



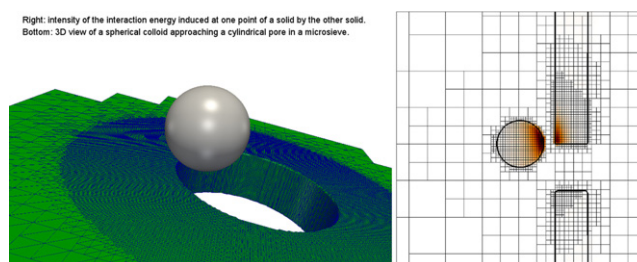
Analytical and numerical computations of the van der Waals force in complex geometries: Application to the filtration of colloidal particles

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HIGHLIGHTS

- ▶ An exact solution for the sphere/wedge vdW interaction energy is derived.
- ▶ The validity of both simple and new models for sphere/pore interactions is assessed.
- ▶ A new numerical tool to compute the van der Waals colloidal interactions is presented.
- ▶ An adaptive mesh refinement strategy is used to discretize the solids.

GRAPHICAL ABSTRACT



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ABSTRACT

Particle capture during the filtration of colloidal dispersions depends on a complex balance between repulsive forces, such as hydrodynamic or electrostatic effects, and attractive forces, amongst them the van der Waals interaction forces. Satisfactory expressions for the latter are thus required in complex geometries. Exact expressions for the geometrical factor involved in the van der Waals interaction energy based on Hamaker's additivity hypothesis are derived for a sphere in interaction with a square wedge, a semi-infinite or finite slit, a semi-infinite slab, a 2D pillar, a rectangular rod, a corner and a rectangular channel. A numerical tool based on an adaptive mesh refinement strategy is presented and used to validate the analytical results. The analytical result for a sphere/wedge system is used to assess the domain of applicability of the sphere/plane model in the vicinity of the edge. The interaction between a sphere and a cylindrical pore in a plate of finite thickness is then simulated and the range of validity of the sphere/wedge system as a model of the sphere/pore system is deduced from the numerical results.

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1. Introduction

The evaluation of the van der Waals force or interaction energy between two or more solids is of crucial importance in many academic and industrial problems. Some examples are the

(de)stabilization of colloidal suspensions in which an equilibrium between the repulsive electrostatic forces and attractive van der Waals interactions is involved (e.g. [1]), the drying of colloidal films to produce surface coatings, the prediction of protein interactions [2] or the filtration of sub-micronic particles in water treatment [3,4].

In the latter problem, particle capture is the result of a complex interplay between hydrodynamic, electrostatic and van der Waals forces. Let us suppose colloids are not too small and the influence of

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