IFPRI Abstract- Annual meeting 2022
Simplified industrial formulations.
Design challenges

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Goals

Our goals within the IFPRI project remain threefold

1. To explore how, moving away from model systems containing spherical colloids with near hard interactions, we can widen the range of rheological responses by changing the properties of the building blocks of the suspensions, so that even in simple formulations a wide range of behaviors can be "built in", i.e. obtaining formulation guidelines to do "more with less" or simplifying formulations from within.
2. To further develop a limited number of rheological and structural tools to interrogate the rheological response of the such dispersions, focusing on
   - Advanced rheological methods
   - High resolution confocal microscopy to probe structural development in situ during flow (4D imaging)
   - Local scale tribological measurements using AFM.
3. Apply these methods to simplified industrial dispersion by industrial partners and compare with the formulation guidelines obtained from (1).

Simplified industrial systems : bottom-up

Model systems with more complex topography : During the past year[1] we achieved one of the main results we were aiming for. A model thermoreversible gel system was designed, using a new synthesis approach for better controlling the grafting for octadecyl grafting to silica particles. This chemistry can be can be combined with different surface roughnesses to influence yielding behavior under shear conditions. For the same particle size, medium viscosity and surface chemistry, but different roughness, the elastic modulus and yield pont can now be varied independently. For the rough system, the elastic response regime (and hence the yield stress in rheological terms) can be increased by almost two orders of magnitudes, while the modulus remains the same. The rough systems are also less thixotropic and recover much faster. The

[1] Work of graduate student Florence Mueller

hypothesis is that interlocking of rough particles inhibits cluster densification, meaning the network structure can resist to shear. Work is ongoing to vary the roughness scale to get scaling relations, and micro-structural imaging and SAXS analysis of the microstructure.

Versatile particle toolbox:The specific goal of having roughness and tunable attractions to control yield stresses and thixotropy by having control over the openness of the aggregate structures has been achieved. An original and practically useful result, which will be submitted for publication.

Advanced rheological measurements: The main advances made in this area over the last year were the final improvements on the setup, image processing routine validation and measurements on both shear thickening systems and thixotropic gels. The key result was that we have new results on tracking of individual particle motion[2], now looking at for rotation at least 3 points in space. Rough particles with only fluorescent asperities are used and have been succesfully studied. The role of microscopic contact mechanics is now made possible by comparing this with single particle AFM methods. For the gels work has focused on identifiying local pastic event in gels, for no not yet the rough ones[3].

Rheoconfocal imaging: To elucidate the link between formulation, the microstructure and the rheology, rheo-confocal measurements are being performed. Last years' progress has focused on tracking particle rotation in stable systems and the local plastic events .

Simplified industrial systems: top down

The following samples have been identified as being relevant for and suggested by the members as systems relevant for a class of problems. They will be characterized by the rheological techniques mentioned above

1. Carbopol dispersions, relevant for thickening of consumer products (suggested by Unilever)
2. Latex suspensions, with $Ti0_2$ and $CaCO_3$ as model coating materials (suggested by Chemours)
3. milled paracetamol and a range of additives (Bentopharm (Clay) and Rhodopol 23 (Xantham gum))
4. Protein samples for understanding protein viscosity in bulk and understanding how processing conditions affects protein stability using interfacial tests (suggested by Merck)

Work has started on sample 1,3 and 4. Sample 2 has arrived. For the results on sample 1 a paper is being readied for publication

Concluding remarks

1. Concerning the bottom up increased complexity of model systems, the essential result has been achieved. Microscopic studies will now lead to a more precise predictive capacity.
2. Top down simplified industrial systems have been identified and are being characterized, a first successful example of the approach and new modeling insights have been achieved.

[2]Work of graduate student Vincent Niggel
[3]Work of graduate student Pierre Lehericy