Research Project Brief

Computational Modeling of Particle Suspensions

The International Fine Particle Research Institute (IFPRI) wishes to fund a research project on computational modeling of particle suspensions. IFPRI has a long history of supporting research in the rheology of Brownian and non-Brownian suspensions, however the last project that we funded focused on simulation of suspension behavior was John Brady's project on Stokesian dynamics which ended in 2004. With this project, we hope to fill this gap in IFPRI's "wet systems" portfolio.

New state-of-the-art simulations incorporate hydrodynamic interactions to generate large-scale (10^6 or more) particle simulations that quantitatively capture macroscopic properties, including sedimentation/stability, processability, dispersibility, flowability) and microstructural changes over time and in flows. With two excellent experimental projects currently in the wet systems portfolio (Jan Vermant, "Simulated Industrial Formulations"; Erin Koos, "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.

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.

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). A long-term goal of this work is towards computer simulations that can be used to guide formulation design and explore large design spaces as the complexity of systems increases through the incorporation of multiple aspects of shape, roughness, polydispersity, heterogeneity, etc. Specific objectives include:

- Provide insight, and ultimately access, to current wet system modeling tools.
- 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.
- 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 the experimental SIFs and Slurry and Pastes project groups to perform coordinated characterization of structure, rheology, and interactions.
- Advance simulations to combine with experiments for model suspension development.