



Original Research Paper

Aggregation of nanoparticles in high ionic strength suspensions: Effect of Hamaker constant and particle concentration

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ARTICLE INFO

Article history:

Received 15 December 2011
 Received in revised form 3 April 2012
 Accepted 17 April 2012
 Available online 3 May 2012

Keywords:

Discrete Element Method (DEM)
 Colloidal suspensions
 van der Waals forces
 Binary mixtures

ABSTRACT

The kinetics of aggregation of nanocolloidal particles in suspensions has been studied using computer simulations based on Discrete Element Method. This study presents the analysis of the influence of Hamaker constant, Brownian forces and particle concentration on the aggregation time of nanoparticles in high ionic strength suspensions. Particle adhesion and cohesion were simulated using the van der Waals force equation. Half the particles were assigned a Hamaker constant of 9.0×10^{-20} J and the other half of the particles had the Hamaker constant varied from case to case with values between 1.0×10^{-20} and 9.0×10^{-20} J. Aggregation times obtained from analysing the number of interparticle contacts and number of singlets in the suspensions have been used to characterise the speed of the aggregation process. The simulation results show that when the strength of the van der Waals interaction increases the aggregation time decreases following a power law. In addition, the presence of Brownian forces speeds up the aggregation process. Finally, the relationship between packing fraction and aggregation times for singlets and contacts has been very well expressed by power laws.

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1. Introduction

The control of long term stability of particulate dispersions is of crucial importance to a wide variety of industries including mineral processing and waste water treatment, and commodities such as paints, pharmaceuticals, and consumer care products. Whilst experimental methods are routinely utilised to assess suspension stability, the ability to simulate suspension behaviour computationally is becoming increasingly important. This is particularly true of samples that are costly (e.g. pharmaceuticals) or hazardous (e.g. biologically active particles), or to probe conditions for which there are not yet well-characterised model experimental analogues.

In the absence of steric stabilisation, polymer bridging, or strong solvent structural forces, the interaction energy between two colloidal particles can be expressed as the sum of attractive van der Waals force and the electric double layer repulsion according to the well known Derjaguin–Landau–Verwey–Overbeek (DLVO) theory [1].

For two identical particles, the electrical double layer interaction energy, V_{edl} (J), as a function of separation distance between particle centres, r (m), is given by:

$$V_{edl} = 2\pi\epsilon\epsilon_0 R\psi_0^2 \exp(-\kappa r) \quad (1)$$

where ϵ is the dielectric constant of the intervening medium, ϵ_0 is the permittivity of free space ($C V^{-1} m^{-1}$), R is the particle radius (m), ψ_0 is the surface potential of the particles (V), and κ is the Debye constant (m^{-1}).

Furthermore, the electric double layer interaction is dependent on the electrolyte concentration through the Debye constant, κ , which may be calculated by:

$$\kappa = \left(\frac{2000 N_A e^2}{\epsilon \epsilon_0 k_B T} \right)^{1/2} \sqrt{I} \quad (2)$$

Here, N_A is the Avogadro number (mol^{-1}), e is the elementary charge on an electron (C), k_B is the Boltzmann constant ($J K^{-1}$), T is the temperature (K), and I is the solution ionic strength ($mol L^{-1}$). The ionic strength is the sum of all electrolyte concentrations and, where c_i and z_i are the concentration ($mol L^{-1}$) and charge of the i th electrolyte species, respectively, can be expressed as:

$$I = \frac{\sum_i c_i z_i^2}{2} \quad (3)$$

According to Eqs. (1) and (2), as the ionic strength increases, through electrolyte concentration or charge, so does the Debye constant. Consequently the exponential decay in the magnitude of the electrical double layer repulsion as a function of particle

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