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Calculation of double layer interaction between colloidal aggregates

Karin Schießl^a, Frank Babick^{b,*}, Michael Stintz^b^a Institut für Strömungsmechanik, TU Dresden, 01062 Dresden, Germany^b Institut für Verfahrenstechnik und Umwelttechnik, TU Dresden, 01062 Dresden, Germany

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ABSTRACT

This paper examines the interaction between the electric double layers of aggregates. Commonly, rather simplified models are used like the approximation of primary particle interaction (APPI), which just considers the interaction of the closest pair of primary particles having a double layer as if they were isolated. However, for nanoparticles the double layer thickness may be in the same order of magnitude as the particle size or even larger, what leads to a considerable double layer overlap inside the aggregates and between two interacting aggregates. Consequently, such approximations will fail. The paper presents a numerical scheme for the double layer interaction of arbitrarily shaped aggregates, which can e.g. help to establish criteria for the applicability of approximate models. The calculation employs a singularity method, which is based on the linearised Poisson–Boltzmann equation. Additionally, a linear model for charge regulation is implemented. The impact of charge regulation and double layer thickness were studied for fractal DLCA aggregates and hexagonal closed-packed aggregates.

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1. Motivation

It is commonly accepted that the macroscopic properties of suspensions are determined by concentration, size and shape of the particles as well as by the interparticle forces. The latter are of particular relevance for colloidal material and affect i. a. the microscopic structure, the viscosity and the stability of the suspension. The interactions between the particles may be attractive or repulsive. The main attractive component is the van-der-Waals interaction, whereas the repulsion is (at least in aqueous systems) primarily due to the interaction between the electric double layers surrounding any charged particle in a liquid medium. For spherical particles the total effect of van-der-Waals and double layer interaction is described by the DLVO theory named after Derjaguin, Landau, Verwey und Overbeek (e.g. [1]).

Particulate material especially with particles in the colloidal size range (<1 µm) is frequently encountered in form of aggregates, e.g. carbon black or fumed silica. The structure of the aggregates strongly depends on factors like the particle concentration, the flow conditions and the interparticle forces in the aggregation process. Consequently there exists a huge variety of potential particle configuration within an aggregate.

Hitherto, there is no clear understanding on how the aggregate structure affects the double layer interaction between two

aggregates. That is mainly due to the absence of simple analytical expressions for the interaction between aggregates and the diversity of aggregate configurations. In particular the formation of double layers inside an aggregate and the interaction with the double layers of neighboring aggregates involves the overlap of the double layers and correspondingly charge regulation. For that reason double layer interaction is intrinsically a many-body phenomenon.

A common approximation (e.g. [2–6]) for the interaction of aggregates is to ignore any interaction term but that of the closest pair of primary particles, which is assumed to have a double layer as in the isolated case (approximation of primary particle interaction – APPI). However, its validity has not been examined sufficiently for aggregates of nanoparticles, i.e. particles whose size is in the typical range of the double layer thickness (e.g. the Debye length of a 0.001 M NaCl solution is 10 nm). There is no quantitative criterion that can be employed. Another approximation consists in adding up all pairwise interactions between the primary particles. As in APPI the individual double layers are considered unchanged compared to the isolated case (e.g. [7,8]). Quantitative limits of this approach are not discussed. Therefore, this paper addresses the calculation of the double layer interaction energy between aggregates by refining an existing calculation scheme [9]. It employs this method for a qualitative discussion on the impact of charge regulation and double layer thickness for selected aggregate geometries. Eventually comparison is made with the approximate solutions.

* Corresponding author.

E-mail address: Frank.Babick@tu-dresden.de (F. Babick).