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A model of fine particles deposition on smooth surfaces: I—Theoretical basis and model development

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Abstract

A model of fine particles deposition from a flowing suspension on smooth surfaces is developed. It is based on a common Eulerian–Lagrangian particle tracking approach, that allows a force-based description of the interactions between particles and surface. Hydrodynamics and particle–wall forces are included, with emphasis on a detailed account of Van der Waals forces. Diffusion has also been included and combined with the Lagrangian approach resulting in a stochastic process. Efficient and physically consistent techniques to solve the resulting stochastic differential equations are discussed, with specific algorithms to manage transition from small to extremely strong forcing function, and to precisely determine when and where particle trajectories reach the boundary. Quantitative evidences of the usefulness of techniques are shown.

Keywords: Colloidal phenomena; Diffusion; Interface; Laminar flow; Stochastic processes; Brownian dynamics

0. Introduction

The deposition of colloidal particles suspended in a fluid on a surface interests many branches of engineering. It can be a key step in a wide range of applications, e.g., fouling of heat exchangers, contamination of nuclear reactors, occlusion of membrane filters, lumen reduction of human veins, deposits in microelectronics processes and paper industry. Accordingly, there is a need of developing methods to predict and control the surface deposition rate of colloidal particles suspended in fluids, both liquid or gas. Many experimental data and models have been published about deposition from aerosols, defined as suspensions of solids or liquid particles in a gas. Several Lagrangian particle tracking models have been developed for aerosol (e.g. McLaughlin, 1989; Fichman et al., 1988; Fan and Ahmadi, 1993; He and Ahmadi, 1999). Adhesion models based on an Eulerian approach have been developed by Young and Leeming (1997) and Guha (1997), among others.

Deposition of colloidal particles dispersed in a flowing liquid has been comparatively less addressed, both experimentally and theoretically. Bowen and Epstein (1979) developed a combined transport and adhesion model based on the interaction forces between particles and surfaces, comparing their predictions to experimental data. Many empirical correlations have been developed from experimental data (Beal, 1978; Epstein, 1988; Vasak et al., 1995). Adomeit and Renz (1996) and Yiantsios and Karabelas (2003) collected experimental data and developed an Eulerian model to predict the deposition rate. In the Eulerian approach particles are assumed to behave like molecules of a diluted tracer. The approach is thus suitable for very small, neutrally buoyant particles up to a few microns, but it becomes more and more inappropriate as the particle dimension or density increase.

Most of the models that we mentioned require empirical parameters to describe experimental data, so they are difficult to extrapolate to different configurations. In this work we aim at developing a predictive model which has the capability of properly accounting for the relevant mechanism of particle transport and adhesion in liquids, without needing adjustable parameters. Here we aim to develop a model which can be applied to a larger range of particle size, from strictly colloidal to inertial particles, to include prediction of cells and microorganisms deposition. For this purpose, we turn to an Eulerian–Lagrangian approach that allows to include forces on the particles that are

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relevant on different particle scales, from inertial to diffusive. The expected result is a simulation model that remains correct as the particle size varies, also in intermediate regimes. Here we focus on the case of non-inertial particles that allows some simplifications typical of the "Brownian dynamics simulations" to alleviate the numerical solution. However, the same approach without simplifications can deal with the case of inertial particles as well, with additional computational cost. In the formulation of our model we also refer to studies of aerosol deposition, because many Lagrangian particle tracking methods have been developed for these systems. In each case, we restrict to the ideal configuration of monodispersed, spherical particles depositing from a diluted aqueous suspension in laminar flow on a non-reactive surface. We consider pH values for which the electrical double layer repulsion is negligible in order to study the situation of purely attractive particle–wall interaction. We compared the results of our simulations to literature experimental data and to analytical results for simplified circumstances in a companion paper. Notwithstanding some restriction, the structure of the model developed can be preserved in further extensions, to generate sub-models to be coupled to CFD in more complex applications.

1. Physical model of adhesion

Particle deposition is traditionally described as a two-step process. The first is considered the wandering of particles through the fluid, driven by particle–fluid interactions and diffusion; all of them may take particles to the wall. The second is the adhesion step due to the interaction forces between particles and surfaces (van de Ven, 1988). Such a scheme is somehow misleading because it assumes a strictly sequential process, where adhesion is seen as an irreversible step that can occur almost exclusively once particles get close enough to the surface (perfect-sink model). In our model, adhesion forces are always operating, the same as hydrodynamic forces and diffusion. As a matter of fact, particle–wall interactions are quite short-ranged if compared to a characteristic extension of flow normal to the wall, so they can affect the trajectories of particles that are sufficiently close to the surface. In contrast, hydrodynamic forces can affect the adhesion up to the contact between particle and surface and even after that, although re-entrainment has not been addressed here.

Fine particles are easily transported by drag, particularly in highly viscous fluids (liquids, compared to gases), so their paths are mostly determined by this mechanism. Significant modifications of the particle path can be induced by gravity, but only in the case of large density differences, or after very long paths. Other hydrodynamic forces can in principle affect the particle fate. These include the lift force, normal to the velocity gradient. We neglected the effects of the virtual mass and Basset forces, both because of the small particles size and the condition of completely developed laminar flow. Thermophoretic effects have been neglected because we study isothermal conditions. Finally, we disregarded autoretardation (Epstein, 1997) and particle reentrainment. Autoretardation is negligible because we consider a dilute suspension of small particles, so

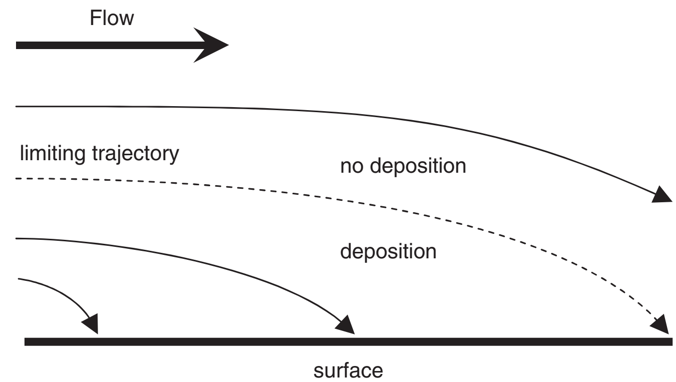

Fig. 1. Schematic picture of the limiting trajectory that separates regions where particle can or cannot reach an attractive surface, within the flow domain, neglecting diffusion.

there will never be an appreciable reduction of the available deposition area due to attached particles. Particle reentrainment has been neglected because several experimental observations report data with negligible (if any) particle detachment. A detailed discussion of forces and phenomena mentioned above can be found in Epstein (1997).

Small particles in liquids are thus very likely to settle on the fluid streamlines, with some delay in case the initial velocity of the particle is markedly different from that of the fluid or the particle has a large density compared to the fluid. However, also in laminar flow, small particles are expected to fluctuate about a mean path because of diffusion, i.e., a Brownian motion superposes to the deterministic path. Such a contribution increases as the particle size decreases. Fluctuations because of Brownian motion must be accounted for in a realistic model because small displacements can be extremely critical in close proximity to a surface, where adhesive–repulsive forces operate. Such forces have a very small region of influence compared to most realistic flow domains, but within their range of influence they are extremely strong and very sensitive to the position.

We expected two mechanisms for particle approach to a surface, depending on the attractive features of the surface. They are qualitatively described in the following, suggesting the crucial role of diffusion in both cases.

First, assuming a purely attractive surface and no diffusion (deterministic path), the action of drag and attractive forces uniquely identifies particle paths, as schematically shown in Fig. 1. The distance from the surface where particle paths can be affected until deposition is very small, compared with a length scale of the flow, like the velocity boundary layer. A limiting trajectory, that depends on the surface extension in the flow direction, can be identified; it separates two regions where particles can or cannot reach the surface, within its length. In this case (attractive surface), diffusion can allow particles to cross the limiting trajectory, in both directions.

Second, diffusion can cause deposition to take place when it is not allowed by repulsive forces. When attractive and repulsive forces reach an equilibrium the particle settles on a different limiting trajectory, shown in Fig. 2, strictly parallel to