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# MODELING FOULING OF ROUGH SURFACES BY COLLOIDAL PARTICLES IN TURBULENT FLOWS

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### **EXTENDED ABSTRACT**

Deposition of colloidal particles is a sensitive issue in the nuclear industry. For instance, fouling of heat exchangers in Pressurized Water Reactor (PWR) occurs in the secondary circuit: due to the corrosion of pipes, colloidal oxide particles (mainly magnetite) are transported in the secondary coolant, and deposit in the broached holes of the tube support plates or on the tubes. As in other industrial applications, this fouling affects the heat transfer efficiency but deposition can also lead to the blockage of some broached holes. In order to prevent fouling or to clean heat exchangers, a better understanding of the fouling mechanisms in heat exchangers is required.

Fouling can be depicted with four simple mechanisms: deposition, resuspension, agglomeration and clogging. Deposition occurs when particles are transported by the fluid towards the surface, where surface interactions may allow or hinder deposition. Resuspension is possible when particles are weakly bounded to the surface, allowing the fluid to drag them away. Agglomeration happens when two colliding particles adhere together, thereby forming an agglomerate which has more inertia than each single particle. Clogging is the last stage of fouling: deposited particles will influence the flow of fluid around them, also changing the geometry of the surface. It appears that each of the previous mechanisms is governed by the coupling of two phenomena: the hydrodynamic transport of particles and the physicochemical interactions between two surfaces. The deposition process is therefore modeled as a two-step process: a transport step and an attachment step.

The transport step has been treated first, since it is the restraining step: no matter how good the attachment step is, if the number of particles reaching the surface is misevaluated, the whole deposition process would be inaccurate. The transport step is modeled using the stochastic Lagrangian model for the hydrodynamic transport (Minier and Peirano, 2001) in Code\_Saturne (a hydrodynamic CFD Code). The model has been refined to take into account some near-wall coherent structures, such as the "sweep" and "ejection" events (Guingo and Minier, 2008a). Three zones are then defined (see Fig. 1): in the core flow, the stochastic Lagrangian model is used; in the logarithmic zone, the interaction with near-wall coherent

structures is modeled; in the viscous sublayer, another Langevin equation is used.



Figure 1: Hydrodynamic model in the near-wall region

The attachment step is modeled using the DLVO theory (Israelachvili, 1991), which takes into account both Lifshitz-Van der Waals forces and electrostatic forces to describe the interaction energy between smooth surfaces. Under electrostatically repulsive conditions, an energy barrier (corresponding to the maximum value of the interaction energy) may appear. This energy barrier, if greater than the kinetic energy of an incoming particle, will prevent deposition from happening.

As far as resuspension is concerned, a three-stage process has been implemented taking into account the effect of surface roughness (Guingo and Minier, 2008b): in the first stage, hydrodynamic drag forces can overcome the adhesion torque (determined with VDW forces only) forcing the particle to roll on the surface; during stage two, the particle rolls on the surface; in the third stage, upon encounter with a large asperity, the particle may be resuspended if its kinetic energy – considered to be converted from the streamwise to the wall-normal direction – is high enough to overcome the adhesion forces.



Figure 2: a three-stage process for resuspension

Agglomeration is not taken into account in the present study, since we are dealing with low particle concentrations. Clogging has not yet been fully investigated, since the effects of a deposit on the flow can be added only once the predictions of deposition and reentrainment phenomena are accurate enough.

This first model yields satisfactory results on the initial deposition rate of particles on surfaces under electrostatically attractive conditions. However, under electrostatically repulsive conditions, discrepancies have been found: no deposition is predicted whereas a non-zero deposition rate is sometimes observed experimentally. In addition, the resuspension model does not account for the pH-dependence of reentrainement observed experimentally.

The purpose of the present study is to discuss the role of hydrodynamic transport, surface chemistry and surface geometry in the deposition and reentrainment process, as well as to assess their relative impact in some industrialrelevant test-cases.

In the experiment of Cerovic et al, 2009, the deposition of hematite particles on polypropylene walls has been measured under varying pH and hydrodynamic conditions: the loop consisted of 7.2m tube network with bends and boxes (more details in Cerovic et al, 2009) inside which hematite particles circulate. The existence of non-zero deposition rate under repulsive conditions in experimental data challenges the numerical predictions. Since satisfactory predictions are obtained in attractive conditions (between pH 4 and pH 7), the transfer of particles towards the wall through hydrodynamic transport is assumed to be accurate and, therefore, such a discrepancy is more likely to be related to the attachment step. In a first study, the effect of surface roughness on the energy barrier and its consequences on the deposition rate have been investigated (Henry et al, 2011). The model proceeds in two steps: firstly, wall-roughness is described using hemispherical asperities placed randomly on a surface inside which asperities play a significant role in the interaction; secondly the interaction energy is determined using the DLVO theory and assuming interaction energies to be additive. Surface roughness has been shown to reduce significantly the energy barrier: interaction energies are roughly proportional to the asperity size, while surface coverage controls the number of asperities in contact with the particle (see Henry et al, 2011). Lowering the energy barrier will enhance the deposition rate under repulsive conditions, which may become non-zero. Figure 3 compares the measured deposition rate to a predicted rate obtained on a simple pipe with or without surface roughness (no description of surface roughness being available, 20 nm asperities have been considered to provide an example).

However, even if surface roughness provides an explanation for non-zero deposition rates under repulsive conditions, it does not account for the nearly steady deposition rate observed experimentally at pH greater than 8. Such a trend in the deposition rate may be linked with the geometrical singularities (bends and boxes) existing in the experiment of Cerovic et al, 2009. Geometrical singularities induce indeed specific local deposition rates, which are much higher than the deposition rate predicted in a simple

pipe. Taking into account both geometrical singularities and surface roughness yields better agreement between predictions and experimental data (see Fig. 4).



Figure 3: Deposition rate of hematite particles on polypropylene walls: (x) experimental measurements from Cerovic et al, 2009, (□) numerical results with smooth surfaces, (•) numerical results with 20nm asperities

covering 4% of the surface





Deposition phenomena being accurately modeled, the issues concerning resuspension phenomena are then dealt with. The pH-dependence of resuspension observed experimentally cannot be reproduced numerically using a model based on VDW forces only, since VDW forces depend neither on the pH conditions nor on the ionic strength of the solution. In order to improve numerical predictions, a model using the DLVO theory has been developed: following the scheme developed for deposition phenomena, surface roughness is described using hemispherical asperities while interaction energies are assumed to be additive. This model yields satisfactory results for the distribution of adhesion forces observed experimentally (see for instance Zhou et al, 2003) and also for the pH dependence of the adhesion force (see for instance Eichenlaub et al, 2006).

From the present study – which highlights the coupled effects of hydrodynamic transport, surface chemistry and

surface geometry on the deposition rate of colloidal particles in turbulent flows - it appears that surface roughness is a promising candidate for the observed non-zero deposition rate in repulsive conditions, but geometrical singularities of the experiment also play a role in the global deposition rate. Predicted adhesion forces have also been shown to depend on both surface roughness (asperity size and surface coverage) and pH. Further detailed calculations have to be performed in order to provide further comparisons with experimental data on the effect of surface roughness and pH on the resuspension of colloidal particles. In the present study, the failure of the DLVO theory to predict some observations was thus assumed to be explained by surface roughness. However, depending on solution conditions, non-DLVO forces such as capillary forces (see Nitschke et al, 2009) or acid-base forces (see van Oss, 1993) may have to be taken into account. The advantage of the present Lagrangian method is that adding a new force to the balance between hydrodynamic and surface forces is rather straightforward.

Since agglomeration has been neglected in this study, the last step towards a better description of the fouling process is to investigate the clogging mechanism (which can be described as a balance between multilayer deposition, deposits cohesion and the influence of deposits on the fluid).

#### NOMENCLATURE

y distance to the wall, m

 $y^{+}$  dimensionless distance to the wall,  $u_{\tau}y/v_{f}$ , dimensionless

 $u_{\tau}$  wall friction velocity, m/s

 $v_{\rm f}$  kinematic viscosity of the fluid, m<sup>2</sup>/s

## ABBREVIATIONS

CFD Computational Fluid Dynamics EDL Electrostatic Double Layer PDF Probability Density Function PWR Pressurized Water Reactor VDW Van der Waals

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