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Monte Carlo modelling of particle resuspension on a flat surface

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ABSTRACT

A model for the resuspension of a monolayer of particles deposited on a flat surface is developed based on a Monte Carlo simulation of the phenomenon. Particles deposited on the surface are attached to it through an adhesion force. A turbulent flow is assumed to be responsible for the resuspension of particles. The stochastic process used for particle resuspension is based on the evaluation of probabilities depending on the ratio between adhesion and aerodynamic forces and using a Metropolis function. Although simple, the present model accounts for the main features of the resuspension flux observed experimentally and by other models. The model is able to clearly show the role that the parameters of the force distributions (both adhesion and turbulent) have on the short- and long-term resuspension flux, and it captures the intrinsic stochastic nature of the resuspension process.

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1. Introduction

The problem of resuspension of already deposited fine particles on a surface has a long history, and has captured the attention of researchers since many decades. Its presence in a wide set of industrial and environmental scenarios makes its study and description an important chapter in aerosol science (Bowling, 1988). In particular, one of the main concerns has been to obtain perfectly clean surfaces for micro and nanoelectronic technology. In addition, there is the problem of the release of radioactive particles to the environment during nuclear accidents (Reeks et al., 1988; Zhang et al., 2013; Stempniewicz et al., 2008).

Furthermore, the problem of the resuspension not only concerns the above domains, but also causes serious difficulties in mining production. Indeed, mining operations are notable in the amount of generated particulates, the extent of polluted areas and toxicity, when compared with other sources of dust and aerosol emissions (Csavina et al., 2012; Stovern et al., 2014).

However, many aspects of the problem still remain as an open question for researchers. The complexity of the problem is based on the difficulties in the measurement of the microscopic adhesion forces that result from the particles–surface interaction through a blend of mechanical stress, chemical bonds and physical attractions. For example, knowledge of the particle size and the surface roughness is crucial for the calculation of the reduction and spread in the adhesion force.

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However, given the serious experimental difficulties in their determination, a theoretical approach to this description is required to model particle–surface interactions. Other difficulties are the different flow conditions and the respective aerodynamic forces involved.

Besides, in practice, many problems of particle resuspension involve the presence of multilayer deposits, which add greater complexity related to mutual obstruction of particles, the formation and eventual resuspension of clusters and the dependence of the resuspension process on the structure of the deposit (Ziskind, 2006; Gradón, 2009; Boor et al., 2013; Henry & Minier, 2014b; Hanus et al., 2007). Many models have been developed in the last two decades. Comprehensive reviews concerning resuspension models can be found in Zhang (2011), Ziskind et al. (1995), Henry & Minier (2014a) and Stempniewicz et al. (2008). In general, theoretical models developed to simulate and predict the resuspension properties are divided into two categories: those based on the balance resulting from the aerodynamic and adhesive forces acting on a particle, called quasi-static models (Reeks & Hall, 2001); and those based on the removing of particles by energy accumulation, described in terms of the accumulation of kinetic energy of the flow, called dynamic models. However, given the large amount of diverse work, the debating points and the models that may not fit in these two raw categories, a new classification has been recently proposed to account for recent developments in resuspension models (Henry & Minier, 2014a).

In most cases, the models reproduce the experimental behavior, characterized by an initial or short-term resuspension, and by a long-term resuspension described by a $1/t$ decay. In general, the condition for the particles to resuspend is that the aerodynamic forces have to be greater than the forces of adhesion. In particular, we want to highlight the kinetic model of Wen & Kasper (1989), based on the analogy between the process of resuspension supported by the balance of forces, and the kinetics of the first order reaction that describes the desorption of molecules from a heterogeneous surface, with a constant resuspension rate. Many models are based on a balance of forces that involves the possibility of instantaneous resuspension of particles when the removal forces are greater than the adhesion forces. Nevertheless, other models allow the movement of the particle on the surface before reentrainment (Guingo & Minier, 2008; Henry et al., 2012; Henry & Minier, 2014b; Fu et al., 2013).

Given the fact that the resuspension phenomenon can be treated as a stochastic process, this paper proposes a model based on a Monte Carlo (MC) simulation. Our aim is to use an algorithm that takes into account the analogy between the release process of particles and first order chemical reactions. With the help of the phenomenological Arrhenius expression for the determination of the resuspension rate, we show that the Metropolis function (Binder & Heermann, 1992), used as the transition probability between configuration states, is able to describe the main features of the resuspended particle flux for the case of a monolayer of particles deposited onto a flat surface and subjected to a turbulent flow. In this case, there will be a process activated by removal forces, as for the case of the kinetic model of Wen & Kasper (1989), instead of being activated by the surface temperature. We consider that the resuspension rate depends on the ratio between the adhesive force and the removal force acting on a particle (Zhang, 2011). We should clarify here that other MC models (Goldasteh et al., 2013; Fu et al., 2013) use the balance between moments of adhesion and hydrodynamic forces. As one can expect, the choice of a force balance or a moment balance approach is related to the assumed motion of particles: rolling, described by moment balance, while sliding and lifting are properly described by a force balance (Ibrahim et al., 2008). As emphasized in a recent review (Henry & Minier, 2014a), the relative importance of rolling and 'burst-type' resuspension (by turbulent flows) depends on the size of particles: small particles which are well embedded in the viscous sublayer are more sensitive to rolling motion while larger particles are more affected by 'burst-type' resuspension.

The main difference between our present model and the models before is that we employ a MC method to deal with resuspension kinetics. As will be explained below, in the present model, the probability of a particle to be released from the surface is not necessary equal to one if the adhesion force is less than the aerodynamic force and, moreover, the probability is not equal to zero if the aerodynamic force is less than the adhesion force. As it will be seen, this model allows recovering the main aspects of the resuspension process. Thus, the novelty here is the inclusion, through a MC method, of the stochastic nature of the removal forces due to the flow and the adhesion forces between particles and the surface.

In the following section, the description of the model and a brief explanation of the Monte Carlo method, are presented. In addition, the type of distribution assumed for aerodynamic and adhesion forces is also presented, along with the rules of the stochastic process applied in the simulation routine. The complete set of the simulation results is displayed in Section 3, which is divided into four subsections that present simulations for monodisperse adhesive forces, rough surfaces, a phase diagram and a final comparison with experimental data for fractional mass resuspension vs. time. Section 4 presents a detailed discussion of all the obtained results and, finally, the conclusions are presented in Section 5.

2. Model description

The model proposed here, as the one of Wen & Kasper (1989), describes the resuspension of particles from a surface as a first order chemical reaction, such as the desorption process from a heterogeneous surface (Zhdanov, 1991). For the expression of the rate constant, empirical or phenomenological equations are used. One of the most used is the Arrhenius Law (Moelwyn Hughes, 1971). In this case, the rate constant k is given as $k(F)=A\exp(-F)$, where A, the preexponential factor, and F, the relative balance between the adhesion force and the removing force in the process, are the apparent Arrhenius parameters.

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