IFPRI BRIEF TEMPLATE

Check One: ☒**Project** ☐**Review** ☐**Collaboration**
☐**Workshop** ☐**Other**

Descriptive Title	Computational Modeling of Colloidal and Non-Brownian Suspensions in Industrial Systems
Working Title[1]	Computational Modeling of Dispersions
Technical Area[2]	W, M
Date	25/6/19 (based on 2018 brief after Slurries & Suspension New Physics Workshop)
Short Description	Recent advances in computational algorithms and resources create new opportunities for computer simulations of Brownian and non-Brownian suspensions. Such state-of-the-art simulations incorporate hydrodynamic interactions to generate large-scale (~10^6 or more) particle simulations that *quantitatively* capture macroscopic properties (rheology, sedimentation) and microstructural changes that accompany processing. Simulations with different particle shapes, sizes, and chemical heterogeneities are now increasingly feasible. There is an immediate opportunity to develop and validate simulations that can be used as modeling platforms for industry-specific problems of processing (e.g., extrusion), aging, stability, and thixotropy. Such models will predict microstructure and rheology, and serve as a starting point to incorporate the effects of electrostatics, solvophobicity (and other DLVO- and non-DLVO like-interactions), shape, and porosity. A long-term goal of this work is towards computer simulations that can be used to design processes (e.g. die geometries) and explore large experimental design spaces as the complexity of model systems increases through the incorporation of multiple aspects of shape, roughness, heterogeneity, etc.
Objectives	Reflect the state of the art of modeling to predict rheological phenomena in industrial systems to understand the gap and define the steps needed to improve the models.

[1] Title used in meeting agendas and file archives
[2] One or more from the following list: W = wet systems; D = dry systems; F = particle formation; SR = size reduction; M = modeling; SE = systems engineering

	Develop and validate simulations against benchmark literature studies, such as shear rheology (e.g., viscosity, viscoelasticity, yielding), delayed consolidation, and microstructural transitions on shearing (e.g. as measured by scattering). Work with an experimental group or groups to perform coordinated characterization of structure, rheology, and interactions of a simplified model system. Advance simulations to combine with experiments for model suspension development.
Scope	In: - Identify key particle properties that affect the models being predictive to a range of industrial systems - Engage the industrial IFPRI members and contractors for validation Out: - Hard spheres in pure water (oversimplified system) - Particle changes by reaction or crystallisation

Recommended Contractors (2 or 3)		
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