

Wet Systems Consultant Report 2021

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2019 wet systems roadmap

Need

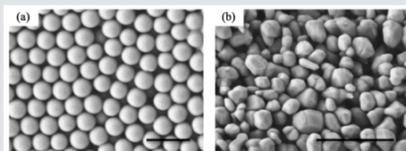
Mechanisms of suspension rheology and stability

How can rheology / flow / jamming be tailored, changed, altered, controlled? e.g. adsorbates, stabilizers, surface chemistry, particle properties (size distribution, shapes, roughness)

Model formulations and model validation

"Is your adhesive hard sphere index-matched monodisperse suspension truly representative of my system?"

Effect of fines, polydispersity, roughness, shape, ...



Lee et al., 2020

Rheology and stability (especially involving changes)

Aging, *formulation changes, sensitivity, feed variability*

Predictable? "How close to edge" is a formulation?

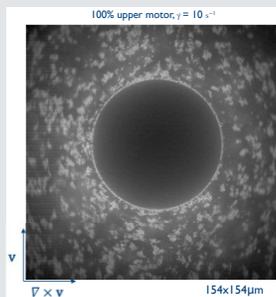
"What can go wrong" / "what just went wrong"?

Informs accelerated testing? (*months / years to days / weeks*)

Processing flows and processability

Extrusion, die slip, static zones

Complex geometries and flows



Current work, opportunity, or need

- Connecting structure, composition, particle characteristics to rheology and function (Slurry and Paste Rheology Project)
- Tailored rheology with interactions, particle roughness (see SIFs project update)
- **Missing: computational models**

- SIFs project with Jan Vermant (year 1)
- Collaboration with Lilian Hsiao (particle roughness)
- Vermant collaboration with Lucio Isa (particle friction, roughness)

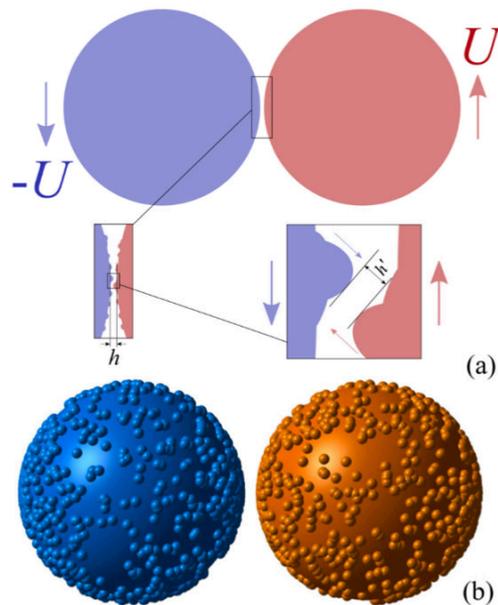
- Opportunity for **computational models** in close coordination with experiments

- Imaging dense suspension flows in complex geometries (see SIFs project update)
- Opportunity for **computational models**
- Microstructure changes in compression (Slurry and Paste Rheology Project)

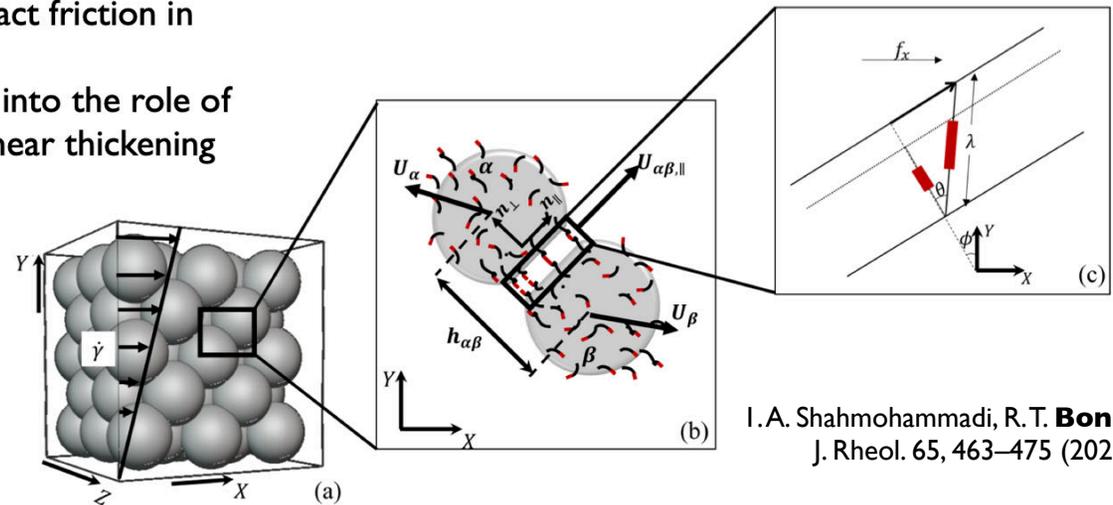
Recent fundamental advances in the field

Adhesive, repulsive elastic, frictional and elastohydrodynamic interparticle forces

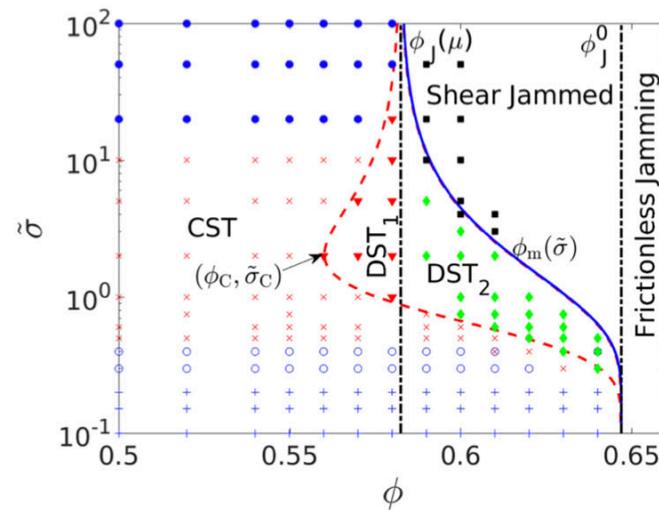
- Role of (lubrication) hydrodynamics versus contact friction in discontinuous shear thickening
- Continuing work and interest in the community into the role of particle contacts, particle surface chemistry in shear thickening



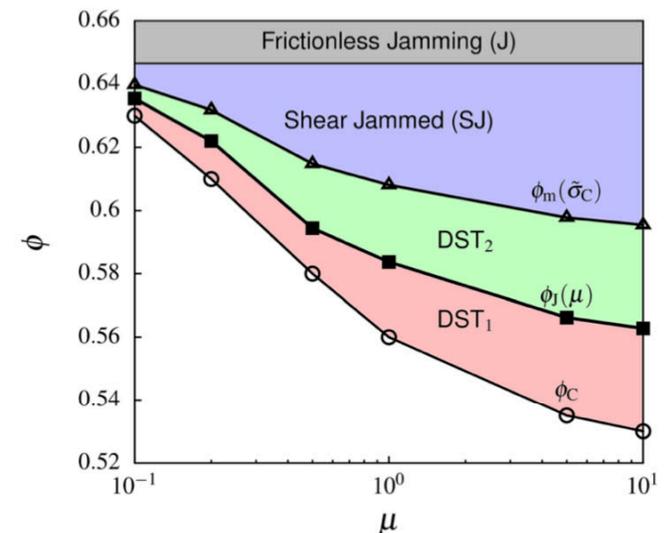
S. **Jamali**, J. F. Brady, Phys. Rev. Lett. 123, 138002 (2019); M. Wang, S. **Jamali**, J. F. Brady, J. Rheol. 64, 379–394 (2020).



I. A. Shahmohammadi, R. T. **Bonnecaze**, J. Rheol. 65, 463–475 (2021).



A. Singh, R. Mari, M. M. Denn, J. F. **Morris**, J. Rheol. 62, 457–468 (2019).

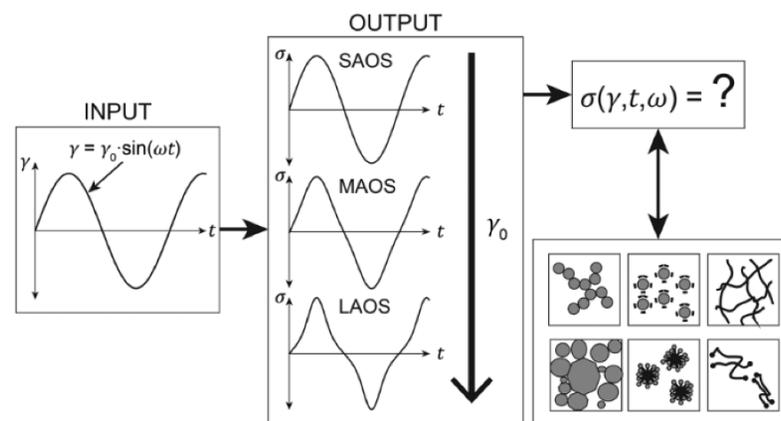
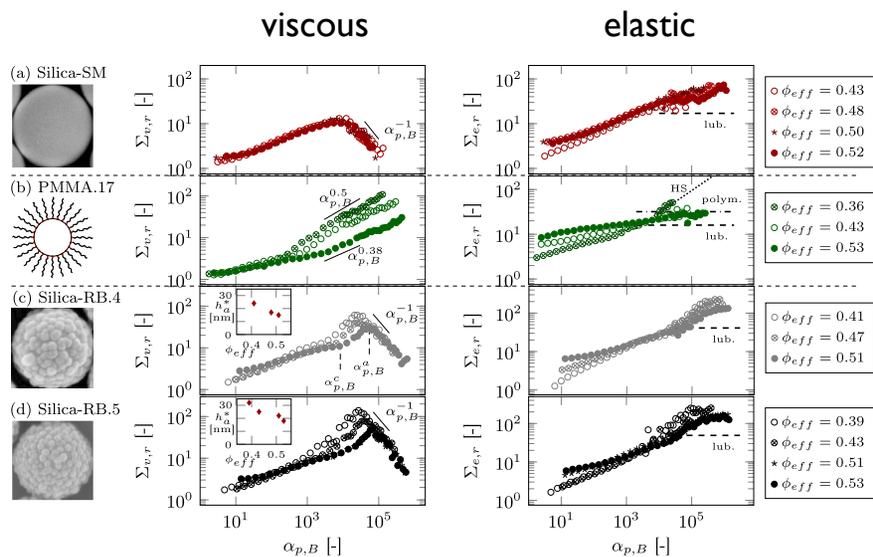


Experimental advances

High frequency rheology

MAOS

Rough Stabilized Smooth



High
concentrat
interparticle
separation small:
15-45nm

Stress Contributions in Colloidal Suspensions

B. Schroyen, C.-P. Hsu, L. Isa, P. Van Puyvelde, J. Vermant, Phys. Rev. Lett. 122, 218001 (2019).

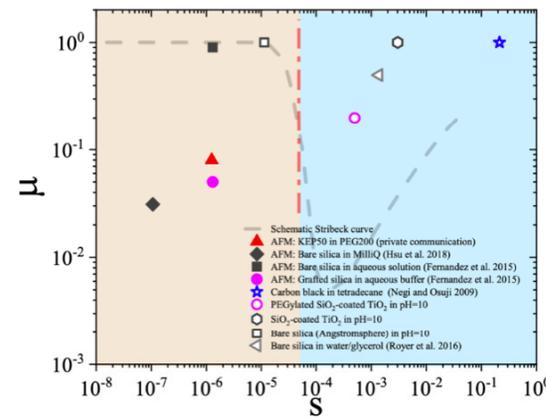
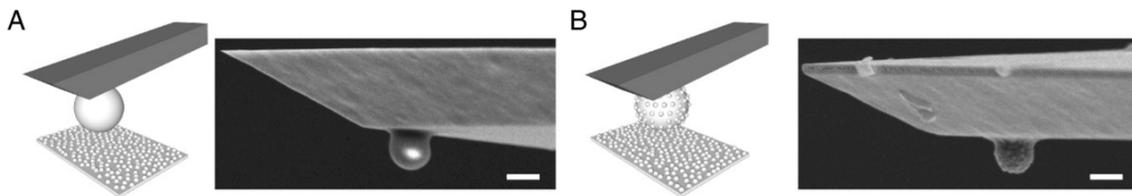
Applications to contact mechanics

Natalia, R. H. Ewoldt, E. Koos, J. Rheol. 64, 625--635 (2020).
Natalia, R. H. Ewoldt, E. Koos, arXiv:2104.05678v1 [cond-mat.soft]

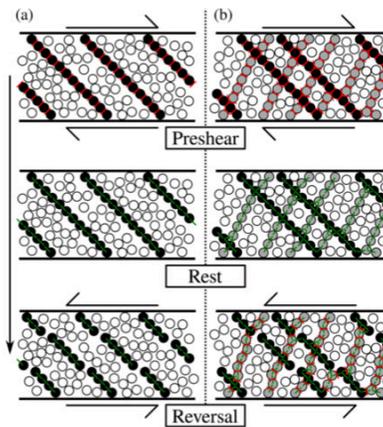
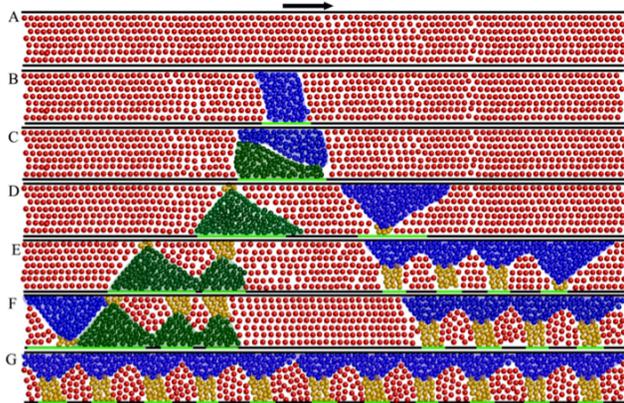
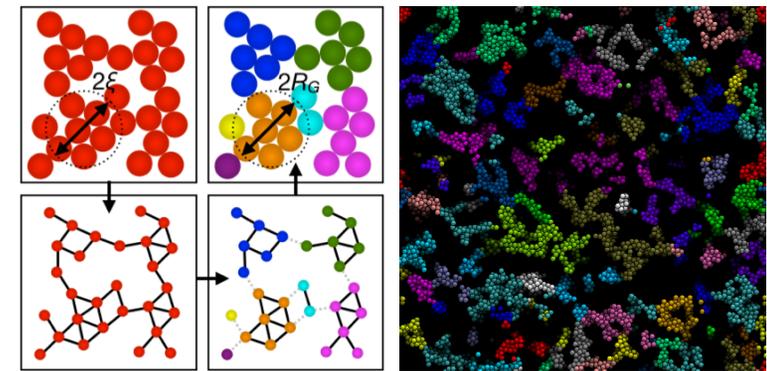
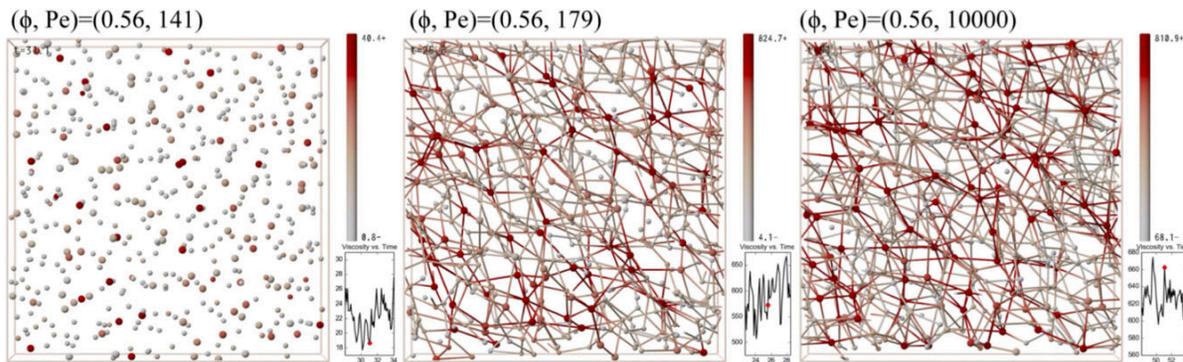
Measurement of friction and interactions

Y. Lee, Y. Luo, S. C. Brown, N. J. Wagner, J. Rheol. 64, 267--282 (2020).

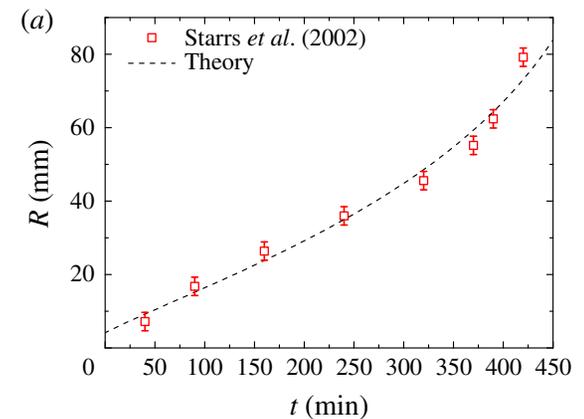
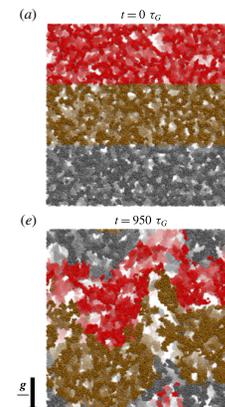
C.-P. Hsu, S. N. Ramakrishna, M. Zanini, N. D. Spencer, L. Isa, Proc. Natl. Acad. Sci. 115, 1--6 (2018).



Area of advance and IFPRI need: Computational modeling



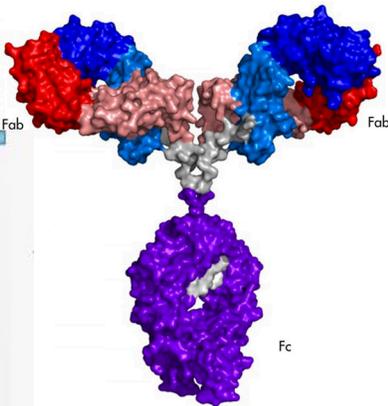
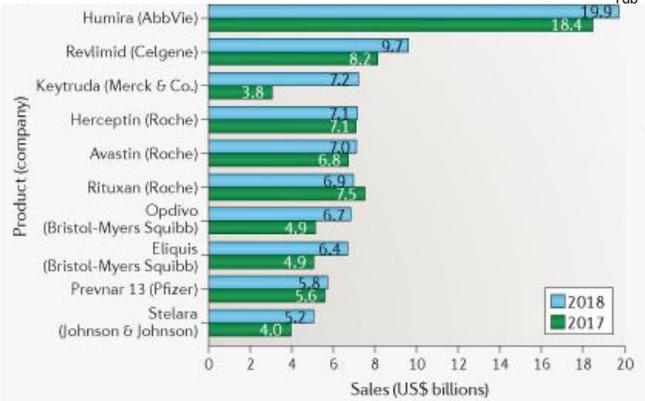
Z.Varga, J. L. Hofmann, J.W. Swan, *J. Fluid Mech.* 856, 1014–1044 (2018).



Connect particle-level physics and chemistry
to processing and formulation

Opportunity: MAb biologics

Global MAb market valued at ~\$135.38 billion in 2018, expected to grow to ~\$213 billion at a CAGR of 12.0% through 2022.

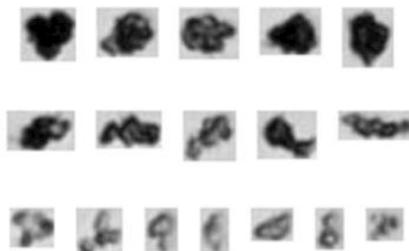
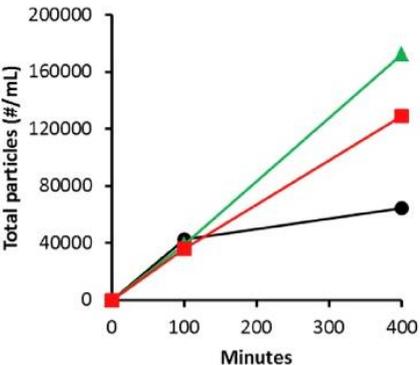


10 mg/mL antibody formulation particle formation



Kiese et al., J. Pharm. Sci., 97, 4347-4366 (2007)

Players in the area: Amgen, Genentech, Medimmune, Janssen, GSK, BMS, ... in close supervision with regulatory bodies (e.g. FDA)



BMI **MFI** **FlowCam**

mAb1
5-10 μm
10-25 μm

- Exogenous particle formation processes, kinetics
- Particle detection and particle characterization
- Interfacial rheology

IFPRI Wet Systems Investigators

PI	Institution	Research portfolio	IFPRI engagement
Lilian Hsiao*	North Carolina State University, Chemical and Biomolecular	Shaped colloids and functionalized surfaces	Active IFPRI collaboration with Vermant, 2019 proposal not selected
Lucio Isa*	ETH, Zürich, Materials	Colloid friction / tribology	Collaborator with Vermant / SIF project
James Swan	MIT, Chemical Engineering	Computational modeling and theory	2018 Workshop attendee Potential collaboration SIFs
Roseanna Zia	Stanford, Chemical Engineering	Computational modeling	2018 Workshop attendee
Roger Bonnecaze	UT Austin, Chemical Engineering	Computational modeling, theory	2018 Report
Emanuela Del Gado	Georgetown, Physics	Modeling and theory of suspensions	None
Jeff Morris	City College of New York, Lehigh Institute	Computational modeling, theory	None
Xavier Chateau	Université Paris-Est / École des Ponts	Pastes, cements	None
Guillaume Ovarlez	Université de Bordeaux	Rheology, shear thickening, non-Brownian suspensions	None
Ron Larson	Michigan	Rheology, computational modeling, 2019 thixotropy review	None
Dan Blair & Jeff Urbach	Georgetown, Physics	Friction and jamming in dense suspensions	2018 proposal not selected (Blair)
George Petekidis	University of Crete / FORTH	Dense suspension rheology	2019 proposal not selected

IFPRI Wet Systems Investigators

PI	Institution	Research portfolio	IFPRI engagement
Safa Jamali	Northeastern, Mechanical Engineering	Computational suspension physics	None
Thibault Divoux	ENS Lyon / CNRS	Fluidization, thixotropy	None
Jaci Conrad	University of Houston, Chemical Engineering	Colloids in confinement and in flow	None
Randy Ewoldt	Illinois Urbana-Champaign, Mechanical Engineering	Non-Newtonian fluid mech, non-linear rheology, yield stress fluids	None
Frank Scheffold	University of Fribourg, Physics	Light scattering, dense suspensions and emulsions	None
Roberto Cerbino	University of Vienna	Differential dynamic microscopy, suspension dynamics	None
Patrick Anderson	TU Eindhoven	Computational / Applied rheology and process modeling	None
Peter Schall	Amsterdam, Physics	Glasses and yielding	None
Luca Cipelletti	University Montpellier	Jamming, glasses, light scattering	None
Roberto Piazza	Politecnico di Milano	Colloidal gels and glasses	None