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Original Research Paper

A DEM-based analysis of the influence of aggregate structure on suspension shear yield stress

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ABSTRACT

This study theoretically examined the effect of aggregate structure on the suspension shear yield stress. The aggregation process of colloidal particles was simulated using the discrete element model (DEM) combined with the well-known DLVO theory. The predicted aggregate structural characteristics, namely the coordination number and inter-particle forces were then used in a modified version of the Flatt and Bowen mechanistic model [6] to calculate the corresponding suspension yield stress. The effect of key parameters such as solid volume fraction, suspension pH and ionic strength on the aggregate structure and hence the yield stress of the suspension was investigated.

The results showed that the yield stress increased significantly under conditions that were favourable for formation of complex net-like aggregate structures, such as high solid volume fractions, pH values near the iso-electric point, and high ionic strengths. In such cases, the mean coordination number reached a maximum value which was considered to be dependent on the particle size and size distribution. The suspension yield stress exhibited a power law dependency on the solid volume fraction. The interconnected network structure developed at high solid volume fractions was found to be the major contributing factor to the observed high suspension yield stress. As the particle–particle repulsion became significant, a decrease in both the number of bonds and the mechanical bonding strength of the aggregate structure was observed. That was considered to be responsible for the reduction in the suspension yield stress. The suspension yield stress became independent of the suspension ionic strength when the ionic strength exceeded the critical coagulation concentration. Satisfactory agreements were obtained between simulation results and the published experimental data.

1. Introduction

Yield stress is an important rheological characteristic of aggregated suspensions, as it dictates the input power-load to render the suspension flowable. In aggregated suspensions, the yield stress is a mechanical rigidity exhibited by the space filling particulate network that is formed due to interactions between colloidal particles. It is therefore closely related to structural properties of the particulate network, in terms of the strength of bonds between particles and the number of bonds that need to be broken. The bonding strength is controlled by inter-particle forces such as electrostatic, van der Waals, and/or steric and other more complex forces, which in turn are controlled by the solution and particle surface properties, such as solution pH and ionic strength. The number of bonds depends on the network structural factors and particle parameters such as size and size distribution, shape, and volume fraction [1,2].

Various theoretical models have been reported for the prediction of suspension yield stress. Generally, these models can be classified according to the calculation approaches into two categories. The first category predicts suspension yield stress based on the tensile strength of a bed of particles, whilst the second approach is based on the force balance on primary particles mainly between inter-particle forces and shear stress.

Rumpf [3] carried out the pioneering research in this field predicting the suspension yield stress by equating the tensile strength of a bed of mono-sized particles to the number of particle bonds per unit area and the bonding strength. Later, Kapur et al. [4] modified the equation of Rumpf [3] by incorporating the contribution from particle size poly-dispersity. However, the model was only valid when the net electrical double layer (EDL) repulsive forces between particles were zero, i.e. at the iso-electric point (IEP). Scales et al. [5] extended Kapur's model [4] to include the effect of particle–particle repulsion using the well-known DLVO theory.

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