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A stochastic approach for the simulation of particle resuspension from rough substrates: Model and numerical implementation

Christophe Henry [a,*], Jean-Pierre Minier [b]

[a] Institute of Fluid-Flow Machinery, Polish Academy of Sciences, ul. Fiszera 14, 80-231 Gdańsk, Poland
[b] EDF R&D, Mécanique des Fluides, Energie et Environnement, 6 quai Watier, 78400 Chatou, France

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ABSTRACT

This paper presents a Lagrangian stochastic model to simulate colloid resuspension from rough surfaces. For that purpose, the extension of a recent proposition is discussed as well as the details of its numerical implementation. The basis of this model is a dynamical approach which reproduces explicitly the different steps involved in a three-stage scenario of particle resuspension where particles are set in motion (first stage); roll/slide along a rough surface due to varying force moments (second stage); and can be detached when a large-scale asperity is hit (third stage). The model treats separately hydrodynamic forces (drag force), adhesion forces (mainly due to interface chemical effects) and surface roughness through a two-level description (small-scale asperities and large-scale asperities) within a unified approach that combines the effects of fluid mechanics, interface chemistry and material properties. A description of the key points of the model brings forward the important role played by the number of small-scale asperities in contact with each particle; the pivot point around which particles can roll; the streamwise kinetic energy acquired as particles roll/slide along the surface; the probability to hit a large-scale asperity and the prediction of the actual detachment. Specific methods to simulate the trajectories of these stochastic processes are detailed and validated in a step-by-step manner with a specific emphasis put on the interplay between adhesion forces and particle dynamics. Finally, once each step has been separately assessed, the complete model is evaluated by comparing predictions to a realistic resuspension test-case for airborne colloids, showing that good and consistent numerical predictions are obtained with reasonable time steps.

1. Introduction

Resuspension (also referred to as reentrainment or detachment) corresponds to the phenomenon where deposited particles, or materials, are being removed from substrates by a flow (either liquid or air). As described in comprehensive reviews (Boor et al., 2013; Gradoń, 2009; Henry & Minier, 2014; Ziskind, 2006; Ziskind et al., 1995), this process is present in a wide range of industrial and environmental situations where, depending on the issues at stake, the incentive can be either to promote or to prevent it. For example, particle resuspension is sometimes needed to remove unwanted materials (such as

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* Corresponding author.
E-mail address: christophe.henry@mines-paris.org (C. Henry).

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dust accumulation on solar cells Mani & Pillai, 2010) whereas reentrainment of hazardous materials should be avoided (extensive studies are available in aerosol science such as radioactive particles in nuclear power plants Stempniewicz & Komen, 2010 or dust with pollutants in an indoor environment Boor et al., 2013).

From a more general point of view, resuspension is one of the processes at play in particle fouling and is often closely related to particle deposition on walls. This explains why particle resuspension needs to be studied as such and also as one part of a complete modelling approach aiming at addressing deposition, agglomeration and up to possible clogging (see a recent detailed review discussing these phenomena from a unified modelling standpoint, Henry et al., 2012).

In the present paper, attention is focussed on the resuspension of colloids exposed to fluid flows. This is a complex issue since, apart from hydrodynamical effects, colloidal particles can also be subject to strong interfacial forces linked with surface physico-chemistry. Therefore, modelling colloidal particle resuspension requires a careful understanding and implementation of both hydrodynamical and adhesion forces to obtain accurate descriptions. Furthermore, inertia effects must be properly accounted for so that the model be applicable for both large-inertia and colloidal particles. In the following, we concentrate on what can be referred to as “mono-layer resuspension”, which means that we mainly address situations where deposited particles on a wall surface form a single layer. Consequently, we consider the case where each particle interacts only with the fluid and with the wall surface independently of other deposited particles. When the rate of deposition is high enough, particles can form what is called “multi-layer deposits” that can exhibit various structures and morphologies and where particles interact also noticeably with other particles. In that case, a flowing fluid can induce “multi-layer resuspension”. Though the situation remains the same (basically, particles are re-entrained from “layers attached to the wall”), the precise phenomenology involved in multi-layer resuspension is far less well known and represents specific issues (Boor et al., 2013; Henry & Minier, 2014; Ziskind, 2006). A detailed discussion of experimental data and of related modelling challenges has been proposed recently (Henry et al., 2012; Henry & Minier, 2014) and multi-layer resuspension is left out of the present work.

1.1. *The reentrainment process*

From a phenomenological point of view, particle resuspension results from a balance between two opposite interactions:

- *Particle-fluid interactions*: deposited particles placed within a moving fluid undergo hydrodynamic forces, such as drag or lift forces, that tend to set them in motion.
- *Particle-surface interactions*: deposited particles are subject to adhesion forces with the surface, also called contact forces, that attach them and tend to prevent motion.

Although correct, this presentation in terms of a direct force balance can be misleadingly simple and the detailed mechanism of particle resuspension has been a long-term object of debate and investigations (Ziskind et al., 1995). However, recent experimental studies have provided new insights into the mechanisms of colloid resuspension from surfaces (Ibrahim et al., 2003; Jiang et al., 2008): it has been shown that the detachment of colloidal particles from surfaces is mainly triggered by particle motion along the surface (rolling and sliding motion) while lift-off forces play a negligible role (Ibrahim et al., 2003). Moreover, experimental studies have also highlighted that the presence of nanoscale roughness can considerably reduce adhesion forces, thus allowing more particles to be resuspended (Audry et al., 2009).

1.2. *Modelling approaches for particle resuspension*

Several approaches have been proposed in the literature to simulate colloid resuspension (Reeks & Hall, 2001; Stempniewicz & Komen, 2010; Ziskind et al., 1995) and these modelling approaches can be classified into two main categories (another classification has been proposed recently by Henry & Minier (2014)):

1. “Quasi-static models” which focus only on the inception of particle motion, i.e. on the rupture of static equilibrium. In such models, it is assumed that each moving particle is necessarily resuspended. In other words, detachment is identified with particle motion. Models belonging to this category can be further separated into two sub-categories depending on how static equilibrium is addressed.
    (a) *Force-balance approaches* (Ziskind, 2006): here, the balance between hydrodynamic and adhesive forces (or moments) is the determining criterion for particle resuspension. In that case, particles are set in motion (rolling or sliding motion) when hydrodynamic forces overcome adhesion forces, leading to their resuspension.
    (b) *Energy-accumulation approaches* (Reeks & Hall, 2001; Stempniewicz & Komen, 2010): here, particle resuspension results from the accumulation of vibrational energy which can reach values higher than the adhesive energy between the particle and the surface, triggering particle motion (and thus detachment in this approach).
2. “Dynamical models” which simulate not only the onset of particle motion but also particle dynamics along the wall (how particles can gain or lose kinetic energy when rolling or sliding). In these approaches, particle motion is not identified with detachment. Therefore, in contrast to quasi-static models, the phenomenological description in terms of the two opposite forces mentioned in the previous subsection is incomplete and must be supplemented with a specific description, or scenario, for particle detachment from the surface.