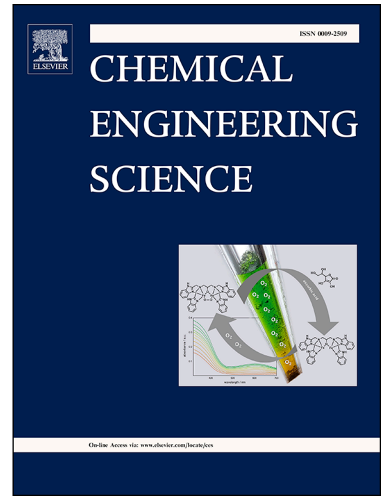
Accepted Manuscript



The rheology of slurries of athermal cohesive micro-particles immersed in fluid: a computational and experimental comparison

Eric Murphy, Gilson Lomboy, Kejin Wang, Sriram Sundararajan, Shankar Subramaniam

PII: S0009-2509(18)30660-2
DOI: https://doi.org/10.1016/j.ces.2018.09.010
Reference: CES 14486

To appear in: *Chemical Engineering Science*

Received Date: 11 May 2018
Accepted Date: 9 September 2018

The rheology of slurries of athermal cohesive micro-particles immersed in fluid: a computational and experimental comparison

Eric Murphy[1], Gilson Lomboy[2], Kejin Wang[3], Sriram Sundararajan[4], Shankar Subramaniam[1,*]

Abstract

Immersed cohesive particles that aggregate under shear are commonly encountered in chemical engineering contexts. This work concerns the rheology of a particular set of systems, cement pastes, that have been difficult to treat from first-principles. In practice, these pastes exhibit large polydispersity with micron to millimeter sized particles, complicated particle shapes, and non-trivial surface morphology and surface chemistry. Simulations utilize the discrete element model, informed by microscale atomic force microscopy measurements of surface topography, surface energy, and friction, and a simplified version of Stokesian Dynamics. Using these simulations, we study simple shear of two cementitious slurries composed of Portland cement and fly ash particles. These computations are then compared with steady-state vane rheometer experiments. This first-principles approach to comparing simulation and experiment allows us to explore how the microscale and macroscale physics are linked. Both computations and experiments agree qualitatively and are well modeled as Bingham plastics. Computations also show the emergence of percolating clusters, responsible for the rheology. Finally, including the mechanisms that are responsible for frustrated particle motions, such as effects of friction and rough walls at experimental scales, are shown to help give quantitatively better comparisons

[*]Corresponding Author: Ph: (515) 294–3698 e-mail: shankar@iastate.edu

[1]Department of Mechanical Engineering, CoMFRE: Multiphase Flow Research and Education, Iowa State University, Ames, IA 50011, USA

[2]Department of Civil and Environmental Engineering, Rowan University, Glassboro, NJ 08028, USA

[3]Department of Civil, Construction, and Environmental Engineering, Iowa State University, Ames, IA 50011, USA

[4]Department of Mechanical Engineering, Iowa State University, Ames, IA 50011, USA