IFPRI Abstract- Annual meeting 2023
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 consolidated one of the main results we were aiming for. A model thermo-reversible 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 point 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. Rheological and optical characterization revealed that rough particle gels exhibit enhanced toughness and self-healing properties. These remarkable properties can be utilized in various applications, such as xerogel fabrication and high-fidelity extrusion 3D printing.[2]. We also characterized the adhesion, rolling and sliding friction on single particles as a function of roughness suing colloidal probe based AFM measurements. These single particle measurements confirmed the concepts which came from macroscopic rheology, i.e. the adhesion strength does not change a lot, suggesting that we have single asperity interactions, but the friction is changed by particle topography, with an interplay of the configuration of the particle brush. .

Based on promising results on percolation and gravitational stability. Roughness is shown to lower the percolation treshold and impart a much improved gravitational stability. we also extended the synthesis protocol to rods, making rough rodlike particles, and preliminary results show substantial improvements when shape and roughness effects are combined.

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 understanding based on single particle measurements yields new insight into how to inapplications .

Advanced rheological measurements: The main focus this year was to obtain data on the rheo-confocal setup for the smooth and rough gels [3]. The focus is understanding better the elasto-plastic response of dense suspensions and gels. The goal of the measurements is to understand how the particle characteristics lead to the occurrence and propagation of plastic events or of strand rupturing. Much efforts has gine and goes into the image processing where we need to use machine learning methods but we get the characteristic length scales and timescales which underlie the behavior of the macroscopic response.

Rheoconfocal imaging: To elucidate the link between formulation, the microstructure and the rheology, rheo-confocal measurements are being performed. Consistent data sets on rough and smooth particle gels have been obtained.

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)

On the carbopol materials we developed a minimalistic model and we tested

[2]This work is submitted and is currently under review
[3]Work of graduate student Pierre Lehéricy

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.