocity, temperature and pressure). In this research context, we will present some results that summarize the deposition of particles at any inlet velocity, and we propose to present all the elements necessary for the numerical study of the indoors dispersion of particles under a RANS k-epsilon model.

2 Method

The numerical study has been made with two software packages. First of all, SolidWorks, on which we carried out the geometrical design of a single empty room with a volume of 8m x 2.5m x 5m, with a door designated as the pollutant inlet, and a window designated as the outlet. These two designations are very important in the configuration stage of the results. We performed the numerical modeling of the fine particle dispersion using ANSYS 2019 R3.
Numerical simulation of this flow is several problematic, because the topology of the flow requires a very fine mesh in a large part of the domain. In order to accurately follow any variation in the mass and aerodynamic fields, especially in the region where the gradients are important.

The size of the mesh affects the quality of the representation of the different variables, as a finer mesh size would ensure better accuracy in the calculation of gradients, but would limit the consideration of roughness and increase calculation times by increasing the number of cells in the mesh. This imposed mesh size is then a compromise between the accuracy of the calculations and its convergence time. An illustration of the final mesh size is shown in the Figure below:

The 3D mesh, consisting of a set of tetrahedral and hexahedral cells, was constructed using the software. The number of meshes was chosen to be as small as possible without degrading the quality of the results. There are 33787 tetrahedrons.

After meshing, we moved on to the configuration of the general parameters, which can be summarized as follows:

- Taking into consideration the energy equation...
- Standard k-epsilon viscosity
- Fluid: Air
- Magnitude of velocity at the entrance (the door): 0.53 m/s
- Temperature: 273k
• Turbulent viscosity: constant
• Number of irritation: 500

3 Digital implementation

3.1 Boundary conditions

Physically a CLS (Surface Boundary Layer) has only one boundary, the ground, but in the calculations we have to delimit in all directions, so let’s use non-physical boundaries. This general presentation then allows us to identify all the points to be taken into consideration. We can then put forward:

• the conditions of entry into the field;
• the conditions of exit from the field;
• the conditions on the ground;
• the conditions at the top of the field;

the conditions of entry into the field

Domain entry conditions must ensure continuity with the surface boundary layer surrounding the modeled field. Indeed, the calculating field is an integral part of the CLS, and must reproduce as well as possible the air flow on flat and rough walls. The entrance conditions that we have to consider are:

• the velocity profile;
And to account for the turbulent characteristics of the CLS:
• the profile of k;
• the profile of $\varepsilon$;

In the literature, CLS modeling is often done under a Rans model $k - \varepsilon$, [1], [4].

the conditions of exit from the field

The outflow boundary condition is used to model the flow outside the calculating field when the flow velocity and pressure are not known before the problem is solved.

The solver extrapolates the necessary information from within the calculating. It is important, however, to understand the limitations of this type of condition. For example, this condition cannot be applied:

- If the problem concerns the inlet pressure condition.
- If we are modeling a compressible flow.

The outflow condition applies for fully developed flows where the diffusion flow for all flow variables in the outlet direction is null.
Consideration of the ground characteristics

In order to model a surface boundary layer with a numerical model, it is necessary to take into account the ground conditions. Indeed, all the profiles characterizing the CLS are dependent on the ground surface condition. All the variables of the surface boundary layer, such as speed and turbulent variables depend on the ruggedness parameter. Consequently, the ground condition will be characterized by these quantities, in accordance with the analytical profiles imposed at the entrance of the domain. This approach is consistently used in the literature [6].

We impose a standard wall law on the floor. The aerodynamic ruggedness (chosen in accordance with the input profiles) is not directly used by the CFD code. ANSYS 19.3 which works with a roughness length which is determined by the relation.

The field summit conditions

During the modeling of a surface boundary layer, most authors impose a condition called symmetry at the field summit [1],[2]. The purpose of the last one is to create a null flux condition for all the CLS quantities (momentum, heat flux, etc.) at the head of the numerical field.

3.2 Digital deployment

The implementation of numerical simulation requires a number of steps detailed below:

1. Create the geometric configuration and generate the mesh,
2. Run the appropriate solver for 3-D modeling,
3. Import and size the mesh,
4. Select the physical models,
5. Define material properties,
6. Define the calculation conditions,
7. Define boundary conditions,
8. Provide an initial solution,
9. Set the solver parameters,
10. Adjust the convergence monitors,
11. Calculate and monitor the solution,
12. Post-Processing :
   a) Interaction with the solver,
   b) Analysis of results: This is the most important part. It is necessary to check the physical consistency 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...
4 Results and Discussion

4.1 Convergence of numerical calculations

The FLUENT code will stop iterations as soon as all calculated residuals are below the value of the convergence entered by the user. This value is to be set according to the desired degree of accuracy of the solution approximated by the calculation code. Figure 3 shows the convergence of the residuals towards the set value, which in our case is less than $10^{-7}$.

4.2 Flow structure

The general structure of the flow in our case where the wind is blowing in a horizontal direction at the field clearly shows the slowing down of the velocities due to the effect of the ground and the walls of the room. The area of air recirculation is visible inside the room.

4.3 Particle behaviour

The deposition of fine particles indoors depends on their transport in the air under the local action of air flows and the various forces that can be exerted on it (molecular diffusion, gravity, radiometric forces). As it depends
Numerical simulation of indoors fine particles deposition

on their interactions with the surface, either the particle will be captured by the surface (and therefore lost to the air) or it will ricochet, the result will depend on the nature and strength of the interaction between the surface and the particle. The figures below show the deposition of particles on the different walls of the room.

5 Conclusion

This article helps to fill in part the lack of studies on fine particle dispersion in the literature. From a methodological viewpoint, the CFD tool is efficient to implement several dispersion schemes according to the different
measures and constraints related to the quality of the area, the surface coating, the characteristics of the particles...etc.

This study could be adapted to also measure vertical particle flows and deposition velocities in complex environments, on the one hand to compare the results of parameterization on other areas covered and on the other hand to provide the literature with further data that is sufficiently well-informed in terms of micro-meteorology. The main obstacle to this adaptation is the response time of the detectors of these particles.

The results obtained will interest the scientific community because they will provide a better understanding of the behaviour of particles indoors under less complex conditions than the outdoor environment. In particular, they can be directly integrated into models to assess, understand and predict the impact of accidental pollutant emissions.

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