Wet Systems Consultant Report 2022

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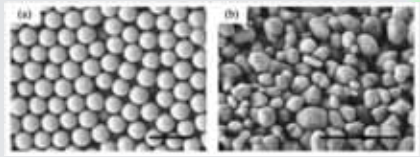
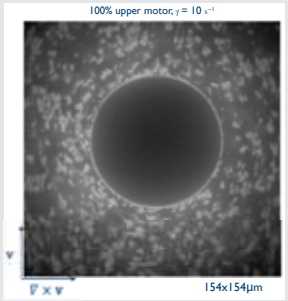
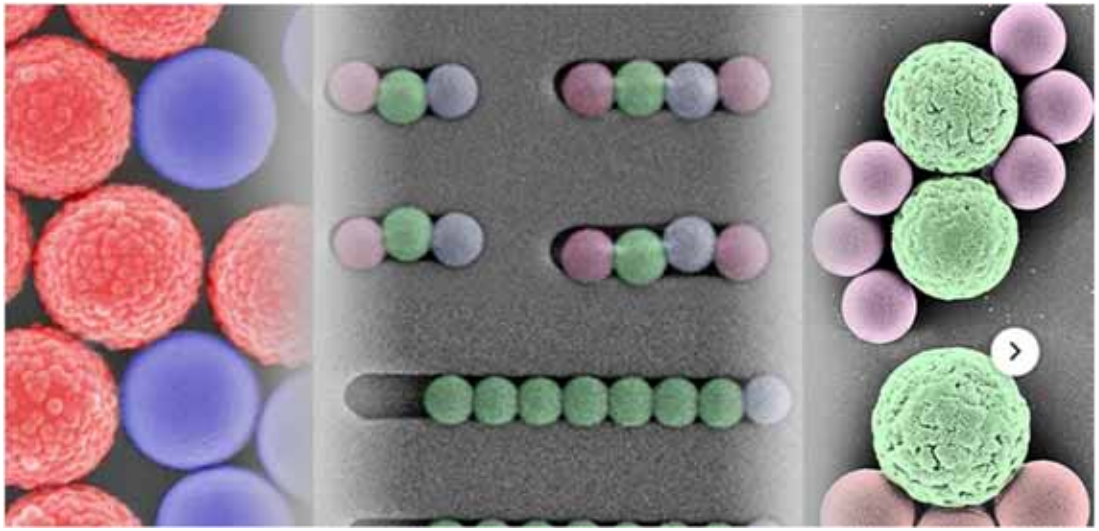
Prepared for

IFPRI
International Fine Particle Research Institute

2018 IFPRI workshop wet systems roadmap

Need	Current work or opportunity
1. 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)	• Connecting structure, composition, particle characteristics to rheology and function (Slurry and Paste Rheology, SIFS projects) • Tailored rheology with interactions, particle roughness (see SIFs project update) • **Missing: computational models**
2. 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	• SIFs project with Jan Vermant (year 2) includes both bottom-up and top-down • Collaboration with Lilian Hsiao (particle roughness) • Vermant collaboration with Lucio Isa (particle friction, roughness)
3. 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*)	• Opportunity for **computational models** in close coordination with experiments
4. Processing flows and **processability** Extrusion, die slip, static zones Complex geometries and flows 	• Imaging dense suspension flows in complex geometries (2021 *SIFs project* update) • Opportunity for **computational models** • Microstructure changes in compression (*Slurry and Paste Rheology Project*)

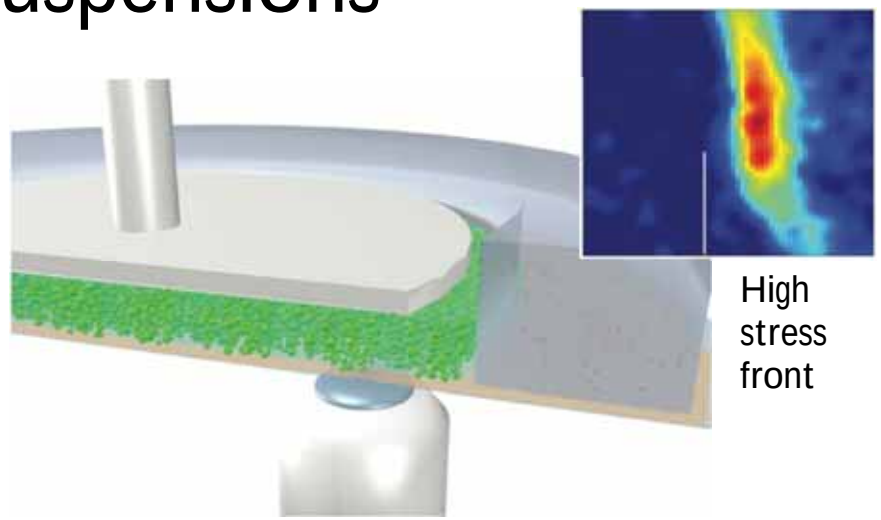
Particle contacts, friction, rheology, stability



Lucio Isa, ETH Zürich
Lilian Hsiao, NCSU

- Mandal, J.; Ramakrishna, S. N.; Spencer, N. D.; Isa, L. Exploring the Roles of Roughness, Friction and Adhesion in Discontinuous Shear Thickening by Means of Thermo-Responsive Particles. *Nat. Commun*. 2021, 12, 1477.
- Pradeep, S.; Nabizadeh, M.; Jacob, A. R.; Jamali, S.; Hsiao, L. C. Jamming Distance Dictates Colloidal Shear Thickening. *Phys. Rev. Lett*. 2021, 127, 158002.

Boundary stress microscopy of shear thickening suspensions



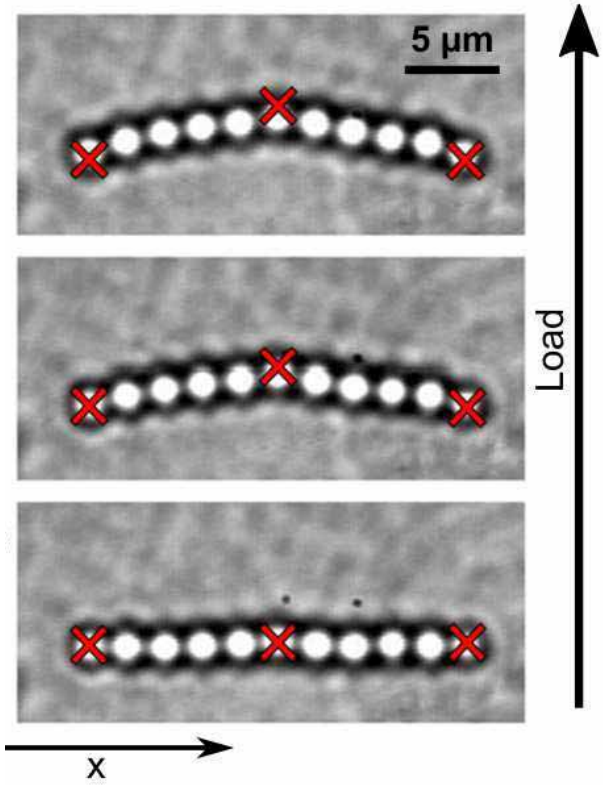
Jeff Urbach and Dan Blair, Georgetown

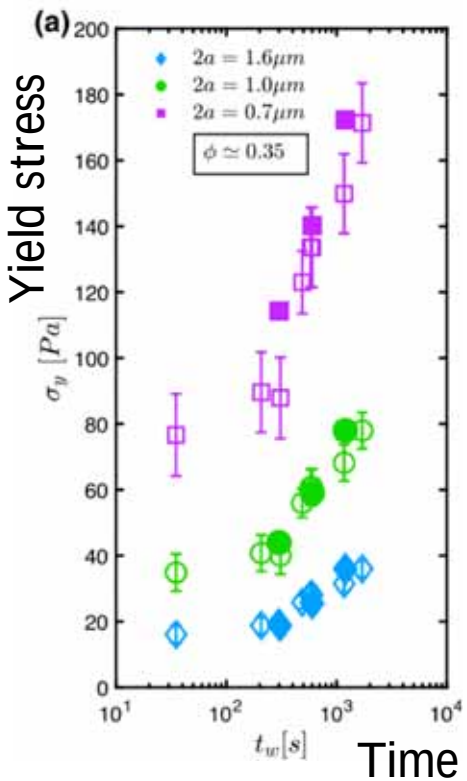
- Rathee, V.; Blair, D. L.; Urbach, J. S. Localized Stress Fluctuations Drive Shear Thickening in Dense Suspensions. *Proc. Natl. Acad. Sci.* 2017, 114, 8740–8745.
- Rathee, V.; Miller, J. M.; Blair, D. L.; Urbach, J. S. Structure of Propagating High Stress Fronts in a Shear Thickening Suspension. arXiv:2203.02482, 2022
- Rathee, V.; Blair, D. L.; Urbach, J. S. Localized Transient Jamming in Discontinuous Shear Thickening. J. Rheol. 2020, 64, 299–307.

Contact mechanics, yield stress aging, and elasticity

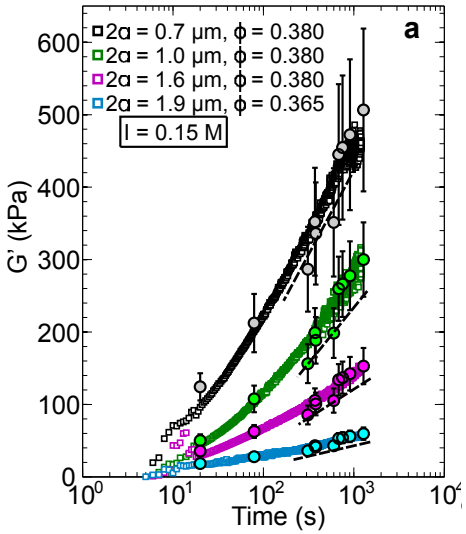
Bonacci, F.; Chateau, X.; Furst, E. M.; Goyon, J.; Lemaître, A. *Phys. Rev. Lett*. 2022, 128, 18003.
Bonacci, F.; Chateau, X.; Furst, E. M.; Fusier, J.; Goyon, J.; Lemaître, A. *Nat. Mater*. 2020, 19, 775–780.

Micromechanics

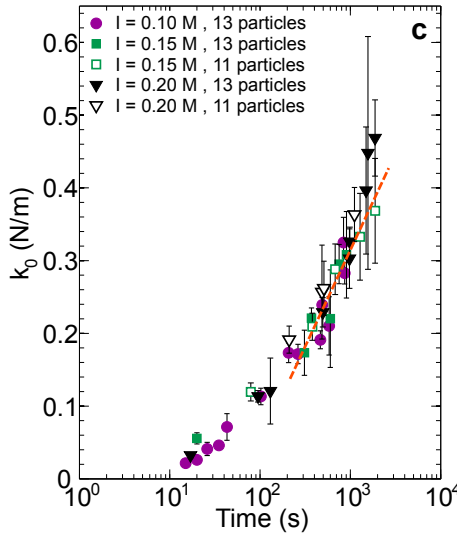


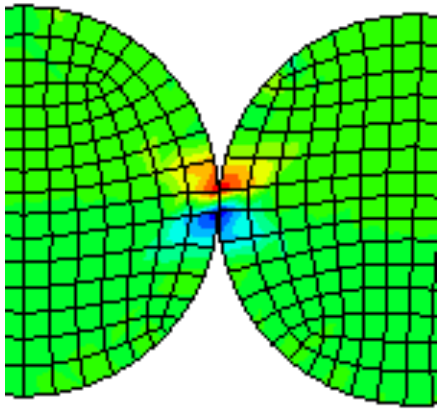


Elastic modulus



Bond rigidity

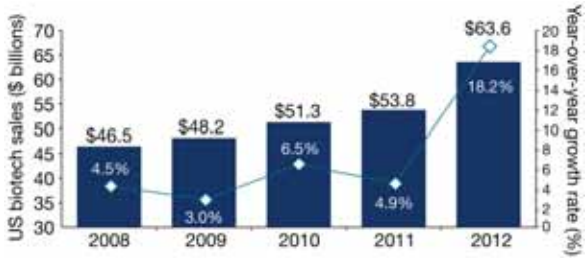




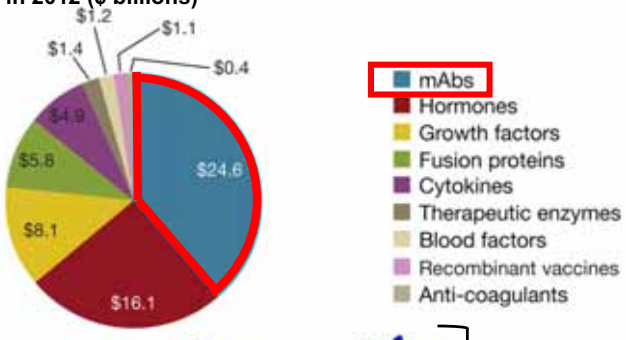
Contact aging

Opportunity: Biologics

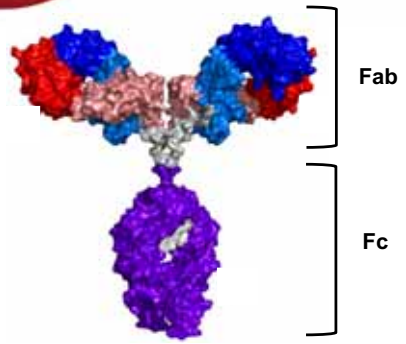
Growth trends in the US biotech market for biologic drugs (2008-2012)



Top nine categories of biologic drugs in terms of US sales in 2012 ($ billions)



Examples of illnesses:
Arthritis, cancer, auto-immune diseases, anthrax, anti-inflammatory disorders, etc.

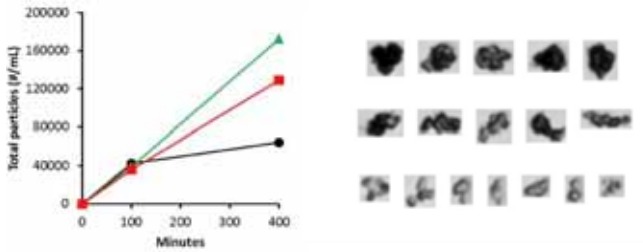


Aggarwal, S., *Nature Biotechnology*, 32, 32-39 (2014)

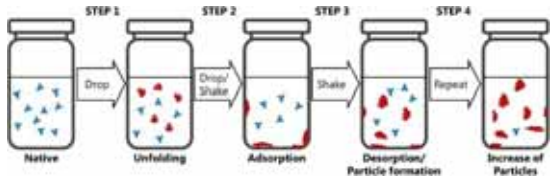
Aggregation time course of a 10 mg/mL antibody formulation with 0-0.01% PS20 stressed by shaking (▲) and stirring (□) at 5 °C

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

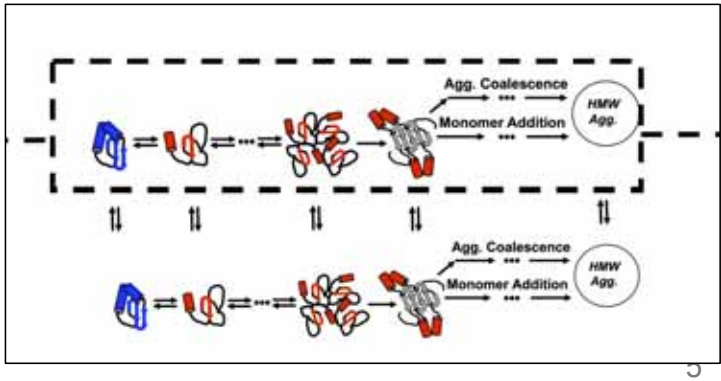
Subvisible particles are created under combination dropping and shaking stress of an 0.9 mg/mL IgG1 at different 1-2 mL fill volumes



Proposed aggregation pathway induced by combination drop and shake stress



Torisu *et al.*, *J. Pharm. Sci.*, 106, 521-529 (2017)



Exogenous particle formation
Particle characterization

Genentech, Medimmune, Janssen, Amgen, GSK, etc.

IFPRI Wet Systems Investigators

PI	Institution	Research portfolio	IFPRI engagement	website
Lilian Hsiao*	North Carolina State University, Chemical and Biomolecular Engineering	Shaped colloids and functionalized surfaces	Active IFPRI collaboration with Vermant, 2019 proposal	http://www.hsiaolab.com
Lucio Isa*	ETH, Zürich, Materials	Colloid friction / tribology	Collaborator with Vermant / SIF project	https://isa.mat.ethz.ch
Roger Bonnecaze	UT Austin, Chemical Enigneering	Computational modeling, theory	2018 Report	https://sites.utexas.edu/bonnecazegroup/
Emanuela Del Gado	Georgetown, Physics	Modeling and theory of suspensions	None	http://delgadolab.georgetown.domains
Jeff Morris	City College of New York, Levich Institute	Computational modeling, theory	None	https://levich.ccny.cuny.edu/morris-laboratory/
Xavier Chateau	Université Paris-Est / École des Ponts	Pastes, cements, contact mechanics	None	https://navier-lab.fr/en/equipe/chateau-xavier/
Guillaume Ovarlez	Université de Bordeaux	Rheology, shear thickening, non-Brownian suspensions	None	https://www.lof.cnrs.fr/guillaume-ovarlez/
Ron Larson	Michigan	Rheology, computational modeling, 2019 thixotropy review	None	http://cheresearch.engin.umich.edu/larson/
Dan Blair & Jeff Urbach	Georgetown, Physics	Friction and jamming in dense suspensions, spatio-temporal cross-corrleation	2018 proposal not selected (Blair)	https://blairlab.georgetown.edu

IFPRI Wet Systems Investigators

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Jaci Conrad	University of Houston, Chemical Engineering	Colloids in confinement and in flow	None	https://www.chee.uh.edu/faculty/conrad
Randy Ewoldt	Illinois Urbana-Champain, Mechanical Engineering	Non-Newtonian fluid mech, non-linear rheology, yield stress fluids	None	https://ewoldt.mechanical.illinois.edu
Frank Scheffold	University of Fribourg, Physics	Light scattering, dense suspensions and emulsions	None	https://www.unifr.ch/phys/en/research/groups/scheffold/
Roberto Cerbino	University of Vienna	Differential dynamic microscopy, suspension dynamics	None	https://sites.google.com/site/cerbino/
Patrick Anderson	TU Eindhoven	Computational / Applied rheology and process modeling	None	https://scholar.google.com/citations?user=m-Q4RrAAAAAJ&hl=en&oi=ao
Peter Schall	Amsterdam, Physics	Glasses and yielding, nanomechnanics, particle interactions	None	https://peterschall.de
Luca Cipelletti	University Montpellier	Jamming, glasses, light scattering	None	https://coulomb.umontpellier.fr/user/luca.cipelletti
Roberto Piazza	Politecnico di Milano	Colloidal gels and glasses	None	https://scholar.google.com/citations?user=lGnqlMYAAAAJ&hl=en&oi=ao
Vinny Manoharan	Harvard	Holographic microscopy of dispersions	None	https://manoharan.seas.harvard.edu
Alex Routh	Cambridge	Film Formation and dispersion drying, Aggregation	None	https://www.ceb.cam.ac.uk/directory/alex-routh

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Jasper Van der Gucht	Wageningen University	Networks, contact networks	None	https://www.wur.nl/en/Research-Results/Chair-groups/Agrotechnology-and-Food-Sciences/Physical-Chemistry-and-Soft-
George Petekidis	University of Crete / FORTH	Dense suspension rheology	2019 proposal not selected	https://www.iesl.forth.gr/en/people/petekidis-george
Joost de Graaf	Institute for Theoretical Physics, Utrecht	Dense suspension rheology	None but collaborating with Kool	https://webspace.science.uu.nl/~graaf156/group.html