PREDICTION OF PARTICLE DEPOSITION IN TURBULENT INDOOR FLOWS WITH A 3D LAGRANGIAN MODEL

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ABSTRACT
This study describes the development of a three dimensional (3D) Lagrangian code of particle transport in indoor turbulent flows. This approach consists of integrating transport equations for each particle at each time step to determine successive positions of the particle. The first challenge was to calculate instantaneous velocities of the airflow. The mean component of these velocities was calculated by a classic CFD code. A stochastic process based on the Gosman and Ioannides method generated the fluctuating component. Corrections were applied to better fit experimental results. The second challenge was the determination of the wall-particle interactions. These interactions were evaluated through the simulation of small-scale experiments to measure particles deposition on real textures encountered in building surfaces. Two kinds of boundary conditions were tested: a particle rebound probability and a critical velocity of rebound. The latter seems more appropriate for simulating the interaction between textures and 5.0 $\mu$m particles.

INDEX TERMS
Particle, Deposition, Wall texture, Boundary condition, Numerical simulation, Lagrangian modeling.

INTRODUCTION
The modern work environment has changed with technical development in our society. French people spend 80 to 90\% of their time inside buildings (CSHPF, 1996), and thus are more exposed to the indoor environment than the outdoors. Public awareness of indoor bacteriological risks has recently increased due to U.S. anthrax events.

Indoor particle pollution modeling tools are important to assess a better prediction of human exposure to particle pollutants. Two levels of particle dispersion modeling exist in building environment. The first, based on a multizone airflow model approach (Crump and Seinfeld, 1981 and Nazaroff and Cass, 1989) considers the room (or building) as a perfectly well mixed zone. This model has a quick response for first analysis but it doesn’t take into account the heterogeneity of particle concentration within the zone. This can be done using the second kind of model, called Lagrangian model, which calculates the trajectory of each particle based on the fluid characteristics. Particle transport through air can be tracked and deposition location can be precisely known.

This study was aimed to develop a three dimensional (3D) Lagrangian code for the simulation of particle dispersion in turbulent indoor flows. First, the reliability of the Gosman and Ioannides (1981) model applied to recalculate the fluctuating component of the fluid velocity, which is needed to determine the particle trajectory, is analysed. Then two kinds of wall-

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particle interaction are described and compared: a particle rebound probability and a critical velocity of rebound.

**METHODOLOGY**

**Lagrangian modeling principle:**

In the Lagrangian method, particles are treated individually by solving the particle motion equation and the bulk of properties of the particulate phase is obtained by averaging a significant number of particles. The particle motion equation, according to Hinze (1987), is:

\[
\frac{\pi}{6} d_p^3 \rho_p \frac{d \bar{U}_p}{dt} = C_d \frac{\pi}{8} d_p^2 \rho_p \left[ \bar{U} - \bar{U}_p \right] \left( \bar{U} - \bar{U}_p \right) + C_a \frac{\pi}{6} d_p \rho_p \left( \frac{d \bar{U}}{dt} - \frac{d \bar{U}_p}{dt} \right) + F_e
\]

where \(d_p\), \(\rho_p\) and \(U_p\) are the diameter, the density and the instantaneous velocity of the particle respectively; \(\rho\) and \(U\) are the density and the instantaneous velocity of the fluid; \(C_d\) is the drag coefficient; \(C_a\) is the added mass coefficient and \(F_e\) represents the external forces.

**Fluid flow characteristics**

In order to determine the instantaneous velocities of the fluid, three different methods may be used to solve the Navier Stokes equations. The first is the Direct Numerical Simulation (DNS) that has the advantage of solving these equations without any hypothesis but requires an extremely fine mesh. As such, it’s only suitable for simple or 2D geometry due to time intensive calculations. The Large Eddy Simulation (LES), based on average turbulence theory solves the Navier-Stokes equations using a coarser grid, but needs additional equations to take into account the energy transfers between small and large eddies. LES models need to be further developed to better suit airflow simulation in buildings. The last model is the Reynolds Averaged Navier-Stokes model. The method for this model consists of introducing time averages of each variable (velocities, pressure and temperature) into the Navier-Stokes equations, and adding additional equations in order to solve the equations system. These models are suitable for complex geometry and are less time consuming than the other, and for this reason are frequently used to model airflow patterns in indoor spaces. Numerous two-equation (\(k-\varepsilon\)) models exist and differ in the transport equations of the turbulent characteristics and in their applicability (Chen, 1995). According to Chen, the Renormalization Group Theory (RNG) model is more accurate then other \(k-\varepsilon\) models for airflow in buildings because it takes into account small and large scales of turbulence differently, although it requires more calculations (iterations) than the standard model to achieve a good convergence. In this study, all the mean quantities, such as the mean fluid velocities, the turbulent kinetic energy, \(k\), and the kinetic energy dissipation rate, \(\varepsilon\), are computed by a Computational Fluid Dynamics (CFD) code using a RNG model.

**Determination of the fluctuating component of the velocity**

In order to obtain the instantaneous velocity of the fluid, we have to calculate at each time step and for each location of a particle the fluctuating component of the fluid velocity based on the turbulent characteristics of the fluid flow. Several models exist and differ in the stochastic method applied. The Gosman and Ioannides (1981) model has served as the basis for numerous authors (Durst, Milojevic and Shonung, 1984 and Mostafa and Mongia, 1987). It calculates the fluctuating component of the fluid velocity from a random variable whose standard deviation, \(\sigma\), is proportional to the turbulent kinetic energy.
The particle motion equation (equation 1) is solved for the entire time that the particle interacts with the turbulent eddy. This time is defined as the minimum between the eddy lifetime and the time required by the particle to pass through the eddy. The eddy lifetime, $t_e$, is a function of the turbulent kinetic energy, $k$, and its dissipation, $\varepsilon$:

$$t_e = \frac{L_e}{(2k/3)^{3/2}} \quad \text{and} \quad L_e = C \frac{k^{2/3}}{\varepsilon}$$

(3)

where $C$ is a constant equal to 0.46 (Chen and Crow, 1983) and $L_e$ is the eddy characteristic length. The time required by the particle to pass through the eddy is given by the following expression:

$$t_r = -\tau \times \ln \left(1 - \frac{L_e}{\tau \times |U - \bar{U}_p|} \right) \quad \text{and} \quad \tau = \frac{\rho_p d_p^2}{18 \mu}$$

(4)

where $\tau$ is the particle relaxation time and $\mu$ is the dynamic viscosity of the fluid. The relaxation time, $t_r$, is the time required by the particle to react to a change in the fluid flow, thus it is well adapted to measure the effect of flow turbulence on particle behavior. The higher the particle relaxation time is, the lower the flow turbulence effect.

Wall-particle interaction

The wall-particle interaction is a complex phenomenon because it involves many parameters. Dahneke (1971) and more recently John (1995) studied this process intensively. When a particle collides with a wall, it can stick to the wall or rebound, depending on the intensity of the adhesion force. This force is difficult to evaluate because it depends on the wall and particle surface characteristics (geometry, hardness and electrostatic polarity) and air dryness. To determine if a rebound occurs, we have defined two rebound criteria. The first one is the stochastic parameter ‘probability of rebound’, $Pr$. If $N$ particles hit a wall, only $Pr \times N$ will stick to the wall; the others will rebound. By calculating a random number at each collision and comparing it to the probability of rebound value (a function of the considered wall-particle couple), the particle behavior is determined. This criterion has no physical value but is well adapted to the Lagrangian method (more precisely to the Gosman and Ioannides (1981) scheme) because the Lagrangian method also requires a large number of particle trajectory calculations. The second criterion is the ‘critical velocity’ below which the particle sticks to the wall. As with the first criterion, it depends on the considered wall-particle couple. It should be added that elastic rebound without energy loss was taken as a first approximation for both criteria to calculate the post-collision particle position.

RESULTS

Before studying the wall-particle interaction, effort was made to determine the reliability of the Gosman and Ioannides (1981) model to predict particle trajectory. The Snyder and Lumley (1972) experiment was simulated in order to compare the behavior of three kinds of particle introduced in a homogeneous turbulent flow. Comparison with the numerical results shows that the model tends to underestimate the particle axial dispersion. Corrections to the
Gosman and Ioannides (1981) model were added by repeating the simulations multiplying the fluctuations by a damping coefficient, $K_{GI}$, evaluated for each particle in order to match the experimental results. Moreover, a direct correlation was determined between this new coefficient, $K_{GI}$, and the particle relaxation time, $\tau$.

$$K_{GI}(\tau) = 4 \times (1 - 4 \times \tau) \quad (5)$$

Figure 1 presents the particle lateral dispersion as a function of time. As expected, numerical and experimental results look similar. The corrected results obtained using this correction factor is shown for the 0.023 s-relaxation time particle as an example; the uncorrected numerical method leads to a quasi non-dispersion, which is in direct contradiction with the experimental results.

![Figure 1. Lateral dispersion of three particle relaxation times versus time.](image)

Figure 2. 5.0 $\mu$m particle deposition on floor as a function of texture.

![Figure 2. 5.0 $\mu$m particle deposition on floor as a function of texture.](image)
The Abadie (2000a, 2000b and 2001) experiment was modeled to evaluate the wall-particle interaction and more precisely to determine the rebound probability and the critical velocity values for a given wall texture-particle couple. This experiment consists of a confined cubic enclosure whose horizontal and vertical walls can be covered by various textures. The selected wall surface panel for the present study is made up of five kinds of textures: from the smoothest and hardest ones like glazing, linoleum and smooth wallpaper, to the roughest and softest like rough wallpaper, and carpet (with cut velvet). A three-bladed propeller suspended from the center of the scale model ceiling and blowing towards the ceiling is employed as a turbulent source. Experimental constants of deposition were determined by regression-fitting of the concentration exponential decay curves. This parameter was used as a reference to calculate the deposition on walls using the global model of Crump and Seinfeld (1983). This global model is a reference to determine particle deposition location in turbulent vessels. By varying the value of the numerical criterion and by comparing the obtained constant of deposition with the experimental value, one can identify the criterion value for the desired texture-particle couple. Figure 2 presents the 5.0 µm-particle deposition on floor as a function of texture for both wall-particle criteria and for the experiment. If the tendencies for both criteria are the same as the global model, the critical velocity criterion seems to be more appropriate to model the wall-particle interaction.

DISCUSSION
The development of the 3D Lagrangian code of particle dispersion brought out two main points. First, the integration of a corrected coefficient to the Gosman and Ioannides (1981) model is consistent with the physics involved in the particle dispersion. The calculation of the fluctuation by the Gosman and Ioannides (1981) model depends only on the fluid characteristics, and its exclusive goal is the determination of the fluctuating part of the velocity without the presence of a solid body. As a result, the fluid instantaneous velocity is the same regardless of the particle type. With the introduction of the coefficient $K_{GI}$, the presence of the particle is then taken into account. For example, the fluid fluctuating velocity is lower for a high relaxation time particle than for a low one.

The second point is that the method employed to evaluate the wall-particle interaction intensity seems reliable and permits an initial approach to model this complex process. Results show that the method clearly highlights the difference in interactions between the textures and their consequences on the deposition location. Despite these encouraging results, deposition on floor is still over-evaluated compared to global model prediction. One improvement will be to consider the energy loss during the wall-particle contact by introducing a restitution coefficient. Taking into account both critical velocity and restitution coefficient would provide a better modeling of the wall-particle interaction.

CONCLUSION AND IMPLICATIONS
A 3D Lagrangian code of particle dispersion in turbulent flows was developed in this study. A correction to a classical model of velocity fluctuating component generation was applied to better fit experimental results. Additional improvement to this part of the code would consist in testing other models of velocity fluctuating component generation or using another approach; for example, Large Eddy Simulation modeling (Chen, Jiang, Beghein et al., 2001) would permit avoiding the use of the artificial velocity fluctuating component calculation.

The most important development from this study concerns the approach used to evaluate the wall-particle interaction. The first step of this method consists of experimentally measuring the constant of deposition for a desired wall-particle couple. Then, using the current database
(available for 5.0 µm-particle) or simulating the experiment for a new kind of particle, the critical velocity (or rebound probability) can be determined. This implies that wall-particle interaction (and particle deposition) for every indoor wall texture can be simulated using both the experimental facility and the numerical code we developed.

This tool is suitable to determine particle dispersion in buildings, to evaluate the main paths followed by particles, to determine the deposition locations and to assess a better prediction of human exposure to particle pollutants.

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