Πανεπιστήμιο Αιγαίου
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Book of Abstracts

9th International Conference of the *Hellenic Society of Rheology*

Honoring Professor L. Gary Leal and Professor Andreas Alexandrou for their contributions to Rheology and Fluid Mechanics

23-27 June, 2019

Pythagorion, Samos, Greece

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Message from the organizers

It is with great pleasure that we welcome all the delegates and accompanying persons to HSR 2019 (9th International Meeting of the Hellenic Society of Rheology), Samos, June 23-27, 2019.

The 1st meeting of the HSR was held in Cyprus, 23 years ago in Nicosia. Since then, the HSR meetings took place in Heraklion (1998 and 2014), Patras (2001), Athens (2004 and 2011), Rhodes (2007), and in Limassol (2017). The main goal of these meetings is to promote scientific interactions at the highest level not only among the members of the Greek Chapter of the Society of Rheology but also among scientists from all over the World. Another objective of the meetings is to provide the forum where students could interact and share their work with the established members of the community.

The HSR-2019 is devoted to Professor L. Gary Leal and Professor Andreas Alexandrou for their contributions to rheology and fluid mechanics. Professor Alexandrou was a founding member of the HSR and served as its President (2005-2007).

The program includes four invited keynote talks by Professors Gerry Fuller (Stanford University, USA), L Gary Leal (University of California, Santa Barbara, USA), Mathew Helgeson (University of Santa Barbara, USA) and Michael Modigell (German University of Oman, Oman), 56 regular talks, and 14 poster presentations. For the first time, the “Best poster award” for students is introduced. Finally, a short course on modern rheology precedes the meeting.

With approximately 70 registered participants from eighteen countries the conference is truly an international event.

We hope that *HSR 2019* will promote scientific exchange, collaboration and interactions between participants.

Kostas Housiadas and Georgios Georgiou

Sunday, June 23, 2019	
20:00-21:00	***Registration at "Doryssa Seaside Resort"***
20:30-22:30	***Welcome Reception at "Doryssa Seaside Resort"***

		Monday, June 24, 2019
	07:45-08:30	***Registration***
	08:00-08:10	*Opening*
Leal symposium - A	08:10-08:50	**G. Fuller**, E.J. Mossige, V. Suja *Evaporation-induced stabilization/destabilization*
	08:50-09:10	**R.I. Tanner**, S. Dai *Edge fracture in non-colloidal suspensions*
	09:10-09:30	A. Maheshwari, C. Aponte-Rivera, E. Gonzalez, A. Sunol, D. Endy, **R. Zia** *The colloidal hydrodynamics and rheology of the cell*
	09:30-09:50	*Coffee break*
	09:50-10:10	**G.J. Elfring** *Active particles in complex fluids*
	10:10-10:30	E. Amah, N. Musunuri, M. Hossain, I. Fischer, **P. Singh** *Numerical simulations of electric field driven hierarchical self-assembly of monolayers of mixtures of particles*
	10:30-10:50	**A. Papadopoulou**, M.K. Tiwari, S. Balabani *Rheology and microstructure of non-aqueous silica particle suspensions*
	10:50-11:20	*Coffee break*
	11:20-11:40	E. Chatzigiannakis, A. Alicke, **J. Vermant** *Dynamics of thin liquid films: Implications for beer foam stability*
	11:40-12:00	Y.H. Huang, A. Kamble, F. Salmon, M. Michelon, B.C. Leopercio, M.S. Carvalho, **J.M. Frostad** *Direct measurement of the dynamic modulus of micro-capsules*
	12:00-12:20	E. Vereroudakis, A. Louhichi, **D. Vlassopoulos** *Rheology sensitively probes water-mediated changes of supramolecular structure*
	12:20-12:40	T. Tomkovic, N. Kuanr, L.L. Schafer, **S.G. Hatzikiriakos** *Rheological properties of amine functionalized polynorbornenes*
	12:40-13:00	**J. Vlachopoulos,** N.D. Polychronopoulos *Moffatt eddies in single screw extrusion*
	13:00	***End of morning sessions***
General session - A	18:00-18:20	N. Cagney, **S. Balabani** *Dynamics of Taylor-Couette flow of shear-thinning fluids*
	18:20-18:40	A. Katsavria, **V. Bontozoglou** *Stability of film flow with high loadings of soluble surfactant: The effect of surface compressibility*
	18:40-19:00	V. Mitsoulas, K. Giannokostas, **Y. Dimakopoulos**, J. Tsamopoulos *Investigation of the scaling of the endothelial surface layer permeability of microvessels through multiscale modeling and simulations*
	19:00-19:20	A.N. Spyropoulos, A.G. Papathanasiou, **A.G. Boudouvis** *2-3-4 spikes competition in the normal field instability of ferrofluids*
	19:20-19:40	**S. Varchanis**, A. Syrakos, P. Moschopoulos, Y. Dimakopoulos, J. Tsamopoulos *3-Dimensional flows of non-Newtonian fluids with free surfaces*
	19:40	***End of evening sessions***
	20:00-23:30	***Dinner at "Elia" restaurant in Pythagorion***

	Tuesday, June 25, 2019	
Leal symposium - B	08:10-08:50	J. Peterson, C. Sasmal, **L. Gary Leal** *The dynamics of bimodal polymer blends in a contraction-expansion slit device*
	08:50-09:10	**M. Doi** *Application of Onsager Machlup integral in solving evolution equations in non-equilibrium systems*
	09:10-09:30	P.M. Mwasame, A.N. Beris, R.B. Diemer, S. Jariwala, **N.J. Wagner** *A constitutive equation for thixotropic suspensions with yield stress by coarse-graining a population balance model & experimental validation*
	09:30-09:50	*Coffee break*
	09:50-10:10	**E.S.G. Shaqfeh**, A. Jain, J. Einarsson, N. Alvarez, Z. Hinton *A study of the effective extensional viscosity in a particle laden viscoelastic solution*
	10:10-10:30	G. D'Avino, **P.L. Maffettone** *Dynamics of particle pair in a viscoelastic fluid under pressure driven flows: Clues for particle ordering in microfluidics*
	10:30-10:50	M. Vlachomitrou, **N. Pelekasis** *A numerical study for the compression only effect of contrast agents*
	10:50-11:10	**E. Antonopoulou**, O. Harlen, M. Walkley, N. Kapur *Drop-on-demand inkjet printing of surfactant solutions*
	11:10-11:40	*Coffee break*
	11:40-12:00	M.A. Hulsen, M.A. Carrozza, M. Hütter, **P.D. Anderson** *Using the contravariant deformation tensor formulation in simulation of viscoelastic fluid flow*
	12:00-12:20	L. Zhou, **L.P. Cook** *Mesoscale modeling of networked fluids*
	12:20-12:40	**J. Gillissen**, Helen Wilson, Christopher Ness, Joseph Peterson, Michael Cates *A tensor model for shear thickening suspensions of spherical particles*
	12:40-13:00	**R.R. Huilgol** *A particle distribution function approach to the equations of continuum mechanics in Cartesian, cylindrical and spherical coordinates: Newtonian and non-Newtonian fluids*
	13:00	***End of morning sessions***
General session - B	17:45-18:05	P. Edera, P. McCall, M. Gardel, V. Trappe, F. Giavazzi, **R. Cerbino** *Tracking-free one- and two-point microrheology of soft materials*
	18:05-18:25	A. Passos, J.M. Sherwood, E. Kaliviotis, **S. Balabani** *Microscale flows of hardened red blood cell suspensions*
	18:25-18:45	K. Kapnisis, H. Seidner, M. Prokopi, D. Pasias, C. Pitsillides, A. Anayiotos, **E. Kaliviotis** *Blood rheology and flow geometry effects*
	18:45-19:05	**D.G. Tsalikis**, A.J. Tsamopoulos, A. Katsarou, V.G. Mavrantzas *Steady shear flow of marginally entangled ring polymer melts through nonequilibrium molecular dynamics simulations*
	19:05-19:25	V. Harmandaris, **P. Bačová**, A.N. Rissanou *Multi-scale dynamic simulations of polymer nanocomposites with inorganic or polymer-based nanoparticles*
	19:25-20:00	***Poster session***
	20:00	***End of evening sessions***
	20:30-23:30	***Conference dinner at "Aphrodite Garden Restaurant" in Pythagorion***

	Wednesday, June 26, 2019	
Alexandrou memorial symposium	08:10-08:50	**M. Modigell** *Professor A.N. Alexandrou's contributions to rheology and semisolid material processing*
	08:50-09:10	**R.R. Huilgol**, A.N. Alexandrou, G.C. Georgiou *Start-up plane Poiseuille flow of a Bingham fluid*
	09:10-09:30	**G.C. Florides**, A.N. Alexandrou, M. Modigell, G.C. Georgiou *Squeeze flow of thixotropic semisolid slurries*
	09:30-09:50	*Coffee break*
	09:50-10:10	J.S. Horner, **A.N. Beris**, N.J. Wagner *Experimental and theoretical investigations of human and animal blood rheology*
	10:10-10:30	**P.S. Stephanou**, I.Ch. Tsimouri, G.C. Georgiou, V.G. Mavrantzas *Understanding the rheological behaviour of blood from a non-equilibrium thermodynamics perspective*
	10:30-10:50	L. Gury, D. Parisi, M. Cloitre, **D. Vlassopoulos** *Comparative rheological study of dense microgel and star polymer suspensions*
	10:50-11:10	T. Tomkovic, **S.G. Hatzikiriakos** *Rheology of poly(ethylene-co-methacrylic acid) ionomers*
	11:10-11:30	**E. Mitsoulis**, A. Neunhäuserer, S. Stieger, W. Friesenbichler *Capillary flow behavior of a rubber compound*
	11:30-12:00	*Coffee break*
General session - C	12:00-12:20	**D.E.V. Andrade**, P. Coussot *The solid-liquid transition of brittle solids: Waxy oil study*
	12:20-12:40	**S. Migliozzi**, P. Angeli, L. Mazzei *A rheological study of the gelation kinetics of non-aqueous carbopol dispersion*
	12:40-13:00	**A. Syrakos**, Y. Dimakopoulos, J. Tsamopoulos *Lid-driven elastoviscoplastic flow in a cavity*
	13:00-13:20	L. Böni, K. Rementzi, Dimitris Vlassopoulos, **P. Fischer** *Slime for defense – biophysical design principles in a marine environment*
	13:20	***End of morning sessions***
	13:30-18:00	***Visit to the Wine Museum in Vathi and excursion/lunch to Mitilinii***

	Thursday, June 27, 2019	
General session - D	08:10-08:50	**M.E. Helgeson** *Toward "Damascus yogurt": using phase separation to understand and control the rheology of colloidal gels*
	08:50-09:10	E. Moghimi, J. Vermant, **G. Petekidis** *Probing the internal dynamics of model colloidal glasses under shear by orthogonal superposition rheometry*
	09:10-09:30	**R. Bitton** *Tuning the mechanical properties of alginate-peptide hydrogels*
	09:30-09:50	*Coffee break*
	09:50-10:10	**Q. Huang**, O. Hassager, J. Ahn, T. Chang, D. Vlassopoulos *Extensional rheology of ring polystyrene melt and linear/ring polystyrene blends*
	10:10-10:30	**D. Ashkenazi**, M. Gottlieb Interfacial viscoelasticity - the effect of polymer chain flexibility and hydrophobicity
	10:30-10:50	**C.O. Klein**, R. Figuli, D.Z. Gunes, J. Ray, O. Schafer, M. Wilhelm *Fat crystallization and solidification as observed by novel combined rheological methods*
	10:50-11:10	**S.J. Gstöhl**, C.M. Schlepütz, J. Wemmer, J. Läuger, M. Stampanoni, P. Fischer, E.J. Windhab *Full spatio-temporal elucidation of sheared multiphase materials*
	11:10-11:40	*Coffee break*
	11:40-12:00	C.S. Valentine, **L.M. Walker** *Probing the nanoscale structure of block copolymer micelle liquid crystals using rheology and mechanical behavior*
	12:00-12:20	**A. Jabbarzadeh** *Effect of additives shape and size on crystallization of polymeric systems*
	12:20-12:40	**S. Costanzo**, L. Scherz, G. Floudas, R. Pasquino, M. Kröger, A.D. Schlüter, D. Vlassopoulos *Hybrid dendronized polymers as molecular objects: viscoelastic properties in the melt*
	12:40-13:00	**T. Athanasiou**, D. Vlassopoulos, G. Petekidis *High-frequency rheometry of polymeric systems*
	13:00-13:20	**E. Chatzigiannakis**, J. Vermant *Drainage dynamics of thin polymer-solution films*
	13:20-13:30	***Closure***
	13:30 – 15:00	***Lunch at "Doryssa Seaside Resort"***
	15:00	***End of HSR-2019 conference***

Poster Session ***Tuesday, June 27, 2019:* 19:25-20:00**
S. Alexandris, D. Vlassopoulos *Shear rheology of marginally entangled polystyrene*
F. Boudjema, Z. Aliche, B. Khelidj, M. Lounis, O. Sokona, F. Khoualdia *Experimental and rheological study of prepared bioformulations*
P. Chatzakis, M. Das, D.G. Papazoglou, **G. Petekidis** *A multimodal light scattering and imaging device for rheological applications*
Y. Damianou, P. Panaseti, C. Xenophontos, G.C. Georgiou *Viscoplastic Couette flow in the presence of wall slip with non-zero slip yield stress*
L. Fusi, A. Farina *Flow of inhomogeneous Bingham fluids*
S.D. Gkormpatsis*, E.A. Gryparis, K.D. Housiadas, A.N. Beris *Steady sphere translation in a viscoelastic fluid with Navier slip on the sphere*
E.A. Gryparis*, S.D. Gkormpatsis, K.D. Housiadas, R.I. Tanner *Viscoelastic planar elongational flow past an infinitely long cylinder*
K.D. Housiadas *The sedimentation of a sphere in a viscoelastic fluid under constant rotation*
P. Moschopoulos*, K. Psaraki, A. Syrakos, Y. Dimakopoulos, J. Tsamopoulos *The dynamic response of elastoviscoplastic fluids under extension*
P. Panaseti, **G.C. Georgiou**, I. Ioannou *Flow of a Herschel-Bulkley fluid with pressure-dependent rheological parameters in an asymmetric channel*
K. Sverdrup*, A. Almgren, N. Nikiforakis *Simulating unsteady flow of viscoplastic fluids in three dimensions with embedded boundaries*
A. Tsiantis, **T.D. Papathanasiou** *Quantitative relationships between the aggregation state and the permeability of fibrous systems*
D. Zablotsky *Shear banding in magnetic colloids studied by LAOS and numerical simulations*

** Eligible for the best student poster award*

Invited Talks

Evaporation-induced stabilization/destabilization

Gerald Fuller, Endre Joachim Mossige, and Vinny Suja
Chemical Engineering, Stanford University, USA

Evaporation of liquid solutions is known to induce important fluid dynamical phenomena. In this presentation, two cases are discussed: soluto-capillary Marangoni flows leading to the stabilization of non-aqueous foams and the inducement of Rayleigh-Taylor instabilities in polymer solutions. The former consequence of evaporation is of concern in viscous oils and lubricants where sustained foams are normally unwanted. In the absence of surfactants and temperature gradients, viscosity is normally implicated as the source of stability. Using a newly developed instrument to capture the thinning of submicron liquid films in space and time, the dynamic fluid film interferometer, it is demonstrated that foam stability in these systems is a result of soluto-capillary Marangoni stresses. These lead to spontaneous dimpling and resistance to coalescence of the top layer of bubbles in these foams.

The second application concerns polymer solutions that are used in the formulation of food and personal products. In this work, polymer solutions ranging from dilute to semi-dilute have been examined and it is demonstrated that spontaneous, evaporation driven Rayleigh-Taylor instabilities will ensue whenever the polymers are higher in density and whenever viscoelastic skin formation at the solution/air interface is avoided. Two aqueous polymer systems have been studied: dextran and polyethylene glycol dissolved in water. The initial state of the solutions is uniform in concentration, but through special lighting and imaging, instabilities in the form of plumes of descending regions of higher polymer concentration are seen to appear from the upper interface where evaporation is taking place. The onset time for plumes to appear can be established and these times are a strong function of polymer concentration and solution viscosity. A simple theory is described wherein the onset times are collapsed onto a single master curve that depends on the ratio of polymer concentration of viscosity. From these results, classical scaling laws of semi-dilute polymer solutions can successfully map the experimental results.

The dynamics of bimodal polymer blends in a contraction-expansion slit device.

Joseph Peterson[1], Chandi Sasmal[2] and **L. Gary Leal**
Department of Chemical Engineering, University of California, Santa Barbara, USA
[1]current address: DAMTP, University of Cambridge, Cambridge, UK
[2]current address: Dept of Chem. Eng, IIT Ropar, Rupnagar, India

We consider the flow of a bimodal polymer blend in a contraction-expansion slit device previously studied experimentally by Mackley and coworkers using a polystyrene blend of a high MW component with MW of 485kg/mol and a low MW component of 67kg/mol. We carry out numerical studies of the flow using a recently derived constitutive model known as the SRDP Model that was developed in collaboration with researchers from Leeds University (Boudara, Peterson, Leal and Read, J. Rheology,**63,** 71 (2019)). The numerical solutions were carried out for parameters intended to match the experimental systems studied in the earlier experimental investigations. Our numerical solutions show that the flow with 10% of the small molecular weight component is stable for flow conditions when the monodisperse high MW melt is predicted to be unstable. This is similar to experimental observations that also show that 10% of the low molecular weight polymer added to the high MW component can stabilize the flow, which is otherwise unstable under the same flow conditions. We also show that a model that assumes that the blend can be treated as a linear superposition of two non-interacting species of the same molecular weights does not capture this effect, but instead predicts unstable flow under very similar conditions to the monodisperse, high MW melt.

Professor A.N. Alexandrou’s contributions to rheology and semisolid material processing

Michael Modigell
Rectorate, German University of Technology in Oman, PO Box 1816, Athaibah PC 130, Muscat, Sultanate of Oman

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Toward “Damascus yogurt”: using phase separation to understand and control the rheology of colloidal gels

Matthew E. Helgeson
University of California, Santa Barbara, USA

Colloidal gels are solid-like particle networks that underlie a number of soft material technologies. It is generally understood that gel rheology is intimately connected to the attractive colloidal forces and heterogeneous distribution of interparticle “bonds” they give rise to. However, most experimental insights into these relationships have been limited by an inability to enact direct and precise control over the colloidal interactions and network structure, leading to correlative, system-dependent and often contradictory models of gelation and gel properties. Here, we review our recent attempts to develop and study colloidal systems in which the attractive colloidal interactions can be carefully tuned with temperature, leading to precise control over the formation and arrested structure of colloidal gels. Inspired by ancient strategies for thermal processing of atomic and molecular materials, we study how a combination of phase separation and gelation can be used to kinetically control and arrest the development of gel structures with systematically varying length scales and densities of heterogeneity. Rheological studies of these gels reveal a remarkable degree of variability in both the linear and nonlinear rheological behavior with varying network heterogeneity at length scales much larger than the individual colloids. Structural measurements show that this behavior arises due to a combination of the phase separation process itself, which proceeds even at rest long after the onset of gelation, as well as the hydrodynamics associated with flow through the heterogeneous gel structure. Overall, our studies highlight the important and underappreciated role of mesoscale heterogeneous structure in determining the rheology of colloidal gels, and ultimately provide new routes for designing gels with novel or superior properties.

Regular Talks

Edge fracture in non-colloidal suspensions

Roger I. Tanner and Shaocong Dai
School of Aerospace, Mechanical and Mechatronic Engineering, University of Sydney, Sydney 2006
Australia

The phenomenon of edge fracture in parallel-plate and cone-plate rheological measurements is encountered when normal stresses are present in the viscometric flows. Using various non-Newtonian fluids it was confirmed [1-4] that the edge fracture instability depended on the second normal stress difference (N_2) and it was found by a simple static analysis based on a second-order fluid model [1] that the critical magnitude of N_2 was described by

$$N_{2c} = 2\Gamma / 3\alpha \tag{1}$$

where Γ is the surface tension coefficient of the sample and α represents the size of the 'flaw' at the sample edge. Keentok and Xue [3] showed experimentally that $\alpha \sim 0.12h$, where h is the gap between the plates at the rim. Hence the result (1) becomes

$$N_{2c} = 5.56\Gamma / h \tag{2}$$

However, it is well known that for non-colloidal suspensions the magnitude of N_2 is proportional to the shear stress, and so the above analyses do not apply and the correlation (2) implies fracture occurs at shear rates about five times lower than observed- essentially suspensions are more stable than expected against edge fracture.

Here we extend the simple analysis if [1] to fluids where the normal stresses are proportional to the (shear rate)^q ; for the second-order, Oldroyd-B and Giesekus models $q = 2$; for non-colloidal suspensions $q = 1$; for other data $q \sim 1.7$. Following the work of Pipkin on viscometric flows, we find instead of (1)

$$N_{2c} = q\Gamma / 3\alpha \tag{3}$$

This would imply, if α is still $0.12h$, that a suspension has a lower critical stress than a matrix fluid. This is not the case, and so it is suggested that instead of basing the 'flaw' size on the gap h it should be based on the size of the particles (d) instead. Some experiments with 40μm particles in a 40% volume fraction suspension suggest that a 'flaw' size of 30μm is needed to obtain agreement between Eq. (3) and experiment. In conclusion, these tests show that the classical treatments of edge fracture [1-4] is very inaccurate for suspensions. If a flaw size of order of the sphere radius is used in the analysis, much better agreement between experiment and prediction is achieved.

References.

1. R.I.Tanner , M.Keentok (1983) J. Rheol.27:47.
2. C.S.Lee,B.C.Tripp, J.J.Magda (1992) Rheol. Acta 42:1389.
3. M.Keentok, S.C. Xue (1999) Rheol. Acta 38:321.
4. E.J.Hemingway, H. Kusumaatmaja, S.M.Fielding (2017) Phys.Rev.Letters 119:028006.

The colloidal hydrodynamics and rheology of the cell

Akshay Maheshwari, Christian Aponte-Rivera, Emma Gonzalez, Alp Sunol, Drew Endy, and **Roseanna Zia**
Chemical Engineering, Stanford University, USA

Many representations of intra-cellular behavior rely on abstractions that do not account for how macromolecules are organized and move inside the crowded, watery cell milieu. For example, linear algebra- and differential equation-based models typically do not represent biomolecules or their spatial positioning and motion. For many questions in biology and medicine these simpler models have been sufficient. However, fundamental gaps in understanding of many cell functions persist; physics may provide a bridge to close such gaps. I will discuss our progress in developing computational and theoretical tools to model spherically confined colloidal suspensions, as a simple model cell, so that biomolecules and their interactions can be physically represented, individually and explicitly. By developing a more robust and fundamentally well-grounded physics model for how macromolecules interact within cells we can contribute to a more physically complete representation of living matter. A primary challenge in models of confined colloidal suspensions is the accurate and efficient representation of many-body hydrodynamic interactions, Brownian motion, and the enclosure itself. To this end, we developed a new "Cellular Stokesian dynamics" framework that accounts for spherically confined many-body hydrodynamic and lubrication interactions, Brownian motion, and active transport. Utilizing this model, we studied diffusion, cooperative motion, and self-organization with confinement and crowding levels representative of a cell interior. I will discuss the qualitative influence of hydrodynamics, confinement and crowding on transport behavior, as well as the consequences of neglecting such influences. Connections to underlying structure are made, and implications for cellular function are discussed.

Active particles in complex fluids

Gwynn J. Elfring
Department of Mechanical Engineering, The University of British Columbia, Canada

Active particles are self-driven objects, biological or otherwise, which convert stored or ambient energy into systematic motion. The motion of small active particles in Newtonian fluids has received considerable attention, with interest ranging from phoretic propulsion to biological locomotion, whereas studies on active bodies immersed in complex fluids are comparatively scarce. In this talk, I will discuss a theoretical formalism for understanding the motion of active particles in complex fluids, based largely on theory developed by Professor Leal (and others) for passive particles, and then discuss the effects of viscoelasticity and shear-thinning rheology in the context of biological locomotion and the propulsion of colloidal Janus particles.

Numerical simulations of electric field driven hierarchical self-assembly of monolayers of mixtures of particles

E. Amah, N. Musunuri, M. Hossain, I. Fischer and **P. Singh**
Department of Mechanical and Industrial Engineering, New Jersey Institute of Technology, Newark, NJ 07102

We numerically study the process of self-assembly of particle mixtures on fluid-liquid interfaces when an electric field is applied in the direction normal to the interface. The inter-particle forces cause mixtures of micron to nano sized particles to self-assemble into molecular-like hierarchical arrangements consisting of composite particles which are organized in a pattern. The minimum electric field intensity required is larger for nanoparticles for which the electric field induced lateral forces must also overcome Brownian forces. As in experiments (for micron sized particles), the structure of a composite particle depends on factors such as the relative sizes and the number ratio of the particles, their polarizabilities, and the electric field intensity. The initial distribution also influenced the final arrangement especially when the speeds with which the two types of particles moved during the self-assembly process differed substantially. For nanoparticle monolayers, the composition of composite particles was relatively more uniform because of the mixing induced by Brownian motion. If the particles sizes differ by a factor of two or more, the composite particle has a larger particle at its core and several smaller particles forming a ring around it. Approximately same sized particles, when their concentrations are approximately equal, form chains (analogous to polymeric molecules) in which positively and negatively polarized particles alternate, but when their concentrations differ, the particles whose concentration is larger form rings around the particles with smaller concentration.

Rheology and microstructure of non-aqueous silica particle suspensions

Anastasia Papadopoulou[1,2], Manish K. Tiwari[1], Stavroula Balabani[2]
[1] Nanoengineered Systems laboratory, [2] FluME
University College London, Department of Mechanical Engineering,
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Silica particle suspensions are encountered in a range of healthcare and industrial formulations. In toothpastes for example silica particles are added to provide certain functions such as abrasion, or as rheology modifiers. Silica particles contain various surface functional groups with the free silanol groups, -OH, playing a key role in controlling the interactions with neighbouring particles or the suspending medium through hydrogen bonding. These interactions significantly affect the microstructure of the suspensions and thus, their rheology. The present work aims to probe the interparticle interactions of non-colloidal silica particle suspensions and their effect on suspension rheology, with particular emphasis on non-aqueous matrices, such as glycerol, commonly employed in novel toothpaste formulations.

Commercial silica particles were suspended in two different solvents, namely glycerol and mineral oil, at different concentrations and their rheology was characterised by means of steady state and oscillatory shear (LAOS) measurements. A stress controlled rotational rheometer (DHR-3, TA Instruments) and a sandblasted parallel plate geometry were used for the rheological characterization. Suspensions of smooth glass spheres were also studied as control systems. Additionally, the microstructure of the sheared suspensions was investigated using an optical shearing system (CSS450, LINKAM). The irregular morphology and surface roughness of the silica particles suspended in glycerol increased suspension viscosity and promoted the onset of shear thinning behaviour at lower particle volume fractions compared to glass spheres. The use of the non-polar solvent (mineral oil) led to the formation of large particle clusters resulting in high yield stress, shear-thinning and viscoelastic behaviour, in contrast to glycerol-based suspensions, where the particles showed better dispersion capacity and Newtonian behaviour for the same particle concentrations. Particle clustering and dispersion were quantified from the optical shearing images using image analysis tools.

Dynamics of thin liquid films: Implications for beer foam stability

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Beer foam stability is believed to be enhanced by a rigid protein-stabilized thin liquid film (TLF) formed between two neighboring CO_2 bubbles. Such a film is expected to hinder drainage, coalescence and even Ostwald ripening [1], which are the main foam destabilization mechanisms. Although the synthesis or addition of certain proteins during the brewing process is common industrial practice, the mechanism by which they act still remains unclear.

The thin film drainage of three commercial beers was evaluated using a newly developed variation of the thin film balance technique coupled with interferometry [2]. The influence of surface tension, particle size, bulk and interfacial rheological properties on TLF stability was assessed by Wilhelmy-plate tensiometry, dynamic light scattering, double-wall ring interfacial rheometry and bulk viscosity measurements.

The surface tension and the bulk viscosity of the different beers did not show large variations. However, their drainage behavior differed significantly. Increased film stability, highly heterogeneous film thicknesses and slower thinning rates were observed for the beers of higher fermentation. Although the comparison between the experimental drainage curves and the predictions of the Reynolds model [3] indicates that the interfaces are highly stress-carrying, the mechanism of stabilization was found to differ. For two of the beers, it was observed that the drainage time increases with the interfacial shear viscoelasticity, while the most stable one was stabilized through Marangoni stresses.

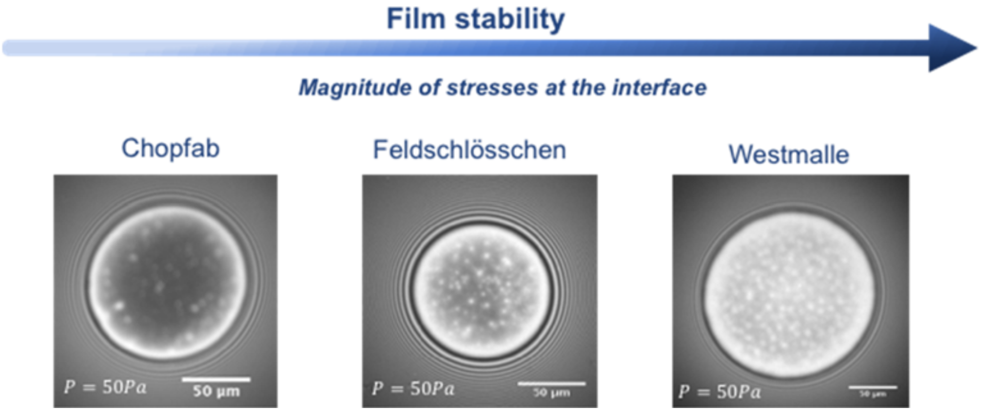

Figure 1. Microinterferometry images of the films of the studied beers. Film stability was found to increase from left to right, being maximum when Marangoni stresses were evident at the interface.

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Direct Measurement of the Dynamic Modulus of Micro-Capsules

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Micro-capsules are increasingly being studied as models for cells, as drug delivery vehicles, and even as devices for enhanced oil recovery form porous substrates. As such, understanding of their mechanical properties is critical for rational design and optimal performance. Here we describe experiments using a Cantilevered-Capillary Force Apparatus to probe the dynamic modulus of micro-capsules under axial compression. The micro-capsules used in this study are approximately 200 microns in diameter and are composed of a sunflower-oil core surrounded by a gellan-gum shell.

Rheology sensitively probes water-mediated changes of supramolecular structure

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Despite the widespread use of alkanes as solvents in supramolecular self-assembly, the role of water in the stability of the formed structures was ignored until recently [1]. This is probably because water is miscible in such solvents in extremely small quantities (typically, less than 0.01% by weight at room temperature). Yet, the presence of humidity may have profound consequences in supramolecular organization, likely due to competing hydrogen-bonding interactions, and rheometry is a very sensitive quantitative tool to explore the relevant structural and dynamic changes [1,2]. Here, we discuss two examples of supramolecular organogelators in apolar solvent dodecane, both based on moieties assembling by means of hydrogen bonding, whose structure and (in particular) dynamics are affected by the presence of humidity: a living polymer formed by bis-urea based monomers (EHUT) 2, 4-bis (2-ethylhexylureido) [2], and a long fiber formed by biphenyl tetracarboxamides (BPTA) [1]. We present linear and nonlinear shear viscoelastic measurements under conditions of controlled humidity and discuss the findings in view of water's interference with the supramolecular organization. Both systems exhibit similar phenomenology: in the absence of water, the plateau modulus is weakly affected, the dynamics significantly slows-down and the transient shear stress exhibits strain haderning. Given that experimenters usually do not account for humidity effects in oily environments, our results suggest that this practice should be reconsidered, at least when dealing with problems involving self-assembly based on hydrogen bonding. Moreover, the results resolve old dilemmas concerning data discrepancies in the literature of surfactants and offer ways to exploit water-mediated interactions for controlling supramolecular structure.

Work in collaboration with N. J. Van Zee, E. W. Meijer (Eindhoven) and L. Bouteiller (Paris).

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Rheological properties of amine functionalized polynorbornenes

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Amine-functionalized polymeric materials are found potentially useful in a wide variety of applications including adhesives, membranes, coatings and energy ion-polymer batteries. Combination of hydroaminoalkylation reaction and ring-opening metathesis polymerization was used to synthesize monodisperse secondary amine-containing polynorbornenes. Various functionalities that exhibit different hydrogen bonding strengths were introduced. Extensive rheological characterization has shown the effect of the substituents in dictating the hydrogen bond ability within the polymeric materials and thereby, influencing their rheological properties (sticky-Rouse and reptation relaxation times as well as the plateau modulus). The detailed rheological study (shear and extensional) has demonstrated clear transition from liquid-like behavior of tertiary amine-containing polynorbornenes to solid-like behavior of secondary amine-containing polymers depending on the side groups and molecular weight.

Moffatt Eddies in Single Screw Extrusion

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A 3D flow analysis package was used to simulate the flow phenomena in a short section of the metering zone of a single screw extruder. The assumption of stationary screw and rotating barrel is used. For sharp flight root corners, in addition to the primary flow field a secondary flow was determined in front of the root of the pushing flight and behind the root of the trailing flight, akin to what is known in the fluid mechanics literature as Moffatt eddies. These have been studied extensively for lid driven cavity flows. In the present work, simulations were carried out for Newtonian and inelastic shear- thinning fluids. In single screw extrusion the flow is fully 3D and the computer simulations show that fluid particles caught in Moffatt eddy regions require travel times which are at least two orders of magnitude larger than the average residence time. This implies high probability of degradation and explains the deposits of thin carbonaceous films and gels, which have been discussed in several publications in the technical literature. The computer simulations show the existence of Moffatt eddies in the presence or absence of pressure gradients. When the screw roots have relatively wide angles no Moffatt eddies are predicted, in agreement with recommendations for good screw design practices. The present work also suggests that Moffatt eddies probably occur in other parts of extrusion equipment, such as in mixing elements and even in extrusion dies which are frequently manufactured having complicated geometries with obstacles and/or sharp corners.

Dynamics of Taylor-Couette flow of shear-thinning fluids

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The flow between two concentric cylinders with the outer one fixed and the inner one rotating (Taylor-Couette flow) has been studied extensively due to its relevance to flow stability analysis as well as many industrial applications. The flow is known to experience a series of bifurcations when the rotational speed is increased, leading to rich flow phenomena. It is also a typical rotational rheometer configuration and can serve as an idealised mixer to study vortex dynamics and mixing due to the well-defined Taylor structures that form following the primary instability and persist up to the onset of turbulence.

Non-Newtonian fluids or particle suspensions commonly employed in process engineering applications can have a strong effect on the primary and higher-order instabilities that are essential for effective mixing. However, there is a lack of experimental studies on the dynamics of such flows and their impact on mixing. We examine the behaviour of Newtonian and non-Newtonian (shear-thinning) fluids in Taylor-Couette flow for a range of Reynolds number spanning the Couette, Taylor Vortex and Wavy Vortex flow regimes, using a combination of Particle-Image Velocimetry and flow visualisation methods. Shear-thinning is found to have a non-monotonic effect on the critical Reynolds number for flow transitions, increases the wavelength (vortex size) and the amplitude of the wavy instability, which have implications for mixing. The work is currently been extended to suspensions of spherical and platelet like particles.

Stability of film flow with high loadings of soluble surfactant: The effect of surface compressibility

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The primary instability of a falling liquid film laden with a soluble surfactant is investigated. Surface properties are derived by Gibb's theory, using a Langmuir or Frumkin isotherm[1]. An eigenvalue problem is formulated for disturbances of arbitrary wavenumber, which is solved numerically by a finite-element method and analytically in the longwave limit[2,3].

Film stabilization, which is known to occur by Marangoni stresses, is found to depend on two key surface properties, the Gibbs elasticity $E_0 = -d\sigma/dln\Gamma$ and the diffusional relaxation frequency $\omega_D = \mathcal{D}(d\Gamma/dc)^{-2}$ (σ: surface tension, c: bulk concentration, Γ: surface concentration). In particular, high E_0 values enhance Marangoni stresses, while high ω_D values enhance mass exchange between the interface and the bulk and thus mitigate them. However, both E_0 and ω_D become singular when surfactant concentrations approach from below the critical for micelle formation (CMC).

The double singularity is resolved by attributing finite compressibility to the adsorbed monolayer[4], i.e. taking the molar area of adsorbed molecules to decrease linearly with surface pressure. The stability analysis using realistic values of surface compressibility[4] indicates enhanced stabilization with the approach to CMC, in comparison to the hard-sphere model.

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Investigation of the scaling of the endothelial surface layer permeability of microvessels through multiscale modeling and simulations

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The effect of the macromolecular layer covering the luminal surface of the vascular endothelium, called endothelial surface layer (ESL) [1], on microcirculation has become increasingly interesting, since it has been described as the main mechanosensor and transducer of fluid shear-stress on endothelial cells. In this study, we investigate the ability of the ESL to allow fluid transition (permeability) by extensive multiscale simulations of blood flow in capillaries. To this end, we introduce a three-phase moving interface model [2] with: (a) the rich-in-RBCs (Red Blood Cells) core represented by a novel viscoplastic constitutive equation [3] which associates the aggregation of erythrocytes into rouleaux with the yield stress value at low shear rates, (b) a dynamically predictable cell-free layer (CFL) adjacent to the vessel walls rich in plasmatic proteins [4], and (c) a porous medium of about 150-500 nm of thickness which corresponds to the glycocalyx layer of the ESL. By modelling the glycocalyx as an ideal spatial arrangement of protein fibers we accurately calculate the core-plasma interface shear stress as well as the macroscopic geometry-defined permeability. The investigation extends to a more realistic model through a microscopic approach incorporating the interaction between blood plasma and glycocalyx fibers. The latter are assumed to be deformable elastic solids. The fluid-structure interaction (FSI) problem is defined on two- and three-dimensional periodic domains utilizing the shear stress and CFL thickness extracted from the macroscopic simulations. Based on the quasiperiodic ultrastructural model of Squire et al. [5] and the periodic bush-structure model of Weinbaum et al. [6] for the geometric representation of the glycocalyx, we construct a realistic computational domain of the solid phase. These microscopic fluid-structure interaction simulations allow for more accurate determination of the dynamically changing shear stress but are costlier than the macroscopic, one-dimensional calculations. Consequently, based on these data we define relationships that yield in great precision the macroscopic time-dependent mechanical and fluid-flowing properties as a function of the respective hemorheological regime. By weighing the computational cost of the FSI method and the accuracy of the two models, we conclude that the permeability of the sieve porous layer can be efficiently determined by the versatile low-level model for blood flow situations where the role of the glycocalyx is relatively inconspicuous. On the other hand, in cases where intensive hemodynamical phenomena are present, the glycocalyx's complex characteristics of elasticity and geometry must be taken into account in the evaluation of the ESL apparent permeability.

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2-3-4 spikes competition in the normal field instability of ferrofluids

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The horizontal free surface of a magnetic liquid (ferrofluid) pool turns unstable when the strength of a vertically applied uniform magnetic field exceeds a threshold. The instability, known as normal field instability or Rosensweig's instability, is accompanied by the formation of liquid spikes either few, in small diameter pools, or many in large diameter pools; in the latter case, the spikes are arranged in hexagonal or square patterns. In small pools where only few spikes - 2, 3 or 4 in this work - can be accommodated, their appearance/disappearance/re-appearance observed in experiments, as applied field strength varies, is investigated by computer-aided bifurcation and linear stability analysis. The equations of three-dimensional capillary magneto-hydrostatics give rise to a three-dimensional free boundary problem which is discretized by the Galerkin/finite element method and solved for multi-spike surface deformation coupled with magnetic field distribution simultaneously with a compact numerical scheme based on Newton iteration. Standard eigenvalue problems are solved in the course of parameter continuation to reveal the multiplicity and the stability of the emerging deformations. The computational predictions reveal selection mechanisms among equilibrium states and explain the corresponding experimental observations and measurements.

3-Dimensional flows of non-Newtonian fluids with free surfaces

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In this study, we propose a new, fully consistent and highly stable finite element formulation for the simulation of Non-Newtonian fluid flows with free surfaces in 3-dimensions. In this numerical scheme, we have coupled our newly proposed FEM method for strong viscoelastic flows [1] with the quasi-elliptic mesh generator [2] of our lab to solve Non-Newtonian fluid flows with free surfaces mapped on highly deformed domains. The Petrov-Galerkin stabilization terms along with the log-conformation representation of the constitutive equation have allowed us to obtain numerically stable solutions at high values of the Weissenberg number using linear interpolation functions for all variables (velocities/position vector/pressure/stresses). In addition, parallel iterative Krylov solvers are employed for the solution of the resulting linear systems, boosting the speed of our numerical simulations. The validity of the presented FEM framework is tested by simulating the extension process of 3-dimensional viscoelastic and elasto-visco-plastic filaments, in which the stress-tensor is predicted by the PTT and Saramito/Herschel-Bulkley constitutive equations, respectively. In order to illustrate the robustness of the proposed formulation, the results are compared to 2-dimensional axisymmetric simulations, where possible. In addition, we perform mesh and time convergence tests illustrating that the proposed method is convergent and features 2nd order accuracy in space and time.

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Application of Onsager Machlup integral in solving evolution equations in non-equilibrium systems

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In 1931, Onsager proposed a variational principle which has become the base of many kinetic equations for non-equilibrium systems [1]. This principle has been shown to be very useful in soft matter physics [2,3]. Here I demonstrate this using two hydrodynamic problems, (a) capillary problem in a tube with corners [4], and (b) free boundary problem in liquid coating [5]. I will show that the existing governing equations (2nd and 4th order non-linear pde) can be derived by the variational principle, and that their approximate solutions are also obtained by the variational principle using the Onsager Machlup integral [6].

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A constitutive equation for thixotropic suspensions with yield stress by coarse-graining a population balance model & experimental validation

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A population balance model appropriate for the shear flow of thixotropic colloidal suspensions with yield stress is derived and tested against experimental data on a model system available in the literature. Modifications are made to account for dynamic arrest at the onset of the yield stress, in addition to enforcing a minimum particle size below which breakage is not feasible. The resulting constitutive model also incorporates a structural based relaxation time, unlike existing phenomenological models that use the inverse of the material shear rate as the relaxation time. The model provides a reasonable representation of experimental data for a model thixotropic suspension in the literature, capturing the important thixotropic timescales. When compared to prevalent structure kinetics models, the coarse-grained population balance equation is shown to be distinct, emphasizing the novelty of utilizing population balances as a basis for thixotropic suspension modeling. The mathematical differences are shown to result from taking a particle viewpoint as opposed to that based on “bonds” rather than particles. The model is applied to experimental data on industrially relevant systems, enabling extracting fundamental information of value to formulators of suspensions. Extensions to handle size distributions are discussed and shown to yield additional information about yielding systems.

Some aspects of this paper are published in AIChE J. DOI 10.1002/aic.15574[1] Mwasame PM, Beris AN, Diemer RB, Wagner NJ. A constitutive equation for thixotropic suspensions with yield stress by coarse-graining a population balance model. Aiche Journal. 2017 Feb;63(2):517-31.

A study of the effective extensional viscosity in a particle laden viscoelastic solution

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Previous studies have now shown in some detail that the effective shear viscosity of particle laden viscoelastic solutions demonstrates shear thickening even at small volume fractions in contrast to the shear thinning, particle free fluid. This thickening is created by increasing particle-induced fluid stress in the fluid surrounding the particles which offsets a reduction in the stresslet contribution to the average shear stress. Since the particle-induced fluid stress is a nonlinear function of flow type, the conclusions from studies on shear flow do not immediately allow prediction of the material properties for other linear flows. Extensional flow is of primary importance in molding, film blowing and fiber drawing applications. We therefore describe a theoretical, computational and experimental examination of the effective extensional viscosity of a particle laden Boger fluid at small and moderate particle volume fraction. The results for numerical calculation for the effective extensional viscosity for single spherical particles (i.e. in the dilute limit) as a function of strain and strain rate (i.e. Deborah number) will be presented for the Oldroyd B, FENE-P and Giesekus models. The results are compared to theories valid for small Deborah number (see Einarsson et al. 2018)[1] as well as a new theory valid for small strain. The effective extensional viscosity calculation is renormalized using the methods described in our previous publication [1]. We compare these predictions to fiber stretching rheometry experiments up to volume fractions of 25% particle loading.

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Dynamics of particle pair in a viscoelastic fluid under pressure driven flows: Clues for particle ordering in microfluidics

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The dynamics of two particles suspended in a viscoelastic fluid and aligned on the centerline of a microfluidic channel is investigated by direct numerical simulations. The fluid is shear-thinning and elastic. The relative particle velocity is studied by varying the interparticle distance, the Weissenberg number, fluid shear-thinning, and particle shape. Concerning the latter aspect, spherical and spheroidal particles with different aspect ratios are considered. Particle attraction or repulsion as well as the equilibrium configurations are identified and correlated to the fluid rheological properties and particle shape. The simulation results provide useful insights to design efficient microfluidics devices to achieve particle ordering, i.e., the formation of equally-spaced particle structures.

A numerical study for the compression only effect of contrast agents

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Contrast agents are gas-filled encapsulated microbubbles that are used in novel biomedical applications such as targeted drug delivery and the medical imaging of vital organs. Their coating is usually a lipid monolayer or polymeric material The former type shells exhibit a strain-softening behavior when subjected to acoustic disturbances which amounts to preferential excursion from equilibrium during expansion, especially at large sound amplitudes. However, experiments have revealed a counter-intuitive behavior of lipid monolayer shells in that a compression only behavior has been reported where they pulsate mainly in the compression phase of their radial time series. We numerically investigate this behavior by solving the

Navier-Stokes and continuity equations for the liquid, whereas the force balance and the kinematic condition are applied on the interface. Besides the membrane stresses, the interfacial model includes the force due to bending as well. We assume constant rheological shell properties that do not depend on the radius of the bubble. The dilatational and the shear viscosity of the membrane are treated separately which allows for a more realistic motion of the interface. The overall problem is solved using the finite element methodology with a hybrid scheme that uses 2D Lagrangian basis functions for the flow domain in conjunction with 1D cubic splines for the interface, in order to resolve the fourth order derivatives corresponding to shell bending. The elliptic mesh generation technique is used for the construction of the computational grid. The numerical results reveal that lipid contrast agents exhibit a compression only behavior when they are initially pre-stressed, provided that the rheological properties of the membrane allow it. The difference between the dilatational and the shear shell viscosity facilitates significantly this effect and the presence of the wall accelerates its appearance. Moreover, it is found that for a given frequency there is a critical threshold in sound amplitude above which the bubble exhibits the compression only response pattern, with the threshold amplitude being reduced as the forcing frequency decreases. The amplitude threshold for the onset of compression only effect is determined from the static buckling threshold and from the threshold for parametric mode excitation.

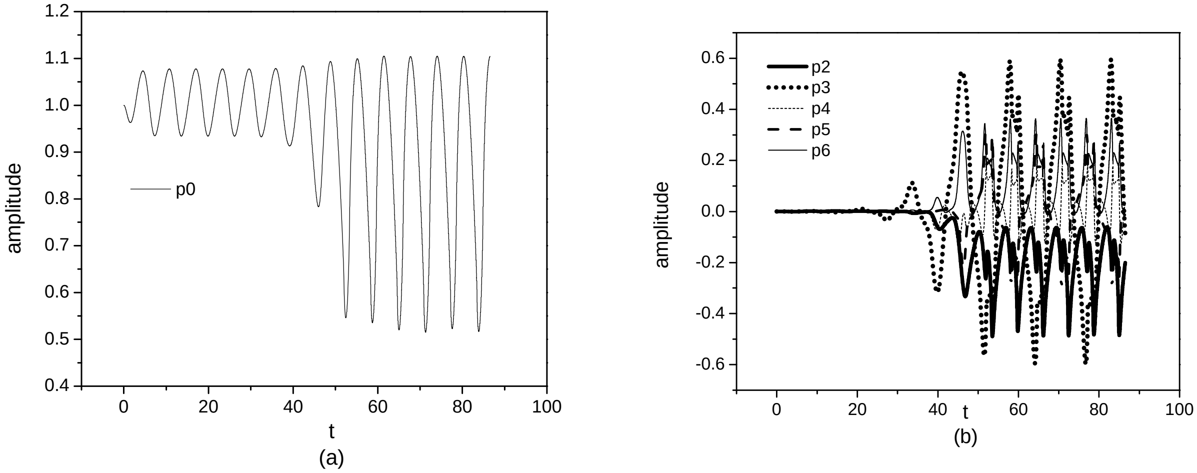

Figure 1. Compression-only effect of a contrast agent for an acoustic disturbance of 1.2MHz frequency and amplitude ε=0.5. Temporal evolution of (a) breathing mode and (b) shape modes.

Drop-on-demand inkjet printing of surfactant solutions

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A key challenge in developing new applications of inkjet technology is to produce inks that can be jetted to form individual droplets and to transport functional components needed for the application. The development of mathematical models that allow fluid jetting behaviour to be determined as a function of fluid properties would allow optimisation to be carried out in-silico before creating the inks and verifying the performance. Surfactants are often added to aqueous inks in order to modify the surface tension.

However, the rapid expansion of the free surface during the fast inkjet jetting process means local areas of surface will be depleted of surfactants leading to surface tension gradients. There is still a mystery on the ink behaviours under such conditions. In this work, experimental studies of the jetting behaviour with the addition of surfactants are presented. Key ink ingredients are identified and are used to investigate the effect of jetting properties in an industrial inkjet print-head. In parallel, we are developing a finite element based numerical simulation of inkjet break-up and drop formation in the presence of surfactants.

Using the contravariant deformation tensor formulation in simulation of viscoelastic fluid flow

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Numerical simulations of viscoelastic fluid flow commonly employ conformation tensor based constitutive models. Standard stabilisation techniques known from convection dominated flows, such as SUPG in finite elements, are required but also insufficient to solve flows at high Weissenberg numbers on fixed grids. The reason is a numerical imbalance of the convection and deformation terms in the conformation tensor equations [1]. The log-conformation representation (LCR) technique, introduced in [1], fixes the imbalance and has become a standard technique to obtain solutions for high Weissenberg numbers. A disadvantage is that the LCR technique involves the spectral decomposition of the conformation tensor, which complicates the use of fully implicit time integration techniques or finding a steady state solution using Newton-Raphson iteration.

Motivated by the introduction of thermal fluctuations, in [2] the conformation tensor models are rewritten in terms of the so-called contravariant deformation tensor. However, it is also suggested that it could help in solving the high Weissenberg problem similar to the LCR-technique. Since the resulting equations do not require a spectral decomposition, Newton-Raphson iteration would be easy to apply. A disadvantage is the inherent time-dependent formulation in terms of on-going rotations, even if the flow is steady.

In this talk, we will show results of our finite element implementation of the contravariant deformation formulation for various conformation tensor models. We consider the standard benchmarks for the flow around a confined cylinder and an initially perturbed shear flow. The stability for high Weissenberg numbers turns out to be very good and comparable to the LCR technique.

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Mesoscale modeling of networked fluids

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Mucins, telechelic polymers, wormlike micelles, and other complex fluid mixtures consist of transiently networked elements at the mesoscale. Modeling these mixtures at the mesoscale has the advantage over macroscale models in that the models capture the local properties (connections, orientations, stretch) of the structural elements. The mesoscale elements are often modeled as bead springs (Hookean or FENE) which can attach to each other to form chains or cross-linked networks. These linkages can break, thus the element connections are continually dynamically breaking and reforming. Long wormlike micelles in concentrated mixtures entangle and thus their motion is confined by nearby worms. This confinement can possibly be captured in models by allowing weak cross-chain attractions. These weaker cross-chain attractions exist in mucins. Models and simulation results for a stochastic mesoscale breaking reforming system will be presented and parameter ranges explored which lead to capturing behaviors of physical interest.

A tensor model for shear thickening suspensions of spherical particles

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Dense suspensions of repulsive particles exhibit shear thickening, when the suspension pressure overcomes the inter-particle repulsive force, and pushes the particles into physical contact, with an enhanced friction, as compared to lubricated contact. Particle contacts sustain forces, that are aligned in the compressive direction of the rate of strain tensor. When this direction is abruptly reversed, the particle contacts disintegrate, and the suspension thins abruptly, and re-thickens gradually, due to the association of particle contacts in the new compressive direction. We use a discrete element method (DEM), to study of the suspension stress and microstructure after shear reversal. The results show, that there is a strong correlation between the time dependent suspension viscosity and the coordination number of frictional contacts Z_f. In order to better understand these dynamics, we develop a second rank tensor model, for the suspension microstructure $\boldsymbol{a}$, defined as the second order moment of the probability distribution function of the separation vector $\boldsymbol{n}$ of the closely interacting particles. The evolution equation of $\boldsymbol{a}$ accounts for the affine rotation of $\boldsymbol{n}$ and for the creation and destruction of interacting particle pairs, through compressive and extensive deformation, which brings particles together and pulls them apart, respectively. The model agrees qualitatively with the DEM simulations, for the time dependent microstructure and stress recovery after shear reversal.

A particle distribution function approach to the equations of continuum mechanics in Cartesian, cylindrical and spherical coordinates: Newtonian and non-Newtonian fluids

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The evolution equations for the particle distribution functions are written in a divergence form applicable in three dimensions. From this set, it is shown that the continuity equation and the equations of motion are satisfied in Cartesian, cylindrical and spherical coordinates for all fluids when additional source terms are added to the equations of evolution in the latter two coordinate systems. If the body forces are present, a new set of source functions is required in each coordinate system and these are described as well. Next, the energy equation is derived by using a separate set of particle distribution functions. Modifications of the relevant equations to be applicable to incompressible fluids is described. The incorporation of boundary conditions and the description of the numerical scheme for the simulation of the flows employing the new approach is given. Validation results obtained through the modelling of a mixed convection flow of a Bingham fluid in a lid-driven square cavity, and the steady flow of a Bingham fluid in a pipe of square

cross-section are presented. Finally, some comments on the theoretical differences between the present approach and the existing formulations regarding Lattice Boltzmann Equations are offered.

Tracking-free one- and two-point microrheology of soft materials

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Passive particle tracking microrheology (PT-μr) is an experimental technique that exploits the thermal motion of tracer particles to probe the local mechanical properties of small amounts of homogeneous (one-point PT-μr) and micro-structured (two-point PT-μr) soft materials [1].

While in one-point PT-μr the trajectories of single particles are analysed to extract their mean squared displacement, in two-point PT-μr the cross correlations between the mean-square displacements of two particles are studied, which provides a means to get rid of artefacts that may arise in PT-μr as a consequence of the interactions of the probes with the sample microstructure. Despite its appealing conceptual simplicity, both approaches require calibration procedures and operating assumptions that constitute a practical barrier to a wider adoption, especially in industrial environments and in particular for two-point PT-μr that requires a large number of accurate measurements and a subtle analysis of the acquired data.

Here, we present a novel approach to passive one-and two-point microrheology that, not requiring particle tracking, unlocks a calibration-free, automated, operator-independent rheological characterisation of soft materials. We first show how Differential Dynamic Microscopy (DDM) [2] can be used to perform one-point microrheology of different homogeneous complex fluids [3] by relying on the multi-scale, temporal correlation study of the image intensity fluctuations that are observed in microscopy experiments as a consequence of the motion of the tracers. In addition, we show how a novel analysis based on optical flow detection, enables one obtaining accurate two-point microrheology data of entangled F-actin solutions [4].

Our results are in good agreement with PT-μr when the latter can be used. In addition, DDM-μr is found to provide reliable information even in cases where PT-μr is not a suitable option, demonstrating tracking-free microrheology as a viable alternative and complement to PT-μr and to other rheological probes.

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Microscale flows of hardened red blood cell suspensions

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Blood is a dense suspension of cellular elements, primarily red blood cells (RBCs). The deformability and aggregation of RBCs are key determinants of blood rheology and hence microcirculatory flow. Diseases such as diabetes mellitus, sickle cell anaemia and malaria alter the morphology and mechanical properties of RBCs leading to microvascular occlusions and impaired organ perfusion. However, the exact role of RBC deformability on local haemodynamics has not been established.

In the present study, we extend our previous work on healthy RBC flows in bifurcating microchannels (Sherwood et al, PLoS One, 2014; Kaliviotis et al, Sci. Rep 2017) to examine the role of deformability on the velocity, haematocrit and aggregation characteristics of RBC suspension microflows. Human RBCs, obtained from donors following an approved ethics protocol, were artificially stiffened using glutaraldehyde (GA) and suspended in solutions of PBS and PBS-Dextran2000 to induce aggregation. RBC suspensions were perfused through straight microchannels (50 x 50 μm^2) at rates varying from 1 -150 s^{-1} and imaged using a bespoke microPIV set up. Velocity and haematocrit profiles were obtained for both aggregating and non- aggregating samples and concentrations varying from 5 to 25%. RBC migration and cell interactions were further probed by means of cell tracking experiments using fluorescently labelled RBCs.

The experiments showed that the loss of deformability alters the velocity and haematocrit profiles of the dense RBC suspensions producing more Newtonian-like velocity profiles. Hardened RBCs were found to concentrate towards the centre of the flow in dense suspensions as opposed to dilute ones highlighting the importance of cell interactions on the resulting suspension microstructure. Aggregation was found to be less pronounced in hardened RBC suspensions compared to healthy ones.

Blood rheology and flow geometry effects

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The rheological properties of blood are influenced by the intensive and extensive properties of its constituent elements. The dominant element in blood is the red blood cell (RBC), and its concentration, elasticity, and tendency to aggregate under certain flow conditions govern the rheological behaviour of the fluid. In various clinical applications blood is forced to flow through devices, the function and/or geometry of which, cause intense alterations in the local flow conditions. One such device is the cardiovascular stent, and the current work aimed to investigate how blood rheology is influenced by the geometry changes caused by the stent presence. Blood samples from healthy volunteers were prepared as RBC suspensions in serum and in phosphate buffer saline at 45% haematocrit. Self-expanding nitinol stents were placed in clear perfluoroalkoxy alkane tubing of I.D. 0.75mm and connected to a syringe/syringe pump arrangement. The samples were tested at various flow rates, covering physiological and extreme conditions. Tests were performed also in non-stented vessels for comparison. For each flow rate, the sample viscosity, RBC aggregation and deformability were estimated. RBC membrane lysis was examined by measuring the serum free haemoglobin concentration. The results indicate that the geometry changes caused by the presence of a stent in a vessel affect the hemorheological characteristics of blood: RBC deformability and aggregation decline, blood viscosity is elevated and membrane lysis is observable. The cause of the observed hemorheological alterations is traced in the complex local flow conditions, in the vicinity of the stent area, which affect the physiological and mechanical properties of the RBC. The stresses developed in the stent area could be sufficiently high to damage the RBC membrane. The results are viewed and discussed from a theoretical perspective, utilising novel and established constitutive models for blood.

Steady shear flow of marginally entangled ring polymer melts through nonequilibrium molecular dynamics simulations

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Atomistic simulations of ring polymer melts under equilibrium conditions have been proven very useful in extracting scaling laws for the conformational and transport properties (chain center-of-mass diffusion coefficient and zero-shear-rate viscosity) of this unique class of polymers in the crossover regime around the entanglement molecular weight M_e [1]. In combination with a detailed geometric analysis, such simulations have also helped tremendously characterize topological constraints in ring polymers developing due to ring-ring but also ring-linear threading (in the presence of any remaining linear impurities) and their connection with the slow relaxation modes observed experimentally [2].

In the present work, we extend this study to nonequilibrium conditions by investigating in a systematic way the flow behavior of ring polymers using as a model system poly(ethylene oxide) (PEO). We have conducted detailed nonequilibrium molecular dynamics (NEMD) simulations of pure ring and linear PEO melts, as well as of ring-linear blends, over a wide range of shear rates covering both the linear and nonlinear regime using the p-SLLOD equations of motion [3]. Through these simulations, we have been able to compute the relevant viscometric functions in shear (shear viscosity and first and second normal stress coefficients) and their dependence on applied shear rate, melt molecular weight and relative concentration of the melt in ring and linear chains.

In addition, selected configurations from the NEMD trajectories have been subjected to a detailed geometric analysis [4,5] to provide information on the effect of flow on the degree of ring-ring and ring-linear threading, and thus on the nature of topological constraints in melts of non-concatenated ring polymers, given the tendency of linear chains to penetrate rings and form a network.

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Multi-scale dynamic dimulations of polymer nanocomposites with inorganic or polymer-based nanoparticles

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Heterogeneous polymer-based nanoparticles comprise a very promising family of materials for a broad range of applications. Here we presented a detailed multi-scale simulation methodology for the study of structure and dynamics of polymer nanocomposites with either polymeric, or inorganic nanoparticles. The proposed methodology consists of atomistic and coarse-grained dynamic simulations. Our goal is to provide direct quantitative studies of structural and dynamical heterogeneities in polymer nanocomposites with different kind of nanoparticles. We examine two different families of polymer nanocomposite systems:

(a) The first concerns, polystyrene (PS) stars and mikto-arm stars of mikto-arm star copolymers with two types of chemically incompatible arms, namely poly(ethylene oxide) (PEO) and PS, [(PS)n(PEO)n], where n is the number of arms.in melt and in blend with linear PS chains by means of atomistic molecular dynamics simulations. By using a particularly designed protocol for the equilibration of the melts, we prepare star melts with a range of functionalities, tuning their mutual penetration. The immiscibility between the two components gives rise to intramolecularly nanostructured particles. The nanostructured objects resemble either "Janus-like" or "patchy-like" particles, depending on the number or the length of the arms (or both) as well as the interaction with the surrounding medium. We further quantify the actual slowing down of the dynamics close to the star core, which is believed to be responsible for the extraordinary viscoelastic properties of the stars. We show that the dynamical heterogeneities related to the star-like architecture are more pronounced in the translational motion in comparison to the rotational dynamics of the star arms.

(b) The second concerns polybutadiene (PB) nanocomposites with inorganic (silica) nanoparticles. We provide a detailed study concerning the structural and dynamical properties of the bound polymer layer in nanocomposite elastomers by using a hierarchical dynamical simulation approach involving atomistic and coarse-grained simulations. Clear thermodynamical (density), structural and dynamical (rheological) heterogeneities are reported. A detailed analysis show that the segmental mobility is characterized by heterogeneities along the chain and also in different layers around the Silica. The results indicate that even in the case of high confinement, where a low percentage of free chains is present, a decoupling between the adsorbed and the middle layer is present. In addition, the dynamics of the bound layer when extending far from the adsorbed layer is characterized by relaxation times at least an order of magnitude lower than the ones in the adsorbed layer.

Overall, through the proposed multi-scale simulation approach we provide, for the first time to our knowledge, a detailed insight into the morphology and dynamics of polymer nanocomposites with inorganic or polymeric nanoparticles.

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Start-up plane Poiseuille flow of a Bingham fluid

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The start-up flow of a Bingham plastic in a channel is considered and Safronchik's solution for the initial evolution of the yield surface and the core velocity is revisited. Stricter time bounds for the validity of the above solution are derived and the solution is extended to include the velocity profile in the evolving yielded zone. Comparisons are made with another approximate solution derived under the assumption that the velocity in the yielded zone is parabolic adjusting with the evolving yield surface. This approximation performs well for small values of the yield surface, or, equivalently for large values of the imposed pressure gradient.

Squeeze flow of thixotropic semisolid slurries

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Semi-solid metal processing (SSM) is a powerful manufacturing technology used to manufacture complex near-net-shaped components with high integrity characteristics. This technology, known also as thixoforming process, implies that the material behaves as a solid when the applied stress lies below the yield stress. Once the yield stress is exceeded, the material behaves either as a shear-thickening or as shear-thinning fluid with a non-linear stress-strain relationship [1-3]. An important issue for the integration of this innovative technology in the production of complex commercial components by the industry is the availability of accurate mathematical and computational tools that could describe both the rheological behavior and the material characteristics of the suspension, which is strongly affected from its internal structure and its evolution during deformation. In contrast to other thixotropic materials, semisolid slurries show partially irreversible rheological characteristics due to the breakage of the welded bonds between the particles [3, 4].

In this work, we investigate further a numerical model based on the Herschel-Bulkley constitutive equation and simulate the classical squeeze flow experiment by including the effects of thixotropy under constant velocity, while the bottom side remains fixed [3, 5]. The yield stress is assumed to vary linearly with the structural parameter which follows a first-order rate equation accounting for the material structure break-down and build-up. The development of the yielded/unyielded regions in relation to material structural changes is analyzed. The numerical model has been tested against available experimental data on a semisolid aluminum alloy.

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Experimental and theoretical investigations of human and animal blood rheology

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Blood is a complex living fluid that has been well engineered through several million years of evolution to provide optimal transport. Despite a consistent makeup across species with minor variations in the constituent sizes and volume fractions, the material properties of blood may change significantly. At stasis and low shear rates, the red blood cells within blood from some species will naturally form coin stack structures called rouleaux. The presence of these structures gives rise to interesting rheological properties including viscoplasticity, viscoelasticity, and thixotropy. Interestingly, the formation of rouleaux is not universal across species and will occur to different extents if at all.

In this work, we provide experimental and modeling results probing the material properties of blood from a range of species through both steady state and transient shear rheology. Using a modified form from a previously developed model for transient blood rheology [1] we work to understand the observed similarities and differences and to connect them better to blood physiology.

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Understanding the rheological behaviour of blood from a non-equilibrium thermodynamics perspective

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Blood is mainly a suspension of elastic particulate cells, among which red blood cells (RBCs) dominate, in plasma (a Newtonian fluid). Under quiescent conditions, when the shear rate is not high enough (~1-5 s^{-1}), RBCs aggregate forming column-like structures called rouleaux. As the shear rate increases, rouleaux break and eventually, after a critical shear rate, only individual RBCs can be observed. An early constitutive model that could predict this dynamical behaviour was the one suggested by Owens and co-workers [1] which considers explicitly the formation and destruction of rouleaux [1]. Also, at physiological haematocrit values and low shear rates, blood exhibits a yield-stress, i.e., it flows only above this critical stress and behaves as elastic solid, otherwise. This behaviour is usually modelled using empirical constitutive equations, such as the Bingham and Herschel-Bulkley models.

In the present work, we use the framework of non-equilibrium thermodynamics, particularly the generalized bracket formalism [2], to derive two constitutive models for blood. Firstly, we derive a constitutive model [3] which accounts for the formation and dissociation of rouleaux and turns out to be very similar to that of Owens and co-workers. However, by explicitly considering a mechanism for the formation and breakage of rouleaux, our model further provides expressions for the aggregation and disaggregation rates, which in the kinetic theory-based network model of Owens were absent and had to be specified separately. Secondly, we derive an elastoviscoplastic model [4] which introduces self-consistently and effortlessly thixotropic effects. The predictions of the new model are in good agreement with available steady-state shear rheological data exhibiting a yield stress, and with time-dependent rheological data exhibiting a hysteresis for blood. The proposed approaches are expected to provide the means to improve our understanding of the rheological behaviour of blood.

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Comparative rheological study of dense microgel and star polymer suspensions

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Dense microgel suspensions exhibit a thermal glass-to-jammed glass transition, characterized by large yield stress and linear dependence of plateau modulus on concentration, as well as other fine differences in flow curves [1]. Shape adjustment in the highly concentrated regime appears to be at the origin of jamming [3]. Hairy particles represent the other archetype soft colloidal system, with the additional feature being their dangling arms [4]. An outstanding challenge in the field is understanding the role of internal microstructure on the dynamic properties of soft colloids and in particular with respect to the possible glass to jamming transition and associated yielding at high concentrations. Here, we address this challenge by systematically investigating highly concentrated suspensions of well-characterized microgels and multiarm star polymers. Whereas both types of particles are able to shrink and deform under the action of osmotic pressure, star polymers can also interpenetrate their arms and, moreover, can be investigated throughout the entire concentration regime up to the dry melt state. We show that the difference in the internal particle microstructure is reflected in distinct rheological signatures of these soft colloids. We focus on linear and nonlinear rheological shear measurements and analysis with additional support from dynamic light scattering. Subtle differences in flow curves and associated velocity profiles are critically discussed and linked to the different features that dictate particle softness. Some generic features associated with the yield stress and strain are also presented.

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Rheology of poly(ethylene-co-methacrylic acid) ionomers

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Using a parallel plate rheometer equipped with a partitioned plate, and an extensional fixture (SER), a full rheological characterization of several commercial ionomers has been carried out including the determination of the linear viscoelastic moduli, the damping function and the tensile stress growth coefficient (extensional viscosity). Particular emphasis has been placed on the effect of ionic association on the rheological behavior, which was studied by comparing the properties of ethylene methacrylic acid copolymer with the corresponding ionomers neutralized with sodium hydroxide. The distribution of the relaxation times to identify the characteristics times such as reptation, Rouse, and sticky-Rouse that is associated with the characteristic life time of the ionic associations has been thoroughly studied. Finally, the experimental rheological data have been fitted to a viscoelastic model (the K-BKZ model).

Capillary flow behavior of a rubber compound

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Rubber compounds are known to be very shear-thinning and possess a strong degree of viscoelasticity. A series of rheological measurements for rubber are carried out using a cone-and-plate rheometer and a high-pressure capillary rheometer in order to study the effect of different die characteristics and temperature. The flow simulations are performed for axisymmetric (capillary dies) extrusion using an integral (K-BKZ) rheological model (with the PSM or Wagner damping function). The effect of rheological properties is investigated and some conclusions are drawn regarding the ability of the integral K-BKZ model to capture well the viscoelastic behavior of rubber.

The solid-liquid transition of brittle solids: Waxy oil study

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At low temperature the waxy oil presents a solid-like behaviour. The paraffin crystals that precipitate during the cooling form a percolated system that entraps the oil and provides a structure to the material. It is known that only 0.5 wt% of precipitated paraffin in oil is enough to yield a solid behaviour to the material in static cooling conditions. The breakage of this structured material and the restart-up flow is a challenge in the real production and transportation of waxy crude oil. Predicting the pressure peak to resume the flow and the time to get the steady state pressure is crucial to project the pipelines, pumps and equipments in the oil and gas industry. At low temperature the way oils are elastoviscoplastic and time-dependent materials and its macroscopic rheological characteristics depend on the amount, morphology and size of wax crystals precipitated in the oil. The interactions between the wax crystals, which are responsible for complex rheological behavior of the waxy oils, have not been fully understood yet. In the current work, using a model waxy oil with rheometric and microscopic analysis and a careful procedure to control the thermal

and shear history of the material, we describe the behaviour of the material in the solid regime. Due to the needle-like morphology of the precipitated paraffin and the bonds between the crystals the material behaves as a brittle solid with a high elastic modulus but a very low critical strain. The creep tests, performed each time if a new sample, show that for stress above the yield stress when the material reaches the critical strain the system presents a collapse. Finally, we show that depending on the wax concentration in oil the material can present an important shear banding that is a crucial point to understand the behaviour of the material after the breakage.

A rheological study of the gelation kinetics of non-aqueous Carbopol dispersions

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Manufacturing processes involving complex non-Newtonian fluids are employed in several industrial applications. Specifically, the design of new continuous mixing operations poses many challenges, especially when dealing with complex fluids, which may undergo rapid changes in rheology due to polymerization, heat transfer or simple homogenization of different phases. For process design purposes, numerical methods, such as computational fluid dynamics, represent a valuable tool to achieve a quicker and more cost-efficient investigation of all the different process variables. When dealing with complex fluids, knowledge of the rheological behaviour at different stages of the process is important for obtaining meaningful results.

In this work we investigate the gelation kinetics of non-aqueous Carbopol® dispersions, currently used in novel formulations of oral health products. We used Fourier Transform Mechanical Spectroscopy (FTMS) to track the evolution of the viscoelastic properties and obtained operating maps in terms of a structural conversion degree X_s, at different solvent compositions and operating temperatures. UV-vis spectroscopy was employed to confirm the mechanism of gelation. It was found that an increase in both the concentration of protic solvent and the gelation temperature increased the gelation rate, thus highlighting a diffusive controlled mechanism of the process. To link the generalized kinetic model with the effective time-evolution of viscosity, the flow behaviour of the mixtures was also tracked at different shear rates in a cone-plate rheometer. The kinetic process appears to be independent of the shear rate applied as well as the final viscoelastic properties of the gels, thus allowing a full description of the flow curves of the mixtures at different gelation degrees. The viscosity model was then implemented in a computational fluid dynamics environment to predict the gelating flow in a small channel.

Lid-driven elastoviscoplastic flow in a cavity

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We implemented the elasto-viscoplastic (EVP) version of the Herschel-Bulkley constitutive model proposed by Saramito [J. Non-Newton. Fluid Mech. 158 (2009) 154-161] into a Finite Volume code and performed numerical simulations of lid-driven EVP flow in a square cavity. The Saramito-Herschel-Bulkley (SHB) model parameters were fitted to Carbopol. The material is initially at rest and driven to steady-state at various lid velocities. The results were compared against corresponding simulations with the classic Herschel-Bulkley (HB) viscoplastic model. We performed the following investigations:

(a) Effect of the lid velocity. The lid velocity affects the relative importance of plasticity, elasticity, and inertia, as quantified by dimensionless numbers (Bingham, Weissenberg, Reynolds). At low lid velocities the plastic character of the flow is accentuated, while at higher velocities elastic effects become more prominent, with an oscillatory evolution in time of the kinetic energy of the fluid until a steady state is reached.
(b) Flow with and without wall slip. In the no-slip case a region of stationary material forms at the bottom of the cavity, which includes "transition" zones where material is formally in a yielded state, but practically behaves as unyielded, being stationary and having stress values that drop towards the yield stress at an ever-decreasing rate. This is not observed in the slip case.
(c) Flow with different initial stress conditions. The material is always initially at rest, but we performed different simulations with either zero initial stress or with non-zero residual stresses close to the yield stress. Different steady states are reached depending on the initial stress condition.
(d) Flow dependence on the elastic modulus. We artificially increased the elastic modulus of the material and observed how fast the EVP results converge to the classic HB results.
(e) Flow cessation. After the steady state had been reached, we suddenly stopped the lid and observed the flow decay. Contrary to purely viscoplastic flow, EVP flow does not cease in finite time but once the material has solidified into an elastic solid there is a perpetual back-and-forth conversion between elastic and kinetic energies, with associated oscillatory motions. Flow decay is much faster in the presence of wall slip, due to friction between the material and the wall.

Slime for defense – biophysical design principles in a marine environment

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Hagfish are genetically one of the oldest living creatures on earth. Neither charming in appearance or task they brought their defense mechanism to perfection during the last 150 million years. When attacked by predators, hagfish excrete a concentrated mucin – protein fiber solution, which forms within milliseconds a large body of slime. Although the slime consists out of vast amounts of water, the diluted mucin and fibers span a cohesive network eventually clogging mouth or gills of the predators and enabling the hagfish to escape. Here, we present both the rheological properties of the slime in defense and escape situations as well as the biophysical principles of slime formation in the saline marine environment. We show that the different rheological responses of the slime under shear and elongational flow lead to strain hardening under attack but shear thinning during escape, promoting the survival chances of the hagfish. Considering the slime as a complex polyelectrolyte, a fine-tuned interaction with the different ions present in seawater must be given to employ the full defense capability of the slime, i.e. the rapid unraveling and network formation of both mucins and skeins under charge screening conditions. By elucidating the molecular and biophysical design principles and their consequences on the rheological properties of the slime, we are able to provide guidelines for tailoring mechanical properties of other mucin-like polyelectrolyte systems.

Probing the internal dynamics of model colloidal glasses under shear by orthogonal superposition rheometry

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Attractive colloidal glasses are unique as their dynamical arrest is due to a combination of entropic crowding effects and formation of attractive bonds. When such systems are subjected to flow, the dynamics of the system are activated in a way which differs from hard sphere glasses which melt through a ‘convective cage release mechanism’. Here, we investigate the microscopic dynamics by measuring the relaxation spectrum during flow using orthogonal superposition rheometry. A small amplitude oscillatory shear deformation is imposed perpendicularly to a steady shear flow and the superposition moduli are measured. At low Péclet number a crossover frequency of the elastic and viscous superposition moduli is detected which represents the relaxation time associated to shear-induced escape of particles from their localization. For the repulsive glass, this is related to shear-induced cage renewal of particles. For attractive glasses, however, when particles escape their localized length (bonds), they move with no further hindrance with the escape time that is independent of the attraction strength and interestingly, although counterintuitively, is faster than that in a purely repulsive glass. This is attributed to the fact that in attractive glasses, particles are localized at much shorter length scales due to bonding. At high Peclet number flows, a second low frequency crossover between elastic and viscous moduli is observed and a low frequency elastic dominated response emerges. This elastic response may originate from the slow relaxation of hydroclusters or be a consequence of the more intricate nature of the superposition moduli. At high frequencies both the elastic and loss moduli probed orthogonally increase relative to the quiescent state due to anisotropic cage deformation that slows down short-time in-cage dynamics. Brownian dynamic simulations are utilized complementary to probe the underlying microscopic dynamics by measuring the mean square displacements (MSD) under flow. The generalized Stokes-Einstein (GSE) relation is used to extract from the MSD the moduli under shear, which are then compared to the experimental orthogonal superposition moduli.

Tuning the mechanical properties of alginate-peptide hydrogels

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Current effort in the engineering of hydrogel synthetic extra cellular matrix (ECM) has focused on installing bioactive molecules (peptides) within the hydrogel. Incorporating biomolecules within the gel may cause a change in the gels’ physical properties, which could indirectly lead to a change in its bioactivity, since hierarchical structural organization and mechanical properties have been shown to affect cellular response.

Covalent bonding peptides to alginates is routinely used to tailor alginate gels biofunctionality, here, we explore the possibility of tuning the mechanical properties of alginate-peptide gels by altering the sequence of the covalently bound peptide.

We present a systematic investigation of the effect of three RGD-containing peptides, G_6KRGDY, A_6KRGDY and V_6KRGDY, on the physical properties of alginate hydrogels by Small angle X-ray scattering (SAXS) and rheology.

Rheology measurements show that the storage modulus (G') of Alginate-A_6KRGDY and Alginate-V_6KRGDY gels, are an order of magnitude higher than that of the alginate–G_6KRGDY gels. SAXS data obtained from alginate-peptide gels indicate there are substantial differences between the nanostructure of

Alginate-A_6KRGDY and Alginate-V_6KRGDY and that of alginate–G6KRGDY exhibiting a correlation between the two.

Our results showed that the ability of peptides to self-assemble in aqueous solutions (i.e. the peptide sequence) is an important factor in tuning the mechanical properties of alginate/peptide gels. Therefore, a detailed structural analysis of the conjugated architecture in solution can be used as a tool to tailor the properties of alginate/peptide hybrid hydrogels.

Extensional rheology of ring polystyrene melt and linear/ring polystyrene blends

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The state-of-the-art understanding of entangled linear polymers is based on the concept of physical network formation from entanglements. The physical network is characterized by a plateau modulus in linear viscoelastic (LVE) measurements. However, linking the two free ends of a linear polymer, thereafter called a ring polymer, has dramatic consequences. For example, non-concatenated rings have much lower zero-shear-rate viscosity compared to their linear entangled counterparts. A plateau modulus is not observed in LVE measurements for ring polymers [1].

Due to the difficulties in synthesis, which leads to very limited amount of samples, well-defined ring polymers have never been studied in extensional flow. In this work, we present the first results of extensional rheology of a ring polystyrene (PS) melt with the molecular weight 185k (Ring-185k). We show that the ring PS is surprisingly strain hardening in extensional flow and reaches the same extensional steady state viscosity as its linear counterpart (Lin-185k) when the stretch rate is fast enough. We further present the extensional rheology of blends made of Ring-185k and Lin-185k, with weight fraction of 5%, 20%, and 30% of Ring-185k, respectively. We show that in the transient stress-strain responses, stress overshoot is observed for the samples containing 20% and 30% Ring-185k, while the stress overshoot is not observed for the pure Ring-185k and Lin-185k.

The present results shed light into the fascinating flow properties of polymers without free ends, while they also advance the state-of-the-art in polymer physics. At the same time, they open the route for understanding the response of folded proteins and chromosome territories under strong external fields.

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Interfacial viscoelasticity - the effect of polymer chain flexibility and hydrophobicity

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Complex fluid interfaces play a crucial role in many biological and industrial process. Understanding the interplay between polymer characteristics and its effect on the mechanical properties of an interface is a prerequisite for a proper design for processes such as foaming, spontaneous emulsification, printing, paint and coating applications to name a few.

The relationship between the phase behavior of polymer monolayers as studied by the classical rectangular Langmuir-Pockels trough, the rheological properties of the interface, and the importance of the detailed test geometry were recently described and analyzed in detail [1] but are still poorly understood. In this contribution, using Brewster's angle microscopy for morphology and layer thickness determination, and Interfacial magnetic rod stress rheometer for shear interfacial rheology measurement - we study how different characteristics such as Tg, hydrophobicity, and molecular weight affect the evolution of the interfacial phases and the formation of elastic interfaces at the air-water interface. When examining glassy polymers such as poly(tert butyl methacrylate) and flexible polymers such as polydimethylsiloxane, profoundly different behavior is observed. Furthermore, hydrophobic polymers with no hydrophilic groups or substitutions such as polystyrene and polybutadiene, exhibit yet a further different behavior in comparison to less hydrophobic polymers.

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Fat crystallization and solidification as observed by novel combined rheological methods

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In this study, the crystallization of fat was observed with novel combined rheological methods. In these methods a rheometer was combined with a molecular spectroscopical method, e.g. dielectric or NMR-relaxometry. The novel setups allow simultaneously monitoring the mechanical rheological and the molecular spectrocopical processes. The methods applied here are Rheo-NMR and Rheo-dielectric spectroscopy, which are sensitive to the polarization and orientation of crystals.

The sample fat used in the presented work is a Palm kernel stearin (PKS) blended with 40% w/w High oleic sunflower oil (HOSO). The crystallization process was induced by changing the temperature. the samples were heated to melt and subsequently cooled down until crystallization and again heated up to the melt state again. The whole process could be followed by the rheological and spectroscopical methods.

Full spatio-temporal elucidation of sheared multiphase materials

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Suspensions, emulsions, foams, and mixtures thereof exhibit complex flow behavior due to microstructural rearrangement and orientation of the disperse phase(s). In nature, landslides and other catastrophic events emphasize the importance to understand multiphasic microstructural evolution under controlled macroscopic mechanical stress or deformation. A causal understanding of complex flow comes when imaging techniques capable of adequately detecting the events couple in synchronism with rheometry.

A full-volume approach to structure elucidation in real-time and under full control of all shear flow parameters is still missing, especially at significant high forces to understand natural and industrial processes better. Current methods are constrained by the mode of deformation, the acquisition speed, and resolution or they are restricted to fewer dimensions when operating in real-time, but most important, there is no complete control or information of rheological quantities [1,2]. To address this shortcoming, we present a method to recover the full volume microstructural evolution by ultrafast µCT X-Ray imaging while controlling or measuring all relevant macroscopic rheological quantities, such as shear stress, shear rate, and normal pressure.

The setup consists of a modified two-motor rheometer in co-rotating mode with a custom 3D printed shear cell to match the requirements for higher stresses. When operated at co-rotation, the differential speed of the motors induce flow within the enclosed material and allow full volume µCT scans, which are acquired synchronously with corresponding rheological data.

To demonstrate the method, we present a study of densely packed glass beads immersed in different Newtonian fluids. Such a dense granular model suspension appears in a wide spectrum, both in nature and industry. It is of current scientific interest since it can show very complex material behavior, especially at high particle concentrations. Recent developments have led to a successful description of granular suspensions by considering a pressure-imposed instead of a volume-imposed flow, also known as frictional rheology [3]. In combination with our method, it is possible to extend the measurement range into unknown territories and explore rheological measurements in synchronism with full volume structural information. We expect that this method can generally answer many open questions concerning the rheology of complex materials.

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Probing the nanoscale structure of block copolymer micelle liquid crystals using rheology and mechanical behavior

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At high polymer concentrations, solvent-selective block copolymer molecules self-assemble into concentrated micellar solutions that form highly-ordered, nanostructured, soft solids. Controlling the solvent quality allows for high densities of deformable (soft) particles to be achieved. These materials have rich phase behavior offering considerable potential in templating, transport properties and nanostructure control through both molecular design and processing. The complexity of the phase diagrams increases as the molecular weight of the block copolymers decreases and fluctuations in micelle aggregation number increase; connecting to the similarly rich phase behaviors observed in concentrated surfactant solutions. The goal of this work is to use rheology to fingerprint and then map out the phase behavior of low molecular weight diblock copolymers in solution. Providing a mechanical probe of structure will guide nanostructural studies (SAXS) by providing realizable search spaces; having rheological data will also aid in processing of these materials. Results will be presented for diblock (Brij) and triblock (Pluronic) copolymer systems in aqueous solution at different temperatures. We will discuss the feasibility of developing rheology fingerprints for these different materials.

Effect of additives shape and size on crystallization of polymeric systems

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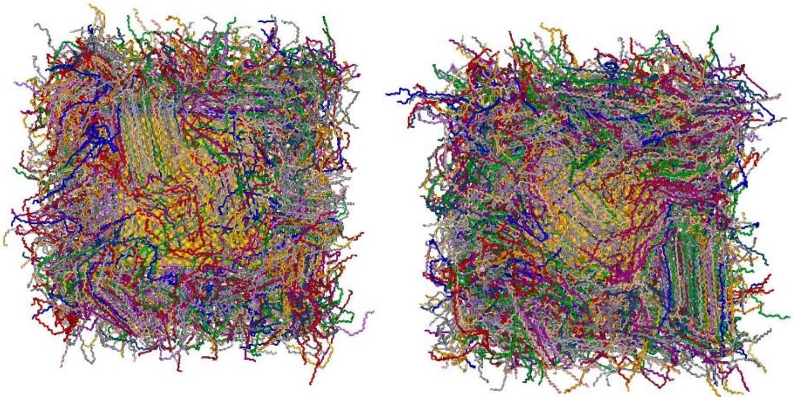
Previously we have studied thermo-mechanical effects including temperature and cooling rate [0], shear rate and strain [0], and surface effects [0] such as roughness on the crystallization of polymers. For polymer processing, particles of various shapes and sizes are often added to polymers as colourants or crystallization agents or when nanocomposite polymers are formulated. Therefore the effect of these solid inclusions in the mixture is of great importance to rheological behaviour and also crystallization kinetics of polymer melts. In this work, large scale molecular simulations are performed and the effect of the shape and size of the particles on crystallization kinetics of polymer matrix has been studied. Hexacontane ($C_{60}H_{122}$) is simulated as a model polymer, and spherical and cubic particles are added to the melt at 500K. The system is then allowed to crystallize at constant pressure condition while cooling it done to 325 K. The results show interesting phenomena where both the shape and size of the particles affect the rate of crystallization. The global and local crystallinity is measured for each case, and the effects of particle size and shape are discussed.



(a) (b)

Fig 1. C60 system crystallized at 325K for 38 ns, with a) cubic and (b) spherical particles added to the melt.

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Hybrid dendronized polymers as molecular objects: viscoelastic properties in the melt

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Two homologous series of dendronized polymers (DPs) of second and third generation, and different degrees of polymerization of the backbone, were synthesized combining two previously reported approaches. Firstly, methacrylate-based DPs of first generation were prepared via radical polymerization of the corresponding methacrylate monomers. The side branches of such first-generation DPs can form hydrogen bonding and π-π stacking, therefore they are referred to as supramolecular DPs. Secondly, the first-generation DPs so prepared were grafted with linear oligoethylene glycol groups, in order to increase the size of the dendrons up to the second and third generation [1]. Due to the different chemical structure of the outermost generations with respect to the inner one, these DPs are termed as "hybrid" DPs. The glycol-based generations do not form supramolecular associations, which control the aging dynamics and viscoelastic properties of the supramolecular DPs. Therefore, the series of hybrid DPs allows for investigating the dynamics of dendronized polymers in the absence of synergistic effects due to supramolecular interactions and topology. We find that the absence of intermolecular peripheral interactions dramatically increases the equilibration time of hybrid DPs compared to the supramolecular ones. Concerning the viscoelastic behavior of the hybrids of second generation, the onset of the global relaxation is observable at low frequencies, in contrast with supramolecular DPs with same generation and same backbone degree of polymerization, for which a clear plateau region was demonstrated elsewhere[2]. The hybrid DPs of third generation display two distinct plateau regions of the storage modulus. Whereas the first one (at higher frequencies) is of order of 10^6 Pa and attributed to the interpenetration of the side branches, the second is of the order of 10^3 Pa, and attributed to the entanglements of the entire hybrid DPs. The low frequency plateau is absent for supramolecular DPs. These results provide ingredients for tailoring the rheology of hyperbranched polymers.

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High-frequency rheometry of polymeric systems.

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We present a versatile sliding plate piezo-operated rheometer for measuring the linear viscoelastic properties of various soft materials at frequencies up to 1 kHz. The sensitive loss angle measuring loop is validated explicitly against reference data from entangled amorphous polymer melts obtained with conventional rotational rheometers by means of time-Temperature Superposition (tTS). This gives confidence in measuring more complex systems where tTS does not apply. We demonstrate the ability to probe the short-time dynamics of hard-sphere colloidal glasses and microgels. Important high-frequency features such as the limiting behavior of the high-frequency elastic modulus, G_∞', the respective moduli crossover related to β-relaxation and the associated limiting, in phase with strain-rate, dynamic viscosity η_∞', are captured. We also show the adaptation of this setup to high-temperature environments and discuss an application associated with the measurement of the plateau modulus of semi-crystalline polymers, something that cannot be achieved by means of tTS. This promising technique can complement the

rheological map of many soft-matter systems and provide direct insights to interactions at nano-metric particle separations.

Drainage dynamics of thin polymer-solution films

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Thin liquid film (TLF) dynamics is considered to be an important (if not deciding) factor when it comes to foam and emulsion stability. When two bubbles/droplets come into close proximity a TLF is usually formed between them, which gradually drains until it ruptures. The role of the interfacial properties on the hydrodynamic drainage process of various systems has received some attention [1,2]. However, to the best of our knowledge, there are no experimental studies regarding how the rheological properties of the bulk liquid (e.g. viscoelasticity, shear thinning) affect the overall drainage process.

In this study, the drainage dynamics of liquid-air films of polymer solutions were examined using a variation of the thin film balance technique which allows us to vary the Capillary number [3]. A standard thin film balance was modified to perform hydrodynamic studies. Constant, as well as dynamic pressure was applied in order to simulate both head-on and glancing collisions. The effect of three parameters on drainage was studied, namely that of driving force, polymer concentration and molecular weight. All parameters were found to influence non-trivially the drainage of the thin liquid films, giving rise to a multitude of phenomena, both with respect to flow instabilities (symmetric-to-asymmetric drainage transitions, cyclic dimpling and vortices), as well as with respect to confinement effects on structure and possibly rheology (thickness variations comparable to the length-scales of the polymer chains).

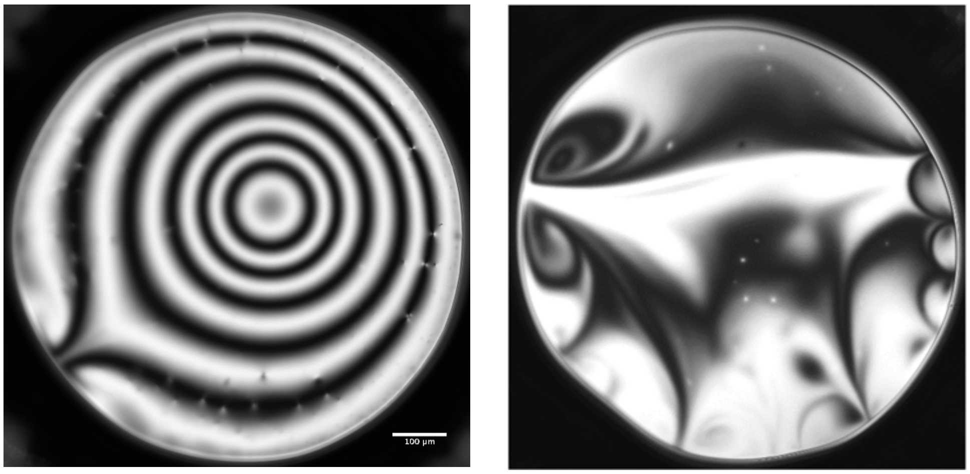

Figure 1. Microinterferometry images of a draining of 1wt% (left) and 10wt% (right) polyisobutylene in hexadecane film under an applied pressure of 400Pa.

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Posters

Shear rheology of marginally entangled polystyrene

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We present a detailed rheological investigation of linear polystyrenes with weight-average molar mass ranging from 10-30 kg/mol, (marginally entangled) and compare them with unentangled bottle-brush polystyrenes. Emphasis is placed on the response of the polymers in simple shear during start-up. To reduce experimental artifacts associated with edge fracture, wall slip and shear banding, we employed a homemade cone-partitioned plate fixture [1]. Reliable data for these polymers could be obtained for Weissenberg numbers below 30. The analysis of the stress overshoot during start-up suggests that in the investigated shear regime the polymers orient but do not stretch. This is corroborated by the fact that the empirical Cox–Merx rule appears to be validated, within experimental error. On the other hand, the (shear) rate dependent steady shear viscosity data exhibit a slope in the range 0,47-0,57. We also measured both the first and second normal stress differences of polymers, hence obtaining the full set of viscometric material functions in nonlinear shear flow. The method is based on the use of a modular cone-partitioned plate (CPP) setup with two different diameters of the inner plate, mounted on a rotational strain-controlled rheometer [2].

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Experimental and rheological study of prepered bioformulations

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The objective of this study is the rheological study of the formulations prepared based on the essential oil (Thymus Serpyllum), extracted and characterized during this work. The Thymus Serpyllum EO harvested from the Khemis Miliana region was extracted by hydrodistillation. The chemical components were determined by the analysis techniques: UV, IR, CGSM. CG (SM) analysis shows that the EO essence contains the following major components: Dehydro-Carvenolide, Limoneme, Sabinene hydrate "cis", Pinocarveol "trans" and α-Pinene Thymol, Carvacol. The two formulations based on Thymus EO (gel and cream) prepared during this study showed stable viscoelastic behavior over time. The results showed that the gel stabilizes after a few days and the preserved cream at room temperature is more stable than at low temperature.

A multimodal light scattering and imaging device for rheological applications

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We present a multimodal light scattering device featuring static and dynamic Small-Angle Light Scattering (SALS), Microscopy (M) and Diffusing Wave Spectroscopy (DWS) able to be performed in combination with rheological experiments. A compact SALS device covering a wide angular (2^o to 30^o) and scattering wavevector q (= $(4\pi n/\lambda)\sin\theta/2$) range (0.4 $m\text{m}^{-1}$ - 6.2 $m\text{m}^{-1}$) that can be easily adapted as a modular accessory to different commercially available rheometers. The apparatus was validated through dilute suspensions measurements by Static Light Scattering (SLS) at rest to extract the form factor, F(q), providing information of the particle size and polydispersity and in concentrated suspensions where the structure factor, S(q), is measured probing the microstructure for a variety of colloidal systems. Similar measurements under steady and oscillatory shear, combining SALS and rheology, allow the link of shear induced structures with the linear and nonlinear mechanical properties. Finally, exploiting the device modularity we utilize the imaging module to image (in 5x magnification) shear induced structures in colloidal gels of spherical and rodlike particles, liquid crystalline polymers (under cross-polarizers) and performed DWS measurements in multiple scattering samples determining their dynamics at rest and under shear.

Viscoplastic Couette flow in the presence of wall slip with non-zero slip yield stress

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The steady-state Couette flow of a yield-stress material obeying the Bingham-plastic constitutive equation is analyzed assuming that slip occurs when the wall shear stress exceeds a threshold value, the slip yield stress. Both cases where either the inner or the outer cylinder is rotating and the other is fixed are studied. The different flow regimes that arise depending on the relative values of the yield stress and the slip yield stress are identified and the various critical angular velocities are determined. Analytical solutions are presented for all possible cases and the implications to this important rheometric flow are discussed.

Flow of inhomogeneous Bingham fluids

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We present a mathematical model for the Poiseuille flow of a Bingham fluid in which the rheological parameters are not constant (inhomogeneous Bingham fluid). Practical applications of this type of fluids are ubiquitous including landslide modeling, mud flow and blood flow. In particular, we consider the following applications:
i) Mud Flow – the fluid is incompressible and inhomogeneous (stratified flow) and the yield stress and the viscosity depend on the density.
ii) Blood Flow – the fluid is homogeneous (constant density) but the yield stress and viscosity depend on the hematocrit, i.e. the concentration of red blood cells
In case i) we assume that the density is not constant in the reference configuration (inhomogeneous body) and we assume that the rheological parameters are constant along each particle's path. In case ii) we assume that mass distribution is homogeneous, but the rheological parameters are functions of the red blood cells distribution. For both cases we formulate the mathematical problem, which is of free boundary type, and we solve the problem numerically to detect the position of the yield surface.

Steady sphere translation in a viscoelastic fluid with Navier slip on the sphere

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We study analytically the effect of slip on the surface of a spherical particle which translates with constant velocity U in a viscoelastic fluid. We consider isothermal and creeping flow conditions and assume that the ambient fluid is viscoelastic and modelled with the Upper Convected Maxwell (UCM), Oldroyd-B, exponential Phan-Thien and Tanner (ePTT), and Giesekus constitutive equations. The solution for all the dependent variables is expanded as an asymptotic power series with the small parameter being the Weissenberg number, $Wi=\lambda U/R$ where λ is the single relaxation time of the fluid and R the radius of the particle. The resulting sequence of equations is solved analytically up to fourth order in Wi. The solution reveals the effect of viscoelasticity and the relevant rheological parameters on the flow variables, as well as the effect of the slip coefficient on the drag force on the particle.

Viscoelastic planar elongational flow past an infinitely long cylinder

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Following our previous work [Housiadas & Tanner, Phys. Fluids, **30**, 073101 (2018)], we study analytically the effect of steady planar elongational flow past an infinitely long circular cylinder using asymptotic methods. The ambient fluid is assumed viscoelastic and modelled with the Upper Convected Maxwell (UCM), Oldroyd-B, exponential Phan-Thien and Tanner (ePTT), Giesekus, and Finite Extensibility Nonlinear Elastic model with the Peterlin approximation (FENE-P) constitutive equations under isothermal and creeping flow conditions. The solution for all the dependent variables is expanded as an asymptotic power series with the small parameter being the Weissenberg number, Wi, which is defined as the product of the single relaxation time of the fluid times the constant rate of elongation. The resulting sequence of equations is solved analytically up to fourth order in the Weissenberg number. The solution derived here is the first analytical result in the literature for the planar elongational flow of viscoelastic fluids past a cylinder. It reveals the effect of viscoelasticity and all the relevant rheological parameters on the flow variables and the extensional viscosity of the fluid.

The sedimentation of a sphere in a viscoelastic fluid under constant rotation

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We study analytically the steady translation of a spherical particle with radius R under constant rotation. The ambient fluid is considered viscoelastic following the FENE-P constitutive model. Creeping and isothermal flow is assumed. The solution of the governing equations is found by applying a regular perturbation scheme with the small parameter being the Weissenberg number $De = U \lambda / R$ where λ is the single relaxation time of the ambient fluid, ω is the externally imposed constant rotation of the particle. A

high-order asymptotic solution is found for all the flow variables, and an expression for the drag force on the particle is derived. Comparison with the literature is performed and discussed.

The dynamic response of elastoviscoplastic fluids under extension

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We study the extension of a yield-stress material that is confined by two coaxial disks initially forming a cylindrical filament when the disks are pulled apart. The material may be an emulsion, suspension or foam, and so it exhibits an elastoviscoplastic response. It follows the Saramito HB [1] model and yields according to the von Mises criterion. The evolution of the bridge shape, particularly its minimum radius, velocity, and stress fields are monitored. Assuming axial symmetry, the governing equations are numerically solved using our newly proposed finite element framework [2], and the discretization mesh is based on a quasi-elliptic set of equations [3]. We investigate the effect of important material properties, like the yield stress, τ_y, the elastic modulus, G and the shear thinning exponent, n, on the filament's shape and minimum radius during the extension. We show that the elastic response of the material is amplified for large upper plate velocities. Thus, the viscoplastic nature of the material prevails for small velocities which can lead to incorrect conclusions whether such materials are indeed elastoviscoplastic. Also, with our simulations, we track the transient evolution of the yielded/unyielded regions inside the filament due to changes in the stress fields. Depending on the material properties, the minimum radius attains its minimum value approximately at the center of the filament or at two symmetric points around the center of the filament.

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Flow of a Herschel-Bulkley fluid with pressure-dependent rheological parameters in an asymmetric channel

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The lubrication flow of a Herschel-Bulkley fluid in a long asymmetric channel, the walls of which are described by two arbitrary functions $h_1(x)$ and $h_2(x)$ such that $h_1(x)<h_2(x)$ and $h_1(x)+h_2(x)$ is linear, is solved extending a recently proposed method, which avoids the lubrication paradox approximating satisfactorily the correct shape of the yield surface at zero order [1,2]. Both the consistency index and the yield stress are assumed to be pressure-dependent. Under the lubrication approximation, the pressure at zero order is a function of x only, is decoupled from the velocity components, and obeys a first-order integro-differential equation. An interesting feature of the asymmetric flow is that the unyielded core (Fig. 1) moves not only in the main flow direction but also in the transverse direction. Explicit expressions for the two yield surfaces defining the asymmetric unyielded core are obtained and the two velocity components in both the yielded and unyielded regions are calculated by means of closed-form expressions in terms of the calculated pressure and the two yield surfaces. The method is applicable in a range of Bingham numbers where the unyielded core extends from the inlet to the outlet plane of the channel. Semi-analytical solutions are derived in the case of an asymmetric channel with h_1=0 and linearly varying h_2. Representative results demonstrating the effects of the Bingham number and the consistency-index and yield-stress growth numbers are discussed.

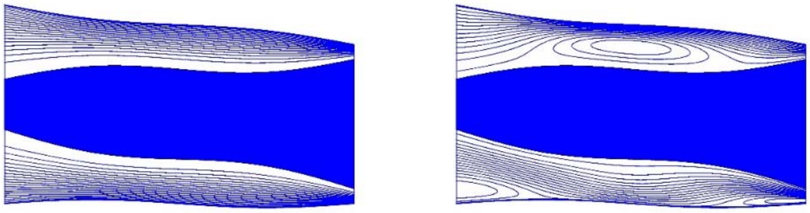

Fig. 1: *Contours of u_x (left) and u_y (right) in a certain asymmetric channel in the case of a Bingham plastic with $Bn=0.2$. The unyielded region is shaded.*

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Simulating unsteady flow of viscoplastic fluids in three dimensions with embedded boundaries

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Although major advances have been made in the field of computational viscoplasticity in recent decades, simulating these fluids is still a problem which requires considerable processing resources. Consequently, most numerical studies are limited to two-dimensional and/or steady-state problems in order to allow reasonable computing time for researchers. In order to address this issue, we have developed a fully three-dimensional, unsteady solver for incompressible flow of viscoplastic fluids. In order to achieve rapid runtimes, the code utilises the highly efficient AMReX framework for structured adaptive mesh refinement and state-of-the-art parallelisation techniques. The fluids are modelled as general Newtonians through apparent viscosity functions, and the implemented rheological equations include Papanastasiou regularised Bingham and Herschel-Bulkley fluids, in addition to de Souza Mendes and Dutra's more recent model. Our latest efforts allow for flow in non-trivial domain geometries through the use of embedded boundaries in the discrete space.

Quantitative relationships between the aggregation state and the permeability of fibrous systems

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We investigate computationally the effect of randomness as well as the effect of fiber aggregation on the hydraulic permeability (Keff) of unidirectional fiber arrays. For this we carry out extensive viscous flow computations in various random fiber arrays which are generated through an NVT Monte-Carlo process, starting from uniform square arrays or from regular arrays of fiber clusters. Up to 10,000 individual fibers are included in each simulation. The extent of aggregation in these arrays is quantified using an integral measure of Ripley's K-function and is shown to correlate with the dimensionless temperature used in the Monte-Carlo algorithm. This metric expresses the deviation of the K-function of any given fiber arrangement from that of a Poisson process at the length scale range of interest. The results demonstrate that the extent of aggregation correlates with the computed permeability as well as with the scatter in the computed values. The latter observation points to a criterion for the selection of properly sized computational unit cells.

Shear banding in magnetic colloids studied by LAOS and numerical simulations

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Magnetic nanoparticles are prospective candidates for various biomedical applications. For these purposes they are injected into the body and interact with different body fluids often experiencing the simultaneous action of magnetic field and shear flow. In these conditions the presence of small amount of magnetic nanoparticles can significantly influence the rheology of the fluid [1-3].

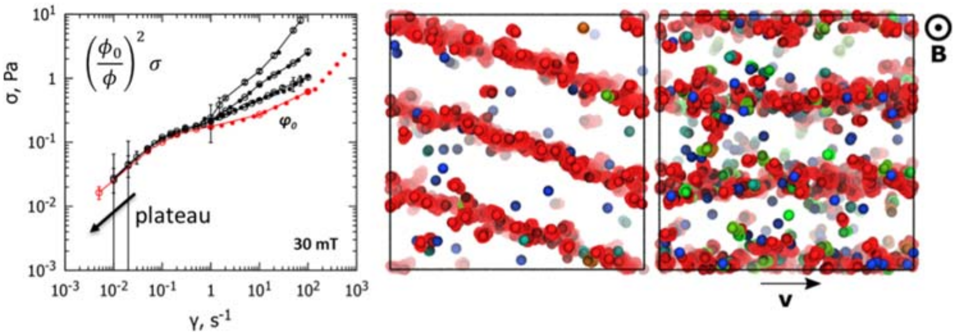

Fig. 1. *Left - monotonic stress curve of a model colloid, right - predicted structural behavior*

Self-assembly is a major route by which colloids are able to spontaneously organize into a variety of large scale structures. Magnetic colloids exhibit field-dependent mechanical response due to complex microstructural transformations that lead to their directional assembly in various aligned mesophases when subjected to electromagnetic fields. This self-assembled system represents unique opportunities for a strongly anisotropic reconfigurable active material susceptible to external stimulation by electromagnetic fields to gain control over the reversible interaction between colloidal particles.

We will report the results of an experimental rheological investigation of the structural behavior of a model magnetic colloid. We will show evidence of at least one mesophase transformations in magnetic colloids under dynamic excitation. Additionally, using hybrid molecular dynamics and multi-particle collision dynamics simulations with explicit coarse-grained hydrodynamics to resolve the coupling of collective hydrodynamic and electromagnetic interactions in colloids outside of equilibrium we observe the self-assembly of magnetic nanoparticles into a hierarchy of aligned mesostructures and elucidate the nature of their transformation. We will present quantitative comparison of our simulated rheometric studies with micromechanical models and experimental data.

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