



IFPRI BRIEF TEMPLATE

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

Descriptive Title	Computational Modeling of Particle Suspensions
Working Title¹	Computational Modeling of Suspensions
Technical Area²	W, M
Date	22/6/2021
Short Description	<p>DEM for dry systems is the “go-to” modelling method of choice. Historically in wet systems there have been few options, however the modeling of Brownian colloidal suspensions has made dramatic advances in the last 10 years. This is a gap in the IFPRI wet systems portfolio.</p> <p>New state-of-the-art simulations incorporate hydrodynamic interactions to generate large-scale ($\sim 10^6$ or more) particle simulations that <i>quantitatively</i> capture macroscopic properties, including sedimentation/stability, processability, dispersibility, flowability) and microstructural changes over time and in flows. With two excellent experiment projects currently in the wet systems portfolio (SIFs, Slurries and Pastes), maximum benefit can be extracted from that work with computational support to give further insights to properties that cannot be disentangled experimentally.</p> <p>Simulations with different particle shapes, sizes, chemical heterogeneities and at high loadings are now increasingly feasible, allowing the model to closely approach the complexity of real product formulations in the SIFs and Slurries and Paste projects.</p> <p>The goal of this project is to bring insights to failure modes that can be experimentally observed but not understood (for example delayed collapse of particle networks) and provide detailed particle-level mechanistic details so that strategies to prevent or predict failure can be developed. Work can also guide formulation decisions, increase the applicability and relevance of the experimental projects by identifying key mechanisms that are difficult or impossible to access experimentally (e.g. role of friction, particle shape and dispersity).</p>

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

	A long-term goal of this work is towards computer simulations that can be used to design processes (e.g. formulations) and explore large design spaces as the complexity of systems increases through the incorporation of multiple aspects of shape, roughness, polydispersity, heterogeneity, etc.
Objectives	<p>Provide insight, and ultimately access, to current wet system modeling tools.</p> <p>Reflect the state of the art of modeling to predict flow phenomena in industrial systems to understand the gap and define the steps needed to improve the models.</p> <p>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).</p> <p>Work with the experimental SIFs and Slurry and Pastes project groups to perform coordinated characterization of structure, rheology, and interactions.</p> <p>Advance simulations to combine with experiments for model suspension development.</p>
Scope	<p>In:</p> <ul style="list-style-type: none"> - 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 <p>Out:</p> <ul style="list-style-type: none"> - Hard spheres in pure water (oversimplified system) - Particle changes by reaction or crystallisation

Recommended Contractors (2 or 3)		
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