

Simulating the aerodynamical resuspension of a granular bed of microparticles

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Abstract. The deposition of micrometric particles in layers on various surfaces (e.g., ventilation ducts, industrial environments, nuclear reactors) has raised concerns due to potential resuspension in enclosed spaces or the atmosphere. While previous studies mainly focused on single-layer deposits, there is limited research on multilayer deposits. The complexity of this phenomenon arises from the granular topography and particle interactions, which can lead to individual or cluster resuspension due to aerodynamic forces or particle impacts. Aerodynamic forces are influenced by factors related to the morphology of the deposit. This work presents a numerical model studying resuspension of a 2D granular bed of microparticles, where adhesive forces are stronger than particle weight. The deposit is subjected to aerodynamic forces that cause detachment. Two deposit types are examined: one with perfectly stacked grains, where adhesion forces are randomly distributed, and another built using a pseudo-dynamic algorithm, controlling porosity. Monte Carlo simulations are used to model the resuspension process, considering aerodynamic and adhesion forces. Results for the simplest bed align with previous experimental studies but require calibration for accurate kinematics. The second deposit type shows promising results, highlighting the importance of deposit topology in particle detachment and resuspension, with a focus on geometric obstruction, a key aspect of the problem.

1 Introduction

The deposition of micrometric particles in successive layers on surfaces, such as those found in ventilation ducts, solar panels, nuclear reactors, and industrial environments, has gained significant attention due to the potential health, safety, and environmental risks associated with particle resuspension [1-4]. While most research has focused on single-layer deposits, there is a lack of studies on multilayer deposits, despite their relevance in real-world applications.

Multilayer systems introduce additional complexities, including particle interactions and deposit topography, complicating resuspension mechanisms. Notable examples include the accumulation of dust or spores in ventilation ducts and radioactive particles in nuclear reactors [5, 6]. Existing models, largely based on single-layer assumptions, fail to adequately predict resuspension in multilayer scenarios due to uncertainties in adhesion force definitions. This highlights the need for further measurements under specific conditions to improve predictive capabilities [5].

Monte Carlo (MC) simulations have proven effective in modelling resuspension in dilute, single-layer systems, by capturing particle dynamics with low computational cost [7, 8]. While several studies focus on multi-layered granular beds dominated by gravity, there is limited literature on microparticle multilayers in resuspension phenomena [9]. The novelty of this study is to extend the use of MC tools for developing a numerical model for resuspension in a multilayer of aerosol particles, where adhesive forces dominate over

gravitational ones. The model accounts for aerodynamic forces and their role in destabilizing particles, providing a better perspective for more accurate representation of resuspension in complex multilayer environments.

2 Layout of the problem

A schematic representation of a granular bed (multilayer) of microparticles subjected to airflow is shown in Figure 1. In general, particles are in contact with each other and/or with the bottom surface, resulting in adhesion forces between them.

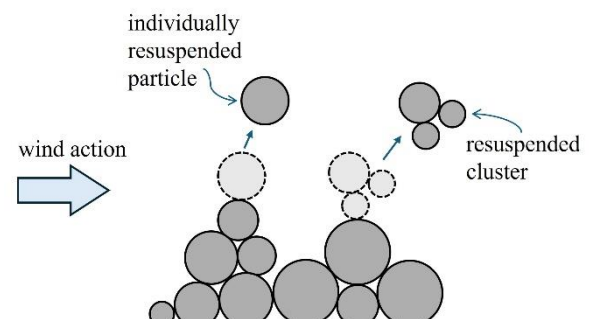


Fig. 1. Sketch of a multilayer showing resuspension.

These forces exceed the weight of the particles, which could lead to high-porosity within the bed. Adhesion plays a crucial role in preventing particle detachment.

Due to the action of aerodynamic force, particles may detach individually or as part of a resuspending cluster. Each time the equilibrium between aerodynamic

and adhesion forces (and/or moments) acting on a particle (or cluster) is broken, the particle (or cluster) may detach from the bed and resuspend.

To model this complex scenario, we use two types of multilayer structures: one is a simple structure with perfectly stacked grains, and the second is generated using a pseudo-dynamic algorithm with a controlled porosity degree. The resuspension process in each bed is modelled using a MC methodology, and the results are compared with previous models and experimental data from other authors.

3 Simplest bed structure

Figure 2 (a) shows a multilayer arrangement of superimposed layers of microparticles subjected to aerodynamic forces in a wind tunnel. Each particle is represented as a cube and assigned an adhesion force, F_{adh} , randomly sampled from a log-normal distribution to reflect the variability observed in experimental systems. The distribution is the same for all layers, and the adhesion force binds each particle to the one directly below it. There are no interactions between lateral neighbors in the same layer. Each layer contains N cubes, and the number of cubes exposed to the airflow remains constant and equal to N in each iteration.

One iteration consists in checking sequentially the *resuspension condition* of the exposed cube in each of the N columns. These exposed cubes are subjected to an aerodynamic force, F_{aero} , sampled from a Gaussian distribution. These are the only cubes that may resuspend individually. Cluster resuspension is not allowed.

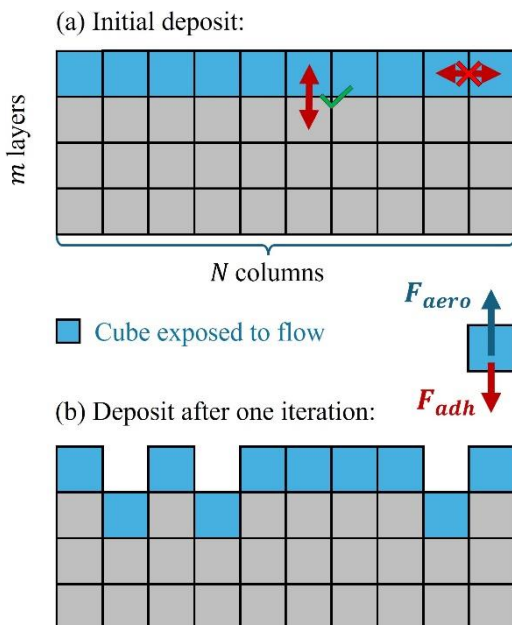


Fig. 2. (a) Sketch of the initial stage of the simplest bed structure representation. (b) Example of the bed's appearance after one iteration.

The aerodynamic forces are calculated using the friction velocity u_* which can be expressed as a function of the wall shear stress τ_w in the wind tunnel, $u_* = \sqrt{\tau_w/\rho}$, where ρ is the fluid density. Thus, the mean of

the Gaussian distribution is $\bar{F}_{aero} = \alpha u_*^2$ and the dispersion is $\sigma_{aero} = \frac{1}{3} \alpha u_*^2$ [10]. Parameter α is determined from experimental comparison between aerodynamic and adhesion forces in each studied case [11]. The simplest choice is $\alpha = 1$ (not affecting the results) and αu_*^2 is considered as an arbitrary force unity, a.u. For the log-normal distribution of adhesion forces, the median, \bar{F}_{adh} , is selected based on this arbitrary force unit, with σ_{adh} , the geometric SD.

3.1 Recreation of Fromentin's results

The above model and the associated rules were previously used by Fromentin as a simplified approach in a semi-empirical model for resuspension [11]. In his approach, the *resuspension condition* is satisfied when the aerodynamic force exceeds the adhesion force.

Due to the formulation of the Fromentin's model, at least two experimental data points are needed to calibrate the mass of a cube, the iteration duration and the particle flowrate.

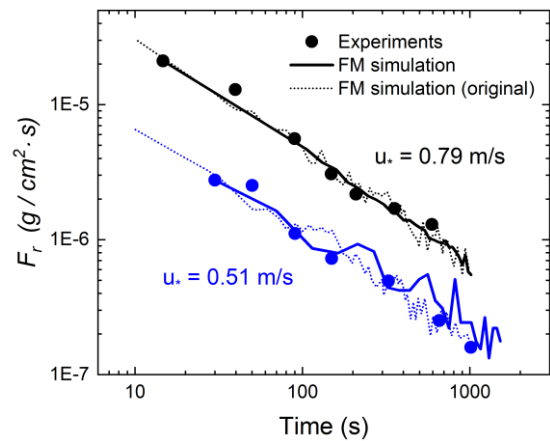


Fig. 3. Recreation of Fromentin's results for Fe_2O_3 particles with 2-4.3 μm , using a log-normal distribution with median 5.5 a.u. and dispersion 2.2.

Following the procedure outlined above and considering the materials studied in [11], we reproduce Fromentin's results for one particular case and two different friction velocities in the tunnel, as shown in Figure 3. The input parameters used for the force distributions are provided in the figure caption. As expected, our results closely match those in [11] and the model describes the experimental behavior quite well. However, the model has some limitations. It requires two experimental points in advance to predict subsequent experimental behavior. Furthermore, it does not account for bed topography, meaning its influence on resuspension is not captured.

3.2 Monte Carlo model

As explained in the Introduction, MC simulation has proven effective in modeling monolayer deposits in previous studies [4, 8]. Extending this approach to multilayer resuspension could be useful for predicting the kinetics of the process while eliminating the need of calibration. Additionally, it enables a statistical

treatment of the problem, capturing the randomness and complexity inherent in particle detachment events.

As discussed elsewhere [4, 8], the MC formulation for particle resuspension uses the analogy between this phenomenon (activated by airflow) and molecular desorption from surfaces (activated by temperature) [12]. Thus, the resuspension rate for particle i is calculated as:

$$r_i = k \cdot e^{\left[\frac{F_{adh,i}}{F_{aero,i}} \right]} \quad (1)$$

where $k = 0.006 \frac{u_*^2}{\nu_{air}}$ is the maximum resuspension rate, and ν_{air} is the air viscosity [13]. The probability for resuspension is $p_i = r_i/r_{sup}$, with r_{sup} being the supreme of r_i [4, 8]. Therefore, the *resuspension condition* in this model is different from that in Fromentin's one. If $p_i > \zeta(0,1)$, resuspension occurs; otherwise, if $p_i \leq \zeta(0,1)$, no resuspension is allowed. $\zeta(0,1)$ is a random number in the (0,1) interval.

Finally, the time increment Δt after each iteration (MC step) is calculated as $\Delta t = -\frac{\ln(\varepsilon)}{r_{sup} N_p(t)}$, where ε is a random number in (0,1) interval, and N_p is the total number of particles in the bed [8]. Using r_{sup} ensures a small enough time increment to capture all events.

Using this MC approach, we simulate the same type of system as in Section 3.1, adopting the same assumptions as in Fromentin's model, except for the *resuspension condition* expressed above. The results are shown in Figure 4. Note that the time scale here is not calibrated by any experimental data. The only required information is the mass represented by each cube represents in the system.

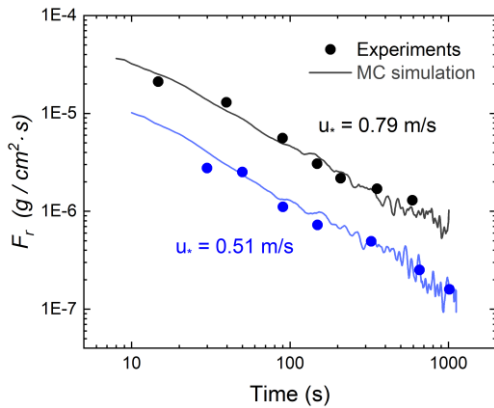


Fig. 4. Comparison of simulations with experiments in [11].

In this way, the MC approach represents a step forward in the characterization of multilayer resuspension. However, the deposit topography is not yet considered in this formulation. The next section addresses this issue to provide a more comprehensive description of the present problem.

4 Bed structure with porosity

A 2D multilayered deposit of microparticles, similar to the one in Figure 1, has been used in previous studies

[14]. Here, we generate the granular bed following the same concept but using a standard pseudo-dynamic (PD) algorithm [15], which provides a more realistic representation of multilayer deposits. We consider two cases: deposits formed by polydisperse microparticles (with sizes sampled from a log-normal distribution) and deposits formed by monodisperse particles. The porosity of the deposit is controlled through a sticking probability, P_s , where higher P_s values lead to looser structure and increased porosity ϕ .

The number of layers in the deposit is varied by adjusting the total number of deposited particles. Adhesive forces between particles are assigned randomly from the same adhesion force distribution as in Section 3. Figure 5 shows two typical deposits generated by the PD algorithm with different porosities.

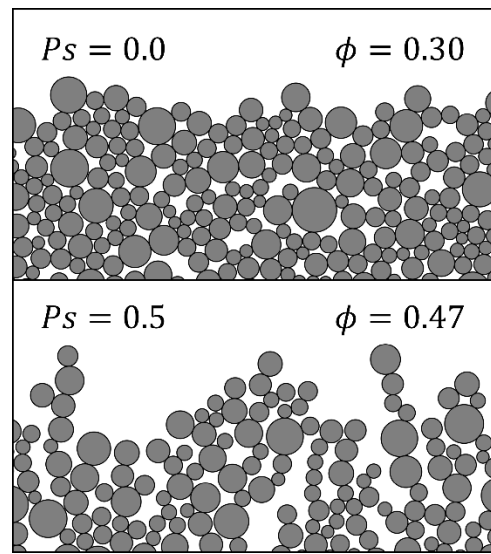


Fig. 5. Microparticle deposit generated by PD algorithm with different porosities as indicated.

Resuspension is modelled using a MC algorithm similar to the one described in the previous section. To initiate a resuspension loop, particles exposed to airflow must first be identified. For simplicity, cluster resuspension is not considered. Thus, candidate particles for detachment must not support any other particle in the array and must be unobstructed. Particle i (with coordinates x_i , y_i , and diameter d_i) is considered obstructed by particle j (with coordinates x_j , y_j , and diameter d_j) if these inequalities are satisfied:

$$y_i < y_j \quad (2)$$

$$\left(x_i - \frac{d_i}{2} \right) - \frac{d_j}{2} < x_j < \left(x_i + \frac{d_i}{2} \right) + \frac{d_j}{2} \quad (3)$$

Once a candidate particle is identified, the *resuspension condition* is evaluated. After completing a full MC step, time is updated, and the number of particles detached from the bed is recorded.

Figure 6 shows the number of resuspended particles, $N_r(t)$, over time for different porosities and both types of deposits: (a) polydisperse and (b) monodisperse. As seen, $N_r(t)$ tends to be higher for the intermediate porosity among the three tested cases. This suggests a competition between two effects: increasing

P_s (i.e., increasing porosity) reduces the number of supporting particles in the arrangement, which favours resuspension. However, higher porosity also leads to looser structures, increasing the likelihood of particles being obstructed by others, which limits their potential for resuspension. Particle flow results are not presented here due to limited statistics. Increasing system size is crucial to obtain flow curves similar to those shown for previous simpler deposit structures.

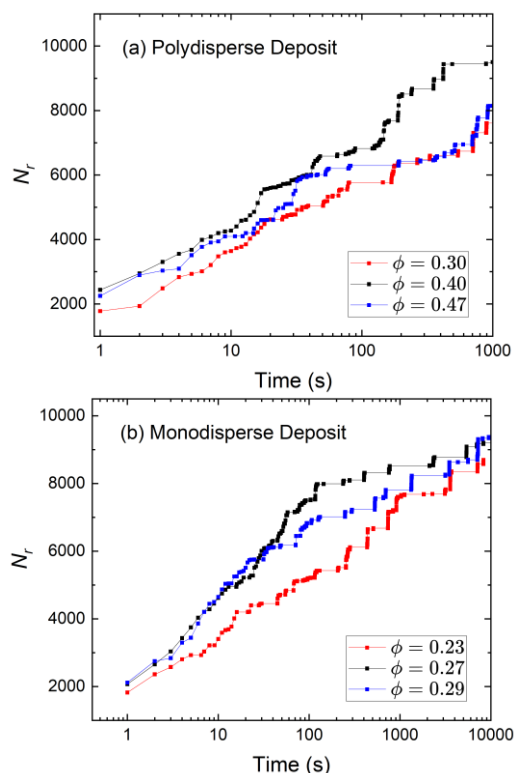


Fig. 6. MC simulation for the number of resuspended particles vs. time for different porosities and both types of deposits.

5 Conclusion

MC simulations of the simplest granular bed demonstrate that the model successfully captures the general behaviour observed in experimental results from previous studies. However, the calibration between each cube-particle and a real particle can only be achieved with prior experimental data. Furthermore, the model does not account for the impact of bed topography on the results. For the second type of granular bed, the results are promising, highlighting the importance of topological structure in particle detachment and resuspension, resembling more realistic multilayered systems. This approach enhances the understanding of geometric obstruction, a critical aspect of the problem. However, further work is needed to assign consistent adhesive forces to the different structures, which will also address other key aspect of the problem.

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Data is available upon request.

All authors contributed equally to this work.

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